A First Course in Optimization

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Contents

Chapter 1

Introduction

1.1 Chapter Summary

We discuss the two basic uses of optimization, some important types of problems and algorithms commonly used to solve these problems, and then review some basic analysis.

1.2 Overview

As its title suggests, this book is designed to be a text for an introductory graduate course in optimization. In this course, the focus is on generality, with emphasis on the fundamental problems of constrained and unconstrained optimization, linear and convex programming, on the fundamental iterative solution algorithms, gradient methods, the Newton-Raphson algorithm and its variants, sequential unconstrained optimization methods, and on the necessary mathematical tools and results that provide the proper foundation for our discussions. We include some applications, such as game theory, but the emphasis is on general problems and the underlying theory.

In the companion text, "Applied and Computational Linear Algebra" (ACLA), we discuss several applications in which optimization plays a role, but is not the primary goal. These types of applications tend to lead to *problems of inference*, as we discuss below. In ACLA the emphasis is on inverse problems involving constrained solutions of large-scale systems of linear equations, and iterative algorithms specifically tailored to such problems.

1.3 Two Types of Applications

Optimization means maximizing or minimizing some function of one or, more often, several variables. The function to be optimized is called the *objective function*. There are two distinct types of applications that lead to optimization problems, which, to give them a name, we shall call *problems of optimization* and *problems of inference*.

1.3.1 Problems of Optimization

On the one hand, there are problems of optimization, which we might also call *natural* optimization problems, in which optimizing the given function is, more or less, the sole and natural objective. The main goal, maximum profits, shortest commute, is not open to question, although the precise function involved will depend on the simplifications adopted as the real-world problem is turned into mathematics. Examples of such problems are a manufacturer seeking to maximize profits, subject to whatever restrictions the situation imposes, or a commuter trying to minimize the time it takes to get to work, subject, of course, to speed limits. In converting the real-world problem to a mathematical problem, the manufacturer may or may not ignore non-linearities such as economies of scale, and the commuter may or may not employ probabilistic models of traffic density. The resulting mathematical optimization problem to be solved will depend on such choices, but the original real-world problem is one of optimization, nevertheless.

Operations Research (OR) is a broad field involving a variety of applied optimization problems. Wars and organized violence have always given impetus to technological advances, most significantly during the twentieth century. An important step was taken when scientists employed by the military realized that studying and improving the use of existing technology could be as important as discovering new technology. Conducting research into on-going operations, that is, doing operations research, led to the search for better, indeed, optimal, ways to schedule ships entering port, to design convoys, to paint the under-sides of aircraft, to hunt submarines, and many other seemingly mundane tasks [111]. Problems having to do with the allocation of limited resources arise in a wide variety of applications, all of which fall under the broad umbrella of OR.

Sometimes we may want to optimize more than one thing; that is, we may have more than one objective function that we wish to optimize. In image processing, we may want to find an image as close as possible to measured data, but one that also has sharp edges. In general, such multiple-objective optimization is not possible; what is best in one respect need not be best in other respects. In such cases, it is common to create a single objective function that is a combination, a sum perhaps, of the

original objective functions, and then to optimize this combined objective function. In this way, the optimizer of the combined objective function provides a sort of compromise.

The goal of simultaneously optimizing more than one objective function, the so-called *multiple-objective function problem*, is a common feature of many economics problems, such as bargaining situations, in which the various parties all wish to steer the outcome to their own advantage. Typically, of course, no single solution will optimize everyone's objective function. Bargaining is then a method for finding a solution that, in some sense, makes everyone equally happy or unhappy. A *Nash equilibrium* is such a solution.

In 1994, the mathematician John Nash was awarded the Nobel Prize in Economics for his work in optimization and mathematical economics. His theory of equilibria is fundamental in the study of bargaining and game theory. In her book *A Beautiful Mind* [128], later made into a movie of the same name starring Russell Crowe, Sylvia Nasar tells the touching story of Nash's struggle with schizophrenia, said to have been made more acute by his obsession with the mysteries of quantum mechanics. Strictly speaking, there is no Nobel Prize in Economics; what he received is "The Central Bank of Sweden Prize in Economic Science in Memory of Alfred Nobel" , which was instituted seventy years after Nobel created his prizes. Nevertheless, it is commonly spoken of as a Nobel Prize.

To illustrate the notion of a Nash equilibrium, imagine that there are J store owners, each selling the same N items. Let p_n^j be the price that the jth seller charges for one unit of the nth item. The vector $p^j = (p_1^j, ..., p_N^j)$ is then the list of prices used by the jth seller. Denote by P the set of all price vectors,

$$P = \{p^1, ..., p^J\}.$$

How happy the jth seller is with his list p^j will depend on what his competitors are charging. For each j denote by $f_j(p^1, p^2, ..., p^J)$ a quantitative measure of how happy the jth seller is with the entire pricing structure. Once the prices are set, it is natural for each individual seller to consider what might happen if he alone were to change his prices. Let the vector $x = (x_1, ..., x_N)$ denote an arbitrary set of prices that the jth seller might decide to use. The function

$$g_j(x|P) = f_j(p^1, ..., p^{j-1}, x, p^{j+1}, ..., p^J)$$

provides a quantitative measure of how happy the jth seller would be if he were to adopt the prices x, while the others continued to use the vectors in P. Note that all we have done is to replace the vector p^j with the variable vector x. The jth seller might then select the vector x for which $g_j(x|P)$ is greatest. The problem, of course, is that once the jth seller has selected his best x, given P, the others may well change their prices also. A Nash

equilibrium is a set of price vectors

$$\hat{P} = \{\hat{p}^1, ..., \hat{p}^J\}$$

with the property that

$$g_j(\hat{p}^j|\hat{P}) \geq g_j(x|\hat{P}),$$

for each j. In other words, once the sellers adopt the prices $\hat{p}_n^j$, no individual seller has any motivation to change his prices. Nash showed that, with certain assumptions made about the behavior of the functions f_j and the set of possible price vectors, there will be such an equilibrium set of price vectors.

1.3.2 Problems of Inference

In addition to natural optimization problems, there are *artificial* optimization problems, often *problems of inference*, for which optimization provides useful tools, but is not the primary objective. These are often problems in which estimates are to be made from observations. Such problems arise in many remote sensing applications, radio astronomy, or medical imaging, for example, in which, for practical reasons, the data obtained are insufficient or too noisy to specify a unique source, and one turns to optimization methods, such as likelihood maximization or least-squares, to provide usable approximations. In such cases, it is not the optimization of a function that concerns us, but the optimization of technique. We cannot know which reconstructed image is the best, in the sense of most closely describing the true situation, but we do know which techniques of reconstruction are "best" in some specific sense. We choose techniques such as likelihood or entropy maximization, or least-mean-squares minimization, because these methods are "optimal" in some sense, not because any single result obtained using these methods is guaranteed to be the best. Generally, these methods are "best"in some average sense; indeed, this is the basic idea in statistical estimation.

Artificial optimization arises, for example, in solving systems of linear equations, $Ax = b$. Suppose, first, that this system has no solution; this *over-determined case* is common in practice, when the entries of the vector b are not perfectly accurate measurements of something. Since we cannot find an exact solution of $Ax = b$, we often turn to a *least squares solution*, which is a vector x that minimizes the function

$$f(x) = \|Ax - b\|.$$

It often happens that there is only one such x, but it can happen that there is more than one.

Suppose now that the system $Ax = b$ has multiple solutions. This *under-determined case* also arises frequently in practice, when the entries of the vector b are measurements, but there aren't enough of them to specify one unique x. In such cases, we can use optimization to help us select one solution from the many possible ones. For example, we can find the *minimum norm* solution, which is the one that minimizes $\|x\|$, subject to $Ax = b$.

We often have a combination of the two situations, in which the entries of b are somewhat inaccurate measurements, but there are not enough of them, so multiple exact solutions exist. Because these measurements are somewhat inaccurate, we may not want an exact solution; such an exact solution may have an unreasonably large norm. In such cases, we may seek a minimizer of the function

$$g(x) = \|Ax - b\|^2 + \epsilon\|x\|^2.$$

Now we are trying to get Ax close to b, but are keeping the norm of x under control at the same time.

As we shall see, in both types of problems, the optimization usually cannot be performed by algebraic means alone and iterative algorithms are required.

The mathematical tools required do not usually depend on which type of problem we are trying to solve. A manufacturer may use the theory of linear programming to maximize profits, while an oncologist may use likelihood maximization to image a tumor and linear programming to determine a suitable spatial distribution of radiation intensities for the therapy. The only difference, perhaps, is that the doctor may have some choice in how, or even whether or not, to involve optimization in solving the medical problems, while the manufacturer's problem is an optimization problem from the start, and a linear programming problem once the mathematical model is selected.

1.4 Types of Optimization Problems

The optimization problems we shall discuss differ, one from another, in the nature of the functions being optimized and the constraints that may or may not be imposed. The constraints may, themselves, involve other functions; we may wish to minimize $f(x)$, subject to the constraint $g(x) \leq 0$. The functions may be differentiable, or not, they may be linear, or not. If they are not linear, they may be convex. They may become linear or convex once we change variables. The various problem types have names, such as Linear Programming, Quadratic Programming, Geometric Programming, and Convex Programming; the use of the term 'programming' is an historical accident and has no connection with computer programming.

All of the problems discussed so far involve functions of one or several real variables. In the Calculus of Variations, the function to be optimized is a *functional*, which is a real-valued function of functions. For example, we may wish to find the curve having the shortest length connecting two given points, say $(0, 0)$ and $(1, 1)$, in R^2. The functional to be minimized is

$$J(y) = \int_0^1 \sqrt{1 + (\frac{dy}{dx})^2} dx.$$

We know that the optimal function is a straight line. In general, the optimal function $y = f(x)$ will satisfy a differential equation, known as the Euler-Lagrange Equation.

1.5 Algorithms

The algorithms we shall study in this course are mainly general-purpose optimization methods. In the companion text ACLA, we focus more on techniques tailored to particular problems.

1.5.1 Root-Finding

One of the first applications of the derivative that we encounter in Calculus I is optimization, maximizing or minimizing a differentiable real-valued function $f(x)$ of a single real variable over x in some interval $[a, b]$. Since $f(x)$ is differentiable, it is continuous, so we know that $f(x)$ attains its maximum and minimum values over the interval $[a, b]$. The standard procedure is to differentiate $f(x)$ and compare the values of $f(x)$ at the places where $f'(x) = 0$ with the values $f(a)$ and $f(b)$. These places include the values of x where the optimal values of $f(x)$ occur. However, we may not be able to solve the equation $f'(x) = 0$ algebraically, and may need to employ numerical, approximate techniques. It may, in fact, be simpler to use an iterative technique to minimize $f(x)$ directly.

Perhaps the simplest example of an iterative method is the *bi-section method* for finding a root of a continuous function of a single real variable.

Let $g : R \to R$ be continuous. Suppose that $g(a) < 0$ and $g(b) > 0$. Then, by the Intermediate Value Theorem, we know that there is a point c in (a, b) with $g(c) = 0$. Let $m = \frac{a+b}{2}$ be the mid-point of the interval. If $g(m) = 0$, then we are done. If $g(m) < 0$, replace a with m; otherwise, replace b with m. Now calculate the mid-point of the new interval and continue. At each step, the new interval is half as big as the old one and still contains a root of $g(x)$. The distance from the left end point to the root is not greater than the length of the interval, which provides a good estimate of the accuracy of the approximation.

1.5.2 Iterative Descent Methods

Suppose that we wish to minimize the real-valued function $f : R^J \rightarrow R$ of J real variables. If f is Gâteaux-differentiable (see the chapter on Differentiation), then the two-sided directional derivative of f, at the point a, in the direction of the unit vector d, is

$$f'(a;d) = \lim_{t \rightarrow 0} \frac{1}{t}[f(a+td) - f(a)] = \langle \nabla f(a), d \rangle.$$

According to the Cauchy-Schwarz Inequality, we have

$$|\langle \nabla f(a), d \rangle| \leq ||\nabla f(a)||\,||d||,$$

with equality if and only if the direction vector d is parallel to the vector $\nabla f(a)$. Therefore, from the point a, the direction of greatest increase of f is $d = \nabla f(a)$, and the direction of greatest decrease is $d = -\nabla f(a)$.

If f is Gâteaux-differentiable, and $f(a) \leq f(x)$, for all x, then $\nabla f(a) = 0$. Therefore, we can, in theory, find the minimum of f by finding the point (or points) $x = a$ where the gradient is zero. For example, suppose we wish to minimize the function

$$f(x,y) = 3x^2 + 4xy + 5y^2 + 6x + 7y + 8.$$

Setting the partial derivatives to zero, we have

$$0 = 6x + 4y + 6,$$

and

$$0 = 4x + 10y + 7.$$

Therefore, minimizing $f(x,y)$ involves solving this system of two linear equations in two unknowns. This is easy, but if f has many variables, not just two, or if f is not a quadratic function, the resulting system will be quite large and may include nonlinear functions, and we may need to employ iterative methods to solve this system. Once we decide that we need to use iterative methods, we may as well consider using them directly on the original optimization problem, rather than to solve the system derived by setting the gradient to zero. We cannot hope to solve all optimization problems simply by setting the gradient to zero and solving the resulting system of equations algebraically.

For $k = 0, 1, ...$, having calculated the current estimate x^k, we select a direction vector d^k such that $f(x^k + \alpha d^k)$ is decreasing, as a function of $\alpha > 0$, and a step-length α_k. Our next estimate is $x^{k+1} = x^k + \alpha_k d^k$. We may choose α_k to minimize $f(x^k + \alpha d^k)$, as a function of α, although this is usually computationally difficult. For (Gâteaux) differentiable f, the gradient, $\nabla f(x)$, is the direction of greatest increase of f, as we move away from the point x. Therefore, it is reasonable, although not required, to select $d^k = -\nabla f(x^k)$ as the new direction vector; then we have a *gradient descent method*.

1.5.3 Solving Systems of Linear Equations

Many of the problems we shall consider involve solving, as least approximately, systems of linear equations. When an exact solution is sought and the number of equations and the number of unknowns are small, methods such as Gauss elimination can be used. It is common, in applications such as medical imaging, to encounter problems involving hundreds or even thousands of equations and unknowns. It is also common to prefer inexact solutions to exact ones, when the equations involve noisy, measured data. Even when the number of equations and unknowns is large, there may not be enough data to specify a unique solution, and we need to incorporate prior knowledge about the desired answer. Such is the case with medical tomographic imaging, in which the images are artificially discretized approximations of parts of the interior of the body.

1.5.4 Imposing Constraints

The iterative algorithms we shall investigate begin with an initial guess x^0 of the solution, and then generate a sequence $\{x^k\}$, converging, in the best cases, to our solution. Suppose we wish to minimize $f(x)$ over all x in R^J having non-negative entries. An iterative algorithm is said to be an *interior-point method* if each vector x^k has non-negative entries.

1.5.5 Operators

Most of the iterative algorithms we shall study involve an *operator*, that is, a function $T : R^J \rightarrow R^J$. The algorithms begin with an initial guess, x^0, and then proceed from x^k to $x^{k+1} = Tx^k$. Ideally, the sequence $\{x^k\}$ converges to the solution to our optimization problem. In gradient descent methods with fixed step-length α, for example, the operator is

$$Tx = x - \alpha\nabla f(x).$$

In problems with non-negativity constraints our solution x is required to have non-negative entries x_j. In such problems, the *clipping* operator T, with $(Tx)_j = \max\{x_j, 0\}$, plays an important role.

A subset C of R^J is *convex* if, for any two points in C, the line segment connecting them is also within C. As we shall see, for any x outside C, there is a point c within C that is closest to x; this point c is called the *orthogonal projection* of x onto C, and we write $c = P_C x$. Operators of the type $T = P_C$ play important roles in iterative algorithms. The clipping operator defined previously is of this type, for C the non-negative orthant of R^J, that is, the set

$$R^J_+ = \{x \in R^J | x_j \geq 0, \, j = 1, ..., J\}.$$

1.5.6 Search Techniques

The objective in linear programming is to minimize a linear function $f(x) = c^T x$ over those vectors $x \geq 0$ in R^J for which $Ax \geq b$. It can be shown easily that the minimum of $f(x)$ occurs at one of a finite number of vectors, the vertices, but evaluating $f(x)$ at every one of these vertices is computationally intractable. Useful algorithms, such as Dantzig's *simplex method*, move from one vertex to another in an efficient way, and, at least most of the time, solve the problem in a fraction of the time that would have been required to check each vertex.

1.5.7 Acceleration

For problems involving many variables, it is important to use algorithms that provide an acceptable approximation of the solution in a reasonable amount of time. For medical tomography image reconstruction in a clinical setting, the algorithm must reconstruct a useful image from scanning data in the time it takes for the next patient to be scanned, which is roughly fifteen minutes. Some of the algorithms we shall encounter work fine on small problems, but require far too much time when the problem is large. Figuring out ways to speed up convergence is an important part of iterative optimization.

1.6 Some Basic Analysis

We close with a review of some of the basic notions from analysis.

1.6.1 Minima and Infima

When we say that we seek the minimum value of a function $f(x)$ over x within some set C we imply that there is a point z in C such that $f(z) \leq f(x)$ for all x in C. Of course, this need not be the case. For example, take the function $f(x) = x$ defined on the real numbers and C the set of positive real numbers. In such cases, instead of looking for the minimum of $f(x)$ over x in C, we may seek the *infimum* or *greatest lower bound* of the values $f(x)$, over x in C.

Definition 1.1 *We say that a number α is the* infimum *of a subset S of R, abbreviated $\alpha = \inf(S)$, or the* greatest lower bound *of S, abbreviated $\alpha = \text{glb}(S)$, if two conditions hold:*

- *1. $\alpha \leq s$, for all s in S; and*
- *2. if $t \leq s$ for all s in S, then $t \leq \alpha$.*

Definition 1.2 *We say that a number β is the* supremum *of a subset S in R, abbreviated $\beta = \sup(S)$, or the* least upper bound *of S, abbreviated $\beta = \text{lub}(S)$, if two conditions hold:*

- *1. $\beta \geq s$, for all s in S; and*
- *2. if $t \geq s$ for all s in S, then $t \geq \beta$.*

In our example of $f(x) = x$ and C the positive real numbers, let $S = \{f(x)|x \in C\}$. Then the infimum of S is $\alpha = 0$, although there is no s in S for which $s = 0$. Whenever there is a point z in C with $\alpha = f(z)$, then $f(z)$ is both the infimum and the minimum of $f(x)$ over x in C.

1.6.2 Limits

We begin with the basic definitions pertaining to limits.

Definition 1.3 *A sequence $\{x^n|n = 1, 2, ...\}$, $x^n \in R^J$, is said to* converge *to $z \in R^J$, or have* limit *z if, given any $\epsilon > 0$, there is $N = N(\epsilon)$, usually depending on ϵ, such that*

$$\|x^n - z\| \leq \epsilon,$$

whenever $n \geq N(\epsilon)$.

Unless otherwise indicated, the notation $\|x\|$ will always refer to the 2-norm of a vector x; that is,

$$\|x\| = \sqrt{\sum_{n=1}^{N} |x_n|^2}.$$

Definition 1.4 *A sequence of real numbers $\{x_n|n = 1, 2, ...\}$ is said to* converge to $+\infty$ *if, given any $b > 0$, there is $N = N(b)$, usually depending on b, such that $x_n \geq b$, whenever $n \geq N(b)$. A sequence of real numbers $\{x_n|n = 1, 2, ...\}$ is said to* converge to $-\infty$ *if the sequence $\{-x_n\}$ converges to $+\infty$.*

Definition 1.5 *Let $f : R^J \to R^M$. We say that $L \in R^M$ is the* limit *of $f(x)$, as $x \to a$ in R^J, if, for every sequence $\{x^n\}$ converging to a, the sequence $\{f(x^n)\}$ in R^M converges to L. We then write*

$$L = \lim_{x \to a} f(x).$$

For $M = 1$, we allow L to be infinite.

Let $f : R^J \to R$ and a be fixed in R^J. Let S be the set consisting of all L, possibly including the infinities, having the property that there is a sequence $\{x^n\}$ in R^J converging to a such that $\{f(x^n)\}$ converges to

L. The set S is never empty; we can always let $x^n = a$ for all n, so that $L = f(a)$ is in S. Therefore, we always have

$$-\infty \leq \inf(S) \leq f(a) \leq \sup(S) \leq +\infty.$$

For example, let $f(x) = 1/x$ for $x \neq 0$, $f(0) = 0$, and $a = 0$. Then $S = \{-\infty, 0, +\infty\}$, $\inf(S) = -\infty$, and $\sup(S) = +\infty$.

Definition 1.6 *The (possibly infinite) number* $\inf(S)$ *is called the* inferior limit *or* lim inf *of* $f(x)$*, as* $x \to a$ *in* R^J*. The (possibly infinite) number* $\sup(S)$ *is called the* superior limit *or* lim sup *of* $f(x)$*, as* $x \to a$ *in* R^J*.*

It follows from these definitions and our previous discussion that

$$\liminf_{x \to a} f(x) \leq f(a) \leq \limsup_{x \to a} f(x).$$

For example, let $f(x) = x$ for $x < 0$ and $f(x) = x + 1$ for $x > 0$. Then we have

$$\limsup_{x \to 0} f(x) = 1,$$

and

$$\liminf_{x \to 0} f(x) = 0.$$

Proposition 1.1 *The inferior limit and the superior limit are in the set* S*.*

Proof: We leave the proof as Exercise 1.3.

1.6.3 Continuity

A basic notion in analysis is that of a continuous function.

Definition 1.7 *We say the function* $f : R^J \to R^M$ *is* continuous *at* $x = a$ *if*

$$f(a) = \lim_{x \to a} f(x).$$

When $M = 1$, $f(x)$ is continuous at $x = a$ if and only if

$$\liminf_{x \to a} f(x) = \limsup_{x \to a} f(x) = f(a).$$

A basic theorem in real analysis is the following:

Theorem 1.1 *Let* $f : R^J \to R$ *be continuous and let* C *be non-empty, closed, and bounded. Then there is* z *in* C *with* $f(z) \leq f(x)$ *for all* x *in* C*.*

We give some examples:

- 1. The function $f(x) = x$ is continuous and the set $C = [0, 1]$ is non-empty, closed and bounded. The minimum occurs at $x = 0$ and the maximum occurs at $x = 1$.
- 2. The set $C = (0, 1]$ is not closed. The function $f(x) = x$ has no minimum value on C, but does have a maximum value $f(1) = 1$.
- 3. The set $C = (-\infty, 0]$ is not bounded and $f(x) = x$ has no minimum value on C. Note also that $f(x) = x$ has no finite infimum with respect to C.

1.6.4 Semi-Continuity

We can generalize the notion of continuity by replacing the limit with the inferior or superior limit.

Definition 1.8 *We say that $f : R^J \to R$ is* lower semi-continuous *(LSC) at $x = a$ if*

$$f(a) = \liminf_{x \to a} f(x).$$

Definition 1.9 *We say that $f : R^J \to R$ is* upper semi-continuous *(USC) at $x = a$ if*

$$f(a) = \limsup_{x \to a} f(x).$$

Note that, if $f(x)$ is LSC (USC) at $x = a$, then $f(x)$ remains LSC (USC) when $f(a)$ is replaced by any lower (higher) value.

1.7 A Word about Prior Information

As we noted earlier, optimization is often used when the data pertaining to a desired mathematical object (a function, a vectorized image, etc.) is not sufficient to specify uniquely one solution to the problem. It is common in remote sensing problems for there to be more than one mathematical solution that fits the measured data. In such cases, it is helpful to turn to optimization, and seek the solution consistent with the data that is closest to what we expect the correct answer to look like. This means that we must somehow incorporate prior knowledge about the desired answer into the algorithm for finding it. In this section we give an example of such a method.

Reconstructing a mathematical object from limited data pertaining to that object is often viewed as an *interpolation* or *extrapolation* problem,

in which we seek to infer the measurements we did not take from those we did. From a purely mathematical point of view, this usually amounts to selecting a function that agrees with the data we have measured. For example, suppose we want a real-valued function $f(x)$ of the real variable x that is consistent with the measurements $f(x_n) = y_n$, for $n = 1, ..., N$; that is, we want to interpolate this data. How we do this should depend on why we want to do it, and on what we may already know about $f(x)$. We can always find a polynomial of degree $N - 1$ or less that is consistent with these measurements, but using this polynomial may not always be a good idea.

To illustrate, imagine that we have $f(0) = y_0$, $f(1) = y_1$ and $f(2) = y_2$. We can always find a polynomial of degree two or less that passes through the three points $(0, y_0)$, $(1, y_1)$, and $(2, y_2)$. If our goal is to interpolate to infer the value $f(0.75)$ or to estimate the integral of $f(x)$ over $[0, 2]$, then this may not be a bad way to proceed. On the other hand, if our objective is to extrapolate to infer the value $f(53)$, then we may be in trouble. Note that if $y_0 = y_1 = y_2 = 0$, then the quadratic is a straight line, the x-axis. If, however, $f(1) = 0.0001$, the quadratic opens downward, while if $f(1) = -0.0001$, the quadratic opens upward. The inferred values of $f(x)$, for large x, will be greatly different in the two cases, even though the original data differed only slightly.

It sometimes happens that, when we plot the data points (x_n, y_n), for $n = 1, ..., N$, we see the suggestion of a pattern. Perhaps this cloud of points nearly resembles a straight line. In this case, it may make more sense to find the straight line that best fits the data, what the statisticians call *the regression line*, rather than to find a polynomial of high degree that fits the data exactly, but that oscillates wildly between the data points. However, before we use the regression line, we should be reasonably convinced that a linear relationship is appropriate, over the region of x values we wish to consider. Again, the linear approximation may be a good one for interpolating to nearby values of x, but not so good for x well outside the region where we have measurements. If we have recorded the temperature every minute, from 10 am until 11 am today, we may see a linear relationship, and the regression line may be useful in estimating what the temperature was at eight seconds after twenty past ten. It probably will be less helpful in estimating what the temperature will be at 7 pm in the evening. For that purpose, prior information about the temperature the previous day may be helpful, which might suggest a sinusoidal model. In all such cases, we want to optimize in some way, but we need to tailor our notion of "best" to the problem at hand, using whatever prior knowledge we may have about the problem.

An important point to keep in mind when applying linear-algebraic methods to measured data is that, while the data is usually limited, the information we seek may not be lost. Although processing the data in

a reasonable way may suggest otherwise, other processing methods may reveal that the desired information is still available in the data. Figure 1.1 illustrates this point.

The original image on the upper right of Figure 1.1 is a discrete rectangular array of intensity values simulating a slice of a head. The data was obtained by taking the two-dimensional discrete Fourier transform of the original image, and then discarding, that is, setting to zero, all these spatial frequency values, except for those in a smaller rectangular region around the origin. The problem then is under-determined. A minimum-norm solution would seem to be a reasonable reconstruction method.

The minimum-norm solution is shown on the lower right. It is calculated simply by performing an inverse discrete Fourier transform on the array of modified discrete Fourier transform values. The original image has relatively large values where the skull is located, but the minimum-norm reconstruction does not want such high values; the norm involves the sum of squares of intensities, and high values contribute disproportionately to the norm. Consequently, the minimum-norm reconstruction chooses instead to conform to the measured data by spreading what should be the skull intensities throughout the interior of the skull. The minimum-norm reconstruction does tell us something about the original; it tells us about the existence of the skull itself, which, of course, is indeed a prominent feature of the original. However, in all likelihood, we would already know about the skull; it would be the interior that we want to know about.

Using our knowledge of the presence of a skull, which we might have obtained from the minimum-norm reconstruction itself, we construct the prior estimate shown in the upper left. Now we use the same data as before, and calculate a minimum-weighted-norm reconstruction, using as the weight vector the reciprocals of the values of the prior image. This minimum-weighted-norm reconstruction is shown on the lower left; it is clearly almost the same as the original image. The calculation of the minimum-weighted norm solution can be done iteratively using the ART algorithm [146].

When we weight the skull area with the inverse of the prior image, we allow the reconstruction to place higher values there without having much of an effect on the overall weighted norm. In addition, the reciprocal weighting in the interior makes spreading intensity into that region costly, so the interior remains relatively clear, allowing us to see what is really present there.

When we try to reconstruct an image from limited data, it is easy to assume that the information we seek has been lost, particularly when a reasonable reconstruction method fails to reveal what we want to know. As this example, and many others, show, the information we seek is often still in the data, but needs to be brought out in a more subtle way.

1.8 Exercises

1.1 *For $n = 1, 2, ...,$ let α_n be defined by*

$$\alpha_n = \inf\{f(x) | \, \|x - a\| \leq \frac{1}{n}\}.$$

Show that the sequence $\{\alpha_n\}$ is increasing, bounded above by $f(a)$ and converges to $\alpha = \liminf_{x \to a} f(x)$.

1.2 *For $n = 1, 2, ...,$ let β_n be defined by*

$$\beta_n = \sup\{f(x) | \, \|x - a\| \leq \frac{1}{n}\}.$$

Show that the sequence $\{\beta_n\}$ is decreasing, bounded below by $f(a)$ and converges to $\beta = \limsup_{x \to a} f(x)$.

1.3 *Prove Proposition 1.1.*

1.9 Course Homework

Do all the exercises in this chapter.

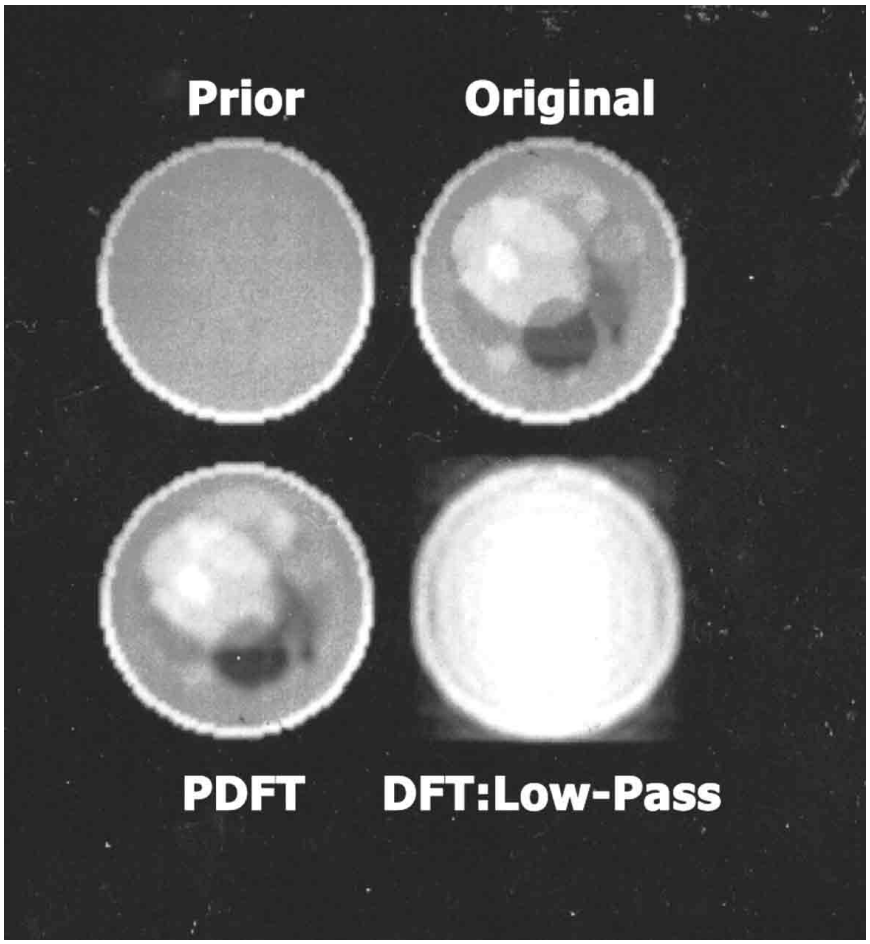

Figure 1.1: Extracting information in image reconstruction.

Chapter 2

Optimization Without Calculus

2.1 Chapter Summary

In our study of optimization, we shall encounter a number of sophisticated techniques, involving first and second partial derivatives, systems of linear equations, nonlinear operators, specialized distance measures, and so on. It is good to begin by looking at what can be accomplished without sophisticated techniques, even without calculus. It is possible to achieve much with powerful, yet simple, inequalities. As someone once remarked, exaggerating slightly, in the right hands, the Cauchy Inequality and integration by parts are all that are really needed.

Students typically encounter optimization problems as applications of differentiation, while the possibility of optimizing without calculus is left unexplored. In this chapter we develop the Arithmetic Mean-Geometric Mean Inequality, abbreviated the AGM Inequality, from the convexity of the logarithm function, use the AGM to derive several important inequalities, including Cauchy's Inequality, and then discuss optimization methods based on the Arithmetic Mean-Geometric Mean Inequality and Cauchy's Inequality.

2.2 The Arithmetic Mean-Geometric Mean Inequality

Let $x_1, ..., x_N$ be positive numbers. According to the famous *Arithmetic Mean-Geometric Mean Inequality*, abbreviated AGM Inequality,

$$G = (x_1 \cdot x_2 \cdot \cdots x_N)^{1/N} \leq A = \frac{1}{N}(x_1 + x_2 + ... + x_N), \tag{2.1}$$

with equality if and only if $x_1 = x_2 = ... = x_N$. To prove this, consider the following modification of the product $x_1 \cdots x_N$. Replace the smallest of the x_n, call it x, with A and the largest, call it y, with $x + y - A$. This modification does not change the arithmetic mean of the N numbers, but the product increases, unless $x = y = A$ already, since $xy \leq A(x + y - A)$ (Why?). We repeat this modification, until all the x_n approach A, at which point the product reaches its maximum.

For example, $2 \cdot 3 \cdot 4 \cdot 6 \cdot 20$ becomes $3 \cdot 4 \cdot 6 \cdot 7 \cdot 15$, and then $4 \cdot 6 \cdot 7 \cdot 7 \cdot 11$, $6 \cdot 7 \cdot 7 \cdot 7 \cdot 8$, and finally $7 \cdot 7 \cdot 7 \cdot 7 \cdot 7$.

2.3 An Application of the AGM Inequality: the Number e

We can use the AGM Inequality to show that

$$\lim_{n\to\infty}(1 + \frac{1}{n})^n = e. \tag{2.2}$$

Let $f(n) = (1 + \frac{1}{n})^n$, the product of the $n + 1$ numbers $1, 1 + \frac{1}{n}, ..., 1 + \frac{1}{n}$. Applying the AGM Inequality, we obtain the inequality

$$f(n) \leq \Big(\frac{n+2}{n+1}\Big)^{n+1} = f(n + 1),$$

so we know that the sequence $\{f(n)\}$ is increasing. Now define $g(n) = (1 + \frac{1}{n})^{n+1}$; we show that $g(n) \leq g(n-1)$ and $f(n) \leq g(m)$, for all positive integers m and n. Consider $(1 - \frac{1}{n})^n$, the product of the $n + 1$ numbers $1, 1 - \frac{1}{n}, ..., 1 - \frac{1}{n}$. Applying the AGM Inequality, we find that

$$\Big(1 - \frac{1}{n+1}\Big)^{n+1} \geq \Big(1 - \frac{1}{n}\Big)^n,$$

or

$$\Big(\frac{n}{n+1}\Big)^{n+1} \geq \Big(\frac{n-1}{n}\Big)^n.$$

Taking reciprocals, we get $g(n) \leq g(n-1)$. Since $f(n) < g(n)$ and $\{f(n)\}$ is increasing, while $\{g(n)\}$ is decreasing, we can conclude that $f(n) \leq g(m)$,

for all positive integers m and n. Both sequences therefore have limits. Because the difference

$$g(n) - f(n) = \frac{1}{n}(1 + \frac{1}{n})^n \to 0,$$

as $n \to \infty$, we conclude that the limits are the same. This common limit we can define as the number e.

2.4 Extending the AGM Inequality

Suppose, once again, that $x_1, ..., x_N$ are positive numbers. Let $a_1, ..., a_N$ be positive numbers that sum to one. Then the *Generalized AGM Inequality* (GAGM Inequality) is

$$x_1^{a_1} x_2^{a_2} \cdots x_N^{a_N} \leq a_1 x_1 + a_2 x_2 + ... + a_N x_N, \tag{2.3}$$

with equality if and only if $x_1 = x_2 = ... = x_N$. We can prove this using the convexity of the function $-\log x$.

A function $f(x)$ is said to be *convex* over an interval (a, b) if

$$f(a_1 t_1 + a_2 t_2 + ... + a_N t_N) \leq a_1 f(t_1) + a_2 f(t_2) + ... + a_N f(t_N),$$

for all positive integers N, all a_n as above, and all real numbers t_n in (a, b). If the function $f(x)$ is twice differentiable on (a, b), then $f(x)$ is convex over (a, b) if and only if the second derivative of $f(x)$ is non-negative on (a, b). For example, the function $f(x) = -\log x$ is convex on the positive x-axis. The GAGM Inequality follows immediately.

2.5 Optimization Using the AGM Inequality

We illustrate the use of the AGM Inequality for optimization through several examples.

2.5.1 Example 1

Find the minimum of the function

$$f(x, y) = \frac{12}{x} + \frac{18}{y} + xy,$$

over positive x and y.

We note that the three terms in the sum have a fixed product of 216, so, by the AGM Inequality, the smallest value of $\frac{1}{3} f(x, y)$ is $(216)^{1/3} = 6$ and occurs when the three terms are equal and each equal to 6, so when $x = 2$ and $y = 3$. The smallest value of $f(x, y)$ is therefore 18.

2.5.2 Example 2

Find the maximum value of the product

$$f(x,y) = xy(72 - 3x - 4y),$$

over positive x and y.

The terms x, y and $72 - 3x - 4y$ do not have a constant sum, but the terms $3x$, $4y$ and $72 - 3x - 4y$ do have a constant sum, namely 72, so we rewrite $f(x,y)$ as

$$f(x,y) = \frac{1}{12}(3x)(4y)(72 - 3x - 4y).$$

By the AGM Inequality, the product $(3x)(4y)(72 - 3x - 4y)$ is maximized when the factors $3x$, $4y$ and $72 - 3x - 4y$ are each equal to 24, so when $x = 8$ and $y = 6$. The maximum value of the product is then 1152.

2.5.3 Example 3

Both of the previous two problems can be solved using the standard calculus technique of setting the two first partial derivatives to zero. Here is an example that is not so easily solved in that way: minimize the function

$$f(x,y) = 4x + \frac{x}{y^2} + \frac{4y}{x},$$

over positive values of x and y. Try taking the first partial derivatives and setting them both to zero. Even if we managed to solve this system of coupled nonlinear equations, deciding if we actually have found the minimum is not easy; take a look at the second derivative matrix, the Hessian matrix. We can employ the AGM Inequality by rewriting $f(x,y)$ as

$$f(x,y) = 4\Big(\frac{4x + \frac{x}{y^2} + \frac{2y}{x} + \frac{2y}{x}}{4}\Big).$$

The product of the four terms in the arithmetic mean expression is 16, so the GM is 2. Therefore, $\frac{1}{4}f(x,y) \geq 2$, with equality when all four terms are equal to 2; that is, $4x = 2$, so that $x = \frac{1}{2}$ and $\frac{2y}{x} = 2$, so $y = \frac{1}{2}$ also. The minimum value of $f(x,y)$ is then 8.

2.6 The Hölder and Minkowski Inequalities

Let $c = (c_1, ..., c_N)$ and $d = (d_1, ..., d_N)$ be vectors with complex entries and let p and q be positive real numbers such that

$$\frac{1}{p} + \frac{1}{q} = 1.$$

The p-norm of c is defined to be

$$\|c\|_p = \Big(\sum_{n=1}^{N} |c_n|^p \Big)^{1/p},$$

with the q-norm of d, denoted $\|d\|_q$, defined similarly.

2.6.1 Hölder's Inequality

Hölder's Inequality is the following:

$$\sum_{n=1}^{N} |c_n d_n| \leq \|c\|_p \|d\|_q,$$

with equality if and only if

$$\Big(\frac{|c_n|}{\|c\|_p} \Big)^p = \Big(\frac{|d_n|}{\|d\|_q} \Big)^q,$$

for each n.

Hölder's Inequality follows from the GAGM Inequality. To see this, we fix n and apply Inequality (2.3), with

$$x_1 = \Big(\frac{|c_n|}{\|c\|_p} \Big)^p,$$

$$a_1 = \frac{1}{p},$$

$$x_2 = \Big(\frac{|d_n|}{\|d\|_q} \Big)^q,$$

and

$$a_2 = \frac{1}{q}.$$

From (2.3) we then have

$$\Big(\frac{|c_n|}{\|c\|_p} \Big) \Big(\frac{|d_n|}{\|d\|_q} \Big) \leq \frac{1}{p} \Big(\frac{|c_n|}{\|c\|_p} \Big)^p + \frac{1}{q} \Big(\frac{|d_n|}{\|d\|_q} \Big)^q.$$

Now sum both sides over the index n.

2.6.2 Minkowski's Inequality

Minkowski's Inequality, which is a consequence of Hölder's Inequality, states that

$$\|c + d\|_p \leq \|c\|_p + \|d\|_p \,;$$

it is the triangle inequality for the metric induced by the p-norm.

To prove Minkowski's Inequality, we write

$$\sum_{n=1}^{N} |c_n + d_n|^p \leq \sum_{n=1}^{N} |c_n|(|c_n + d_n|)^{p-1} + \sum_{n=1}^{N} |d_n|(|c_n + d_n|)^{p-1}.$$

Then we apply Hölder's Inequality to both of the sums.

2.7 Cauchy's Inequality

For the choices $p = q = 2$, Hölder's Inequality becomes the famous Cauchy Inequality, which we rederive in a different way in this section. For simplicity, we assume now that the vectors have real entries and for notational convenience later we use x_n and y_n in place of c_n and d_n.

Let $x = (x_1, ..., x_N)$ and $y = (y_1, ..., y_N)$ be vectors with real entries. The *inner product* of x and y is

$$\langle x, y \rangle = x_1 y_1 + x_2 y_2 + ... + x_N y_N. \tag{2.4}$$

The 2-norm of the vector x, which we shall simply call the *norm* of the vector x is

$$\|x\|_2 = \|x\| = \sqrt{\langle x, x \rangle}.$$

Cauchy's Inequality is

$$|\langle x, y \rangle| \leq \|x\| \, \|y\|, \tag{2.5}$$

with equality if and only if there is a real number a such that $x = ay$.

To prove Cauchy's Inequality, we begin with the fact that, for every real number t,

$$0 \leq \|x - ty\|^2 = \|x\|^2 - (2\langle x, y \rangle)t + \|y\|^2 t^2.$$

This quadratic in the variable t is never negative, so cannot have two real roots. It follows that the term under the radical sign in the quadratic equation must be non-positive, that is,

$$(2\langle x, y \rangle)^2 - 4\|y\|^2 \|x\|^2 \leq 0. \tag{2.6}$$

We have equality in (2.6) if and only if the quadratic has a double real root, say $t = a$. Then we have

$$\|x - ay\|^2 = 0.$$

As an aside, suppose we had allowed the variable t to be complex. Clearly $\|x - ty\|$ cannot be zero for any non-real value of t. Doesn't this contradict the fact that every quadratic has two roots in the complex plane?

The Pólya-Szegö Inequality

We can interpret Cauchy's Inequality as providing an upper bound for the quantity

$$\Big(\sum_{n=1}^{N} x_n y_n\Big)^2.$$

The *Pólya-Szegö Inequality* provides a lower bound for the same quantity. Let $0 < m_1 \leq x_n \leq M_1$ and $0 < m_2 \leq y_n \leq M_2$, for all n. Then

$$\sum_{n=1}^{N} x_n^2 \sum_{n=1}^{N} y_n^2 \leq \frac{M_1 M_2 + m_1 m_2}{4 m_1 m_2 M_1 M_2} \Big(\sum_{n=1}^{N} x_n y_n\Big)^2. \tag{2.7}$$

2.8 Optimizing using Cauchy's Inequality

We present two examples to illustrate the use of Cauchy's Inequality in optimization.

2.8.1 Example 4

Find the largest and smallest values of the function

$$f(x, y, z) = 2x + 3y + 6z, \tag{2.8}$$

among the points (x, y, z) with $x^2 + y^2 + z^2 = 1$.

From Cauchy's Inequality we know that

$$49 = (2^2 + 3^2 + 6^2)(x^2 + y^2 + z^2) \geq (2x + 3y + 6z)^2,$$

so that $f(x, y, z)$ lies in the interval $[-7, 7]$. We have equality in Cauchy's Inequality if and only if the vector $(2, 3, 6)$ is parallel to the vector (x, y, z), that is

$$\frac{x}{2} = \frac{y}{3} = \frac{z}{6}.$$

It follows that $x = t$, $y = \frac{3}{2}t$, and $z = 3t$, with $t^2 = \frac{4}{49}$. The smallest value of $f(x, y, z)$ is -7, when $x = -\frac{2}{7}$, and the largest value is $+7$, when $x = \frac{2}{7}$.

2.8.2 Example 5

The simplest problem in estimation theory is to estimate the value of a constant c, given J data values $z_j = c + v_j$, $j = 1, ..., J$, where the v_j are random variables representing additive noise or measurement error.

Assume that the expected values of the v_j are $E(v_j) = 0$, the v_j are uncorrelated, so $E(v_j v_k) = 0$ for j different from k, and the variances of the v_j are $E(v_j^2) = \sigma_j^2 > 0$. A *linear* estimate of c has the form

$$\hat{c} = \sum_{j=1}^{J} b_j z_j. \tag{2.9}$$

The estimate $\hat{c}$ is *unbiased* if $E(\hat{c}) = c$, which forces $\sum_{j=1}^{J} b_j = 1$. The *best* linear unbiased estimator, the BLUE, is the one for which $E((\hat{c} - c)^2)$ is minimized. This means that the b_j must minimize

$$E\Big(\sum_{j=1}^{J}\sum_{k=1}^{J} b_j b_k v_j v_k\Big) = \sum_{j=1}^{J} b_j^2 \sigma_j^2, \tag{2.10}$$

subject to

$$\sum_{j=1}^{J} b_j = 1. \tag{2.11}$$

To solve this minimization problem, we turn to Cauchy's Inequality.

We can write

$$1 = \sum_{j=1}^{J} b_j = \sum_{j=1}^{J} (b_j \sigma_j)\frac{1}{\sigma_j}.$$

Cauchy's Inequality then tells us that

$$1 \leq \sqrt{\sum_{j=1}^{J} b_j^2 \sigma_j^2}\sqrt{\sum_{j=1}^{J} \frac{1}{\sigma_j^2}},$$

with equality if and only if there is a constant, say λ, such that

$$b_j \sigma_j = \lambda \frac{1}{\sigma_j},$$

for each j. So we have

$$b_j = \lambda \frac{1}{\sigma_j^2},$$

for each j. Summing on both sides and using Equation (2.11), we find that

$$\lambda = 1/\sum_{j=1}^{J} \frac{1}{\sigma_j^2}.$$

The BLUE is therefore

$$\hat{c} = \lambda \sum_{j=1}^{J} \frac{z_j}{\sigma_j^2}. \tag{2.12}$$

When the variances σ_j^2 are all the same, the BLUE is simply the arithmetic mean of the data values z_j.

2.8.3 Example 6

One of the fundamental operations in signal processing is the filtering the data vector $x = \gamma s + n$, to remove the noise component n, while leaving the signal component s relatively unaltered [45]. This can be done either to estimate γ, the amount of the signal vector s present, or to detect if the signal is present at all, that is, to decide if $\gamma = 0$ or not. The noise is typically known only through its *covariance matrix* Q, which is the positive-definite, symmetric matrix having for its entries $Q_{jk} = E(n_j n_k)$. The filter usually is linear and takes the form of an estimate of γ:

$$\hat{\gamma} = b^T x.$$

We want $|b^T s|^2$ large, and, on average, $|b^T n|^2$ small; that is, we want $E(|b^T n|^2) = b^T E(nn^T)b = b^T Q b$ small. The best choice is the vector b that maximizes the *gain* of the filter, that is, the ratio

$$|b^T s|^2 / b^T Q b.$$

We can solve this problem using the Cauchy Inequality.

Definition 2.1 *Let S be a square matrix. A non-zero vector u is an* eigenvector *of S if there is a scalar λ such that $Su = \lambda u$. Then the scalar λ is said to be an* eigenvalue *of S associated with the eigenvector u.*

Definition 2.2 *The* transpose*, $B = A^T$, of an M by N matrix A is the N by M matrix having the entries $B_{n,m} = A_{m,n}$.*

Definition 2.3 *A square matrix S is* symmetric *if $S^T = S$.*

A basic theorem in linear algebra is that, for any symmetric N by N matrix S, R^N has an orthonormal basis consisting of mutually orthogonal, norm-one eigenvectors of S. If we then define U to be the matrix whose columns are these eigenvectors and L the diagonal matrix with the associated eigenvalues on the diagonal, we can easily see that U is an *orthogonal matrix*, that is, $U^T U = I$. We can then write

$$S = ULU^T; \tag{2.13}$$

this is the *eigenvalue/eigenvector decomposition* of S. The eigenvalues of a symmetric S are always real numbers.

Definition 2.4 *A J by J symmetric matrix Q is* non-negative definite *if, for every x in R^J, we have $x^TQx \geq 0$. If $x^TQx > 0$ whenever x is not the zero vector, then Q is said to be positive definite.*

We leave it to the reader to show that the eigenvalues of a non-negative (positive) definite matrix are always non-negative (positive).

A covariance matrix Q is always non-negative definite, since

$$x^TQx = E(|\sum_{j=1}^{J} x_j n_j|^2). \tag{2.14}$$

Therefore, its eigenvalues are non-negative; typically, they are actually positive, as we shall assume now. We then let $C = U\sqrt{L}U^T$, the symmetric square root of Q. The Cauchy Inequality then tells us that

$$|b^Ts|^2 = |b^TCC^{-1}s|^2 \leq [b^TCC^Tb][s^T(C^{-1})^TC^{-1}s],$$

with equality if and only if the vectors C^Tb and $C^{-1}s$ are parallel. It follows that

$$b = \alpha(CC^T)^{-1}s = \alpha Q^{-1}s,$$

for any constant α. It is standard practice to select α so that $b^Ts = 1$, therefore $\alpha = 1/s^TQ^{-1}s$ and the optimal filter b is

$$b = \frac{1}{s^TQ^{-1}s}Q^{-1}s.$$

2.9 An Inner Product for Square Matrices

The *trace* of a square matrix M, denoted tr$M$, is the sum of the entries down the main diagonal. Given square matrices A and B with real entries, the trace of the product B^TA defines an inner product, that is

$$\langle A, B\rangle = \text{tr}(B^TA),$$

where the superscript T denotes the transpose of a matrix. This inner product can then be used to define a norm of A, called the *Frobenius norm*, by

$$\|A\|_F = \sqrt{\langle A, A\rangle} = \sqrt{\text{tr}(A^TA)}. \tag{2.15}$$

From the eigenvector/eigenvalue decomposition, we know that, for every symmetric matrix S, there is an orthogonal matrix U such that

$$S = UD(\lambda(S))U^T,$$

where $\lambda(S) = (\lambda_1, ..., \lambda_N)$ is a vector whose entries are eigenvalues of the symmetric matrix S, and $D(\lambda(S))$ is the diagonal matrix whose entries are the entries of $\lambda(S)$. Then we can easily see that

$$\|S\|_F = \|\lambda(S)\|.$$

Denote by $[\lambda(S)]$ the vector of eigenvalues of S, ordered in non-increasing order. We have the following result.

Theorem 2.1 (Fan's Theorem) *Any real symmetric matrices S and R satisfy the inequality*

$$\mathrm{tr}(SR) \leq \langle [\lambda(S)], [\lambda(R)] \rangle,$$

with equality if and only if there is an orthogonal matrix U such that

$$S = UD([\lambda(S)])U^T,$$

and

$$R = UD([\lambda(R)])U^T.$$

From linear algebra, we know that S and R can be simultaneously diagonalized if and only if they commute; this is a stronger condition than simultaneous diagonalization.

If S and R are diagonal matrices already, then Fan's Theorem tells us that

$$\langle \lambda(S), \lambda(R) \rangle \leq \langle [\lambda(S)], [\lambda(R)] \rangle.$$

Since any real vectors x and y are $\lambda(S)$ and $\lambda(R)$, for some symmetric S and R, respectively, we have the following
Hardy-Littlewood-Polya Inequality:

$$\langle x, y \rangle \leq \langle [x], [y] \rangle.$$

Most of the optimization problems discussed in this chapter fall under the heading of Geometric Programming, which we shall present in a more formal way in a subsequent chapter.

2.10 Discrete Allocation Problems

Most of the optimization problems we consider in this book are *continuous* problems, in the sense that the variables involved are free to take on values within a continuum. A large branch of optimization deals with *discrete* problems. Typically, these discrete problems can be solved, in principle, by an exhaustive checking of a large, but finite, number of possibilities; what is needed is a faster method. The *optimal allocation* problem is a good example of a discrete optimization problem.

We have n different jobs to assign to n different people. For $i = 1, ..., n$ and $j = 1, ..., n$ the quantity C_{ij} is the cost of having person i do job j. The n by n matrix C with these entries is the *cost matrix*. An *assignment* is a selection of n entries of C so that no two are in the same column or the same row; that is, everybody gets one job. Our goal is to find an assignment that minimizes the total cost.

We know that there are $n!$ ways to make assignments, so one solution method would be to determine the cost of each of these assignments and select the cheapest. But for large n this is impractical. We want an algorithm that will solve the problem with less calculation. The algorithm we present here, discovered in the 1930's by two Hungarian mathematicians, is called, appropriately, the Hungarian Method.

To illustrate, suppose there are three people and three jobs, and the cost matrix is

$$C = \begin{bmatrix} 53 & 96 & 37 \\ 47 & 87 & 41 \\ 60 & 92 & 36 \end{bmatrix}. \tag{2.16}$$

The number 41 in the second row, third column indicates that it costs 41 dollars to have the second person perform the third job.

The algorithm is as follows:

- **Step 1:** Subtract the minimum of each row from all the entries of that row. This is equivalent to saying that each person charges a minimum amount just to be considered, which must be paid regardless of the allocation made. All we can hope to do now is to reduce the remaining costs. Subtracting these fixed costs, which do not depend on the allocations, does not change the optimal solution.

  The new matrix is then

$$\begin{bmatrix} 16 & 59 & 0 \\ 6 & 46 & 0 \\ 24 & 56 & 0 \end{bmatrix}. \tag{2.17}$$

- **Step 2:** Subtract each column minimum from the entries of its column. This is equivalent to saying that each job has a minimum cost, regardless of who performs it, perhaps for materials, say, or a permit. Subtracting those costs does not change the optimal solution. The matrix becomes

$$\begin{bmatrix} 10 & 13 & 0 \\ 0 & 0 & 0 \\ 18 & 10 & 0 \end{bmatrix}. \tag{2.18}$$

- **Step 3:** Draw a line through the smallest number of rows and columns that results in all zeros being covered by a line; here I have put in boldface the entries covered by a line. The matrix becomes

$$\begin{bmatrix} 10 & 13 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 18 & 10 & \mathbf{0} \end{bmatrix}. \tag{2.19}$$

  We have used a total of two lines, one row and one column. What we are searching for is a set of zeros such that each row and each column contains a zero. Then n lines will be required to cover the zeros.

- **Step 4:** If the number of lines just drawn is n we have finished; the zeros just covered by a line tell us the assignment we want. Since n lines are needed, there must be a zero in each row and in each column. In our example, we are not finished.

- **Step 5:** If, as in our example, the number of lines drawn is fewer than n, determine the smallest entry not yet covered by a line (not boldface, here). It is 10 in our example. Then subtract this number from all the uncovered entries and add it to all the entries covered by both a vertical and horizontal line.

  This rather complicated step can be explained as follows. It is equivalent to, first, subtracting this smallest entry from all entries of each row not yet completely covered by a line, whether or not the entry is zero, and second, adding this quantity to every column covered by a line. This second step has the effect of restoring to zero those zero values that just became negative. As we have seen, subtracting the same quantity from every entry of a row does not change the optimal solution; we are just raising the fixed cost charged by certain of the participants. Similarly, adding the same quantity to each entry of a column just increases the cost of the job, regardless of who performs it, so does not change the optimal solution.

  Our matrix becomes

$$\begin{bmatrix} 0 & 3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 10 \\ 8 & 0 & \mathbf{0} \end{bmatrix}. \tag{2.20}$$

  Now return to Step 3.

In our example, when we return to Step 3 we find that we need three lines now and so we are finished. There are two optimal allocations: one is to assign the first job to the first person, the second job to the second person, and the third job to the third person, for a total cost of 176 dollars; the other optimal allocation is to assign the second person to the first job, the third person to the second job, and the first person to the third job, again with a total cost of 176 dollars.

2.11 Exercises

2.1 *Let A be the arithmetic mean of a finite set of positive numbers, with x the smallest of these numbers, and y the largest. Show that*

$$xy \leq A(x + y - A),$$

with equality if and only if $x = y = A$.

2.2 *Minimize the function*

$$f(x) = x^2 + \frac{1}{x^2} + 4x + \frac{4}{x},$$

over positive x. Note that the minimum value of $f(x, y)$ is not the one suggested by the AGM Inequality, as applied to the four terms taken together.

2.3 *Find the maximum value of $f(x, y) = x^2y$, if x and y are restricted to positive real numbers for which $6x + 5y = 45$.*

2.4 *Find the smallest value of*

$$f(x) = 5x + \frac{16}{x} + 21,$$

over positive x.

2.5 *Find the smallest value of the function*

$$f(x) = \sqrt{x^2 + y^2},$$

among those values of x and y satisfying $3x - y = 20$.

2.6 *Find the maximum and minimum values of the function*

$$f(x) = \sqrt{100 + x^2} - x$$

over non-negative x.

2.7 *Multiply out the product*

$$(x + y + z)(\frac{1}{x} + \frac{1}{y} + \frac{1}{z})$$

and deduce that the least value of this product, over non-negative x, y, and z, is 9. Use this to find the least value of the function

$$f(x) = \frac{1}{x} + \frac{1}{y} + \frac{1}{z},$$

over non-negative x, y, and z having a constant sum c.

2.8 *The* harmonic mean *of positive numbers $a_1, ..., a_N$ is*

$$H = [(\frac{1}{a_1} + ... + \frac{1}{a_N})/N]^{-1}.$$

Prove that the geometric mean G is not less than H.

2.9 *Prove that*

$$(\frac{1}{a_1} + ... + \frac{1}{a_N})(a_1 + ... + a_N) \geq N^2,$$

with equality if and only if $a_1 = ... = a_N$.

2.10 *Show that the Equation (2.13), $S = ULU^T$, can be written as*

$$S = \lambda_1 u^1 (u^1)^T + \lambda_2 u^2 (u^2)^T + ... + \lambda_N u^N (u^N)^T, \tag{2.21}$$

and

$$S^{-1} = \frac{1}{\lambda_1} u^1 (u^1)^T + \frac{1}{\lambda_2} u^2 (u^2)^T + ... + \frac{1}{\lambda_N} u^N (u^N)^T. \tag{2.22}$$

2.11 *Let Q be positive-definite, with positive eigenvalues*

$$\lambda_1 \geq ... \geq \lambda_N > 0$$

and associated mutually orthogonal norm-one eigenvectors u^n. Show that

$$x^T Q x \leq \lambda_1,$$

for all vectors x with $\|x\| = 1$, with equality if $x = u^1$. Hints: use

$$1 = \|x\|^2 = x^T x = x^T I x,$$

$$I = u^1 (u^1)^T + ... + u^N (u^N)^T,$$

and Equation (2.21).

2.12 *Relate Example 4 to eigenvectors and eigenvalues.*

2.13 Young's Inequality *Suppose that p and q are positive numbers greater than one such that $\frac{1}{p} + \frac{1}{q} = 1$. If x and y are positive numbers, then*

$$xy \leq \frac{x^p}{p} + \frac{y^q}{q},$$

with equality if and only if $x^p = y^q$. Hint: use the GAGM Inequality.

2.14 ([133]) *For given constants c and d, find the largest and smallest values of $cx + dy$ taken over all points (x, y) of the ellipse*

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1.$$

2.15 ([133]) *Find the largest and smallest values of $2x + y$ on the circle $x^2 + y^2 = 1$. Where do these values occur? What does this have to do with eigenvectors and eigenvalues?*

2.16 *When a real M by N matrix A is stored in the computer it is usually vectorized; that is, the matrix*

$$A = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2N} \\ . & & & \\ . & & & \\ . & & & \\ A_{M1} & A_{M2} & \dots & A_{MN} \end{bmatrix}$$

becomes

$$\mathbf{vec}(A) = (A_{11}, A_{21}, ..., A_{M1}, A_{12}, A_{22}, ..., A_{M2}, ..., A_{MN})^T.$$

Show that the dot product $\mathbf{vec}(A) \cdot \mathbf{vec}(B) = \mathbf{vec}(B)^T \mathbf{vec}(A)$ can be obtained by

$$\mathbf{vec}(A) \cdot \mathbf{vec}(B) = \text{trace}\,(AB^T) = \text{trace}\,(B^T A).$$

2.17 *Apply the Hungarian Method to solve the allocation problem with the cost matrix*

$$C = \begin{bmatrix} 90 & 75 & 75 & 80 \\ 35 & 85 & 55 & 65 \\ 125 & 95 & 90 & 105 \\ 45 & 110 & 95 & 115 \end{bmatrix}. \tag{2.23}$$

2.12 Course Homework

In this chapter, the homework exercises for the course are Exercises 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 2.10, 2.11, and 2.17.

Chapter 3

Geometric Programming

3.1 Chapter Summary

Geometric Programming (GP) involves the minimization of functions of a special type, known as posynomials. The first systematic treatment of geometric programming appeared in the book [80], by Duffin, Peterson and Zener, the founders of geometric programming. As we shall see, the Generalized Arithmetic-Geometric Mean Inequality plays an important role in the theoretical treatment of geometric programming. In this chapter we introduce the notions of duality and cross-entropy distance, and begin our study of iterative algorithms.

3.2 An Example of a GP Problem

The following optimization problem was presented originally by Duffin, *et al.* [80] and discussed by Peressini *et al.* in [136]. It illustrates well the type of problem considered in geometric programming. Suppose that 400 cubic yards of gravel must be ferried across a river in an open box of length t_1, width t_2 and height t_3. Each round-trip cost ten cents. The sides and the bottom of the box cost 10 dollars per square yard to build, while the ends of the box cost twenty dollars per square yard. The box will have no salvage value after it has been used. Determine the dimensions of the box that minimize the total cost.

With $t = (t_1, t_2, t_3)$, the cost function is

$$g(t) = \frac{40}{t_1 t_2 t_3} + 20t_1t_3 + 10t_1t_2 + 40t_2t_3, \tag{3.1}$$

which is to be minimized over $t_j > 0$, for $j = 1, 2, 3$. The function $g(t)$ is an example of a posynomial.

3.3 Posynomials and the GP Problem

Functions $g(t)$ of the form

$$g(t) = \sum_{i=1}^{n} c_i \Big(\prod_{j=1}^{m} t_j^{a_{ij}} \Big), \tag{3.2}$$

with $t = (t_1, ..., t_m)$, the $t_j > 0$, $c_i > 0$ and a_{ij} real, are called *posynomials*. The *geometric programming problem*, denoted (GP), is to minimize a given posynomial over positive t. In order for the minimum to be greater than zero, we need some of the a_{ij} to be negative.

We denote by $u_i(t)$ the function

$$u_i(t) = c_i \prod_{j=1}^{m} t_j^{a_{ij}}, \tag{3.3}$$

so that

$$g(t) = \sum_{i=1}^{n} u_i(t). \tag{3.4}$$

For any choice of $\delta_i > 0$, $i = 1, ..., n$, with

$$\sum_{i=1}^{n} \delta_i = 1,$$

we have

$$g(t) = \sum_{i=1}^{n} \delta_i \Big(\frac{u_i(t)}{\delta_i} \Big). \tag{3.5}$$

Applying the Generalized Arithmetic-Geometric Mean (GAGM) Inequality, we have

$$g(t) \geq \prod_{i=1}^{n} \Big(\frac{u_i(t)}{\delta_i} \Big)^{\delta_i}. \tag{3.6}$$

Therefore,

$$g(t) \geq \prod_{i=1}^{n} \Big(\frac{c_i}{\delta_i} \Big)^{\delta_i} \left(\prod_{i=1}^{n} \prod_{j=1}^{m} t_j^{a_{ij}\delta_i} \right), \tag{3.7}$$

or

$$g(t) \geq \prod_{i=1}^{n} \Big(\frac{c_i}{\delta_i} \Big)^{\delta_i} \Big(\prod_{j=1}^{m} t_j^{\sum_{i=1}^{n} a_{ij}\delta_i} \Big), \tag{3.8}$$

Suppose that we can find $\delta_i > 0$ with

$$\sum_{i=1}^{n} a_{ij}\delta_i = 0, \tag{3.9}$$

for each j. Then the inequality in (3.8) becomes

$$g(t) \geq v(\delta), \tag{3.10}$$

for

$$v(\delta) = \prod_{i=1}^{n} \left(\frac{c_i}{\delta_i}\right)^{\delta_i}. \tag{3.11}$$

3.4 The Dual GP Problem

The *dual geometric programming problem*, denoted (DGP), is to maximize the function $v(\delta)$, over all *feasible* $\delta = (\delta_1, ..., \delta_n)$, that is, all positive δ for which

$$\sum_{i=1}^{n} \delta_i = 1, \tag{3.12}$$

and

$$\sum_{i=1}^{n} a_{ij}\delta_i = 0, \tag{3.13}$$

for each $j = 1, ..., m$. Clearly, we have

$$g(t) \geq v(\delta), \tag{3.14}$$

for any positive t and feasible δ. Of course, there may be no feasible δ, in which case (DGP) is said to be *inconsistent*.

As we have seen, the inequality in (3.14) is based on the GAGM Inequality. We have equality in the GAGM Inequality if and only if the terms in the arithmetic mean are all equal. In this case, this says that there is a constant λ such that

$$\frac{u_i(t)}{\delta_i} = \lambda, \tag{3.15}$$

for each $i = 1, ..., n$. Using the fact that the δ_i sum to one, it follows that

$$\lambda = \sum_{i=1}^{n} u_i(t) = g(t), \tag{3.16}$$

and

$$\delta_i = \frac{u_i(t)}{g(t)}, \tag{3.17}$$

for each $i = 1, ..., n$. As the theorem below asserts, if t^* is positive and minimizes $g(t)$, then δ^*, the associated δ from Equation (3.17), is feasible and solves (DGP). Since we have equality in the GAGM Inequality now, we have

$$g(t^*) = v(\delta^*).$$

The main theorem in geometric programming is the following.

Theorem 3.1 *If $t^* > 0$ minimizes $g(t)$, then (DGP) is consistent. In addition, the choice*

$$\delta_i^* = \frac{u_i(t^*)}{g(t^*)} \tag{3.18}$$

is feasible and solves (DGP). Finally,

$$g(t^*) = v(\delta^*); \tag{3.19}$$

that is, there is no duality gap.

Proof: We have

$$\frac{\partial u_i}{\partial t_j}(t^*) = \frac{a_{ij} u_i(t^*)}{t_j^*}, \tag{3.20}$$

so that

$$t_j^* \frac{\partial u_i}{\partial t_j}(t^*) = a_{ij} u_i(t^*), \tag{3.21}$$

for each $j = 1, ..., m$. Since t^* minimizes $g(t)$, we have

$$0 = \frac{\partial g}{\partial t_j}(t^*) = \sum_{i=1}^{n} \frac{\partial u_i}{\partial t_j}(t^*), \tag{3.22}$$

so that, from Equation (3.21), we have

$$0 = \sum_{i=1}^{n} a_{ij} u_i(t^*), \tag{3.23}$$

for each $j = 1, ..., m$. It follows that δ^* is feasible. Since we have equality in the GAGM Inequality, we know

$$g(t^*) = v(\delta^*). \tag{3.24}$$

Therefore, δ^* solves (DGP). This completes the proof. ∎

3.5 Solving the GP Problem

The theorem suggests how we might go about solving (GP). First, we try to find a feasible δ^* that maximizes $v(\delta)$. This means we have to find a positive solution to the system of $m+1$ linear equations in n unknowns, given by

$$\sum_{i=1}^{n} \delta_i = 1, \tag{3.25}$$

and

$$\sum_{i=1}^{n} a_{ij}\delta_i = 0, \tag{3.26}$$

for $j = 1, ..., m$, such that $v(\delta)$ is maximized. As we shall see, the *multiplicative algebraic reconstruction technique* (MART) is an iterative procedure that we can use to find such δ. If there is no such vector, then (GP) has no minimizer. Once the desired δ^* has been found, we set

$$\delta_i^* = \frac{u_i(t^*)}{v(\delta^*)}, \tag{3.27}$$

for each $i = 1, ..., n$, and then solve for the entries of t^*. This last step can be simplified by taking logs; then we have a system of linear equations to solve for the values $\log t_j^*$.

3.6 Solving the DGP Problem

The iterative multiplicative algebraic reconstruction technique MART can be used to minimize the function $v(\delta)$, subject to linear equality constraints, provided that the matrix involved has nonnegative entries. We cannot apply the MART yet, because the matrix A^T does not satisfy these conditions.

3.6.1 The MART

The Kullback-Leibler, or KL distance [113] between positive numbers a and b is

$$KL(a, b) = a \log \frac{a}{b} + b - a. \tag{3.28}$$

We also define $KL(a, 0) = +\infty$ and $KL(0, b) = b$. Extending to nonnegative vectors $a = (a_1, ..., a_J)^T$ and $b = (b_1, ..., b_J)^T$, we have

$$KL(a, b) = \sum_{j=1}^{J} KL(a_j, b_j) = \sum_{j=1}^{J} \left(a_j \log \frac{a_j}{b_j} + b_j - a_j \right).$$

The MART is an iterative algorithm for finding a non-negative solution of the system $Px = y$, for an I by J matrix P with non-negative entries and vector y with positive entries. We also assume that

$$p_j = \sum_{i=1}^{I} P_{ij} > 0,$$

for all $i = 1, ..., I$. When discussing the MART, we say that the system $Px = y$ is *consistent* when it has non-negative solutions. We consider two different versions of the MART.

MART I

The iterative step of the first version of MART, which we shall call MART I, is the following: for $k = 0, 1, ...,$ and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \Big(\frac{y_i}{(Px^k)_i} \Big)^{P_{ij}/m_i},$$

for $j = 1, ..., J$, where the parameter m_i is defined to be

$$m_i = \max\{P_{ij} | j = 1, ..., J\}.$$

The MART I algorithm converges, in the consistent case, to the non-negative solution for which the KL distance $KL(x, x^0)$ is minimized.

MART II

The iterative step of the second version of MART, which we shall call MART II, is the following: for $k = 0, 1, ...,$ and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \Big(\frac{y_i}{(Px^k)_i} \Big)^{P_{ij}/p_j n_i},$$

for $j = 1, ..., J$, where the parameter n_i is defined to be

$$n_i = \max\{P_{ij} p_j^{-1} | j = 1, ..., J\}.$$

The MART II algorithm converges, in the consistent case, to the non-negative solution for which the KL distance

$$\sum_{j=1}^{J} p_j KL(x_j, x_j^0)$$

is minimized.

3.6.2 Using the MART to Solve the DGP Problem

The entries on the bottom row of A^T are all one, as is the bottom entry of the column vector u, since these entries correspond to the equation $\sum_{i=1}^{I} \delta_i = 1$. By adding suitably large positive multiples of this last equation to the other equations in the system, we obtain an equivalent system, $B^T\delta = s$, for which the new matrix B^T and the new vector s have only positive entries. Now we can apply the MART I algorithm to the system $B^T\delta = s$, letting $P = B^T$, $p_i = \sum_{j=1}^{J+1} B_{ij}$, $\delta = x$, $x^0 = c$ and $y = s$. In the consistent case, the MART I algorithm will find the non-negative solution that minimizes $KL(x, x^0)$, so we select $x^0 = c$. Then the MART I algorithm finds the non-negative δ^* satisfying $B^T\delta^* = s$, or, equivalently, $A^T\delta^* = u$, for which the KL distance

$$KL(\delta, c) = \sum_{i=1}^{I} \Big(\delta_i \log \frac{\delta_i}{c_i} + c_i - \delta_i\Big)$$

is minimized. Since we know that

$$\sum_{i=1}^{I} \delta_i = 1,$$

it follows that minimizing $KL(\delta, c)$ is equivalent to maximizing $v(\delta)$. Using δ^*, we find the optimal t^* solving the GP problem.

For example, the linear system of equations $A^T\delta = u$ corresponding to the posynomial in Equation (3.1) is

$$A^T\delta = u = \begin{bmatrix} -1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 1 \\ -1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \\ \delta_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

Adding two times the last row to the other rows, the system becomes

$$B^T\delta = s = \begin{bmatrix} 1 & 3 & 3 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 3 & 2 & 3 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \\ \delta_4 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 1 \end{bmatrix}.$$

The matrix B^T and the vector s are now positive. We are ready to apply the MART.

The MART iteration is as follows. With $j = k(\mathrm{mod}\,(J+1)) + 1$, $m_j = \max\{B_{ij}\,|i = 1, 2, ..., I\}$ and $k = 0, 1, ...$, let

$$\delta_i^{k+1} = \delta_i^k \Big(\frac{s_j}{(B^T\delta^k)_j}\Big)^{m_j^{-1}B_{ij}}.$$

The optimal δ^* is $\delta^* = (.4, .2, .2, .2)^T$, the optimal t^* is $t^* = (2, 1, .5)$, and the lowest cost is one hundred dollars.

3.7 Constrained Geometric Programming

Consider now the following variant of the problem of transporting the gravel across the river. Suppose that the bottom and the two sides will be constructed for free from scrap metal, but only four square yards are available. The cost function to be minimized becomes

$$g_0(t) = \frac{40}{t_1 t_2 t_3} + 40 t_2 t_3, \tag{3.29}$$

and the constraint is

$$g_1(t) = \frac{t_1 t_3}{2} + \frac{t_1 t_2}{4} \leq 1. \tag{3.30}$$

With $\delta_1 > 0$, $\delta_2 > 0$, and $\delta_1 + \delta_2 = 1$, we write

$$g_0(t) = \delta_1 \frac{40}{\delta_1 t_1 t_2 t_3} + \delta_2 \frac{40 t_2 t_3}{\delta_2}. \tag{3.31}$$

Since $0 \leq g_1(t) \leq 1$, we have

$$g_0(t) \geq \Big(\delta_1 \frac{40}{\delta_1 t_1 t_2 t_3} + \delta_2 \frac{40 t_2 t_3}{\delta_2}\Big)\Big(g_1(t)\Big)^{\lambda}, \tag{3.32}$$

for any positive λ. The GAGM Inequality then tells us that

$$g_0(t) \geq \left(\Big(\frac{40}{\delta_1 t_1 t_2 t_3}\Big)^{\delta_1}\Big(\frac{40 t_2 t_3}{\delta_2}\Big)^{\delta_2}\right)\Big(g_1(t)\Big)^{\lambda}, \tag{3.33}$$

so that

$$g_0(t) \geq \left(\Big(\frac{40}{\delta_1}\Big)^{\delta_1}\Big(\frac{40}{\delta_2}\Big)^{\delta_2}\right) t_1^{-\delta_1} t_2^{\delta_2 - \delta_1} t_3^{\delta_2 - \delta_1}\Big(g_1(t)\Big)^{\lambda}. \tag{3.34}$$

From the GAGM Inequality, we also know that, for $\delta_3 > 0$, $\delta_4 > 0$ and $\lambda = \delta_3 + \delta_4$,

$$\Big(g_1(t)\Big)^{\lambda} \geq (\lambda)^{\lambda}\left(\Big(\frac{1}{2\delta_3}\Big)^{\delta_3}\Big(\frac{1}{4\delta_4}\Big)^{\delta_4}\right) t_1^{\delta_3+\delta_4} t_2^{\delta_4} t_3^{\delta_3}. \tag{3.35}$$

Combining the inequalities in (3.34) and (3.35), we obtain

$$g_0(t) \geq v(\delta) t_1^{-\delta_1+\delta_3+\delta_4} t_2^{-\delta_1+\delta_2+\delta_4} t_3^{-\delta_1+\delta_2+\delta_3}, \tag{3.36}$$

with

$$v(\delta) = \Big(\frac{40}{\delta_1}\Big)^{\delta_1}\Big(\frac{40}{\delta_2}\Big)^{\delta_2}\Big(\frac{1}{2\delta_3}\Big)^{\delta_3}\Big(\frac{1}{4\delta_4}\Big)^{\delta_4}\Big(\delta_3 + \delta_4\Big)^{\delta_3+\delta_4}, \tag{3.37}$$

and $\delta = (\delta_1, \delta_2, \delta_3, \delta_4)$. If we can find a positive vector δ with

$$\begin{aligned} \delta_1 + \delta_2 &= 1, \\ \delta_3 + \delta_4 &= \lambda, \\ -\delta_1 + \delta_3 + \delta_4 &= 0, \\ -\delta_1 + \delta_2 + \delta_4 &= 0 \\ -\delta_1 + \delta_2 + \delta_3 &= 0, \end{aligned} \tag{3.38}$$

then

$$g_0(t) \geq v(\delta). \tag{3.39}$$

In this particular case, there is a unique positive δ satisfying the equations (3.38), namely

$$\delta_1^* = \frac{2}{3}, \delta_2^* = \frac{1}{3}, \delta_3^* = \frac{1}{3}, \text{and } \delta_4^* = \frac{1}{3}, \tag{3.40}$$

and

$$v(\delta^*) = 60. \tag{3.41}$$

Therefore, $g_0(t)$ is bounded below by 60. If there is t^* such that

$$g_0(t^*) = 60, \tag{3.42}$$

then we must have

$$g_1(t^*) = 1, \tag{3.43}$$

and equality in the GAGM Inequality. Consequently,

$$\frac{3}{2}\frac{40}{t_1^* t_2^* t_3^*} = 3(40 t_2^* t_3^*) = 60, \tag{3.44}$$

and

$$\frac{3}{2} t_1^* t_3^* = \frac{3}{4} t_1^* t_2^* = K. \tag{3.45}$$

Since $g_1(t^*) = 1$, we must have $K = \frac{3}{2}$. We solve these equations by taking logarithms, to obtain the solution

$$t_1^* = 2,\ t_2^* = 1, \text{ and } t_3^* = \frac{1}{2}. \tag{3.46}$$

The change of variables $t_j = e^{x_j}$ converts the constrained (GP) problem into a constrained convex programming problem. The theory of the constrained (GP) problem can then be obtained as a consequence of the theory for the convex problem, which we shall consider in a later chapter.

3.8 Exercises

3.1 *Show that there is no solution to the problem of minimizing the function*

$$g(t_1, t_2) = \frac{2}{t_1 t_2} + t_1 t_2 + t_1, \tag{3.47}$$

over $t_1 > 0$, $t_2 > 0$.

3.2 *Minimize the function*

$$g(t_1, t_2) = \frac{1}{t_1 t_2} + t_1 t_2 + t_1 + t_2, \tag{3.48}$$

over $t_1 > 0$, $t_2 > 0$. *This will require some iterative numerical method for solving equations.*

3.3 *Program the MART algorithm and use it to verify the assertions made previously concerning the solutions of the two numerical examples.*

3.9 Course Homework

Do Exercises 3.1 and 3.3.

Chapter 4

Convex Sets

4.1 Chapter Summary

Convex sets and convex functions play important roles in optimization. In this chapter we survey the basic facts concerning the geometry of convex sets. We begin with the geometry of R^J.

4.2 The Geometry of Real Euclidean Space

We denote by R^J the real Euclidean space consisting of all J-dimensional column vectors $x = (x_1, ..., x_J)^T$ with real entries x_j; here the superscript T denotes the transpose of the 1 by J matrix (or, row vector) $(x_1, ..., x_J)$.

4.2.1 Inner Products

For $x = (x_1, ..., x_J)^T$ and $y = (y_1, ..., y_J)^T$ in R^J, the dot product $x \cdot y$ is defined to be

$$x \cdot y = \sum_{j=1}^{J} x_j y_j. \tag{4.1}$$

Note that we can write

$$x \cdot y = y^T x = x^T y, \tag{4.2}$$

where juxtaposition indicates matrix multiplication. The 2-norm, or *Euclidean norm*, or *Euclidean length*, of x is

$$||x||_2 = \sqrt{x \cdot x} = \sqrt{x^T x}. \tag{4.3}$$

The *Euclidean distance* between two vectors x and y in R^J is $||x - y||_2$.

The space R^J, along with its dot product, is an example of a finite-dimensional Hilbert space.

Definition 4.1 *Let V be a real vector space. The scalar-valued function $\langle u, v\rangle$ is called an* inner product *on V if the following four properties hold, for all u, w, and v in V, and all real c:*

$$\langle u + w, v\rangle = \langle u, v\rangle + \langle w, v\rangle; \tag{4.4}$$

$$\langle cu, v\rangle = c\langle u, v\rangle; \tag{4.5}$$

$$\langle v, u\rangle = \langle u, v\rangle; \tag{4.6}$$

and

$$\langle u, u\rangle \geq 0, \tag{4.7}$$

with equality in Inequality (4.7) if and only if $u = 0$.

The dot product of vectors is an example of an inner product. The properties of an inner product are precisely the ones needed to prove Cauchy's Inequality, which then holds for any inner product. We shall favor the dot product notation $u \cdot v$ for the inner product of vectors, although we shall occasionally use the matrix multiplication form, $v^T u$ or the inner product notation $\langle u, v\rangle$.

4.2.2 Cauchy's Inequality

Cauchy's Inequality, also called the Cauchy-Schwarz Inequality, tells us that

$$|\langle x, y\rangle| \leq ||x||_2 ||y||_2, \tag{4.8}$$

with equality if and only if $y = \alpha x$, for some scalar α. The Cauchy-Schwarz Inequality holds for any inner product.

A simple application of Cauchy's inequality gives us

$$||x + y||_2 \leq ||x||_2 + ||y||_2; \tag{4.9}$$

this is called the *Triangle Inequality*. We say that the vectors x and y are *mutually orthogonal* if $\langle x, y\rangle = 0$.

The *Parallelogram Law* is an easy consequence of the definition of the 2-norm:

$$||x + y||_2^2 + ||x - y||_2^2 = 2||x||_2^2 + 2||y||_2^2. \tag{4.10}$$

It is important to remember that Cauchy's Inequality and the Parallelogram Law hold only for the 2-norm.

4.3 A Bit of Topology

Having the norm allows us to define the distance between two points x and y in R^J as $||x-y||$. Being able to talk about how close points are to each other enables us to define continuity of functions on R^J and to consider topological notions of closed set, open set, interior of a set and boundary of a set.

Definition 4.2 *A subset B of R^J is* closed *if, whenever x^k is in B for each non-negative integer k and $||x-x^k|| \to 0$, as $k \to +\infty$, then x is in B.*

For example, $B = [0,1]$ is closed as a subset of R, but $B = (0,1)$ is not.

Definition 4.3 *We say that $d \geq 0$ is the* distance from the point x to the set B *if, for every $\epsilon > 0$, there is b_ϵ in B, with $||x-b_\epsilon||_2 < d+\epsilon$, and no b in B with $||x-b||_2 < d$.*

The distance from the point 0 in R to the set $(0,1)$ is zero, while its distance to the set $(1,2)$ is one. It follows easily from the definitions that, if B is closed and $d = 0$, then x is in B.

Definition 4.4 *The* closure *of a set B is the set of all points x whose distance from B is zero.*

The closure of the interval $B = (0,1)$ is $[0,1]$.

Definition 4.5 *A subset U of R^J is* open *if its complement, the set of all points not in U, is closed.*

Definition 4.6 *Let C be a subset of R^J. A point x in C is said to be an* interior point *of set C if there is $\epsilon > 0$ such that every point z with $||x-z|| < \epsilon$ is in C. The* interior *of the set C, written int(C), is the set of all interior points of C. It is also the largest open set contained within C.*

For example, the open interval $(0,1)$ is the interior of the intervals $(0,1]$ and $[0,1]$. A set C is open if and only if $C = \text{int}(C)$.

Definition 4.7 *A point x in R^J is said to be a* boundary point *of set C if, for every $\epsilon > 0$, there are points y_ϵ in C and z_ϵ not in C, both depending on the choice of ϵ, with $||x-y_\epsilon|| < \epsilon$ and $||x-z_\epsilon|| < \epsilon$. The* boundary *of C is the set of all boundary points of C. It is also the intersection of the closure of C with the closure of its complement.*

For example, the points $x = 0$ and $x = 1$ are boundary points of the set $(0,1]$.

Definition 4.8 *For $k = 0, 1, 2, ...$, let x^k be a vector in R^J. The sequence of vectors $\{x^k\}$ is said to* converge *to the vector z if, given any $\epsilon > 0$, there is positive integer n, usually depending on ϵ, such that, for every $k > n$, we have $||z - x^k|| \leq \epsilon$. Then we say that z is the* limit of the sequence.

For example, the sequence $\{x^k = \frac{1}{k+1}\}$ in R converges to $z = 0$. The sequence $\{(-1)^k\}$ alternates between 1 and -1, so does not converge. However, the subsequence associated with odd k converges to $z = -1$, while the subsequence associated with even k converges to $z = 1$. The values $z = -1$ and $z = 1$ are called *subsequential limit points*, or, sometimes, *cluster points* of the sequence.

Definition 4.9 *A sequence $\{x^k\}$ of vectors in R^J is said to be* bounded *if there is a constant $b > 0$, such that $||x^k|| \leq b$, for all k.*

A fundamental result in analysis is the following.

Proposition 4.1 *Every convergent sequence of vectors in R^J is bounded. Every bounded sequence of vectors in R^J has at least one convergent subsequence, therefore, has at least one cluster point.*

4.4 Convex Sets in R^J

In preparation for our discussion of linear and nonlinear programming, we consider some of the basic concepts from the geometry of convex sets.

4.4.1 Basic Definitions

We begin with the basic definitions.

Definition 4.10 *A vector z is said to be a* convex combination *of the vectors x and y if there is α in the interval $[0, 1]$ such that $z = (1-\alpha)x+\alpha y$.*

Definition 4.11 *A nonempty set C in R^J is said to be* convex *if, for any distinct points x and y in C, and for any real number α in the interval $(0, 1)$, the point $(1 - \alpha)x + \alpha y$ is also in C; that is, C is closed to convex combinations.*

For example, the unit ball B in R^J, consisting of all x with $||x||_2 \leq 1$, is convex, while the surface of the ball, the set of all x with $||x||_2 = 1$, is not convex.

Definition 4.12 *The* convex hull *of a set S, denoted conv(S), is the smallest convex set containing S.*

Proposition 4.2 *The convex hull of a set S is the set C of all convex combinations of members of S.*

Definition 4.13 *A subset S of R^J is a* subspace *if, for every x and y in S and scalars α and β, the linear combination $\alpha x + \beta y$ is again in S.*

A subspace is necessarily a convex set.

Definition 4.14 *The* orthogonal complement *of a subspace S is the set*

$$S^{\perp} = \{u | u^T s = 0, \text{for every } s \in S\}, \tag{4.11}$$

the set of all vectors u in R^J that are orthogonal to every member of S.

For example, in R^3, the x, y-plane is a subspace and has for its orthogonal complement the z-axis.

Definition 4.15 *A subset M of R^J is a* linear manifold *if there is a subspace S and a vector b such that*

$$M = S + b = \{x | x = s + b, \text{for some } s \text{ in } S\}.$$

Any linear manifold is convex.

Definition 4.16 *For a fixed column vector a with Euclidean length one and a fixed scalar γ the* hyperplane *determined by a and γ is the set*

$$H(a, \gamma) = \{z | \langle a, z \rangle = \gamma\}.$$

The hyperplanes $H(a, \gamma)$ are linear manifolds, and the hyperplanes $H(a, 0)$ are subspaces.

Definition 4.17 *Given a subset C of R^J, the* affine hull *of C, denoted aff(C), is the smallest linear manifold containing C.*

For example, let C be the line segment connecting the two points $(0, 1)$ and $(1, 2)$ in R^2. The affine hull of C is the straight line whose equation is $y = x + 1$.

Definition 4.18 *The* dimension of a subset *of R^J is the dimension of its affine hull, which is the dimension of the subspace of which it is a translate.*

The set C above has dimension one. A set containing only one point is its own affine hull, since it is a translate of the subspace $\{0\}$.

In R^2, the line segment connecting the points $(0, 1)$ and $(1, 2)$ has no interior; it is a one-dimensional subset of a two-dimensional space and can contain no two-dimensional ball. But, the part of this set without its two end points is a sort of interior, called the *relative interior*.

Definition 4.19 *The* relative interior *of a subset C of R^J, denoted $ri(C)$, is the interior of C, as defined by considering C as a subset of its affine hull.*

Since a set consisting of a single point is its own affine hull, it is its own relative interior.

Definition 4.20 *A point x in a convex set C is said to be an* extreme point *of C if the set obtained by removing x from C remains convex.*

Said another way, $x \in C$ is an extreme point of C if x is not a convex combination of two other points in C; that is, x cannot be written as

$$x = (1 - \alpha)y + \alpha z, \tag{4.12}$$

for y and z in C, $y, z \neq x$ and $\alpha \in (0, 1)$. For example, the point $x = 1$ is an extreme point of the convex set $C = [0, 1]$. Every point on the boundary of a sphere in R^J is an extreme point of the sphere. The set of all extreme points of a convex set is denoted $\text{Ext}(C)$.

Definition 4.21 *A non-zero vector d is said to be a* direction of unboundedness *of a convex set C if, for all x in C and all $\gamma \geq 0$, the vector $x + \gamma d$ is in C.*

For example, if C is the non-negative orthant in R^J, then any non-negative vector d is a direction of unboundedness.

Definition 4.22 *A vector a is* normal *to a convex set C at the point s in C if*

$$\langle a, c - s \rangle \leq 0, \tag{4.13}$$

for all c in C.

Definition 4.23 *Let C be convex and s in C. The* normal cone *to C at s, denoted $N_C(s)$, is the set of all vectors a that are normal to C at s.*

4.4.2 Orthogonal Projection onto Convex Sets

The following proposition is fundamental in the study of convexity and can be found in most books on the subject; see, for example, the text by Goebel and Reich [95].

Proposition 4.3 *Given any nonempty closed convex set C and an arbitrary vector x in R^J, there is a unique member of C closest to x, denoted $P_C x$, the orthogonal (or metric) projection of x onto C.*

Proof: If x is in C, then $P_C x = x$, so assume that x is not in C. Then $d > 0$, where d is the distance from x to C. For each positive integer n, select c_n in C with $||x - c_n||_2 < d + \frac{1}{n}$. Then the sequence $\{c_n\}$ is bounded; let c^* be any cluster point. It follows easily that $||x - c^*||_2 = d$ and that c^* is in C. If there is any other member c of C with $||x - c||_2 = d$, then, by the Parallelogram Law, we would have $||x - (c^* + c)/2||_2 < d$, which is a contradiction. Therefore, c^* is $P_C x$. ∎

For example, if $C = U$, the unit ball, then $P_C x = x/||x||_2$, for all x such that $||x||_2 > 1$, and $P_C x = x$ otherwise. If C is R^J_+, the nonnegative cone of R^J, consisting of all vectors x with $x_j \geq 0$, for each j, then $P_C x = x_+$, the vector whose entries are $\max(x_j, 0)$. For any closed, convex set C, the distance from x to C is $||x - P_C x||$.

If a nonempty set S is not convex, then the orthogonal projection of a vector x onto S need not be well defined; there may be more than one vector in S closest to x. In fact, it is known that a set S is convex if and only if, for every x not in S, there is a unique point in S closest to x; this is Motzkin's Theorem (see [16], p. 447). Note that there may well be some x for which there is a unique closest point in S, but if S is not convex, then there must be at least one point without a unique closest point in S.

Lemma 4.1 *For $H = H(a, \gamma)$, $z = P_H x$ is the vector*

$$z = P_H x = x + (\gamma - \langle a, x \rangle)a. \tag{4.14}$$

We shall use this fact in our discussion of the ART algorithm.

For an arbitrary nonempty closed convex set C in R^J, the orthogonal projection $T = P_C$ is a nonlinear operator, unless, of course, C is a subspace. We may not be able to describe $P_C x$ explicitly, but we do know a useful property of $P_C x$.

Proposition 4.4 *For a given x, a vector z in C is $P_C x$ if and only if*

$$\langle c - z, z - x \rangle \geq 0, \tag{4.15}$$

for all c in the set C.

Proof: Let c be arbitrary in C and α in $(0, 1)$. Then

$$||x - P_C x||_2^2 \leq ||x - (1 - \alpha)P_C x - \alpha c||_2^2 = ||x - P_C x + \alpha(P_C x - c)||_2^2$$

$$= ||x - P_C x||_2^2 - 2\alpha\langle x - P_C x, c - P_C x \rangle + \alpha^2 ||P_C x - c||_2^2. \tag{4.16}$$

Therefore,

$$-2\alpha\langle x - P_C x, c - P_C x \rangle + \alpha^2 ||P_C x - c||_2^2 \geq 0, \tag{4.17}$$

so that

$$2\langle x - P_C x, c - P_C x\rangle \leq \alpha ||P_C x - c||_2^2. \tag{4.18}$$

Taking the limit, as $\alpha \to 0$, we conclude that

$$\langle c - P_C x, P_C x - x\rangle \geq 0. \tag{4.19}$$

If z is a member of C that also has the property

$$\langle c - z, z - x\rangle \geq 0, \tag{4.20}$$

for all c in C, then we have both

$$\langle z - P_C x, P_C x - x\rangle \geq 0, \tag{4.21}$$

and

$$\langle z - P_C x, x - z\rangle \geq 0. \tag{4.22}$$

Adding on both sides of these two inequalities lead to

$$\langle z - P_C x, P_C x - z\rangle \geq 0. \tag{4.23}$$

But,

$$\langle z - P_C x, P_C x - z\rangle = -||z - P_C x||_2^2, \tag{4.24}$$

so it must be the case that $z = P_C x$. This completes the proof. ∎

4.5 Some Results on Projections

The characterization of the orthogonal projection operator P_C given by Proposition 4.4 has a number of important consequences.

Corollary 4.1 *Let S be any subspace of R^J. Then, for any x in R^J and s in S, we have*

$$\langle P_S x - x, s\rangle = 0. \tag{4.25}$$

Proof: Since S is a subspace, $s + P_S x$ is again in S, for all s, as is cs, for every scalar c. ∎

This corollary enables us to prove the Decomposition Theorem.

Theorem 4.1 *Let S be any subspace of R^J and x any member of R^J. Then there are unique vectors s in S and u in $S^\perp$ such that $x = s + u$. The vector s is $P_S x$ and the vector u is $P_{S^\perp} x$.*

Proof: For the given x we take $s = P_S x$ and $u = x - P_S x$. Corollary 4.1 assures us that u is in $S^\perp$. Now we need to show that this decomposition is unique. To that end, suppose that we can write $x = s_1 + u_1$, with s_1 in S and u_1 in $S^\perp$. Then Proposition 4.4 tells us that, since $s_1 - x$ is orthogonal to every member of S, s_1 must be $P_S x$. ∎

This theorem is often presented in a slightly different manner.

Theorem 4.2 *Let A be a real I by J matrix. Then every vector b in R^I can be written uniquely as $b = Ax + w$, where $A^T w = 0$.*

To derive Theorem 4.2 from Theorem 4.1, we simply let $S = \{Ax | x \in R^J\}$. Then $S^\perp$ is the set of all w such that $A^T w = 0$. It follows that w is the member of the null space of A^T closest to b.

Here are additional consequences of Proposition 4.4.

Corollary 4.2 *Let S be any subspace of R^J, d a fixed vector, and V the linear manifold $V = S + d = \{v = s + d | s \in S\}$, obtained by translating the members of S by the vector d. Then, for every x in R^J and every v in V, we have*

$$\langle P_V x - x, v - P_V x \rangle = 0. \tag{4.26}$$

Proof: Since v and $P_V x$ are in V, they have the form $v = s + d$, and $P_V x = \hat{s} + d$, for some s and $\hat{s}$ in S. Then $v - P_V x = s - \hat{s}$. ∎

Corollary 4.3 *Let H be the hyperplane $H(a, \gamma)$. Then, for every x, and every h in H, we have*

$$\langle P_H x - x, h - P_H x \rangle = 0. \tag{4.27}$$

Corollary 4.4 *Let S be a subspace of R^J. Then $(S^\perp)^\perp = S$.*

Proof: Every x in R^J has the form $x = s + u$, with s in S and u in $S^\perp$. Suppose x is in $(S^\perp)^\perp$. Then $u = 0$. ∎

4.6 Linear and Affine Operators on R^J

If A is a J by J real matrix, then we can define an operator T by setting $Tx = Ax$, for each x in R^J; here Ax denotes the multiplication of the matrix A and the column vector x.

Definition 4.24 *An operator T is said to be a* linear operator *if*

$$T(\alpha x + \beta y) = \alpha Tx + \beta Ty, \tag{4.28}$$

for each pair of vectors x and y and each pair of scalars α and β.

Any operator T that comes from matrix multiplication, that is, for which $Tx = Ax$, is linear.

Lemma 4.2 *For $H = H(a, \gamma)$, $H_0 = H(a, 0)$, and any x and y in R^J, we have*

$$P_H(x + y) = P_H x + P_H y - P_H 0, \tag{4.29}$$

so that

$$P_{H_0}(x + y) = P_{H_0} x + P_{H_0} y, \tag{4.30}$$

that is, the operator P_{H_0} is an additive operator. In addition,

$$P_{H_0}(\alpha x) = \alpha P_{H_0} x, \tag{4.31}$$

so that P_{H_0} is a linear operator.

Definition 4.25 *If A is a J by J real matrix and d is a fixed nonzero vector in R^J, the operator defined by $Tx = Ax + d$ is an* affine linear operator.

Lemma 4.3 *For any hyperplane $H = H(a, \gamma)$ and $H_0 = H(a, 0)$,*

$$P_H x = P_{H_0} x + P_H 0, \tag{4.32}$$

so P_H is an affine linear operator.

Lemma 4.4 *For $i = 1, ..., I$ let H_i be the hyperplane $H_i = H(a^i, \gamma_i)$, $H_{i0} = H(a^i, 0)$, and P_i and P_{i0} the orthogonal projections onto H_i and H_{i0}, respectively. Let T be the operator $T = P_I P_{I-1} \cdots P_2 P_1$. Then $Tx = Bx + d$, for some square matrix B and vector d; that is, T is an affine linear operator.*

4.7 The Fundamental Theorems

The Separation Theorem and the Support Theorem provide the foundation for the geometric approach to the calculus of functions of several variables.

A real-valued function $f(x)$ defined for real x has a derivative at $x = x_0$ if and only if there is a unique line through the point $(x_0, f(x_0))$ tangent to the graph of $f(x)$ at that point. If $f(x)$ is not differentiable at x_0, there may be more than one such tangent line, as happens with the function $f(x) = |x|$ at $x_0 = 0$. For functions of several variables the geometric view of differentiation involves tangent hyperplanes.

4.7.1 Basic Definitions

Definition 4.26 *Let S be a subset of R^J and $f : S \to [-\infty, \infty]$ a function defined on S. The subset of R^{J+1} defined by*

$$\text{epi}(f) = \{(x, \gamma) | f(x) \leq \gamma\}$$

is the epi-graph *of f. Then we say that f is* convex *if its epi-graph is a convex set.*

Alternative definitions of convex function are presented in the exercises.

Definition 4.27 *The* effective domain *of a convex function f, denoted* $\text{dom}(f)$*, is the projection onto R^J of its epi-graph; that is,*

$$\text{dom}(f) = \{x |\, (x, \gamma) \in \text{epi}(f)\} = \{x |\, f(x) < +\infty\}.$$

The effective domain of a convex function is a convex set.

Definition 4.28 *A convex function $f(x)$ is* proper *if there is no x for which $f(x) = -\infty$ and some x for which $f(x) < +\infty$.*

The important role played by hyperplanes tangent to the epigraph of f motivates our study of the relationship between hyperplanes and convex sets.

4.7.2 The Separation Theorem

The Separation Theorem, sometimes called the Geometric Hahn-Banach Theorem, is an easy consequence of the existence of orthogonal projections onto closed convex sets.

Theorem 4.3 (The Separation Theorem) *Let C be a closed nonempty convex set in R^J and x a point not in C. Then there is non-zero vector a in R^J and real number α such that*

$$\langle a, c\rangle \leq \alpha < \langle a, x\rangle,$$

for every c in C.

Proof: Let $z = P_C x$, $a = x - z$, and $\alpha = \langle a, z\rangle$. Then using Proposition 4.4, we have

$$\langle -a, c - z\rangle \geq 0,$$

or, equivalently,

$$\langle a, c\rangle \leq \langle a, z\rangle = \alpha\,,$$

for all c in C. But, we also have

$$\langle a, x\rangle = \langle a, x - z\rangle + \langle a, z\rangle = ||x - z||^2 + \alpha > \alpha.$$

This completes the proof. ∎

4.7.3 The Support Theorem

The Separation Theorem concerns a closed convex set C and a point x outside the set C, and asserts the existence of a hyperplane separating the two. Now we concerned with a point z on the boundary of a convex set C, such as the point $(x, f(x))$ on the boundary of the epigraph of f. The Support Theorem asserts the existence of a hyperplane through such a point, having the convex set entirely contained in one of its half-spaces. If we knew a priori that the point z is $P_C x$ for some x outside C, then we could simply take the vector $a = x - z$ as the normal to the desired hyperplane. The essence of the Support Theorem is to provide such a normal vector without assuming that $z = P_C x$.

For the proofs that follow we shall need the following definitions.

Definition 4.29 *For subsets A and B of R^J, and scalar γ, let the set $A + B$ consist of all vectors v of the form $v = a + b$, and γA consist of all vectors w of the form $w = \gamma a$, for some a in A and b in B. Let x be a fixed member of R^J. Then the set $x + A$ is the set of all vectors y such that $y = x + a$, for some a in A.*

Lemma 4.5 *Let B be the unit ball in R^J, that is, B is the set of all vectors u with $||u|| \leq 1$. Let S be an arbitrary subset of R^J. Then x is in the interior of S if and only if there is some $\epsilon > 0$ such that $x + \epsilon B \subseteq S$, and y is in the closure of S if and only if, for every $\epsilon > 0$, the set $y + \epsilon B$ has nonempty intersection with S.*

We begin with the *Accessibility Lemma*. Note that the relative interior of any non-empty convex set is always non-empty (see [140], Theorem 6.2).

Lemma 4.6 (The Accessibility Lemma) *Let C be a convex set. Let x be in the relative interior of C and y in the closure of C. Then, for all scalars α in the interval $(0, 1]$, the point $(1 - \alpha)x + \alpha y$ is in the relative interior of C.*

Proof: If the dimension of C is less than J, we can transform the problem into a space of smaller dimension. Therefore, without loss of generality, we can assume that the dimension of C is J, its affine hull is all of R^J, and its relative interior is its interior. Let α be fixed, and $B = \{z \,|\, ||z|| \leq 1\}$. We have to show that there is some $\epsilon > 0$ such that the set $(1-\alpha)x + \alpha y + \epsilon B$ is a subset of the set C. We know that y is in the set $C + \epsilon B$ for every $\epsilon > 0$, since y is in the closure of C. Therefore, for all $\epsilon > 0$ we have

$$(1 - \alpha)x + \alpha y + \epsilon B \subseteq (1 - \alpha)x + \alpha(C + \epsilon B) + \epsilon B$$

$$= (1 - \alpha)x + (1 + \alpha)\epsilon B + \alpha C$$

$$= (1 - \alpha)[x + \epsilon(1 + \alpha)(1 - \alpha)^{-1} B] + \alpha C.$$

Since x is in the interior of the set C, we know that

$$[x + \epsilon(1+\alpha)(1-\alpha)^{-1}B] \subseteq C,$$

for ϵ small enough. This completes the proof. ∎

Now we come to the Support Theorem.

Theorem 4.4 (Support Theorem) *Let C be convex, and let z be on the boundary of C. Then there is a non-zero vector a in R^J with $\langle a, z\rangle \geq \langle a, c\rangle$, for all c in C.*

Proof: If the dimension of C is less than J, then every point of C is on the boundary of C. Let the affine hull of C be $M = S + b$. Then the set $C - b$ is contained in the subspace S, which, in turn, can be contained in a hyperplane through the origin, $H(a, 0)$. Then

$$\langle a, c\rangle = \langle a, b\rangle,$$

for all c in C. So we focus on the case in which the dimension of C is J, in which case the interior of C must be non-empty.

Let y be in the interior of C, and, for each $s > 1$, let $z_s = y + s(z - y)$. Note that z_s is not in the closure of C, for any $s > 1$, by the Accessibility Lemma, since z is not in the interior of C. By the Separation Theorem, there are vectors b_s such that

$$\langle b_s, c\rangle < \langle b_s, z_s\rangle,$$

for all c in C. For convenience, we assume that $||b_s|| = 1$, and that $\{s_k\}$ is a sequence with $s_k > 1$ and $\{s_k\} \to 1$, as $k \to \infty$. Let $a_k = b_{s_k}$. Then there is a subsequence of the $\{a_k\}$ converging to some a, with $||a|| = 1$, and

$$\langle a, c\rangle \leq \langle a, z\rangle,$$

for all c in C. This completes the proof. ∎

If we knew that there was a vector x not in C, such that $z = P_C x$, then we could choose $a = x - z$, as in the proof of the Separation Theorem. The point of the Support Theorem is that we cannot assume, a priori, that there is such an x. Once we have the vector a, however, any point $x = z + \lambda a$, for $\lambda \geq 0$, has the property that $z = P_C x$.

4.8 Theorems of the Alternative

The following theorem is a good illustration of a type of theorem known as *Theorems of the Alternative*. These theorems assert that precisely one of two problems will have a solution. The proof illustrates how we should go about proving such theorems.

Theorem 4.5 (Gale I)[92] *Precisely one of the following is true:*

- **(1)** *there is x such that $Ax = b$;*
- **(2)** *there is y such that $A^T y = 0$ and $b^T y = 1$.*

Proof: First, we show that it is not possible for both to be true at the same time. Suppose that $Ax = b$ and $A^T y = 0$. Then $b^T y = x^T A^T y = 0$, so that we cannot have $b^T y = 1$. By Theorem 4.1, the fundamental decomposition theorem from linear algebra, we know that, for any b, there are unique x and w with $A^T w = 0$ such that $b = Ax + w$. Clearly, $b = Ax$ if and only if $w = 0$. Also, $b^T y = w^T y$. Therefore, if alternative **(1)** does not hold, we must have w non-zero, in which case $A^T y = 0$ and $b^T y = 1$, for $y = w/||w||^2$, so alternative **(2)** holds. ∎

In this section we consider several other theorems of this type.

Theorem 4.6 (Farkas' Lemma)[87] *Precisely one of the following is true:*

- **(1)** *there is $x \geq 0$ such that $Ax = b$;*
- **(2)** *there is y such that $A^T y \geq 0$ and $b^T y < 0$.*

Proof: We can restate the lemma as follows: there is a vector y with $A^T y \geq 0$ and $b^T y < 0$ if and only if b is not a member of the convex set $C = \{Ax | x \geq 0\}$. If b is not in C, which is closed and convex, then, by the Separation Theorem, there is a non-zero vector a and real α with

$$a^T b < \alpha \leq a^T Ax = (A^T a)^T x,$$

for all $x \geq 0$. Since $(A^T a)^T x$ is bounded below, as x runs over all non-negative vectors, it follows that $A^T a \geq 0$. Choosing $x = 0$, we have $\alpha \leq 0$. Then let $y = a$. Conversely, if $Ax = b$ does have a non-negative solution x, then $A^T y \geq 0$ implies that $y^T Ax = y^T b \geq 0$. ∎

The next theorem can be obtained from Farkas' Lemma.

Theorem 4.7 (Gale II)[92] *Precisely one of the following is true:*

- **(1)** *there is x such that $Ax \leq b$;*
- **(2)** *there is $y \geq 0$ such that $A^T y = 0$ and $b^T y < 0$.*

Proof: First, if both are true, then $0 \leq y^T(b - Ax) = y^T b - 0 = y^T b$, which is a contradiction. Now assume that **(2)** does not hold. Therefore, for every $y \geq 0$ with $A^T y = 0$, we have $b^T y \geq 0$. Let $B = [\, A \quad b \,]$. Then the system $B^T y = [\, 0 \quad -1 \,]^T$ has no non-negative solution. Applying Farkas' Lemma, we find that there is a vector $w = [\, z \quad \gamma \,]^T$ with $Bw \geq 0$ and $[\, 0 \quad -1 \,]\, w < 0$. So, $Az + \gamma b \geq 0$ and $\gamma > 0$. Let $x = -\frac{1}{\gamma} z$ to get $Ax \leq b$, so that **(1)** holds. ∎

Theorem 4.8 (Gordan)[97] *Precisely one of the following is true:*

- **(1)** *there is x such that $Ax < 0$;*
- **(2)** *there is $y \geq 0$, $y \neq 0$, such that $A^T y = 0$.*

Proof: First, if both are true, then $0 < -y^T Ax = 0$, which cannot be true. Now assume that there is no non-zero $y \geq 0$ with $A^T y = 0$. Then, with $e = (1, 1, ..., 1)^T$, $C = [\, A \quad e \,]$, and $d = (0, 0, ..., 0, 1)^T$, there is no non-negative solution of $C^T y = d$. From Farkas' Lemma we then know that there is a vector $z = [\, u \quad \gamma \,]^T$, with $Cz = Au + \gamma e \geq 0$, and $d^T z < 0$. Then $Ax < 0$ for $x = -u$. ∎

Here are several more theorems of the alternative.

Theorem 4.9 (Stiemke I)[149] *Precisely one of the following is true:*

- **(1)** *there is x such that $Ax \leq 0$ and $Ax \neq 0$;*
- **(2)** *there is $y > 0$ such that $A^T y = 0$.*

Theorem 4.10 (Stiemke II)[149] *Let c be a fixed non-zero vector. Precisely one of the following is true:*

- **(1)** *there is x such that $Ax \leq 0$ and $c^T x \geq 0$ and not both $Ax = 0$ and $c^T x = 0$;*
- **(2)** *there is $y > 0$ such that $A^T y = c$.*

Theorem 4.11 (Gale III)[92] *Let c be a fixed non-zero vector. Precisely one of the following is true:*

- **(1)** *there is $x \geq 0$ such that $Ax \geq 0$ and $c^T x < 0$;*
- **(2)** *there is $y \geq 0$ such that $A^T y \leq c$.*

Proof: First, note that we cannot have both true at the same time, since we would then have

$$0 < x^T (c - A^T y) = c^T x - (Ax)^T y \leq c^T x,$$

which is a contradiction. Now suppose that **(2)** does not hold. Then there is no $w \geq 0$ such that

$$[\, A^T \quad I \,]\, w = c.$$

By Farkas' Lemma (Theorem 4.6), it follows that there is x with

$$\begin{bmatrix} A \\ I \end{bmatrix} x \geq 0,$$

and $c^T x < 0$. Therefore, $Ax \geq 0$, $Ix = x \geq 0$, and $c^T x < 0$; therefore, **(1)** holds. ∎

Theorem 4.12 (Von Neumann)[132] *Precisely one of the following is true:*

- **(1)** *there is* $x \geq 0$ *such that* $Ax > 0$*;*
- **(2)** *there is* $y \geq 0$*,* $y \neq 0$*, such that* $A^T y \leq 0$*.*

Proof: If both were true, then we would have

$$0 < (Ax)^T y = x^T (A^T y),$$

so that $A^T y \leq 0$ would be false. Now suppose that **(2)** does not hold. Then there is no $y \geq 0$, $y \neq 0$, with $A^T y \leq 0$. Consequently, there is no $y \geq 0$, $y \neq 0$, such that

$$\begin{bmatrix} A^T \\ -u^T \end{bmatrix} y = \begin{bmatrix} A^T y \\ -u^T y \end{bmatrix} \leq \begin{bmatrix} 0 \\ -1 \end{bmatrix},$$

where $u^T = (1, 1, ..., 1)$. By Theorem 4.11, there is

$$z = \begin{bmatrix} x \\ \alpha \end{bmatrix} \geq 0,$$

such that

$$[\, A \quad -u \,]\, z = [\, A \quad -u \,] \begin{bmatrix} x \\ \alpha \end{bmatrix} \geq 0,$$

and

$$[\, 0 \quad -1 \,]\, z = [\, 0 \quad -1 \,] \begin{bmatrix} x \\ \alpha \end{bmatrix} = -\alpha < 0.$$

Therefore, $\alpha > 0$ and $(Ax)_i - \alpha \geq 0$ for each i, and so $Ax > 0$ and **(1)** holds. ∎

Theorem 4.13 (Tucker)[152] *Precisely one of the following is true:*

- **(1)** *there is* $x \geq 0$ *such that* $Ax \geq 0$*,* $Ax \neq 0$*;*
- **(2)** *there is* $y > 0$ *such that* $A^T y \leq 0$*.*

Theorem 4.14 (Theorem 21.1, [140]) *Let* C *be a convex set, and let* $f_1, ..., f_m$ *be proper convex functions, with* $ri(C) \subseteq dom(f_i)$*, for each* i*. Precisely one of the following is true:*

- **(1)** *there is* $x \in C$ *such that* $f_i(x) < 0$*, for* $i = 1, ..., m$*;*
- **(2)** *there are* $\lambda_i \geq 0$*, not all equal to zero, such that*

$$\lambda_1 f_1(x) + ... + \lambda_m f_m(x) \geq 0,$$

for all x *in* C*.*

Theorem 4.14 is fundamental in proving Helly's Theorem:

Theorem 4.15 (Helly's Theorem) [140] *Let $\{C_i \,|i = 1, ..., I\}$ be a finite collection of (not necessarily closed) convex sets in R^N. If every subcollection of $N+1$ or fewer sets has non-empty intersection, then the entire collection has non-empty intersection.*

For instance, in the two-dimensional plane, if a finite collection of lines is such that every two intersect and every three have a common point of intersection, then they all have a common point of intersection. There is another version of Helly's Theorem that applies to convex inequalities.

Theorem 4.16 *Let there be given a system of the form*

$$f_1(x) < 0, ..., f_k(x) < 0, f_{k+1}(x) \leq 0, ..., f_m(x) \leq 0,$$

where the f_i are convex functions on R^J, and the inequalities may be all strict or all weak. If every subsystem of $J+1$ or fewer inequalities has a solution in a given convex set C, then the entire system has a solution in C.

4.9 Another Proof of Farkas' Lemma

In the previous section, we proved Farkas' Lemma, Theorem 4.6, using the Separation Theorem, the proof of which, in turn, depended here on the existence of the orthogonal projection onto any closed convex set. It is possible to prove Farkas' Lemma directly, along the lines of Gale [92].

Suppose that $Ax = b$ has no non-negative solution. If, indeed, it has no solution whatsoever, then $b = Ax + w$, where $w \neq 0$ and $A^T w = 0$. Then we take $y = -w/||w||^2$. So suppose that $Ax = b$ does have solutions, but not any non-negative ones. The approach is to use induction on the number of columns of the matrix involved in the lemma.

If A has only one column, denoted a^1, then $Ax = b$ can be written as

$$x_1 a^1 = b.$$

Assuming that there are no non-negative solutions, it must follow that $x_1 < 0$. We take $y = -b$. Then

$$b^T y = -b^T b = -||b||^2 < 0,$$

while

$$A^T y = (a^1)^T(-b) = \frac{-1}{x_1} b^T b > 0.$$

Now assume that the lemma holds whenever the involved matrix has no more than $m-1$ columns. We show the same is true for m columns.

If there is no non-negative solution of the system $Ax = b$, then clearly there are no non-negative real numbers $x_1, x_2, ..., x_{m-1}$ such that

$$x_1 a^1 + x_2 a^2 + ... + x_{m-1} a^{m-1} = b,$$

where a^j denotes the jth column of the matrix A. By the induction hypothesis, there must be a vector v with

$$(a^j)^T v \geq 0,$$

for $j = 1, ..., m-1$, and $b^T v < 0$. If it happens that $(a^m)^T v \geq 0$ also, then we are done. If, on the other hand, we have $(a^m)^T v < 0$, then let

$$c^j = (a^j)^T a^m - (a^m)^T a^j,\ j = 1, ..., m-1,$$

and

$$d = (b^T v) a^m - ((a^m)^T v) b.$$

Then there are no non-negative real numbers $z_1, ..., z_{m-1}$ such that

$$z_1 c^1 + z_2 c^2 + ... + z_{m-1} c^{m-1} = d, \tag{4.33}$$

since, otherwise, it would follow from simple calculations that

$$\frac{-1}{(a^m)^T v}\Big([\sum_{j=1}^{m-1} z_j((a^j)^T v)] - b^T v\Big) a^m - \sum_{j=1}^{m-1} z_j((a^m)^T v) a^j = b.$$

Close inspection of this shows all the coefficients to be non-negative, which implies that the system $Ax = b$ has a non-negative solution, contrary to our assumption. It follows, therefore, that there can be no non-negative solution to the system in Equation (4.33).

By the induction hypothesis, it follows that there is a vector u such that

$$(c^j)^T u \geq 0,\ j = 1, ..., m-1,$$

and

$$d^T u < 0.$$

Now let

$$y = ((a^m)^T u) v - ((a^m)^T v) u.$$

We can easily verify that

$$(a^j)^T y = (c^j)^T u \geq 0,\ j = 1, ..., m-1,$$

$$b^T y = d^T u < 0,$$

and

$$(a^m)^T y = 0,$$

so that

$$A^T y \geq 0,$$

and

$$b^T y < 0.$$

This completes the proof.

4.10 Exercises

4.1 *Prove Proposition 4.2.*

4.2 *Show that the subset of R^J consisting of all vectors x with $||x||_2 = 1$ is not convex.*

4.3 *Let $\|x\|_2 = \|y\|_2 = 1$ and $z = \frac{1}{2}(x + y)$ in R^J. Show that $\|z\|_2 < 1$ unless $x = y$. Show that this conclusion does not hold if the* two-norm $\|\cdot\|_2$ *is replaced by the* one-norm*, defined by*

$$\|x\|_1 = \sum_{j=1}^{J} |x_j|.$$

4.4 *Let C be the set of all vectors x in R^J with $\|x\|_2 \leq 1$. Let K be a subset of C obtained by removing from C any number of its members for which $\|x\|_2 = 1$. Show that K is convex. Consequently, every x in C with $\|x\|_2 = 1$ is an extreme point of C.*

4.5 *Prove that every subspace of R^J is convex, and every linear manifold is convex.*

4.6 *Prove that every hyperplane $H(a, \gamma)$ is a linear manifold.*

4.7 *(a) Let C be a circular region in R^2. Determine the normal cone for a point on its circumference. (b) Let C be a rectangular region in R^2. Determine the normal cone for a point on its boundary.*

4.8 *Prove Lemmas 4.2, 4.3 and 4.4.*

4.9 *Let C be a convex set and $f : C \subseteq R^J \to (-\infty, \infty]$. Prove that $f(x)$ is a convex function, according to Definition 4.26, if and only if, for all x and y in C, and for all $0 < \alpha < 1$, we have*

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha) f(y).$$

4.10 *Let $f : R^J \to [-\infty, \infty]$. Prove that $f(x)$ is a convex function if and only if, for all $0 < \alpha < 1$, we have*

$$f(\alpha x + (1-\alpha)y) < \alpha b + (1-\alpha)c,$$

whenever $f(x) < b$ and $f(y) < c$.

4.11 *Show that the vector a is orthogonal to the hyperplane $H = H(a, \gamma)$; that is, if u and v are in H, then a is orthogonal to $u - v$.*

4.12 *Given a point s in a convex set C, where are the points x for which $s = P_C x$?*

4.13 *Let C be a closed non-empty convex set in R^J, x a vector not in C, and $d > 0$ the distance from x to C. Let*

$$\sigma_C(a) = \sup_{x \in C} \langle a, x \rangle,$$

the support function of C. Show that

$$d = \max_{||a|| \leq 1} \{\langle a, x \rangle - \sigma_C(a)\}.$$

Hints: Consider the unit vector $\frac{1}{d}(x - P_C x)$, and use Cauchy's Inequality and Proposition 4.4.

Remark: If, in the definition of the support function, we take the vectors a to be unit vectors, with $a = (\cos\theta, \sin\theta)$, for $0 \leq \theta < 2\pi$, then we can define the function

$$f(\theta) = \sup_{(x,y) \in C} x\cos\theta + y\sin\theta.$$

In [123] Tom Marzetta considers this function, as well as related functions of θ, such as the radius of curvature function, and establishes relationships between the behavior of these functions and the convex set itself.

4.14 (Rådström Cancellation [15])

- *(a) Show that, for any subset S of R^J, we have $2S \subseteq S + S$, and $2S = S + S$ if S is convex.*
- *(b) Find three finite subsets of R, say A, B, and C, with A not contained in B, but with the property that $A + C \subseteq B + C$. Hint: try to find an example where the set C is $C = \{-1, 0, 1\}$.*
- *(c) Show that, if A and B are convex, B is closed, and C is bounded, then $A + C \subseteq B + C$ implies that $A \subseteq B$. Hint: Note that, under these assumptions, $2A + C = A + (A + C) \subseteq 2B + C$.*

4.11 Course Homework

Do all the exercises in this chapter.

Chapter 5

Linear Programming

5.1 Chapter Summary

The term *linear programming* (LP) refers to the problem of optimizing a linear function of several variables over linear equality or inequality constraints. In this chapter we present the problem and establish the basic facts, including weak and strong duality. We then turn to a discussion of the simplex method, the most well known method for solving LP problems. We begin with a review of basic linear algebra. For a much more detailed discussion, consult [129].

5.2 Basic Linear Algebra

In this section we discuss bases and dimension, systems of linear equations, Gaussian elimination, and the notions of basic and non-basic variables.

5.2.1 Bases and Dimension

The notions of a basis and of linear independence are fundamental in linear algebra. Let $\mathcal{V}$ be a vector space.

Definition 5.1 *A collection of vectors* $\{u^1, ..., u^N\}$ *in* $\mathcal{V}$ *is* linearly independent *if there is no choice of scalars* $\alpha_1, ..., \alpha_N$*, not all zero, such that*

$$0 = \alpha_1 u^1 + ... + \alpha_N u^N. \tag{5.1}$$

Definition 5.2 *The* span *of a collection of vectors* $\{u^1, ..., u^N\}$ *in* $\mathcal{V}$ *is the set of all vectors* x *that can be written as linear combinations of the* u^n*; that is, for which there are scalars* $c_1, ..., c_N$*, such that*

$$x = c_1 u^1 + ... + c_N u^N. \tag{5.2}$$

Definition 5.3 *A collection of vectors* $\{w^1, ..., w^N\}$ *in* $\mathcal{V}$ *is called a* spanning set *for a subspace* S *if the set* S *is their span.*

Definition 5.4 *A collection of vectors* $\{u^1, ..., u^N\}$ *in* $\mathcal{V}$ *is called a* basis *for a subspace* S *if the collection is linearly independent and* S *is their span.*

Definition 5.5 *A collection of vectors* $\{u^1, ..., u^N\}$ *in* $\mathcal{V}$ *is called* orthonormal *if* $\|u^n\|_2 = 1$*, for all* n*, and* $\langle u^m, u^n\rangle = 0$*, for* $m \neq n$*.*

Suppose that S is a subspace of $\mathcal{V}$, that $\{w^1, ..., w^N\}$ is a spanning set for S, and $\{u^1, ..., u^M\}$ is a linearly independent subset of S. Beginning with w_1, we augment the set $\{u^1, ..., u^M\}$ with w_j if w_j is not in the span of the u_m and the w_k previously included. At the end of this process, we have a linearly independent spanning set, and therefore, a basis, for S (Why?). Similarly, beginning with w_1, we remove w_j from the set $\{w^1, ..., w^N\}$ if w_j is a linear combination of the w_k, $k = 1, ..., j-1$. In this way we obtain a linearly independent set that spans S, hence another basis for S. The following lemma will allow us to prove that all bases for a subspace S have the same number of elements.

Lemma 5.1 *Let* $W = \{w^1, ..., w^N\}$ *be a spanning set for a subspace* S *in* R^I*, and* $V = \{v^1, ..., v^M\}$ *a linearly independent subset of* S*. Then* $M \leq N$*.*

Proof: Suppose that $M > N$. Let $B_0 = \{w^1, ..., w^N\}$. To obtain the set B_1, form the set $C_1 = \{v_1, w_1, ..., w_N\}$ and remove the first member of C_1 that is a linear combination of members of C_1 that occur to its left in the listing; since v_1 has no members to its left, it is not removed. Since W is a spanning set, v_1 is a linear combination of the members of W, so that some member of W is a linear combination of v_1 and the members of W that precede it in the list; remove the first member of W for which this is true.

We note that the set B_1 is a spanning set for S and has N members. Having obtained the spanning set B_k, with N members and whose first k members are $v_k, ..., v_1$, we form the set $C_{k+1} = B_k \cup \{v_{k+1}\}$, listing the members so that the first $k+1$ of them are $\{v_{k+1}, v_k, ..., v_1\}$. To get the set B_{k+1} we remove the first member of C_{k+1} that is a linear combination of the members to its left; there must be one, since B_k is a spanning set, and so v_{k+1} is a linear combination of the members of B_k. Since the set V is linearly independent, the member removed is from the set W. Continuing in this fashion, we obtain a sequence of spanning sets $B_1, ..., B_N$, each with N members. The set B_N is $B_N = \{v_1, ..., v_N\}$ and v_{N+1} must then be a linear combination of the members of B_N, which contradicts the linear independence of V. ∎

Corollary 5.1 *Every basis for a subspace S has the same number of elements.*

Definition 5.6 *The* dimension *of a subspace S is the number of elements in any basis.*

5.2.2 The Rank of a Matrix

Let A by an I by J matrix and x a J by 1 column vector. The equation $Ax = b$ tells us that the vector b is a linear combination of the columns of the matrix A, with the entries of the vector x as the coefficients; that is,

$$b = x_1 a^1 + x_2 a^2 + ... + x_J a^J,$$

where a^j denotes the jth column of A. Similarly, when we write the product $C = AB$, we are saying that the kth column of C is a linear combination of the columns of A, with the entries of the kth column of B as coefficients. It will be helpful to keep this in mind when reading the proof of the next lemma.

Lemma 5.2 *For any matrix A, the maximum number of linearly independent rows equals the maximum number of linearly independent columns.*

Proof: Suppose that A is an I by J matrix, and that $K \leq J$ is the maximum number of linearly independent columns of A. Select K linearly independent columns of A and use them as the K columns of an I by K matrix U. Since every column of A must be a linear combination of these K selected ones, there is a K by J matrix M such that $A = UM$. From $A^T = M^T U^T$ we conclude that every column of A^T is a linear combination of the K columns of the matrix M^T. Therefore, there can be at most K linearly independent columns of A^T. ∎

Definition 5.7 *The* rank *of A is the maximum number of linearly independent rows or of linearly independent columns of A.*

5.2.3 Systems of Linear Equations

Consider the system of three linear equations in five unknowns given by

$$\begin{array}{rrrrrl} x_1 & +2x_2 & & +2x_4 & +x_5 & = 0 \\ -x_1 & -x_2 & +x_3 & +x_4 & & = 0\,. \\ x_1 & +2x_2 & -3x_3 & -x_4 & -2x_5 & = 0 \end{array} \tag{5.3}$$

This system can be written in matrix form as $Ax = 0$, with A the coefficient matrix

$$A = \begin{bmatrix} 1 & 2 & 0 & 2 & 1 \\ -1 & -1 & 1 & 1 & 0 \\ 1 & 2 & -3 & -1 & -2 \end{bmatrix}, \tag{5.4}$$

and $x = (x_1, x_2, x_3, x_4, x_5)^T$. Applying Gaussian elimination to this system, we obtain a second, simpler, system with the same solutions:

$$\begin{array}{rrrrrl} x_1 & & & -2x_4 & +x_5 & = 0 \\ & x_2 & & +2x_4 & & = 0\,. \\ & & x_3 & +x_4 & +x_5 & = 0 \end{array} \tag{5.5}$$

From this simpler system we see that the variables x_4 and x_5 can be freely chosen, with the other three variables then determined by this system of equations. The variables x_4 and x_5 are then independent, the others dependent. The variables x_1, x_2 and x_3 are then called *basic variables*. To obtain a basis of solutions we can let $x_4 = 1$ and $x_5 = 0$, obtaining the solution $x = (2, -2, -1, 1, 0)^T$, and then choose $x_4 = 0$ and $x_5 = 1$ to get the solution $x = (-1, 0, -1, 0, 1)^T$. Every solution to $Ax = 0$ is then a linear combination of these two solutions. Notice that which variables are basic and which are non-basic is somewhat arbitrary, in that we could have chosen as the non-basic variables any two whose columns are independent.

Having decided that x_4 and x_5 are the non-basic variables, we can write the original matrix A as $A = [\,B \quad N\,]$, where B is the square invertible matrix

$$B = \begin{bmatrix} 1 & 2 & 0 \\ -1 & -1 & 1 \\ 1 & 2 & -3 \end{bmatrix}, \tag{5.6}$$

and N is the matrix

$$N = \begin{bmatrix} 2 & 1 \\ 1 & 0 \\ -1 & -2 \end{bmatrix}. \tag{5.7}$$

With $x_B = (x_1, x_2, x_3)^T$ and $x_N = (x_4, x_5)^T$ we can write

$$Ax = Bx_B + Nx_N = 0, \tag{5.8}$$

so that

$$x_B = -B^{-1}Nx_N. \tag{5.9}$$

5.2.4 Real and Complex Systems of Linear Equations

A system $Ax = b$ of linear equations is called a *complex system*, or a *real system* if the entries of A, x and b are complex, or real, respectively. For any matrix A, we denote by A^T and $A^\dagger$ the transpose and conjugate transpose of A, respectively.

Any complex system can be converted to a real system in the following way. A complex matrix A can be written as $A = A_1 + iA_2$, where A_1 and A_2 are real matrices and $i = \sqrt{-1}$. Similarly, $x = x^1 + ix^2$ and $b = b^1 + ib^2$, where x^1, x^2, b^1 and b^2 are real vectors. Denote by $\tilde{A}$ the real matrix

$$\tilde{A} = \begin{bmatrix} A_1 & -A_2 \\ A_2 & A_1 \end{bmatrix}, \tag{5.10}$$

by $\tilde{x}$ the real vector

$$\tilde{x} = \begin{bmatrix} x^1 \\ x^2 \end{bmatrix}, \tag{5.11}$$

and by $\tilde{b}$ the real vector

$$\tilde{b} = \begin{bmatrix} b^1 \\ b^2 \end{bmatrix}. \tag{5.12}$$

Then x satisfies the system $Ax = b$ if and only if $\tilde{x}$ satisfies the system $\tilde{A}\tilde{x} = \tilde{b}$.

Definition 5.8 *A square matrix A is* symmetric *if $A^T = A$ and* Hermitian *if $A^\dagger = A$.*

Definition 5.9 *A non-zero vector x is said to be an* eigenvector *of the square matrix A if there is a scalar λ such that $Ax = \lambda x$. Then λ is said to be an* eigenvalue *of A.*

If x is an eigenvector of A with eigenvalue λ, then the matrix $A - \lambda I$ has no inverse, so its determinant is zero; here I is the identity matrix with ones on the main diagonal and zeros elsewhere. Solving for the roots of the determinant is one way to calculate the eigenvalues of A. For example, the eigenvalues of the Hermitian matrix

$$B = \begin{bmatrix} 1 & 2+i \\ 2-i & 1 \end{bmatrix} \tag{5.13}$$

are $\lambda = 1 + \sqrt{5}$ and $\lambda = 1 - \sqrt{5}$, with corresponding eigenvectors $u = (\sqrt{5}, 2 - i)^T$ and $v = (\sqrt{5}, i - 2)^T$, respectively. Then $\tilde{B}$ has the same eigenvalues, but both with multiplicity two. Finally, the associated eigenvectors of $\tilde{B}$ are

$$\begin{bmatrix} u^1 \\ u^2 \end{bmatrix}, \tag{5.14}$$

and

$$\begin{bmatrix} -u^2 \\ u^1 \end{bmatrix}, \tag{5.15}$$

for $\lambda = 1 + \sqrt{5}$, and

$$\begin{bmatrix} v^1 \\ v^2 \end{bmatrix}, \tag{5.16}$$

and

$$\begin{bmatrix} -v^2 \\ v^1 \end{bmatrix}, \tag{5.17}$$

for $\lambda = 1 - \sqrt{5}$.

5.3 Primal and Dual Problems

The fundamental problem in linear programming is to minimize the function

$$f(x) = c^T x, \tag{5.18}$$

over the *feasible set* F, that is, the convex set of all $x \geq 0$ with $Ax = b$. Shortly, we shall present an algebraic description of the extreme points of the feasible set F, in terms of *basic feasible solutions*, show that there are at most finitely many extreme points of F and that every member of F can be written as a convex combination of the extreme points, plus a direction of unboundedness. These results will be used to prove the basic theorems about the primal and dual linear programming problems and to describe the simplex algorithm.

Associated with the basic problem in LP, called the *primary problem*, there is a second problem, the *dual problem*. Both of these problems can be written in two equivalent ways, the canonical form and the standard form.

5.3.1 An Example

Consider the problem of maximizing the function $f(x_1, x_2) = x_1 + 2x_2$, over all $x_1 \geq 0$ and $x_2 \geq 0$, for which the inequalities

$$x_1 + x_2 \leq 40,$$

and

$$2x_1 + x_2 \leq 60$$

are satisfied. The set of points satisfying all four inequalities is the quadrilateral with vertices $(0,0)$, $(30,0)$, $(20,20)$, and $(0,40)$; draw a picture. Since the level curves of the function f are straight lines, the maximum value must occur at one of these vertices; in fact, it occurs at $(0,40)$ and the maximum value of f over the constraint set is 80. Rewriting the problem as minimizing the function $-x_1 - 2x_2$, subject to $x_1 \geq 0$, $x_2 \geq 0$,

$$-x_1 - x_2 \geq -40,$$

and

$$-2x_1 - x_2 \geq -60,$$

the problem is now in what is called *primal canonical form.*

5.3.2 Canonical and Standard Forms

Let b and c be fixed vectors and A a fixed matrix. The problem

$$\text{minimize } z = c^T x, \text{ subject to } Ax \geq b, x \geq 0 \text{ (PC)} \tag{5.19}$$

is the so-called *primary problem* of LP, in *canonical form.* The *dual problem* in canonical form is

$$\text{maximize } w = b^T y, \text{ subject to } A^T y \leq c, y \geq 0. \text{ (DC)} \tag{5.20}$$

The primary problem, in *standard form*, is

$$\text{minimize } z = c^T x, \text{ subject to } Ax = b, x \geq 0 \text{ (PS)} \tag{5.21}$$

with the dual problem in standard form given by

$$\text{maximize } w = b^T y, \text{ subject to } A^T y \leq c. \text{ (DS)} \tag{5.22}$$

Notice that the dual problem in standard form does not require that y be nonnegative. Note also that (PS) makes sense only if the system $Ax = b$ has solutions. For that reason, we shall assume, for the standard problems, that the I by J matrix A has at least as many columns as rows, so $J \geq I$, and A has full rank I.

If we are given the primary problem in canonical form, we can convert it to standard form by augmenting the variables, that is, by defining

$$u_i = (Ax)_i - b_i, \tag{5.23}$$

for $i = 1, ..., I$, and rewriting $Ax \geq b$ as

$$\tilde{A}\tilde{x} = b, \tag{5.24}$$

for $\tilde{A} = [\, A \quad -I \,]$ and $\tilde{x} = [x^T u^T]^T$.

If we are given the primary problem in standard form, we can convert it to canonical form by writing the equations as inequalities, that is, by replacing $Ax = b$ with the two matrix inequalities $Ax \geq b$, and $(-A)x \geq -b$.

5.3.3 Weak Duality

Consider the problems (PS) and (DS). Say that x is *feasible* if $x \geq 0$ and $Ax = b$. Let F be the set of feasible x. Say that y is *feasible* if $A^T y \leq c$. The *Weak Duality Theorem* is the following:

Theorem 5.1 *Let x and y be feasible vectors. Then*

$$z = c^T x \geq b^T y = w. \tag{5.25}$$

Corollary 5.2 *If z is not bounded below, then there are no feasible y.*

Corollary 5.3 *If x and y are both feasible, and $z = w$, then both x and y are optimal for their respective problems.*

The proof of the theorem and its corollaries are left as exercises.

The nonnegative quantity $c^T x - b^T y$ is called the *duality gap*. The *complementary slackness condition* says that, for optimal x and y, we have

$$x_j(c_j - (A^T y)_j) = 0, \tag{5.26}$$

for each j, which says that the duality gap is zero. Primal-dual algorithms for solving linear programming problems are based on finding sequences $\{x^k\}$ and $\{y^k\}$ that drive the duality gap down to zero [129].

5.3.4 Strong Duality

The *Strong Duality Theorems* make a stronger statement. One such theorem is the following.

Theorem 5.2 *If one of the problems (PS) or (DS) has an optimal solution, then so does the other and $z = w$ for the optimal vectors.*

Before we consider the proof of the theorem, we need a few preliminary results.

Definition 5.10 *A point x in F is said to be a* basic feasible solution *if the columns of A corresponding to positive entries of x are linearly independent.*

Recall that, for (PS), we assume that $J \geq I$ and the rank of A is I. Consequently, if, for some nonnegative vector x, the columns j for which x_j is positive are linearly independent, then x_j is positive for at most I values of j. Therefore, a basic feasible solution can have at most I positive entries. For a given set of entries, there can be at most one basic feasible solution for which precisely those entries are positive. Therefore, there can be only finitely many basic feasible solutions.

Now let x be an arbitrary basic feasible solution. Denote by B an invertible matrix obtained from A by deleting $J-I$ columns associated with zero entries of x. Note that, if x has fewer than I positive entries, then some of the columns of A associated with zero values of x_j are retained. The entries of an arbitrary vector y corresponding to the columns not deleted are called the *basic variables*. Then, assuming that the columns of B are the first I columns of A, we write $y^T = (y_B^T, y_N^T)$, and

$$A = [\, B \quad N \,], \tag{5.27}$$

so that $Ay = By_B + Ny_N$, $Ax = Bx_B = b$, and $x_B = B^{-1}b$.

The following theorems are taken from the book by Nash and Sofer [129]. We begin with a characterization of the extreme points of F (recall Definition 4.20).

Theorem 5.3 *A point x is in Ext(F) if and only if x is a basic feasible solution.*

Proof: Suppose that x is a basic feasible solution, and we write $x^T = (x_B^T, 0^T)$, $A = [\, B \quad N \,]$. If x is not an extreme point of F, then there are $y \neq x$ and $z \neq x$ in F, and α in $(0, 1)$, with

$$x = (1 - \alpha)y + \alpha z. \tag{5.28}$$

Then $y^T = (y_B^T, y_N^T)$, $z^T = (z_B^T, z_N^T)$, and $y_N \geq 0$, $z_N \geq 0$. From

$$0 = x_N = (1 - \alpha)y_N + (\alpha)z_N \tag{5.29}$$

it follows that

$$y_N = z_N = 0, \tag{5.30}$$

and $b = By_B = Bz_B = Bx_B$. But, since B is invertible, we have $x_B = y_B = z_B$. This is a contradiction, so x must be in Ext(F).

Conversely, suppose that x is in Ext(F). Since x is in F, we know that $Ax = b$ and $x \geq 0$. By reordering the variables if necessary, we may assume that $x^T = (x_B^T, x_N^T)$, with $x_B > 0$ and $x_N = 0$; we do not know that x_B is a vector of length I, however, so when we write $A = [\, B \quad N \,]$, we do not know that B is square.

If the columns of B are linearly independent, then, by definition, x is a basic feasible solution. If the columns of B were not linearly independent, we could construct $y \neq x$ and $z \neq x$ in F, such that

$$x = \frac{1}{2}y + \frac{1}{2}z, \tag{5.31}$$

as we now show. If $\{B_1, B_2, ..., B_K\}$ are the columns of B and are linearly dependent, then there are constants $p_1, p_2, ..., p_K$, not all zero, with

$$p_1 B_1 + ... + p_K B_K = 0. \tag{5.32}$$

With $p^T = (p_1, ..., p_K)$, we have

$$B(x_B + \alpha p) = B(x_B - \alpha p) = Bx_B = b, \tag{5.33}$$

for all $\alpha \in (0, 1)$. We then select α so small that both $x_B + \alpha p > 0$ and $x_B - \alpha p > 0$. Let

$$y^T = (x_B^T + \alpha p^T, 0^T) \tag{5.34}$$

and

$$z^T = (x_B^T - \alpha p^T, 0^T). \tag{5.35}$$

Therefore x is not an extreme point of F, which is a contradiction. This completes the proof. ∎

Corollary 5.4 *There are at most finitely many basic feasible solutions, so there are at most finitely many members of Ext(F).*

Theorem 5.4 *If F is not empty, then Ext(F) is not empty. In that case, let $\{v^1, ..., v^M\}$ be the members of Ext(F). Every x in F can be written as*

$$x = d + \alpha_1 v^1 + ... + \alpha_M v^M, \tag{5.36}$$

for some $\alpha_m \geq 0$, with $\sum_{m=1}^{M} \alpha_m = 1$, and some direction of unboundedness, d.

Proof: We consider only the case in which F is bounded, so there is no direction of unboundedness; the unbounded case is similar. Let x be a feasible point. If x is an extreme point, fine. If not, then x is not a basic feasible solution and the columns of A that correspond to the positive entries of x are not linearly independent. Then we can find a vector p such that $Ap = 0$ and $p_j = 0$ if $x_j = 0$. If $|\epsilon|$ is small enough, $x + \epsilon p$ is in F and $(x + \epsilon p)_j = 0$ if $x_j = 0$. Our objective now is to find another member of F that has fewer positive entries than x has.

We can alter ϵ in such a way that eventually $y = x + \epsilon p$ has at least one more zero entry than x has. To see this, let

$$-\epsilon = \frac{x_k}{p_k} = \min\{\frac{x_j}{p_j} | x_j > 0, p_j > 0\}.$$

Then the vector $x + \epsilon p$ is in F and has fewer positive entries than x has. Repeating this process, we must eventually reach the point at which there is no such vector p. At this point, we have obtained a basic feasible solution, which must then be an extreme point of F. Therefore, the set of extreme points of F is not empty.

The set G of all x in F that can be written as in Equation (5.36) is a closed set. Consequently, if there is x in F that cannot be written in this way, there is a ball of radius r, centered at x, having no intersection with G. We can then repeat the previous construction to obtain a basic feasible solution that lies within this ball. But such a vector would be an extreme point of F, and so would have to be a member of G, which would be a contradiction. Therefore, every member of F can be written according to Equation (5.36). ∎

Proof of the Strong Duality Theorem: Suppose now that x_* is a solution of the problem (PS) and $z_* = c^T x_*$. Without loss of generality, we may assume that x_* is a basic feasible solution, hence an extreme point of F (Why?). Then we can write

$$x_*^T = ((B^{-1}b)^T, 0^T), \tag{5.37}$$

$$c^T = (c_B^T, c_N^T), \tag{5.38}$$

and $A = [\, B \quad N \,]$. We shall show that

$$y_* = (B^{-1})^T c_B,$$

which depends on x_* via the matrix B, and

$$z_* = c^T x_* = y_*^T b = w_*.$$

Every feasible solution has the form

$$x^T = ((B^{-1}b)^T, 0^T) + ((B^{-1}Nv)^T, v^T), \tag{5.39}$$

for some $v \geq 0$. From $c^T x \geq c^T x_*$ we find that

$$(c_N^T - c_B^T B^{-1} N)(v) \geq 0, \tag{5.40}$$

for all $v \geq 0$. It follows that

$$c_N^T - c_B^T B^{-1} N = 0. \tag{5.41}$$

Now let $y_* = (B^{-1})^T c_B$, or $y_*^T = c_B^T B^{-1}$. We show that y_* is feasible for (DS); that is, we show that

$$A^T y_* \leq c^T. \tag{5.42}$$

Since

$$y_*^T A = (y_*^T B, y_*^T N) = (c_B^T, y_*^T N) = (c_B^T, c_B^T B^{-1} N) \tag{5.43}$$

and

$$c_N^T \geq c_B^T B^{-1} N, \tag{5.44}$$

we have

$$y_*^T A \leq c^T, \tag{5.45}$$

so y_* is feasible for (DS). Finally, we show that

$$c^T x_* = y_*^T b. \tag{5.46}$$

We have

$$y_*^T b = c_B^T B^{-1} b = c^T x_*. \tag{5.47}$$

This completes the proof. ∎

5.3.5 Gale's Strong Duality Theorem

Another strong duality theorem is due to David Gale [92].

Theorem 5.5 Gale's Strong Duality Theorem *If both problems (PC) and (DC) have feasible solutions, then both have optimal solutions and the optimal values are equal.*

Proof: We show that there are non-negative vectors x and y such that $Ax \geq b$, $A^T y \leq c$, and $b^T y - c^T x \geq 0$. It will then follow that $z = c^T x = b^T y = w$, so that x and y are both optimal. In matrix notation, we want to find $x \geq 0$ and $y \geq 0$ such that

$$\begin{bmatrix} A & 0 \\ 0 & -A^T \\ -c^T & b^T \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \geq \begin{bmatrix} b \\ -c \\ 0 \end{bmatrix}. \tag{5.48}$$

We assume that there are no $x \geq 0$ and $y \geq 0$ for which the inequalities in (5.48) hold. Then, according to Theorem 4.11, there are non-negative vectors s and t, and non-negative scalar ρ such that

$$\begin{bmatrix} -A^T & 0 & c \\ 0 & A & -b \end{bmatrix} \begin{bmatrix} s \\ t \\ \rho \end{bmatrix} \geq 0, \tag{5.49}$$

and

$$\begin{bmatrix} -b^T & c^T & 0 \end{bmatrix} \begin{bmatrix} s \\ t \\ \rho \end{bmatrix} < 0. \tag{5.50}$$

Note that ρ cannot be zero, for then we would have $A^T s \leq 0$ and $At \geq 0$. Taking feasible vectors x and y, we would find that $s^T Ax \leq 0$, which implies that $b^T s \leq 0$, and $t^T A^T y \geq 0$, which implies that $c^T t \geq 0$. Therefore, we could not also have $c^T t - b^T s < 0$.

Writing out the inequalities, we have

$$\rho c^T t \geq s^T At \geq s^T(\rho b) = \rho s^T b.$$

Using $\rho > 0$, we find that

$$c^T t \geq b^T s,$$

which is a contradiction. Therefore, there do exist $x \geq 0$ and $y \geq 0$ such that $Ax \geq b$, $A^T y \leq c$, and $b^T y - c^T x \geq 0$. ∎

5.4 Some Examples

We give two well known examples of LP problems.

5.4.1 The Diet Problem

There are nutrients indexed by $i = 1, ..., I$ and our diet must contain at least b_i units of the ith nutrient. There are J foods, indexed by $j = 1, ..., J$, and one unit of the jth food cost c_j dollars and contains A_{ij} units of the ith nutrient. The problem is to minimize the cost, while obtaining at least the minimum amount of each nutrient.

Let $x_j \geq 0$ be the amount of the jth food that we consume. Then we need $Ax \geq b$, where A is the matrix with entries A_{ij}, b is the vector with entries b_i and x is the vector with entries $x_j \geq 0$. With c the vector with entries c_j, the total cost of our food is $z = c^T x$. The problem is then to minimize $z = c^T x$, subject to $Ax \geq b$ and $x \geq 0$. This is the primary LP problem, in canonical form.

5.4.2 The Transport Problem

We must ship products from sources to destinations. There are I sources, indexed by $i = 1, ..., I$, and J destinations, indexed by $j = 1, ..., J$. There are a_i units of product at the ith source, and we must have at least b_j units reaching the jth destination. The customer will pay C_{ij} dollars to get one unit from i to j. Let x_{ij} be the number of units of product to go from the ith source to the jth destination. The producer wishes to maximize income, that is,

$$\text{maximize } \sum_{i,j} C_{ij} x_{ij},$$

subject to

$$x_{ij} \geq 0,$$

$$\sum_{i=1}^{I} x_{ij} \geq b_j,$$

and

$$\sum_{j=1}^{J} x_{ij} \leq a_i.$$

Obviously, we must assume that

$$\sum_{i=1}^{I} a_i \geq \sum_{j=1}^{J} b_j.$$

This problem is not yet in the form of the LP problems considered so far. It also introduces a new feature, namely, it may be necessary to have x_{ij} a non-negative integer, if the products exist only in whole units. This leads to *integer programming*.

5.5 The Simplex Method

In this section we sketch the main ideas of the simplex method. For further details see [129].

Begin with a basic feasible solution of (PS) $\hat{x}$. Assume, as previously, that

$$A = [\, B \quad N \,], \tag{5.51}$$

where B is an I by I invertible matrix obtained by deleting from A some (but perhaps not all) columns associated with zero entries of $\hat{x}$. As before, we assume the variables have been ordered so that the zero entries of $\hat{x}$ have the highest index values. The entries of an arbitrary x corresponding to the first I columns are the basic variables. We write $x^T = (x_B^T, x_N^T)$, and so that $\hat{x}_N = 0$, $A\hat{x} = B\hat{x}_B = b$, and $\hat{x}_B = B^{-1}b$. The current value of z is

$$\hat{z} = c_B^T \hat{x}_B = c_B^T B^{-1} b.$$

We are interested in what happens to z as x_N takes on positive entries.

For any feasible x we have $Ax = b = Bx_B + Nx_n$, so that

$$x_B = B^{-1}b - B^{-1}Nx_N,$$

and

$$z = c^T x = c_B^T x_B + c_N^T x_N = c_B^T (B^{-1}b - B^{-1}Nx_N) + c_N^T x_N.$$

Therefore,

$$z = c_B^T B^{-1} b + (c_N^T - c_B^T B^{-1} N) x_N = \hat{z} + r^T x_N,$$

where

$$r^T = (c_N^T - c_B^T B^{-1} N).$$

The vector r is called the *reduced cost vector*. We define the vector $y^T = c_B^T B^{-1}$ of *simplex multipliers*, and write

$$z - \hat{z} = r^T x_N = (c_N^T - y^T N) x_N.$$

We are interested in how z changes as we move away from $\hat{x}$ and permit x_N to have positive entries.

If x_N is non-zero, then z changes by $r^T x_N$. Therefore, if $r \geq 0$, the current $\hat{z}$ cannot be made smaller by letting x_N have some positive entries; the current $\hat{x}$ is then optimal. Initially, at least, r will have some negative entries, and we use these as a guide in deciding how to select x_N.

Keep in mind that the vectors x_N and r have length $J - I$ and the jth column of N is the $(I + j)$th column of A.

Select an index j such that

$$r_j < 0, \tag{5.52}$$

and r_j is the most negative of the negative entries of r. Then x_{I+j} is called the *entering variable*. Compute $d^j = B^{-1} a^j$, where a^j is the $(I + j)$th column of A, which is the jth column of N. If we allow $(x_N)_j = x_{I+j}$ to be positive, then

$$x_B = B^{-1} b - x_{I+j} B^{-1} a^j = B^{-1} b - x_{I+j} d^j.$$

We need to make sure that x_B remains non-negative, so we need

$$(B^{-1} b)_i - x_{I+j} d_i^j \geq 0,$$

for all indices $i = 1, ..., I$. If the ith entry d_i^j is negative, then $(x_B)_i$ increases as x_{I+j} becomes positive; if $d_i^j = 0$, then $(x_B)_i$ remains unchanged. The problem arises when d_i^j is positive.

Find an index s in $\{1, ..., I\}$ for which

$$\frac{(B^{-1} b)_s}{d_s^j} = \min\{\frac{(B^{-1} b)_i}{d_i^j} : d_i^j > 0\}. \tag{5.53}$$

Then x_s is the *leaving variable*, replacing x_{I+j}; that is, the new set of indices corresponding to new basic variables will now include $I + j$, and no longer include s. The new entries of $\hat{x}$ are $\hat{x}_s = 0$ and

$$\hat{x}_{I+j} = \frac{(B^{-1} b)_s}{d_s^j}.$$

We then rearrange the columns of A to redefine B and N, and rearrange the positions of the entries of x, to get the new basic variables vector x_B, the new x_N and the new c. Then we repeat the process.

It is helpful to note that when the columns of A are rearranged and a new B is defined, the new B differs from the old B in only one column. Therefore

$$B_{\text{new}} = B_{\text{old}} - uv^T, \tag{5.54}$$

where u is the column vector that equals the old column minus the new one, and v is the column of the identity matrix corresponding to the column of B_{old} being altered. The inverse of B_{new} can be obtained fairly easily from the inverse of B_{old} using the Sherman-Morrison-Woodbury Identity:

The Sherman-Morrison-Woodbury Identity:

$$(B - uv^T)^{-1} = B^{-1} + \alpha(B^{-1}u)(v^T B^{-1}), \tag{5.55}$$

where

$$\alpha = \frac{1}{1 - v^T B^{-1} u}.$$

We shall illustrate this in the example below.

5.6 An Example of the Simplex Method

Consider once again the problem of maximizing the function $f(x_1, x_2) = x_1 + 2x_2$, over all $x_1 \geq 0$ and $x_2 \geq 0$, for which the inequalities

$$x_1 + x_2 \leq 40,$$

and

$$2x_1 + x_2 \leq 60$$

are satisfied. In (PS) form, the problem is to minimize the function $-x_1 - 2x_2$, subject to $x_1 \geq 0$, $x_2 \geq 0$, $x_3 \geq 0$, $x_4 \geq 0$,

$$-x_1 - x_2 - x_3 = -40,$$

and

$$-2x_1 - x_2 - x_4 = -60.$$

The matrix A is then

$$A = \begin{bmatrix} -1 & -1 & -1 & 0 \\ -2 & -1 & 0 & -1 \end{bmatrix}, \tag{5.56}$$

the matrix B is

$$B = \begin{bmatrix} -1 & -1 \\ -2 & -1 \end{bmatrix}, \tag{5.57}$$

with inverse

$$B^{-1} = \begin{bmatrix} 1 & -1 \\ -2 & 1 \end{bmatrix}, \tag{5.58}$$

and the matrix N is

$$N = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{5.59}$$

The vector b is $b = (-40, -60)^T$. A general vector x is $x = (x_1, x_2, x_3, x_4)^T$, with $x_B = (x_1, x_2)^T$ and $x_N = (x_3, x_4)^T$, and $c = (-1, -2, 0, 0)^T$, with $c_B = (-1, -2)^T$ and $c_N = (0, 0)^T$. The *feasible set* of points satisfying all four inequalities is the quadrilateral in R^2 with vertices $(0, 0)$, $(30, 0)$, $(20, 20)$, and $(0, 40)$. In R^4, these vertices correspond to the vectors $(0, 0, 40, 60)^T$, $(30, 0, 10, 0)^T$, $(20, 20, 0, 0)^T$, and $(0, 40, 0, 20)^T$. Since we have chosen to start with x_1 and x_2 as our basic variables, we let our starting vector be $\hat{x} = (20, 20, 0, 0)^T$, so that $\hat{x}_B = B^{-1}b = (20, 20)^T$, and $\hat{x}_N = (0, 0)^T$. Then we find that $y^T = c_B^T B^{-1} = (3, -1)^T$, and $y^T N = (-3, 1)^T$. The reduced cost vector is then

$$r^T = c_N^T - y^T N = (0, 0)^T - (-3, 1)^T = (3, -1)^T.$$

Since r^T has a negative entry in its second position, $j = 2$, we learn that the entering variable is going to be $x_{2+j} = x_4$. The fourth column of A is $(0, -1)^T$, so the vector d^2 is

$$d^2 = B^{-1}(0, -1)^T = (1, -1)^T.$$

Therefore, we must select a new positive value for x_4 that satisfies

$$(20, 20) \geq x_4(1, -1).$$

The single positive entry of d^2 is the first one, from which we conclude that the leaving variable will be x_1. We therefore select as the new values of the variables $\hat{x}_1 = 0$, $\hat{x}_2 = 40$, $\hat{x}_3 = 0$, and $\hat{x}_4 = 20$. We then reorder the variables as $x = (x_4, x_2, x_3, x_1)^T$ and rearrange the columns of A accordingly. Having done this, we see that we now have

$$B = B_{\text{new}} = \begin{bmatrix} 0 & -1 \\ -1 & -1 \end{bmatrix}, \tag{5.60}$$

with inverse

$$B^{-1} = \begin{bmatrix} 1 & -1 \\ -1 & 0 \end{bmatrix}, \tag{5.61}$$

and the matrix N is

$$N = \begin{bmatrix} -1 & -1 \\ 0 & -2 \end{bmatrix}. \tag{5.62}$$

Since

$$B_{\text{new}} = B_{\text{old}} - \begin{bmatrix} -1 \\ -1 \end{bmatrix} [\, 1 \quad 0 \,],$$

we can apply the Sherman-Morrison-Woodbury Identity to get B_{new}^{-1}.

The reduced cost vector is now $r^T = (2, 1)^T$. Since it has no negative entries, we have reached the optimal point; the solution is $\hat{x}_1 = 0$, $\hat{x}_2 = 40$, with slack variables $\hat{x}_3 = 0$ and $\hat{x}_4 = 20$.

5.7 Another Example of the Simplex Method

The following example is taken from Fang and Puthenpura [86]. Minimize the function

$$f(x_1, x_2, x_3, x_4, x_5, x_6) = -x_1 - x_2 - x_3,$$

subject to

$$2x_1 + x_4 = 1;$$

$$2x_2 + x_5 = 1;$$

$$2x_3 + x_6 = 1;$$

and $x_i \geq 0$, for $i = 1, ..., 6$. The variables x_4, x_5, and x_6 appear to be slack variables, introduced to obtain equality constraints.

Initially, we define the matrix A to be

$$A = \begin{bmatrix} 2 & 0 & 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 0 & 0 & 1 \end{bmatrix}, \tag{5.63}$$

$b = (1, 1, 1)^T$, $c = (-1, -1, -1, 0, 0, 0)^T$ and $x = (x_1, x_2, x_3, x_4, x_5, x_6)^T$.

Suppose we begin with x_4, x_5, and x_6 as the basic variables. We then rearrange the entries of the vector of unknowns so that

$$x = (x_4, x_5, x_6, x_1, x_2, x_3)^T.$$

Now we have to rearrange the columns of A as well; the new A is

$$A = \begin{bmatrix} 1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 0 & 0 & 2 \end{bmatrix}. \tag{5.64}$$

The vector c must also be redefined; the new one is $c = (0, 0, 0, -1, -1, -1)^T$, so that $c_N = (-1, -1, -1)^T$ and $c_B = (0, 0, 0)^T$.

For this first step of the simplex method we have

$$B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and

$$N = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

Note that one advantage in choosing the slack variables as the basic variables is that it is easy then to find the corresponding basic feasible solution, which is now

$$\hat{x} = \begin{bmatrix} \hat{x}_4 \\ \hat{x}_5 \\ \hat{x}_6 \\ \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{bmatrix} = \begin{bmatrix} \hat{x}_B \\ \hat{x}_N \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

The reduced cost vector r is then

$$r = (-1, -1, -1)^T;$$

since it has negative entries, the current basic feasible solution is not optimal.

Suppose that we select a non-basic variable with negative reduced cost, say x_1, which, we must remember, is the fourth entry of the redefined x, so $j = 1$ and $I + j = 4$. Then x_1 is the entering basic variable, and the vector d^1 is then

$$d^1 = B^{-1}a^j = (1, 0, 0)^T.$$

The only positive entry of d^1 is the first one, which means, according to Equation (5.53), that the exiting variable should be x_4. Now the new set of basic variables is $\{x_5, x_6, x_1\}$ and the new set of non-basic variables is $\{x_2, x_3, x_4\}$. The new matrices B and N are

$$B = \begin{bmatrix} 0 & 0 & 2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

and

$$N = \begin{bmatrix} 0 & 0 & 1 \\ 2 & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix}.$$

Continuing through two more steps, we find that the optimal solution is $-3/2$, and it occurs at the vector

$$x = (x_1, x_2, x_3, x_4, x_5, x_6)^T = (1/2, 1/2, 1/2, 0, 0, 0)^T.$$

5.8 Some Possible Difficulties

In the first example of the simplex method, we knew all four of the vertices of the feasible region, so we could choose any one of them to get our initial basic feasible solution. We chose to begin with x_1 and x_2 as our basic variables, which meant that the slack variables were zero and our first basic feasible solution was $\hat{x} = (20, 20, 0, 0)^T$. In the second example, we chose the slack variables to be the initial basic variables, which made it easy to find the initial basic feasible solution. Generally, however, finding an initial basic feasible solution may not be easy.

You might think that we can always simply take the slack variables as our initial basic variables, so that the initial B is just the identity matrix, and the initial basic feasible solution is merely the concatenation of the column vectors b and 0, as in the second example. The following example shows why this may not always work.

5.8.1 A Third Example:

Consider the problem of minimizing the function $z = 2x_1 + 3x_2$, subject to

$$3x_1 + 2x_2 = 14,$$

$$2x_1 - 4x_2 - x_3 = 2,$$

$$4x_1 + 3x_2 + x_4 = 19,$$

and $x_i \geq 0$, for $i = 1, ..., 4$. The matrix A is now

$$A = \begin{bmatrix} 3 & 2 & 0 & 0 \\ 2 & -4 & -1 & 0 \\ 4 & 3 & 0 & 1 \end{bmatrix}. \tag{5.65}$$

There are only two slack variables, so we cannot construct our set of basic variables using only slack variables, since the matrix B must be square. We cannot begin with $\hat{x}_1 = \hat{x}_2 = 0$, since this would force $\hat{x}_3 = -2$, which is not permitted. We can choose $\hat{x}_2 = 0$ and solve for the other three, to get $\hat{x}_1 = \frac{14}{3}$, $\hat{x}_3 = \frac{22}{3}$, and $\hat{x}_4 = \frac{1}{3}$. This is relatively easy only because the problem is artificially small. The point here is that, for realistically large LP problems, finding a place to begin the simplex algorithm may not be a simple matter. For more on this matter, see [129].

In both of our first two examples, finding the inverse of the matrix B is easy, since B is only 2 by 2, or 3 by 3. In larger problems, finding B^{-1}, or better, solving $y^T B = c_B^T$ for y^T, is not trivial and can be an expensive part of each iteration. The Sherman-Morrison-Woodbury identity is helpful here.

5.9 Topics for Projects

The simplex method provides several interesting topics for projects.

- **1.** Investigate the issue of finding a suitable starting basic feasible solution. Reference [129] can be helpful in this regard.
- **2.** How can we reduce the cost associated with solving $y^T B = c_B^T$ for y^T at each step of the simplex method?
- **3.** Suppose that, instead of needing the variables to be nonnegative, we need each x_i to lie in the interval $[\alpha_i, \beta_i]$. How can we modify the simplex method to incorporate these constraints?
- **4.** Investigate the role of linear programming and the simplex method in graph theory and networks, with particular attention to the transport problem.
- **5.** There is a sizable literature on the computational complexity of the simplex method. Investigate this issue and summarize your findings.

5.10 Exercises

5.1 *Prove Theorem 5.1 and its corollaries.*

5.2 *Let $W = \{w^1, ..., w^N\}$ be a spanning set for a subspace S in R^I, and $V = \{v^1, ..., v^M\}$ a linearly independent subset of S. Let A be the matrix whose columns are the v^m, B the matrix whose columns are the w^n. Show that there is an N by M matrix C such that $A = BC$. Prove Lemma 5.1 by showing that, if $M > N$, then there is a non-zero vector x with $Cx = Ax = 0$.*

5.3 *Complete the calculation of the optimal solution for the problem in the second example of the simplex method.*

5.4 *Consider the following problem, taken from [86]. Minimize the function*

$$f(x_1, x_2, x_3, x_4) = -3x_1 - 2x_2,$$

subject to

$$x_1 + x_2 + x_3 = 40,$$
$$2x_1 + x_2 + x_4 = 60,$$

and

$$x_j \geq 0,$$

for $j = 1, ..., 4$. Use the simplex method to find the optimum solution. Take as a starting vector $x^0 = (0, 0, 40, 60)^T$.

5.5 *Redo the first example of the simplex method, starting with the vertex* $x_1 = 0$ *and* $x_2 = 0$.

5.6 *Consider the LP problem of maximizing the function* $f(x_1, x_2) = x_1 + 2x_2$, *subject to*

$$-2x_1 + x_2 \leq 2,$$
$$-x_1 + 2x_2 \leq 7,$$
$$x_1 \leq 3,$$

and $x_1 \geq 0$, $x_2 \geq 0$. *Start at* $x_1 = 0$, $x_2 = 0$. *You will find that you have a choice for the entering variable; try it both ways.*

5.7 *Carry out the next two steps of the simplex algorithm for the second example given earlier.*

5.8 *Apply the simplex method to the problem of minimizing* $z = -x_1 - 2x_2$, *subject to*

$$-x_1 + x_2 \leq 2,$$
$$-2x_1 + x_2 \leq 1,$$

and $x_1 \geq 0$, $x_2 \geq 0$.

5.11 Course Homework

Do Exercises 5.5, 5.6 and 5.7.

Chapter 6

Matrix Games and Optimization

6.1 Chapter Summary

The theory of two-person games is largely the work of John von Neumann, and was developed somewhat later by von Neumann and Morgenstern [132] as a tool for economic analysis. Two-person zero-sum games provide a nice example of optimization and an opportunity to apply some of the linear algebra and linear programming tools previously discussed. In this chapter we introduce the idea of two-person matrix games and use results from linear programming to prove the Fundamental Theorem of Game Theory.

6.2 Two-Person Zero-Sum Games

A two-person game is called a *constant-sum game* if the total payout is the same, each time the game is played. In such cases, we can subtract half the total payout from the payout to each player and record only the difference. Then the total payout appears to be zero, and such games are called *zero-sum games*. We can then suppose that whatever one player wins is paid by the other player. Except for the final section, we shall consider only two-person, zero-sum games.

6.3 Deterministic Solutions

In this two-person game, the first player, call him P1, selects a row of the I by J real matrix A, say i, and the second player selects a column of A, say j. The second player, call her P2, pays the first player A_{ij}. If some $A_{ij} < 0$,

then this means that the first player pays the second. Since whatever the first player wins, the second loses, and vice versa, we need only one matrix to summarize the situation.

6.3.1 Optimal Pure Strategies

In our first example, the matrix is

$$A = \begin{bmatrix} 7 & 8 & 4 \\ 4 & 7 & 2 \end{bmatrix}. \tag{6.1}$$

The first player notes that by selecting row $i = 1$, he will get at least 4, regardless of which column the second player plays. The second player notes that, by playing column $j = 3$, she will pay the first player no more than 4, regardless of which row the first player plays. If the first player then begins to play $i = 1$ repeatedly, and the second player notices this consistency, she will still have no motivation to play any column except $j = 3$, because the other pay-outs are both worse than 4. Similarly, so long as the second player is playing $j = 3$ repeatedly, the first player has no motivation to play anything other than $i = 1$, since he will be paid less if he switches. Therefore, both players adopt a *pure strategy* of $i = 1$ and $j = 3$. This game is said to be *deterministic* and the entry $A_{1,3} = 4$ is a *saddle-point* because it is the maximum of its column and the minimum of its row. Not all such two-person games have saddle-points, however.

6.3.2 An Exercise

6.1 *Show that, in this case, we have*

$$\max_i \min_j A_{ij} = 4 = \min_j \max_i A_{ij}.$$

6.3.3 Optimal Randomized Strategies

Consider now the two-person game with pay-off matrix

$$A = \begin{bmatrix} 4 & 1 \\ 2 & 3 \end{bmatrix}. \tag{6.2}$$

The first player notes that by selecting row $i = 2$, he will get at least 2, regardless of which column the second player plays. The second player notes that, by playing column $j = 2$, she will pay the first player no more than 3, regardless of which row the first player plays. If both begin by playing in this conservative manner, the first player will play $i = 2$ and the second player will play $j = 2$.

If the first player plays $i = 2$ repeatedly, and the second player notices this consistency, she will be tempted to switch to playing column $j = 1$,

thereby losing only 2, instead of 3. If she makes the switch and the first player notices, he will be motivated to switch his play to row $i = 1$, to get a pay-off of 4, instead of 2. The second player will then soon switch to playing $j = 2$ again, hoping that the first player sticks with $i = 1$. But the first player is not stupid, and quickly returns to playing $i = 2$. There is no saddle-point in this game.

For such games, it makes sense for both players to select their play at random, with the first player playing $i = 1$ with probability p and $i = 2$ with probability $1 - p$, and the second player playing column $j = 1$ with probability q and $j = 2$ with probability $1-q$. These are called *randomized strategies*.

When the first player plays $i = 1$, he expects to get $4q+(1-q) = 3q+1$, and when he plays $i = 2$ he expects to get $2q + 3(1 - q) = 3 - q$. Since he plays $i = 1$ with probability p, he expects to get

$$p(3q + 1) + (1 - p)(3 - q) = 4pq - 2p - q + 3 = (4p - 1)q + 3 - 2p.$$

He notices that if he selects $p = \frac{1}{4}$, then he expects to get $\frac{5}{2}$, regardless of what the second player does. If he plays something other than $p = \frac{1}{4}$, his expected winnings will depend on what the second player does. If he selects a value of p less than $\frac{1}{4}$, and $q = 1$ is selected, then he wins $2p + 2$, but this is less than $\frac{5}{2}$. If he selects $p > \frac{1}{4}$ and $q = 0$ is selected, then he wins $3 - 2p$, which again is less than $\frac{5}{2}$. The maximum of these minimum pay-offs occurs when $p = \frac{1}{4}$ and the *max-min* win is $\frac{5}{2}$.

Similarly, the second player, noticing that

$$p(3q + 1) + (1 - p)(3 - q) = (4q - 2)p + 3 - q,$$

sees that she will pay out $\frac{5}{2}$ if she takes $q = \frac{1}{2}$. If she selects a value of q less than $\frac{1}{2}$, and $p = 0$ is selected, then she pays out $3 - q$, which is more than $\frac{5}{2}$. If, on the other hand, she selects a value of q that is greater than $\frac{1}{2}$, and $p = 1$ is selected, then she will pay out $3q+1$, which again is greater than $\frac{5}{2}$. The only way she can be certain to pay out no more than $\frac{5}{2}$ is to select $q = \frac{1}{2}$. The minimum of these maximum pay-outs occurs when she chooses $q = \frac{1}{2}$, and the *min-max* pay-out is $\frac{5}{2}$.

This leads us to the question of whether or not there will always be probability vectors for the players that will lead to the equality of the max-min win and the min-max pay-out.

We make a notational change at this point. From now on the letters p and q will denote probability column vectors, and not individual probabilities, as previously.

6.3.4 The Min-Max Theorem

Let A be an I by J pay-off matrix. Let

$$P = \{p = (p_1, ..., p_I) \,|\, p_i \geq 0, \sum_{i=1}^{I} p_i = 1\},$$

$$Q = \{q = (q_1, ..., q_J) \,|\, q_j \geq 0, \sum_{j=1}^{J} q_j = 1\},$$

and

$$R = A(Q) = \{Aq \,|\, q \in Q\}.$$

The first player selects a vector p in P and the second selects a vector q in Q. The expected pay-off to the first player is

$$E = \langle p, Aq \rangle = p^T Aq.$$

Let

$$m_0 = \max_{p \in P} \min_{r \in R} \langle p, r \rangle,$$

and

$$m^0 = \min_{r \in R} \max_{p \in P} \langle p, r \rangle;$$

the interested reader may want to prove that the maximum and minimum exist. Clearly, we have

$$\min_{r \in R} \langle p, r \rangle \leq \langle p, r \rangle \leq \max_{p \in P} \langle p, r \rangle,$$

for all $p \in P$ and $r \in R$. It follows that $m_0 \leq m^0$. The Min-Max Theorem, also known as the Fundamental Theorem of Game Theory, asserts that $m_0 = m^0$.

Theorem 6.1 The Fundamental Theorem of Game Theory *Let A be an arbitrary real I by J matrix. Then there are vectors $\hat{p}$ in P and $\hat{q}$ in Q such that*

$$p^T A\hat{q} \leq \hat{p}^T A\hat{q} \leq \hat{p}^T Aq, \tag{6.3}$$

for all p in P and q in Q.

The quantity $\omega = \hat{p}^T A\hat{q}$ is called the *value of the game*. Notice that if P1 knows that P2 plays according to the mixed-strategy vector q, P1 could examine the entries $(Aq)_i$, which are his expected pay-offs should he play strategy i, and select the one for which this expected pay-off is largest. However, if P2 notices what P1 is doing, she can abandon $\hat{q}$ to her

advantage. When $q = \hat{q}$, it follows from the inequalities in (6.3), by taking p to have the ith entry equal to one and the rest zero, that

$$(A\hat{q})_i \leq \omega$$

for all i, and

$$(A\hat{q})_i = \omega$$

for all i for which $\hat{p}_i > 0$.

There are a number of different proofs of the Fundamental Theorem. In a later chapter, we present a proof using Fenchel Duality. For the remainder of this chapter we consider various proofs, focusing mainly on linear algebra methods, linear programming, and theorems of the alternative.

6.4 Symmetric Games

A game is said to be *symmetric* if the available strategies are the same for both players, and if the players switch strategies, the outcomes switch also. In other words, the pay-off matrix A is skew-symmetric, that is, A is square and $A_{ji} = -A_{ij}$. For symmetric games, we can use Theorem 4.12 to prove the existence of a randomized solution.

First, we show that there is a probability vector $\hat{p} \geq 0$ such that $\hat{p}^T A \geq 0$. Then we show that

$$p^T A\hat{p} \leq 0 = \hat{p}^T A\hat{p} \leq \hat{p}^T Aq,$$

for all probability vectors p and q. It will then follow that $\hat{p}$ and $\hat{q} = \hat{p}$ are the optimal mixed strategies.

If there is no non-zero $x \geq 0$ such that $x^T A \geq 0$, then there is no non-zero $x \geq 0$ such that $A^T x \geq 0$. Then, by Theorem 4.12, we know that there is $y \geq 0$ with $Ay < 0$; obviously y is not the zero vector, in this case. Since $A^T = -A$, it follows that $y^T A > 0$. Consequently, there is a non-zero $x \geq 0$, such that $x^T A \geq 0$; it is $x = y$. This is a contradiction. So $\hat{p}$ exists.

Since the game is symmetric, we have

$$\hat{p}^T A\hat{p} = (\hat{p}^T A\hat{p})^T = \hat{p}^T A^T \hat{p} = -\hat{p}^T A\hat{p},$$

so that $\hat{p}^T A\hat{p} = 0$.

For any probability vectors p and q we have

$$p^T A\hat{p} = \hat{p}^T A^T p = -\hat{p}^T Ap \leq 0,$$

and

$$0 \leq \hat{p}^T Aq.$$

We conclude that the mixed strategies $\hat{p}$ and $\hat{q} = \hat{p}$ are optimal.

6.4.1 An Example of a Symmetric Game

We present now a simple example of a symmetric game and compute the optimal randomized strategies.

Consider the pay-off matrix

$$A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{6.4}$$

This matrix is skew-symmetric, so the game is symmetric. Let $\hat{p}^T = [1, 0]$; then $\hat{p}^T A = [0, 1] \geq 0$. We show that $\hat{p}$ and $\hat{q} = \hat{p}$ are the optimal randomized strategies. For any probability vectors $p^T = [p_1, p_2]$ and $q^T = [q_1, q_2]$, we have

$$p^T A\hat{p} = -p_2 \leq 0,$$

$$\hat{p}^T A\hat{p} = 0,$$

and

$$\hat{p}^T Aq = q_2 \geq 0.$$

It follows that the pair of strategies $\hat{p} = \hat{q} = [1, 0]^T$ are optimal randomized strategies.

6.4.2 Comments on the Proof of the Min-Max Theorem

In [92], Gale proves the existence of optimal randomized solutions for an arbitrary matrix game by showing that there is associated with such a game a symmetric matrix game and that an optimal randomized solution exists for one if and only if such exists for the other.

6.5 Positive Games

As Gale notes in [92], it is striking that two fundamental mathematical tools in linear economic theory, linear programming and game theory, developed simultaneously, and independently, in the years following the Second World War. More remarkable still was the realization that these two areas are closely related. Gale's proof of the Min-Max Theorem, which relates the game to a linear programming problem and employs his Strong Duality Theorem, provides a good illustration of this close connection.

If the I by J pay-off matrix A has only positive entries, we can use Gale's Strong Duality Theorem 5.5 for linear programming to prove the Min-Max Theorem.

Let b and c be the vectors whose entries are all one. Consider the LP problem of minimizing $z = c^T x$, over all $x \geq 0$ with $A^T x \geq b$; this is the (PC) problem. The (DC) problem is then to maximize $w = b^T y$, over all

$y \geq 0$ with $Ay \leq c$. Since A has only positive entries, both (PC) and (DC) are feasible, so, by Gale's Strong Duality Theorem 5.5, we know that there are feasible non-negative vectors $\hat{x}$ and $\hat{y}$ and non-negative μ such that

$$\hat{z} = c^T\hat{x} = \mu = b^T\hat{y} = \hat{w}.$$

Since $\hat{x}$ cannot be zero, μ must be positive.

6.5.1 Some Exercises

6.2 *Show that the vectors $\hat{p} = \frac{1}{\mu}\hat{x}$ and $\hat{q} = \frac{1}{\mu}\hat{y}$ are probability vectors and are optimal randomized strategies for the matrix game.*

6.3 *Given an arbitrary I by J matrix A, there is $\alpha > 0$ so that the matrix B with entries $B_{ij} = A_{ij} + \alpha$ has only positive entries. Show that any optimal randomized probability vectors for the game with pay-off matrix B are also optimal for the game with pay-off matrix A.*

It follows from these exercises that there exist optimal randomized solutions for any matrix game.

6.5.2 Comments

This proof of the Min-Max Theorem shows that we can associate with a given matrix game a linear programming problem. It follows that we can use the simplex method to find optimal randomized solutions for matrix games. It also suggests that a given linear programming problem can be associated with a matrix game; see Gale [92] for more discussion of this point.

6.6 Learning the Game

In our earlier discussion we saw that the matrix game involving the pay-off matrix

$$A = \begin{bmatrix} 4 & 1 \\ 2 & 3 \end{bmatrix} \tag{6.5}$$

is not deterministic. The best thing the players can do is to select their play at random, with the first player playing $i = 1$ with probability p and $i = 2$ with probability $1 - p$, and the second player playing column $j = 1$ with probability q and $j = 2$ with probability $1 - q$. If the first player, call him P1, selects $p = \frac{1}{4}$, then he expects to get $\frac{5}{2}$, regardless of what the second player, call her P2, does; otherwise his fortunes depend on what P2 does. His optimal mixed-strategy (column) vector is $[1/4, 3/4]^T$. Similarly, the

second player notices that the only way she can be certain to pay out no more than $\frac{5}{2}$ is to select $q = \frac{1}{2}$. The minimum of these maximum pay-outs occurs when she chooses $q = \frac{1}{2}$, and the *min-max* pay-out is $\frac{5}{2}$.

Because the pay-off matrix is two-by-two, we are able to determine easily the optimal mixed-strategy vectors for each player. When the pay-off matrix is larger, finding the optimal mixed-strategy vectors is not a simple matter. As we have seen, one approach is to obtain these vectors by solving a related linear-programming problem. In this section we consider other approaches to finding the optimal mixed-strategy vectors.

6.6.1 An Iterative Approach

In [92] Gale presents an iterative approach to learning how best to play a matrix game. The assumptions are that the game is to be played repeatedly and that the two players adjust their play as they go along, based on the earlier plays of their opponent.

Suppose, for the moment, that P1 knows that P2 is playing the randomized strategy q, where, as earlier, we denote by p and q probability column vectors. The entry $(Aq)_i$ of the column vector Aq is the expected pay-off to P1 if he plays strategy i. It makes sense for P1 then to find the index i for which this expected pay-off is largest and to play that strategy every time. Of course, if P2 notices what P1 is doing, she will abandon q to her advantage.

After the game has been played n times, the players can examine the previous plays and make estimates of what the opponent is doing. Suppose that P1 has played strategy i n_i times, where $n_i \geq 0$ and $n_1 + n_2 + ... + n_I = n$. Denote by p^n the probability column vector whose ith entry is n_i/n. Similarly, calculate q^n. These two probability vectors summarize the tendencies of the two players over the first n plays. It seems reasonable that an attempt to learn the game would involve these probability vectors.

For example, P1 could see which entry of q^n is the largest, assume that P2 is most likely to play that strategy the next time, and play his best strategy against that play of P2. However, if there are several strategies for P2 to choose, it is still unlikely that P2 will choose this strategy the next time. Perhaps P1 could do better by considering his long-run fortunes and examining the vector Aq^n of expected pay-offs. In the exercise below, you are asked to investigate this matter.

6.6.2 An Exercise

6.4 *Suppose that both players are attempting to learn how best to play the game by examining the vectors p^n and q^n after n plays. Devise an algorithm for the players to follow that will lead to optimal mixed strategies for both. Simulate repeated play of a particular matrix game to see how*

your algorithm performs. If the algorithm does its job, but does it slowly, that is, it takes many plays of the game for it to begin to work, investigate how it might be speeded up.

6.7 Non-Constant-Sum Games

In this final section we consider non-constant-sum games. These are more complicated and the mathematical results more difficult to obtain than in the constant-sum games. Such non-constant-sum games can be used to model situations in which the players may both gain by cooperation, or, when speaking of economic actors, by collusion [78]. We begin with the most famous example of a non-constant-sum game, the Prisoners' Dilemma.

6.7.1 The Prisoners' Dilemma

Imagine that you and your partner are arrested for robbing a bank and both of you are guilty. The two of you are held in separate rooms and given the following options by the district attorney: (1) if you confess, but your partner does not, you go free, while he gets three years in jail; (2) if he confesses, but you do not, he goes free and you get the three years; (3) if both of you confess, you each get two years; (4) if neither of you confesses, each of you gets one year in jail. Let us call you player number one, and your partner player number two. Let strategy one be to remain silent, and strategy two be to confess.

Your pay-off matrix is

$$A = \begin{bmatrix} -1 & -3 \\ 0 & -2 \end{bmatrix}, \tag{6.6}$$

so that, for example, if you remain silent, while your partner confesses, your pay-off is $A_{1,2} = -3$, where the negative sign is used because jail time is undesirable. From your perspective, the game has a deterministic solution; you should confess, assuring yourself of no more than two years in jail. Your partner views the situation the same way and also should confess. However, when the game is viewed, not from one individual's perspective, but from the perspective of the pair of you, we see that by sticking together you each get one year in jail, instead of each of you getting two years; if you cooperate, you both do better.

6.7.2 Two Pay-Off Matrices Needed

In the case of non-constant-sum games, one pay-off matrix is not enough to capture the full picture. Consider the following example of a non-constant-

sum game. Let the matrix

$$A = \begin{bmatrix} 5 & 4 \\ 3 & 6 \end{bmatrix} \tag{6.7}$$

be the pay-off matrix for Player One (P_1), and

$$B = \begin{bmatrix} 5 & 6 \\ 7 & 2 \end{bmatrix} \tag{6.8}$$

be the pay-off matrix for Player Two (P_2); that is, $A_{1,2} = 4$ and $B_{2,1} = 7$ means that if P_1 plays the first strategy and P_2 plays the second strategy, then P_1 gains four and P_2 gains seven. Notice that the total pay-off for each play of the game is not constant, so we require two matrices, not one.

Player One, considering only the pay-off matrix A, discovers that the best strategy is a randomized strategy, with the first strategy played three quarters of the time. Then P_1 has expected gain of $\frac{9}{2}$. Similarly, Player Two, applying the same analysis to his pay-off matrix, B, discovers that he should also play a randomized strategy, playing the first strategy five sixths of the time; he then has an expected gain of $\frac{16}{3}$. However, if P_1 switches and plays the first strategy all the time, while P_2 continues with his randomized strategy, P_1 expects to gain $\frac{29}{6} > \frac{27}{6}$, while the expected gain of P_2 is unchanged. This is very different from what happens in the case of a constant-sum game; there, the sum of the expected gains is constant, and equals zero for a zero-sum game, so P_1 would not be able to increase his expected gain, if P_2 plays his optimal randomized strategy.

6.7.3 An Example: Illegal Drugs in Sports

In a recent article in Scientific American [144], Michael Shermer uses the model of a non-constant-sum game to analyze the problem of doping, or illegal drug use, in sports, and to suggest a solution. He is a former competitive cyclist and his specific example comes from the Tour de France. He is the first player, and his opponent the second player. The choices are to cheat by taking illegal drugs or to stay within the rules. The assumption he makes is that a cyclist who sticks to the rules will become less competitive and will be dropped from his team.

Currently, the likelihood of getting caught is low, and the penalty for cheating is not too high, so, as he shows, the rational choice is for everyone to cheat, as well as for every cheater to lie. He proposes changing the pay-off matrices by increasing the likelihood of being caught, as well as the penalty for cheating, so as to make sticking to the rules the rational choice.

6.8 Course Homework

Do all the exercises in this chapter.

Chapter 7

Differentiation

7.1 Chapter Summary

The definition of the derivative of a function $g : D \subseteq R \to R$ is a familiar one. In this chapter we examine various ways in which this definition can be extended to functions $f : D \subseteq R^J \to R$ of several variables. Here D is the domain of the function f and we assume that $\text{int}(D)$ is not empty.

7.2 Directional Derivative

We begin with one- and two-sided directional derivatives.

7.2.1 Definitions

The function $g(x) = |x|$ does not have a derivative at $x = 0$, but it has *one-sided directional derivatives* there. The one-sided directional derivative of $g(x)$ at $x = 0$, in the direction of $x = 1$, is

$$g'_+(0;1) = \lim_{t \downarrow 0} \frac{1}{t}[g(0+t) - g(0)] = 1, \tag{7.1}$$

and in the direction of $x = -1$, it is

$$g'_+(0;-1) = \lim_{t \downarrow 0} \frac{1}{t}[g(0-t) - g(0)] = 1. \tag{7.2}$$

However, the two-sided derivative of $g(x) = |x|$ does not exist at $x = 0$.

We can extend the concept of one-sided directional derivatives to functions of several variables.

Definition 7.1 *Let $f : D \subseteq R^J \to R$ be a real-valued function of several variables, let a be in int(D), and let d be a unit vector in R^J. The* one-sided directional derivative *of $f(x)$, at $x = a$, in the direction of d, is*

$$f'_+(a;d) = \lim_{t \downarrow 0} \frac{1}{t}[f(a+td) - f(a)]. \tag{7.3}$$

Definition 7.2 *The* two-sided directional derivative *of $f(x)$ at $x = a$, in the direction of d, is*

$$f'(a;d) = \lim_{t \to 0} \frac{1}{t}[f(a+td) - f(a)]. \tag{7.4}$$

If the two-sided directional derivative exists then we have

$$f'(a;d) = f'_+(a;d) = -f'_+(a;-d).$$

Given $x = a$ and d, we define the function $\phi(t) = f(a+td)$, for t such that $a + td$ is in D. The derivative of $\phi(t)$ at $t = 0$ is then

$$\phi'(0) = \lim_{t \to 0} \frac{1}{t}[\phi(t) - \phi(0)] = f'(a;d). \tag{7.5}$$

7.3 Partial Derivatives

For $j = 1, ..., J$, denote by e^j the vector whose entries are all zero, except for a one in the jth position.

Definition 7.3 *If $f'(a;e^j)$ exists, then it is $\frac{\partial f}{\partial x_j}(a)$, the* partial derivative *of $f(x)$, at $x = a$, with respect to x_j, the jth entry of the variable vector x.*

Definition 7.4 *If the partial derivative, at $x = a$, with respect to x_j, exists for each j, then the* gradient *of $f(x)$, at $x = a$, is the vector $\nabla f(a)$ whose entries are $\frac{\partial f}{\partial x_j}(a)$.*

7.4 Some Examples

We consider some examples of directional derivatives.

7.4.1 Example 1.

For $(x, y) \neq (0, 0)$, let

$$f(x,y) = \frac{2xy}{x^2 + y^2},$$

and define $f(0, 0) = 1$. Let $d = (\cos\theta, \sin\theta)$. Then it is easy to show that $\phi(t) = \sin 2\theta$, for $t \neq 0$, and $\phi(0) = 1$. If θ is such that $\sin 2\theta = 1$, then $\phi(t)$ is constant, and $\phi'(0) = 0$. But, if $\sin 2\theta \neq 1$, then $\phi(t)$ is discontinuous at $t = 0$, so $\phi(t)$ is not differentiable at $t = 0$. Therefore, $f(x, y)$ has a two-sided directional derivative at $(x, y) = (0, 0)$ only in certain directions.

7.4.2 Example 2.

[91] For $(x, y) \neq (0, 0)$, let

$$f(x, y) = \frac{2xy^2}{x^2 + y^4},$$

and $f(0, 0) = 0$. Again, let $d = (\cos\theta, \sin\theta)$. Then we have

$$\phi'(0) = \frac{2\sin^2\theta}{\cos\theta},$$

for $\cos\theta \neq 0$. If $\cos\theta = 0$, then $f(x)$ is the constant zero in that direction, so $\phi'(0) = 0$. Therefore, the function $f(x, y)$ has a two-sided directional derivative at $(x, y) = (0, 0)$, for every vector d. Note that the two partial derivatives are both zero at $(x, y) = (0, 0)$, so $\nabla f(0, 0) = 0$. Note also that, since $f(y^2, y) = 1$ for all $y \neq 0$, the function $f(x, y)$ is not continuous at $(0, 0)$.

7.5 Gâteaux Derivative

Just having a two-sided directional derivative for every d is not sufficient, in most cases; we need something stronger.

Definition 7.5 *If $f(x)$ has a two-sided directional derivative at $x = a$, for every vector d, and, in addition,*

$$f'(a; d) = \langle \nabla f(a), d \rangle,$$

for each d, then $f(x)$ is Gâteaux-differentiable at $x = a$, and $\nabla f(a)$ is the Gâteaux derivative of $f(x)$ at $x = a$, also denoted $f'(a)$.

Example 2 above showed that it is possible for $f(x)$ to have a two-sided directional derivative at $x = a$, for every d, and yet fail to be Gâteaux-differentiable.

From Cauchy's Inequality, we know that

$$|f'(a; d)| = |\langle \nabla f(a), d \rangle| \leq ||\nabla f(a)||_2 \, ||d||_2,$$

and that $f'(a; d)$ attains its most positive value when the direction d is a positive multiple of $\nabla f(a)$. This is the motivation for steepest descent optimization.

For ordinary functions $g : D \subseteq R \to R$, we know that differentiability implies continuity. It is possible for $f(x)$ to be Gâteaux-differentiable at $x = a$ and yet not be continuous at $x = a$; see Ortega and Rheinboldt [134]. This means that the notion of Gâteaux-differentiability is too weak. In order to have a nice theory of multivariate differentiation, the notion of derivative must be strengthened. The stronger notion we seek is Fréchet differentiability.

7.6 Fréchet Derivative

The notion of Fréchet differentiability is the one appropriate for our purposes.

7.6.1 The Definition

Definition 7.6 *We say that $f(x)$ is* Fréchet-differentiable *at $x = a$ and $\nabla f(a)$ is its Fréchet derivative if*

$$\lim_{||h||\to 0} \frac{1}{||h||}|f(a+h) - f(a) - \langle \nabla f(a), h\rangle| = 0.$$

Notice that the limit in the definition of the Fréchet derivative involves the norm of the incremental vector h, which is where the power of the Fréchet derivative arises. Also, since the norm and the associated inner product can be changed, so can the Fréchet derivative; see Exercise 7.1 for an example. The corresponding limit in the definition of the Gâteaux derivative involves only the scalar t, and therefore requires no norm and makes sense in any vector space.

7.6.2 Properties of the Fréchet Derivative

It can be shown that if $f(x)$ is Fréchet-differentiable at $x = a$, then $f(x)$ is continuous at $x = a$. If $f(x)$ is Gâteaux-differentiable at each point in an open set containing $x = a$, and $\nabla f(x)$ is continuous at $x = a$, then $\nabla f(a)$ is also the Fréchet derivative of $f(x)$ at $x = a$. Since the continuity of $\nabla f(x)$ is equivalent to the continuity of each of the partial derivatives, we learn that $f(x)$ is Fréchet-differentiable at $x = a$ if it is Gâteaux-differentiable in a neighborhood of $x = a$ and the partial derivatives are continuous at $x = a$. If $\nabla f(x)$ is continuous in a neighborhood of $x = a$, the function $f(x)$ is said to be *continuously differentiable*.

7.7 The Chain Rule

For fixed a and d in R^J, the function $\phi(t) = f(a + td)$, defined for the real variable t, is a composition of the function $f : R^J \to R$ itself and the function $g : R \to R^J$ defined by $g(t) = a + td$; that is, $\phi(t) = f(g(t))$. Writing

$$f(a + td) = f(a_1 + td_1, a_2 + td_2, ..., a_J + td_J),$$

and applying the Chain Rule, we find that

$$f'(a; d) = \phi'(0) = \frac{\partial f}{\partial x_1}(a)d_1 + ... + \frac{\partial f}{\partial x_J}(a)d_J;$$

that is,

$$f'(a;d) = \phi'(0) = \langle \nabla f(a), d \rangle.$$

But we know that $f'(a;d)$ is not always equal to $\langle \nabla f(a), d \rangle$. This means that the Chain Rule is not universally true and must involve conditions on the function f. Clearly, unless the function f is Gâteaux-differentiable, the chain rule cannot hold. For an in-depth treatment of this matter, consult Ortega and Rheinboldt [134].

7.8 Exercises

7.1 *Let Q be a real, positive-definite symmetric matrix. Define the Q-inner product on R^J to be*

$$\langle x, y \rangle_Q = x^T Q y = \langle x, Qy \rangle,$$

and the Q-norm to be

$$||x||_Q = \sqrt{\langle x, x \rangle_Q}.$$

Show that, if $\nabla f(a)$ is the Fréchet derivative of $f(x)$ at $x = a$, for the usual Euclidean norm, then $Q^{-1}\nabla f(a)$ is the Fréchet derivative of $f(x)$ at $x = a$, for the Q-norm. Hint: use the inequality

$$\sqrt{\lambda_J}||h||_2 \leq ||h||_Q \leq \sqrt{\lambda_1}||h||_2,$$

where λ_1 and λ_J denote the greatest and smallest eigenvalues of Q, respectively.

7.2 ([15], Ex. 10, p. 134) *For (x, y) not equal to $(0, 0)$, let*

$$f(x, y) = \frac{x^a y^b}{x^p + y^q},$$

with $f(0, 0) = 0$. In each of the five cases below, determine if the function is continuous, Gâteaux, Fréchet or continuously differentiable at $(0, 0)$.

- *1)* $a = 2$, $b = 3$, $p = 2$, *and* $q = 4$;
- *2)* $a = 1$, $b = 3$, $p = 2$, *and* $q = 4$;
- *3)* $a = 2$, $b = 4$, $p = 4$, *and* $q = 8$;
- *4)* $a = 1$, $b = 2$, $p = 2$, *and* $q = 2$;
- *5)* $a = 1$, $b = 2$, $p = 2$, *and* $q = 4$.

Chapter 8

Convex Functions

8.1 Chapter Summary

In this chapter we investigate further the properties of convex functions of one and several variables, in preparation for our discussion of iterative optimization algorithms.

8.2 Functions of a Single Real Variable

We begin by recalling some of the basic results concerning functions of a single real variable.

8.2.1 Fundamental Theorems

- The Intermediate Value Theorem:

  Theorem 8.1 *Let $f(x)$ be continuous on the interval $[a, b]$. If d is between $f(a)$ and $f(b)$, then there is c between a and b with $f(c) = d$.*

- The Mean Value Theorem (MVT):

  Theorem 8.2 *Let $f(x)$ be continuous on the closed interval $[a, b]$ and differentiable on (a, b). Then, there is c in (a, b) with*

  $$f(b) - f(a) = f'(c)(b - a).$$

- The Extended Mean Value Theorem (EMVT):

Theorem 8.3 *Let $f(x)$ be twice differentiable on the interval (u, v) and let a and b be in (u, v). Then there is c between a and b with*

$$f(b) = f(a) + f'(a)(b-a) + \frac{1}{2}f''(c)(b-a)^2.$$

- A MVT for Integrals:

Theorem 8.4 *Let $g(x)$ be continuous and $h(x)$ integrable with constant sign on the interval $[a, b]$. Then there is c in (a, b) such that*

$$\int_a^b g(x)h(x)dx = g(c)\int_a^b h(x)dx.$$

If $f(x)$ is a function with $f''(x) > 0$ for all x and $f'(a) = 0$, then, from the EMVT, we know that $f(b) > f(a)$, unless $b = a$, so that $x = a$ is a global minimizer of the function $f(x)$. As we shall see, such functions are strictly convex.

8.2.2 Some Proofs

We begin with a proof of the Mean Value Theorem for Integrals. Since $g(x)$ is continuous on the interval $[a, b]$, it takes on its minimum value, say m, and its maximum value, say M, and, by the Intermediate Value Theorem, $g(x)$ also takes on any value in the interval $[m, M]$. Assume, without loss of generality, that $h(x) \geq 0$, for all x in the interval $[a, b]$, so that $\int_a^b h(x)dx \geq 0$. Then we have

$$m\int_a^b h(x)dx \leq \int_a^b g(x)h(x)dx \leq M\int_a^b h(x)dx,$$

which says that the ratio

$$\frac{\int_a^b g(x)h(x)dx}{\int_a^b h(x)dx}$$

lies in the interval $[m, M]$. Consequently, there is a value c in (a, b) for which $g(c)$ has the value of this ratio. This completes the proof.

Now we present two proofs of the EMVT. We begin by using integration by parts, with $u(x) = f'(x)$ and $v(x) = x - b$, to get

$$f(b) - f(a) = \int_a^b f'(x)dx = f'(x)(x-b)|_a^b - \int_a^b f''(x)(x-b)dx,$$

or

$$f(b) - f(a) = -f'(a)(a-b) - \int_a^b f''(x)(x-b)dx.$$

Then, using the MVT for integrals, with $g(x) = f''(x)$ assumed to be continuous, and $h(x) = x - b$, we have

$$f(b) = f(a) + f'(a)(b-a) - f''(c)\int_a^b (x-b)dx,$$

from which the assertion of the theorem follows immediately.

A second proof of the EMVT is as follows. Let a and b be fixed and set

$$F(x) = f(x) + f'(x)(b-x) + A(b-x)^2,$$

for some constant A to be determined. Then $F(b) = f(b)$. Select A so that $F(a) = f(b)$. Then $F(b) = F(a)$, so there is c in (a, b) with $F'(c) = 0$, by the MVT, or, more simply, from Rolle's Theorem. Therefore,

$$0 = F'(c) = f'(c) + f''(c)(b-c) + f'(c)(-1) - 2A(b-c) = (f''(c) - 2A)(b-c).$$

So $A = \frac{1}{2}f''(c)$ and

$$F(x) = f(x) + f'(x)(b-x) + \frac{1}{2}f''(c)(b-x)^2,$$

from which we get

$$F(a) = f(b) = f(a) + f'(a)(b-a) + \frac{1}{2}f''(c)(b-a)^2.$$

This completes the second proof.

8.2.3 Lipschitz Continuity

Let $f : R \to R$ be a differentiable function. From the Mean-Value Theorem we know that

$$f(b) = f(a) + f'(c)(b-a), \tag{8.1}$$

for some c between a and b. If there is a constant L with $|f'(x)| \leq L$ for all x, that is, the derivative is bounded, then we have

$$|f(b) - f(a)| \leq L|b-a|, \tag{8.2}$$

for all a and b; functions that satisfy Equation (8.2) are said to be *L-Lipschitz*.

8.2.4 The Convex Case

We focus now on the special case of convex functions. Earlier, we said that a function $g : S \to [-\infty, \infty]$ is convex if its epi-graph is a convex set, in which case the effective domain of the function g must be a convex set. For a real-valued function g defined on the whole real line we have several conditions on g that are equivalent to being a convex function.

Proposition 8.1 *The following are equivalent:*
1) the epi-graph of $g(x)$ is convex;
2) for all points $a < x < b$

$$g(x) \leq \frac{g(b) - g(a)}{b - a}(x - a) + g(a); \tag{8.3}$$

3) for all points $a < x < b$

$$g(x) \leq \frac{g(b) - g(a)}{b - a}(x - b) + g(b); \tag{8.4}$$

4) for all points a and b in R and for all α in the interval $(0, 1)$

$$g((1 - \alpha)a + \alpha b) \leq (1 - \alpha)g(a) + \alpha g(b). \tag{8.5}$$

The proof of Proposition 8.1 is left as an exercise.

As a result of Proposition 8.1, we can use the following definition of a convex real-valued function.

Definition 8.1 *A function $g : R \to R$ is called* convex *if, for each pair of distinct real numbers a and b, the line segment connecting the two points $A = (a, g(a))$ and $B = (b, g(b))$ is on or above the graph of $g(x)$; that is, for every α in $(0, 1)$,*

$$g((1 - \alpha)a + \alpha b) \leq (1 - \alpha)g(a) + \alpha g(b).$$

If the inequality is always strict, then $g(x)$ is strictly convex.

The function $g(x) = x^2$ is a simple example of a convex function. If $g(x)$ is convex on an open set in R, then $g(x)$ is continuous there, as well ([136], p. 47).It follows from Proposition 8.1 that, if $g(x)$ is convex, then, for every triple of points $a < x < b$, we have

$$\frac{g(x) - g(a)}{x - a} \leq \frac{g(b) - g(a)}{b - a} \leq \frac{g(b) - g(x)}{b - x}. \tag{8.6}$$

Therefore, for fixed a, the ratio

$$\frac{g(x) - g(a)}{x - a}$$

is an increasing function of x, and, for fixed b, the ratio

$$\frac{g(b) - g(x)}{b - x}$$

is an increasing function of x.

If $g(x)$ is a differentiable function, then convexity can be expressed in terms of properties of the derivative, $g'(x)$; for every triple of points $a < x < b$, we have

$$g'(a) \leq \frac{g(b) - g(a)}{b - a} \leq g'(b). \tag{8.7}$$

If $g(x)$ is differentiable and convex, then $g'(x)$ is an increasing function. In fact, the converse is also true, as we shall see shortly.

Recall that the line tangent to the graph of $g(x)$ at the point $x = a$ has the equation

$$y = g'(a)(x - a) + g(a). \tag{8.8}$$

Theorem 8.5 *For the differentiable function $g(x)$, the following are equivalent:*
1) $g(x)$ is convex;
2) for all a and x we have

$$g(x) \geq g(a) + g'(a)(x - a); \tag{8.9}$$

3) the derivative, $g'(x)$, is an increasing function, or, equivalently,

$$(g'(x) - g'(a))(x - a) \geq 0, \tag{8.10}$$

for all a and x.

Proof: Assume that $g(x)$ is convex. If $x > a$, then

$$g'(a) \leq \frac{g(x) - g(a)}{x - a}, \tag{8.11}$$

while, if $x < a$, then

$$\frac{g(a) - g(x)}{a - x} \leq g'(a). \tag{8.12}$$

In either case, the inequality in (8.9) holds. Now, assume that the inequality in (8.9) holds. Then

$$g(x) \geq g'(a)(x - a) + g(a), \tag{8.13}$$

and

$$g(a) \geq g'(x)(a - x) + g(x). \tag{8.14}$$

Adding the two inequalities, we obtain

$$g(a) + g(x) \geq (g'(x) - g'(a))(a - x) + g(a) + g(x), \tag{8.15}$$

from which we conclude that

$$(g'(x) - g'(a))(x - a) \geq 0. \tag{8.16}$$

So $g'(x)$ is increasing. Finally, we assume the derivative is increasing and show that $g(x)$ is convex. If $g(x)$ is not convex, then there are points $a < b$ such that, for all x in (a, b),

$$\frac{g(x) - g(a)}{x - a} > \frac{g(b) - g(a)}{b - a}. \tag{8.17}$$

By the Mean Value Theorem there is c in (a, b) with

$$g'(c) = \frac{g(b) - g(a)}{b - a}. \tag{8.18}$$

Select x in the interval (a, c). Then there is d in (a, x) with

$$g'(d) = \frac{g(x) - g(a)}{x - a}. \tag{8.19}$$

Then $g'(d) > g'(c)$, which contradicts the assumption that $g'(x)$ is increasing. This concludes the proof. ∎

If $g(x)$ is twice differentiable, we can say more. If we multiply both sides of the inequality in (8.16) by $(x - a)^{-2}$, we find that

$$\frac{g'(x) - g'(a)}{x - a} \geq 0, \tag{8.20}$$

for all x and a. This inequality suggests the following theorem.

Theorem 8.6 *If $g(x)$ is twice differentiable, then $g(x)$ is convex if and only if $g''(x) \geq 0$, for all x.*

Proof: According to the Mean Value Theorem, as applied to the function $g'(x)$, for any points $a < b$ there is c in (a, b) with $g'(b) - g'(a) = g''(c)(b - a)$. If $g''(x) \geq 0$, the right side of this equation is nonnegative, so the left side is also. Now assume that $g(x)$ is convex, which implies that $g'(x)$ is an increasing function. Since $g'(x + h) - g'(x) \geq 0$ for all $h > 0$, it follows that $g''(x) \geq 0$. ∎

The following result, as well as its extension to higher dimensions, will be helpful in our study of iterative optimization.

Theorem 8.7 *Let $h(x)$ be convex and differentiable and its derivative, $h'(x)$, non-expansive, that is,*

$$|h'(b) - h'(a)| \leq |b - a|, \tag{8.21}$$

for all a and b. Then $h'(x)$ is firmly non-expansive, which means that

$$(h'(b) - h'(a))(b - a) \geq (h'(b) - h'(a))^2. \tag{8.22}$$

Proof: Assume that $h'(b) - h'(a) \neq 0$, since the alternative case is trivial. If $h'(x)$ is non-expansive, then the inequality in (8.20) tells us that

$$0 \leq \frac{h'(b) - h'(a)}{b - a} \leq 1,$$

so that

$$\frac{b - a}{h'(b) - h'(a)} \geq 1.$$

Now multiply both sides by $(h'(b) - h'(a))^2$. ∎

In the next section we extend these results to functions of several variables.

8.3 Functions of Several Real Variables

In this section we consider the continuity and differentiability of a function of several variables. For more details, see the chapter on differentiability.

8.3.1 Continuity

In addition to real-valued functions $f : R^N \to R$, we shall also be interested in vector-valued functions $F : R^N \to R^M$, such as $F(x) = \nabla f(x)$, whose range is in R^N, not in R.

Definition 8.2 *We say that $F : R^N \to R^M$ is* continuous *at $x = a$ if*

$$\lim_{x \to a} f(x) = f(a);$$

that is, $\|f(x) - f(a)\|_2 \to 0$, as $\|x - a\|_2 \to 0$.

Definition 8.3 *We say that $F : R^N \to R^M$ is L-*Lipschitz*, or an L-*Lipschitz continuous function*, if there is $L > 0$ such that*

$$\|F(b) - F(a)\|_2 \leq L\|b - a\|_2, \tag{8.23}$$

for all a and b in R^N.

8.3.2 Differentiability

Let $F : D \subseteq R^N \rightarrow R^M$ be a R^M-valued function of N real variables, defined on domain D with nonempty interior int(D).

Definition 8.4 *The function $F(x)$ is said to be* (Frechet) differentiable *at point x^0 in int(D) if there is an M by N matrix $F'(x^0)$ such that*

$$\lim_{h \rightarrow 0} \frac{1}{||h||_2}[F(x^0 + h) - F(x^0) - F'(x^0)h] = 0. \tag{8.24}$$

It can be shown that, if F is differentiable at $x = x^0$, then F is continuous there as well [91].

If $f : R^J \rightarrow R$ is differentiable, then $f'(x^0) = \nabla f(x^0)$, the gradient of f at x^0. The function $f(x)$ is differentiable if each of its first partial derivatives is continuous. If the derivative $f' : R^J \rightarrow R^J$ is, itself, differentiable, then $f'' : R^J \rightarrow R^J$, and $f''(x) = H(x) = \nabla^2 f(x)$, the Hessian matrix whose entries are the second partial derivatives of f. The function $f(x)$ will be twice differentiable if each of the second partial derivatives is continuous. In that case, the mixed second partial derivatives are independent of the order of the variables, the Hessian matrix is symmetric, and the chain rule applies.

Let $f : R^J \rightarrow R$ be a differentiable function. From the Mean-Value Theorem ([91], p. 41) we know that, for any two points a and b, there is α in $(0, 1)$ such that

$$f(b) = f(a) + \langle \nabla f((1 - \alpha)a + \alpha b), b - a \rangle. \tag{8.25}$$

If there is a constant L with $||\nabla f(x)||_2 \leq L$ for all x, that is, the gradient is bounded in norm, then we have

$$|f(b) - f(a)| \leq L||b - a||_2, \tag{8.26}$$

for all a and b; such functions are then *L-Lipschitz*.

We can study multivariate functions $f : R^J \rightarrow R$ by using them to construct functions of a single real variable, given by

$$\phi(t) = f(x^0 + t(x - x^0)),$$

where x and x^0 are fixed (column) vectors in R^J. If $f(x)$ is differentiable, then

$$\phi'(t) = \langle \nabla f(x^0 + t(x - x^0)), x - x^0 \rangle.$$

If $f(x)$ is twice continuously differentiable, then

$$\phi''(t) = (x - x^0)^T \nabla^2 f(x^0 + t(x - x^0))(x - x^0).$$

8.3.3 Finding Maxima and Minima

Suppose $g : R^J \rightarrow R$ is differentiable and attains its minimum value. We want to minimize the function $g(x)$. Solving $\nabla g(x) = 0$ to find the optimal $x = x^*$ may not be easy, so we may turn to an iterative algorithm for finding roots of $\nabla g(x)$, or one that minimizes $g(x)$ directly. In the latter case, we may again consider a steepest descent algorithm of the form

$$x^{k+1} = x^k - \gamma \nabla g(x^k), \tag{8.27}$$

for some $\gamma > 0$. We denote by T the operator

$$Tx = x - \gamma \nabla g(x). \tag{8.28}$$

Then, using $\nabla g(x^*) = 0$, we find that

$$||x^* - x^{k+1}||_2 = ||Tx^* - Tx^k||_2. \tag{8.29}$$

We would like to know if there are choices for γ that imply convergence of the iterative sequence. As in the case of functions of a single variable, for functions $g(x)$ that are *convex*, the answer is yes.

8.3.4 Lower Semi-Continuity

We begin with a definition.

Definition 8.5 *An extended-real-valued function f from R^J to $[-\infty, \infty]$ is* lower semi-continuous *if $f(x) = \liminf f(y)$, as $y \rightarrow x$.*

The following theorem shows the importance of lower semi-continuity.

Theorem 8.8 ([140], Theorem 7.1) *Let f be an arbitrary function from R^J to $[-\infty, \infty]$. Then the following conditions are equivalent:*

- **1.** *f is lower semi-continuous throughout R^J;*
- **2.** *for every real α, the set $\{x | f(x) \leq \alpha\}$ is closed;*
- **3.** *the epi-graph of $f(x)$ is closed.*

As an example, consider the function $f(x)$ defined for $0 \leq x < 1$ by $f(x) = 2 - x$, and for $1 < x \leq 2$ by $f(x) = x + 1$. If we define $f(1) = 1$, then $f(x)$ becomes lower semi-continuous and the epi-graph becomes closed. However, if we define $f(1) = 2$, the function is no longer lower semi-continuous and its epi-graph is no longer closed.

8.3.5 The Convex Case

We begin with some definitions.

Definition 8.6 *The function $g(x) : R^J \rightarrow R$ is said to be* convex *if, for each pair of distinct vectors a and b and for every α in the interval $(0, 1)$ we have*

$$g((1-\alpha)a + \alpha b) \leq (1-\alpha)g(a) + \alpha g(b). \tag{8.30}$$

If the inequality is always strict, then $g(x)$ is called strictly convex.

The function $g(x)$ is convex if and only if, for every x and z in R^J and real t, the function $f(t) = g(x + tz)$ is a convex function of t. Therefore, the theorems for the multi-variable case can also be obtained from previous results for the single-variable case.

Definition 8.7 *A convex function $g : R^J \rightarrow [-\infty, +\infty]$ is* proper *if there is no x with $g(x) = -\infty$ and some x with $g(x) < +\infty$.*

Definition 8.8 *The* effective domain *of g is dom(g)=$D = \{x|g(x) < +\infty\}$.*

Definition 8.9 *A proper convex function g is* closed *if it is lower semi-continuous.*

A proper convex function g is closed if and only if its epi-graph is a closed set. If g is convex and finite on an open subset of dom(g), then g is continuous there, as well ([140]).

8.3.6 Subdifferentials and Subgradients

Suppose that $g : R^J \rightarrow (-\infty, +\infty]$ is convex and $g(x)$ is finite for x in the non-empty closed convex set C. Applying the Support Theorem to the epigraph of g, we obtain the following theorem.

Theorem 8.9 *If x^0 is an interior point of the set C, then there is a non-zero vector d with*

$$g(x) \geq g(x^0) + \langle d, x - x^0 \rangle,$$

for all x.

Proof: The point $(x^0, g(x^0))$ is a boundary point of the epigraph of g. According to the Support Theorem, there is a non-zero vector $a = (b, c)$ in R^{J+1}, with b in R^J and c real, such that

$$\langle b, x \rangle + cr = \langle a, (x, r) \rangle \leq \langle a, (x^0, g(x^0)) \rangle = \langle b, x^0 \rangle + cg(x^0),$$

for all (x, r) in the epigraph of g, that is, all (x, r) with $g(x) \leq r$. The real number c cannot be positive, since $\langle b, x\rangle + cr$ is bounded above, while r can be increased arbitrarily. Also c cannot be zero: if $c = 0$, then b cannot be zero and we would have $\langle b, x\rangle \leq \langle b, x^0\rangle$ for all x in C. But, since x^0 is in the interior of C, there is $t > 0$ such that $x = x^0 + tb$ is in C. So $c < 0$. We then select $d = -\frac{1}{c}b$. ∎

Note that it can happen that $b = 0$; therefore $d = 0$ is possible; see Exercise 8.2.

Definition 8.10 *A vector d is said to be a* subgradient *of the function $g(x)$ at $x = x^0$ if, for all x, we have*

$$g(x) \geq g(x^0) + \langle d, x - x^0\rangle.$$

The collection of all subgradients of g at $x = x^0$ is called the subdifferential *of g at $x = x^0$, denoted $\partial g(x^0)$. The domain of ∂g is the set dom $\partial g = \{x|\partial g(x) \neq \emptyset\}$.*

Theorem 8.9 says that the subdifferential of a convex function at an interior point of its domain is non-empty. If the subdifferential consists of a single vector, then g is differentiable at $x = x^0$ and that single vector is its gradient at $x = x^0$.

Note that, by the chain rule, $f'(t) = \nabla g(x + tz) \cdot z$, for the function $f(t) = g(x + tz)$.

Theorem 8.10 *Let $g : R^J \to R$ be differentiable. The following are equivalent:*
1) $g(x)$ is convex;
2) for all a and b we have

$$g(b) \geq g(a) + \langle \nabla g(a), b - a\rangle\,; \tag{8.31}$$

3) for all a and b we have

$$\langle \nabla g(b) - \nabla g(a), b - a\rangle \geq 0. \tag{8.32}$$

As in the case of functions of a single variable, we can say more when the function $g(x)$ is twice differentiable. To guarantee that the second derivative matrix is symmetric, we assume that the second partial derivatives are continuous. Note that, by the chain rule again, $f''(t) = z^T \nabla^2 g(x + tz)z$.

Theorem 8.11 *Let each of the second partial derivatives of $g(x)$ be continuous, so that $g(x)$ is twice continuously differentiable. Then $g(x)$ is convex if and only if the second derivative matrix $\nabla^2 g(x)$ is non-negative definite, for each x.*

Suppose that $g(x) : R^J \to R$ is convex and the function $F(x) = \nabla g(x)$ is L-Lipschitz. We have the following analog of Theorem 8.7.

Theorem 8.12 *Let $h(x)$ be convex and differentiable and its derivative, $\nabla h(x)$, non-expansive, that is,*

$$||\nabla h(b) - \nabla h(a)||_2 \leq ||b - a||_2, \tag{8.33}$$

for all a and b. Then $\nabla h(x)$ is firmly non-expansive, which means that

$$\langle \nabla h(b) - \nabla h(a), b - a\rangle \geq ||\nabla h(b) - \nabla h(a)||_2^2. \tag{8.34}$$

Unlike the proof of Theorem 8.7, the proof of this theorem is not trivial. In [96] Golshtein and Tretyakov prove the following theorem, from which Theorem 8.12 follows immediately.

Theorem 8.13 *Let $g : R^J \to R$ be convex and differentiable. The following are equivalent:*

$$||\nabla g(x) - \nabla g(y)||_2 \leq ||x - y||_2; \tag{8.35}$$

$$g(x) \geq g(y) + \langle \nabla g(y), x - y\rangle + \frac{1}{2}||\nabla g(x) - \nabla g(y)||_2^2; \tag{8.36}$$

and

$$\langle \nabla g(x) - \nabla g(y), x - y\rangle \geq ||\nabla g(x) - \nabla g(y)||_2^2. \tag{8.37}$$

Proof: The only difficult step in the proof is showing that Inequality (8.35) implies Inequality (8.36). To prove this part, let $x(t) = (1 - t)y + tx$, for $0 \leq t \leq 1$. Then

$$g'(x(t)) = \langle \nabla g(x(t)), x - y\rangle, \tag{8.38}$$

so that

$$\int_0^1 \langle \nabla g(x(t)) - \nabla g(y), x - y\rangle dt = g(x) - g(y) - \langle \nabla g(y), x - y\rangle. \tag{8.39}$$

Therefore,

$$g(x) - g(y) - \langle \nabla g(y), x - y\rangle \leq$$

$$\int_0^1 ||\nabla g(x(t)) - \nabla g(y)||_2 ||x(t) - y||_2 dt \tag{8.40}$$

$$\leq \int_0^1 ||x(t) - y||_2^2 dt = \int_0^1 ||t(x-y)||_2^2 dt = \frac{1}{2}||x-y||_2^2, \tag{8.41}$$

according to Inequality (8.35). Therefore,

$$g(x) \leq g(y) + \langle \nabla g(y), x - y \rangle + \frac{1}{2}||x-y||_2^2. \tag{8.42}$$

Now let $x = y - \nabla g(y)$, so that

$$g(y - \nabla g(y)) \leq g(y) + \langle \nabla g(y), \nabla g(y) \rangle + \frac{1}{2}||\nabla g(y)||_2^2. \tag{8.43}$$

Consequently,

$$g(y - \nabla g(y)) \leq g(y) - \frac{1}{2}||\nabla g(y)||_2^2. \tag{8.44}$$

Therefore,

$$\inf g(x) \leq g(y) - \frac{1}{2}||\nabla g(y)||_2^2, \tag{8.45}$$

or

$$g(y) \geq \inf g(x) + \frac{1}{2}||\nabla g(y)||_2^2. \tag{8.46}$$

Now fix y and define the function $h(x)$ by

$$h(x) = g(x) - g(y) - \langle \nabla g(y), x - y \rangle. \tag{8.47}$$

Then $h(x)$ is convex, differentiable, and non-negative,

$$\nabla h(x) = \nabla g(x) - \nabla g(y), \tag{8.48}$$

and $h(y) = 0$, so that $h(x)$ attains its minimum at $x = y$. Applying Inequality (8.46) to the function $h(x)$, with z in the role of x and x in the role of y, we find that

$$\inf h(z) = 0 \leq h(x) - \frac{1}{2}||\nabla h(x)||_2^2. \tag{8.49}$$

From the definition of $h(x)$, it follows that

$$0 \leq g(x) - g(y) - \langle \nabla g(y), x - y \rangle - \frac{1}{2}||\nabla g(x) - \nabla g(y)||_2^2. \tag{8.50}$$

This completes the proof of the implication. ∎

If $g(x)$ is convex and $f(x) = \nabla g(x)$ is L-Lipschitz, then $\frac{1}{L}\nabla g(x)$ is non-expansive, so, by Theorem 8.12, it is firmly non-expansive. It follows that, for $\gamma > 0$, the operator

$$Tx = x - \gamma \nabla g(x) \tag{8.51}$$

is averaged, whenever $0 < \gamma < \frac{2}{L}$. By the KM Theorem 17.2, the iterative sequence $x^{k+1} = Tx^k = x^k - \gamma \nabla g(x^k)$ converges to a minimizer of $g(x)$, whenever minimizers exist.

8.4 Exercises

8.1 *Prove Proposition 8.1.*

8.2 *Show that, if $\hat{x}$ minimizes the function $g(x)$ over all x in R^J, then $x = 0$ is in the sub-differential $\partial g(\hat{x})$.*

8.3 *If $f(x)$ and $g(x)$ are convex functions on R^J, is $f(x) + g(x)$ convex? Is $f(x)g(x)$ convex?*

8.4 *Let $\iota_C(x)$ be the indicator function of the closed convex set C, that is,*

$$\iota_C(x) = \begin{cases} 0, \text{ if } x \in C; \\ +\infty, \text{ if } x \notin C. \end{cases}$$

Show that the sub-differential of the function ι_C at a point c in C is the normal cone to C at the point c, that is, $\partial \iota_C(c) = N_C(c)$, for all c in C.

8.5 *[156] Let $g(t)$ be a strictly convex function for $t > 0$. For $x > 0$ and $y > 0$, define the function*

$$f(x, y) = xg(\frac{y}{x}).$$

Use induction to prove that

$$\sum_{n=1}^{N} f(x_n, y_n) \geq f(x_+, y_+),$$

for any positive numbers x_n and y_n, where $x_+ = \sum_{n=1}^{N} x_n$. Also show that equality obtains if and only if the finite sequences $\{x_n\}$ and $\{y_n\}$ are proportional.

8.6 *Use the result in Exercise 8.5 to obtain Cauchy's Inequality. Hint: let $g(t) = -\sqrt{t}$.*

8.7 *Use the result in Exercise 8.5 to obtain Hölder's Inequality. Hint: let $g(t) = -t^{1/q}$.*

8.8 *Use the result in Exercise 8.5 to obtain Minkowski's Inequality. Hint: let $g(t) = -(t^{1/p} + 1)^p$.*

8.9 *Use the result in Exercise 8.5 to obtain* **Milne's Inequality***:*

$$x_+ y_+ \geq \Big(\sum_{n=1}^{N} (x_n + y_n) \Big) \Big(\sum_{n=1}^{N} \frac{x_n y_n}{x_n + y_n} \Big).$$

Hint: let $g(t) = -\frac{t}{1+t}$.

8.10 *For $x > 0$ and $y > 0$, let $f(x, y)$ be the* **Kullback-Leibler function**,

$$f(x, y) = KL(x, y) = x\Big(\log \frac{x}{y}\Big) + y - x.$$

Use Exercise 8.5 to show that

$$\sum_{n=1}^{N} KL(x_n, y_n) \geq KL(x_+, y_+).$$

Compare this result with Lemma 14.5.

8.5 Course Homework

Do all the exercises in this chapter.

Chapter 9

Fenchel Duality

9.1 Chapter Summary

The duality between convex functions on R^J and their tangent hyperplanes is made explicit through the Legendre-Fenchel transformation. In this chapter we discuss this transformation, state and prove Fenchel's Duality Theorem, and investigate some of its applications.

9.2 The Legendre-Fenchel Transformation

Throughout this section $f : C \subseteq R^J \to R$ is a closed, proper, convex function defined on a non-empty, closed convex set C.

9.2.1 The Fenchel Conjugate

For each fixed vector a in R^J, the affine function $h(x) = \langle a, x\rangle - \gamma$ is beneath the function $f(x)$ if $f(x) - h(x) \geq 0$, for all x; that is,

$$f(x) - \langle a, x\rangle + \gamma \geq 0,$$

or

$$\gamma \geq \langle a, x\rangle - f(x). \tag{9.1}$$

This leads us to the following definition, involving the maximum of the right side of the inequality in (9.1), for each fixed a.

Definition 9.1 *The* conjugate function *associated with f is the function*

$$f^*(a) = \sup_{x\in C}(\langle a, x\rangle - f(x)). \tag{9.2}$$

We then define C^* to be the set of all a for which $f^*(a)$ is finite. For each fixed a, the value $f^*(a)$ is the smallest value of γ for which the affine function $h(x) = \langle a, x\rangle - \gamma$ is beneath $f(x)$ for $x \in C$. The passage from f to f^* is the *Legendre-Fenchel Transformation*. Now we repeat this process with $f^*(a)$ in the role of $f(x)$.

9.2.2 The Conjugate of the Conjugate

For each fixed vector x, the affine function $c(a) = \langle a, x\rangle - \gamma$ is beneath the function $f^*(a)$ if $f^*(a) - c(a) \geq 0$, for all $a \in C^*$; that is,

$$f^*(a) - \langle a, x\rangle + \gamma \geq 0,$$

or

$$\gamma \geq \langle a, x\rangle - f^*(a). \tag{9.3}$$

This leads us to the following definition, involving the maximum of the right side of the inequality in (9.3), for each fixed x.

Definition 9.2 *The conjugate function associated with f^* is the function*

$$f^{**}(x) = \sup_a(\langle a, x\rangle - f^*(a)). \tag{9.4}$$

For each fixed x, the value $f^{**}(x)$ is the smallest value of γ for which the affine function $c(a) = \langle a, x\rangle - \gamma$ is beneath $f^*(a)$.

Applying the Separation Theorem to the epigraph of the closed, proper, convex function $f(x)$, it can be shown ([140], Theorem 12.1) that $f(x)$ is the point-wise supremum of all the affine functions beneath $f(x)$; that is,

$$f(x) = \sup_{a,\gamma}\{h(x) | f(x) \geq h(x)\}.$$

Therefore,

$$f(x) = \sup_a \Big(\langle a, x\rangle - f^*(a)\Big).$$

This says that

$$f^{**}(x) = f(x). \tag{9.5}$$

9.2.3 Some Examples of Conjugate Functions

- The exponential function $f(x) = \exp(x) = e^x$ has conjugate

$$\exp^*(a) = \begin{cases} a\log a - a, \text{ if } a > 0; \\ 0, \text{ if } a = 0; \\ +\infty, \text{ if } a < 0. \end{cases} \tag{9.6}$$

- The function $f(x) = -\log x$, for $x > 0$, has the conjugate function $f^*(a) = -1 - \log(-a)$, for $a < 0$.
- The function $f(x) = \frac{|x|^p}{p}$ has conjugate $f^*(a) = \frac{|a|^q}{q}$, where $p > 0$, $q > 0$, and $\frac{1}{p} + \frac{1}{q} = 1$.
- Let $\psi_C(x)$ be the *indicator function* of the closed convex set C, that is,
$$\psi_C(x) = \begin{cases} 0, \text{ if } x \in C; \\ +\infty, \text{ if } x \notin C. \end{cases}$$
Then
$$\psi_C^*(a) = \sup_{x \in C} \langle a, x \rangle,$$
which is the *support function* of the set C, usually denoted $\sigma_C(a)$.
- Let $C = \{x| \ ||x||_2 \leq 1\}$, so that the function $\phi(a) = \|a\|_2$ satisfies
$$\phi(a) = \sup_{x \in C} \langle a, x \rangle.$$
Then
$$\phi(a) = \sigma_C(a) = \psi_C^*(a).$$
Therefore,
$$\phi^*(x) = \sigma_C^*(x) = \psi_C^{**}(x) = \psi_C(x) = \begin{cases} 0, \text{ if } x \in C; \\ +\infty, \text{ if } x \notin C. \end{cases}$$

9.2.4 Conjugates and Sub-gradients

We know from the definition of $f^*(a)$ that
$$f^*(a) \geq \langle a, z \rangle \ - f(z),$$
for all z, and, moreover, $f^*(a)$ is the supremum of these values, taken over all z. If a is a member of the sub-differential $\partial f(x)$, then, for all z, we have
$$f(z) \geq f(x) + \langle a, z - x \rangle,$$
so that
$$\langle a, x \rangle - f(x) \geq \langle a, z \rangle - f(z).$$
It follows that
$$f^*(a) = \langle a, x \rangle \ - f(x),$$
so that
$$f(x) + f^*(a) = \langle a, x \rangle.$$

If $f(x)$ is a differentiable convex function, then a is in the sub-differential $\partial f(x)$ if and only if $a = \nabla f(x)$. Then we can say

$$f(x) + f^*(\nabla f(x)) = \langle \nabla f(x), x \rangle. \tag{9.7}$$

The conjugate of a differentiable function $f : C \subseteq R^J \rightarrow R$ can then be defined as follows [140]. Let D be the image of the set C under the mapping ∇f. Then, for all $a \in D$ define

$$f^*(a) = \langle a, (\nabla f)^{-1}(a) \rangle - f((\nabla f)^{-1}(a)).$$

9.2.5 The Conjugate of a Concave Function

A function $g : D \subseteq R^J \rightarrow R$ is *concave* if $f(x) = -g(x)$ is convex. One might think that the conjugate of a concave function g is simply the negative of the conjugate of $-g$, but not quite.

The affine function $h(x) = \langle a, x \rangle - \gamma$ is above the concave function $g(x)$ if $h(x) - g(x) \geq 0$, for all $x \in D$; that is,

$$\langle a, x \rangle - \gamma - g(x) \geq 0,$$

or

$$\gamma \leq \langle a, x \rangle - g(x). \tag{9.8}$$

The conjugate function associated with g is the function

$$g^*(a) = \inf_x(\langle a, x \rangle - g(x)). \tag{9.9}$$

For each fixed a, the value $g^*(a)$ is the largest value of γ for which the affine function $h(x) = \langle a, x \rangle - \gamma$ is above $g(x)$.

It follows, using $f(x) = -g(x)$, that

$$g^*(a) = \inf_x(\langle a, x \rangle + f(x)) = -\sup_x(\langle -a, x \rangle - f(x)) = -f^*(-a).$$

9.3 Fenchel's Duality Theorem

Let $f(x)$ be a proper convex function on $C \subseteq R^J$ and $g(x)$ a proper concave function on $D \subseteq R^J$, where C and D are closed convex sets with non-empty intersection. Fenchel's Duality Theorem deals with the problem of minimizing the difference $f(x) - g(x)$ over $x \in C \cap D$.

We know from our discussion of conjugate functions and differentiability that

$$-f^*(a) \leq f(x) - \langle a, x \rangle,$$

and

$$g^*(a) \leq \langle a, x \rangle - g(x).$$

Therefore,

$$f(x) - g(x) \geq g^*(a) - f^*(a),$$

for all x and a, and so

$$\inf_x \Big(f(x) - g(x)\Big) \geq \sup_a \Big(g^*(a) - f^*(a)\Big).$$

We let C^* be the set of all a such that $f^*(a)$ is finite, with D^* similarly defined.

The Fenchel Duality Theorem, in its general form, as found in [120] and [140], is as follows.

Theorem 9.1 *Assume that $C \cap D$ has points in the relative interior of both C and D, and that either the epigraph of f or that of g has non-empty interior. Suppose that*

$$\mu = \inf_{x \in C \cap D} \Big(f(x) - g(x)\Big)$$

is finite. Then

$$\mu = \inf_{x \in C \cap D} \Big(f(x) - g(x)\Big) = \max_{a \in C^* \cap D^*} \Big(g^*(a) - f^*(a)\Big),$$

where the maximum on the right is achieved at some $a_0 \in C^* \cap D^*$.

If the infimum on the left is achieved at some $x_0 \in C \cap D$, then

$$\max_{x \in C} \Big(\langle x, a_0\rangle - f(x)\Big) = \langle x_0, a_0\rangle - f(x_0),$$

and

$$\min_{x \in D} \Big(\langle x, a_0\rangle - g(x)\Big) = \langle x_0, a_0\rangle - g(x_0).$$

The conditions on the interiors are needed to make use of sub-differentials. For simplicity, we shall limit our discussion to the case of differentiable $f(x)$ and $g(x)$.

9.3.1 Fenchel's Duality Theorem: Differentiable Case

We suppose now that there is $x_0 \in C \cap D$ such that

$$\inf_{x \in C \cap D}(f(x) - g(x)) = f(x_0) - g(x_0),$$

and that

$$\nabla(f - g)(x_0) = 0,$$

or

$$\nabla f(x_0) = \nabla g(x_0). \tag{9.10}$$

Let $\nabla f(x_0) = a_0$. From the equation

$$f(x) + f^*(\nabla f(x)) = \langle \nabla f(x), x \rangle$$

and Equation (9.10),we have

$$f(x_0) - g(x_0) = g^*(a_0) - f^*(a_0),$$

from which it follows that

$$\inf_{x \in C \cap D} (f(x) - g(x)) = \sup_{a \in C^* \cap D^*} (g^*(a) - f^*(a)).$$

This is Fenchel's Duality Theorem.

9.3.2 Optimization over Convex Subsets

Suppose now that $f(x)$ is convex and differentiable on R^J, but we are only interested in its values on the non-empty closed convex set C. Then we redefine $f(x) = +\infty$ for x not in C. The affine function $h(x) = \langle a, x \rangle - \gamma$ is beneath $f(x)$ for all x if and only if it is beneath $f(x)$ for $x \in C$. This motivates our defining the conjugate function now as

$$f^*(a) = \sup_{x \in C} \langle a, x \rangle - f(x).$$

Similarly, let $g(x)$ be concave on D and $g(x) = -\infty$ for x not in D. Then we define

$$g^*(a) = \inf_{x \in D} \langle a, x \rangle - g(x).$$

Let

$$C^* = \{a |\, f^*(a) < +\infty\},$$

and define D^* similarly. We can use Fenchel's Duality Theorem to minimize the difference $f(x) - g(x)$ over the intersection $C \cap D$.

To illustrate the use of Fenchel's Duality Theorem, consider the problem of minimizing the convex function $f(x)$ over the convex set D. Let $C = R^J$ and $g(x) = 0$, for all x. Then

$$f^*(a) = \sup_{x \in C} \Big(\langle a, x \rangle - f(x) \Big) = \sup_{x} \Big(\langle a, x \rangle - f(x) \Big),$$

and

$$g^*(a) = \inf_{x \in D} \Big(\langle a, x \rangle - g(x) \Big) = \inf_{x \in D} \langle a, x \rangle.$$

The supremum is unconstrained and the infimum is with respect to a linear functional. Then, by Fenchel's Duality Theorem, we have

$$\max_{a \in C^* \cap D^*} (g^*(a) - f^*(a)) = \inf_{x \in D} f(x).$$

9.4 An Application to Game Theory

In this section we complement our earlier discussion of matrix games by illustrating the application of the Fenchel Duality Theorem to prove the Min-Max Theorem for two-person games.

9.4.1 Pure and Randomized Strategies

In a two-person game, the first player selects a row of the matrix A, say i, and the second player selects a column of A, say j. The second player pays the first player A_{ij}. If some $A_{ij} < 0$, then this means that the first player pays the second. As we discussed previously, there need not be optimal pure strategies for the two players and it may be sensible for them, over the long run, to select their strategies according to some random mechanism. The issues then are which vectors of probabilities will prove optimal and do such optimal probability vectors always exist. The Min-Max Theorem, also known as the Fundamental Theorem of Game Theory, asserts that such optimal probability vectors always exist.

9.4.2 The Min-Max Theorem

In [120], Luenberger uses the Fenchel Duality Theorem to prove the Min-Max Theorem for two-person games. His formulation is in Banach spaces, while we shall limit our discussion to finite-dimensional spaces.

Let A be an I by J pay-off matrix, whose entries represent the payoffs from the second player to the first. Let

$$P = \{p = (p_1, ..., p_I) \,|\, p_i \geq 0, \sum_{i=1}^{I} p_i = 1\},$$

$$S = \{s = (s_1, ..., s_I) \,|\, s_i \geq 0, \sum_{i=1}^{I} s_i \leq 1\},$$

and

$$Q = \{q = (q_1, ..., q_J) \,|\, q_j \geq 0, \sum_{j=1}^{J} q_j = 1\}.$$

The set S is the convex hull of the set P.

The first player selects a vector p in P and the second selects a vector q in Q. The expected pay-off to the first player is

$$E = \langle p, Aq \rangle.$$

Let

$$m_0 = \max_{p \in P} \min_{q \in Q} \langle p, Aq \rangle,$$

and

$$m^0 = \min_{q \in Q} \max_{p \in P} \langle p, Aq \rangle.$$

Clearly, we have

$$\min_{q \in Q} \langle p, Aq \rangle \leq \langle p, Aq \rangle \leq \max_{p \in P} \langle p, Aq \rangle,$$

for all $p \in P$ and $q \in Q$. It follows that $m_0 \leq m^0$. We show that $m_0 = m^0$.

Define

$$f(x) = \max_{p \in P} \langle p, x \rangle,$$

which is equivalent to

$$f(x) = \max_{s \in S} \langle s, x \rangle.$$

Then f is convex and continuous on R^I. We want $\min_{q \in Q} f(Aq)$.

We apply Fenchel's Duality Theorem, with $f = f$, $g = 0$, $D = A(Q)$, and $C = R^I$. Now we have

$$\inf_{x \in C \cap D} (f(x) - g(x)) = \min_{q \in Q} f(Aq).$$

We claim that the following are true:

- **1)** $D^* = R^I$;
- **2)** $g^*(a) = \min_{q \in Q} \langle a, Aq \rangle$;
- **3)** $C^* = S$;
- **4)** $f^*(a) = 0$, for all a in S.

The first two claims are immediate. To prove the third one, we take a vector $a \in R^I$ that is not in S. Then, by the separation theorem, we can find $x \in R^I$ and $\alpha > 0$ such that

$$\langle x, a \rangle > \alpha + \langle x, s \rangle,$$

for all $s \in S$. Then

$$\langle x, a \rangle - \max_{s \in S} \langle x, s \rangle \geq \alpha > 0.$$

Now take $k > 0$ large and $y = kx$. Since

$$\langle y, s \rangle = k \langle x, s \rangle,$$

we know that

$$\langle y, a \rangle - \max_{s \in S} \langle y, s \rangle = \langle y, a \rangle - f(y) > 0$$

and can be made arbitrarily large by taking $k > 0$ large. It follows that $f^*(a)$ is not finite if a is not in S, so that $C^* = S$.

As for the fourth claim, if $a \in S$, then

$$\langle y, a\rangle - \max_{s\in S}\langle y, s\rangle$$

achieves its maximum value of zero at $y = 0$, so $f^*(a) = 0$.

Finally, we have

$$\min_{q\in Q}\max_{p\in P}\langle p, Aq\rangle = \min_{q\in Q} f(Aq) = \max_{a\in S} g^*(a) = \max_{a\in S}\min_{q\in Q}\langle p, Aq\rangle.$$

Therefore,

$$\min_{q\in Q}\max_{p\in P}\langle p, Aq\rangle = \max_{p\in P}\min_{q\in Q}\langle p, Aq\rangle.$$

Chapter 10

Convex Programming

10.1 Chapter Summary

Convex programming (CP) refers to the minimization of a convex function of one or several variables over a convex set. The convex set is often defined in terms of inequalities involving other convex functions. We begin by describing the basic problems of CP. We then discuss characterizations of the solutions given by the Karush-Kuhn-Tucker (KKT) Theorem, the concept of duality, and use these tools to solve certain CP problems.

10.2 The Primal Problem

Let f and g_i, $i = 1, ..., I$, be convex functions defined on a non-empty closed convex subset C of R^J. The *primal problem* in *convex programming* (CP) is the following:

$$\text{minimize } f(x), \text{ subject to } g_i(x) \leq 0, \text{ for } i = 1, ..., I. \quad \text{(P)} \tag{10.1}$$

For notational convenience, we define $g(x) = (g_1(x), ..., g_I(x))$. Then (P) becomes

$$\text{minimize } f(x), \text{ subject to } g(x) \leq 0. \quad \text{(P)} \tag{10.2}$$

The *feasible set* for (P) is

$$F = \{x | g(x) \leq 0\}. \tag{10.3}$$

Definition 10.1 *The problem (P) is said to be* consistent *if F is not empty, and* super-consistent *if there is x in F with $g_i(x) < 0$ for all $i = 1, ..., I$. Such a point x is then called a* Slater point.

10.2.1 The Perturbed Problem

For each z in R^I let

$$MP(z) = \inf\{f(x)|x \in C, g(x) \leq z\}, \tag{10.4}$$

and $MP = MP(0)$. The convex programming problem (P(z)) is to minimize the function $f(x)$ over x in C with $g(x) \leq z$. The feasible set for (P(z)) is

$$F(z) = \{x|g(x) \leq z\}. \tag{10.5}$$

We shall be interested in properties of the function $MP(z)$, in particular, how the function $MP(z)$ behaves as z moves away from $z = 0$.

For example, let $f(x) = x^2$; the minimum occurs at $x = 0$. Now consider the perturbed problem, minimize $f(x) = x^2$, subject to $x \leq z$. For $z \leq 0$, the minimum of the perturbed problem occurs at $x = z$, and we have $MP(z) = z^2$. For $z > 0$ the minimum of the perturbed problem is the global minimum, which is at $x = 0$, so $MP(z) = 0$. The global minimum of $MP(z)$ also occurs at $z = 0$.

We have the following theorem concerning the function $MP(z)$; see the exercises for related results.

Theorem 10.1 *The function $MP(z)$ is convex and its domain, the set of all z for which $F(z)$ is not empty, is convex. If (P) is super-consistent, then $z = 0$ is an interior point of the domain of $MP(z)$.*

Proof: See [136], Theorem 5.2.6. ∎

From Theorem 8.9 we know that if (P) is super-consistent, then there is a vector d such that

$$MP(z) \geq MP(0) + \langle d, z - 0\rangle. \tag{10.6}$$

In fact, we can show that, in this case, $d \leq 0$. Suppose that $d_i > 0$ for some i. Since $z = 0$ is in the interior of the domain of $MP(z)$, there is $r > 0$ such that $F(z)$ is not empty for all z with $||z|| < r$. Let $w_j = 0$ for $j \neq i$ and $w_i = r/2$. Then $F(w)$ is not empty and $MP(0) \geq MP(w)$, since $F \subseteq F(w)$. But from Equation (10.6) we have

$$MP(w) \geq MP(0) + \frac{r}{2}d_i > MP(0). \tag{10.7}$$

This is a contradiction, and we conclude that $d \leq 0$.

10.2.2 The Sensitivity Vector

From now on we shall use $\lambda^* = -d$ instead of d. For $z \geq 0$ we have $MP(z) \leq MP(0)$, and

$$\langle \lambda^*, z\rangle \geq MP(0) - MP(z) \geq 0. \tag{10.8}$$

The quantity $\langle \lambda^*, z \rangle$ measures how much $MP(z)$ changes as we increase z away from $z = 0$; for that reason, λ^* is called the *sensitivity vector*, as well as the vector of *Lagrange multipliers*.

10.2.3 The Lagrangian Function

The Lagrangian function for the problem (P) is the function

$$L(x, \lambda) = f(x) + \sum_{i=1}^{I} \lambda_i g_i(x), \tag{10.9}$$

defined for all x in C and $\lambda \geq 0$.

10.3 From Constrained to Unconstrained

In addition to being a measure of the sensitivity of $MP(z)$ to changes in z, the vector λ^* can be used to convert the original constrained minimization problem (P) into an unconstrained one.

Theorem 10.2 *If the problem (P) has a sensitivity vector $\lambda^* \geq 0$, in particular, when (P) is super-consistent, then*

$$MP(0) = \inf_{x \in C} \Big(f(x) + \langle \lambda^*, g(x) \rangle \Big) = \inf_{x \in C} L(x, \lambda^*). \tag{10.10}$$

Proof: For any x in the set C, the set $F(g(x))$ is non-empty, and

$$MP(g(x)) + \langle \lambda^*, g(x) \rangle \geq MP(0). \tag{10.11}$$

Since

$$f(x) \geq MP(g(x)), \tag{10.12}$$

it follows that

$$f(x) + \langle \lambda^*, g(x) \rangle \geq MP(0). \tag{10.13}$$

Therefore,

$$\inf_{x \in C} \Big(f(x) + \langle \lambda^*, g(x) \rangle \Big) \geq MP(0). \tag{10.14}$$

But

$$\inf_{x \in C} \Big(f(x) + \langle \lambda^*, g(x) \rangle \Big) \leq \inf_{x \in C, g(x) \leq 0} \Big(f(x) + \langle \lambda^*, g(x) \rangle \Big), \tag{10.15}$$

and

$$\inf_{x\in C, g(x)\leq 0}\Big(f(x)+\langle\lambda^*, g(x)\rangle\Big) \leq \inf_{x\in C, g(x)\leq 0} f(x) = MP(0), \quad (10.16)$$

since $\lambda^* \geq 0$ and $g(x) \leq 0$. ∎

Note that the theorem tells us that the two sides of Equation (10.10) are equal, but we cannot conclude from the theorem that if both sides have a minimizer then the minimizers are the same vector.

10.4 Saddle Points

To prepare for our discussion of the Karush-Kuhn-Tucker Theorem and duality, we consider the notion of *saddle points*.

10.4.1 The Primal and Dual Problems

Suppose that X and Y are two non-empty sets and $K : X \times Y \to (-\infty, \infty)$ is a function of two variables. For each x in X, define the function $f(x)$ by the *supremum*

$$f(x) = \sup_y K(x, y), \quad (10.17)$$

where the supremum, abbreviated "sup" , is the least upper bound of the real numbers $K(x, y)$, over all y in Y. Then we have

$$K(x, y) \leq f(x), \quad (10.18)$$

for all x. Similarly, for each y in Y, define the function $g(y)$ by

$$g(y) = \inf_x K(x, y); \quad (10.19)$$

here the infimum is the greatest lower bound of the numbers $K(x, y)$, over all x in X. Then we have

$$g(y) \leq K(x, y), \quad (10.20)$$

for all y in Y. Putting together (10.18) and (10.20), we have

$$g(y) \leq K(x, y) \leq f(x), \quad (10.21)$$

for all x and y. Now we consider two problems: the *primal problem* is minimizing $f(x)$ and the *dual problem* is maximizing $g(y)$.

Definition 10.2 *The pair* $(\hat{x}, \hat{y})$ *is called a* saddle point *for the function* $K(x, y)$ *if, for all* x *and* y*, we have*

$$K(\hat{x}, y) \leq K(\hat{x}, \hat{y}) \leq K(x, \hat{y}). \tag{10.22}$$

The number $K(\hat{x}, \hat{y})$ *is called the* saddle value*.*

For example, the function $K(x, y) = x^2 - y^2$ has $(0, 0)$ for a saddle point, with saddle value zero.

10.4.2 The Main Theorem

We have the following theorem, with the proof left to the reader.

Theorem 10.3 *Let* $(\hat{x}, \hat{y})$ *be a saddle point for* $K(x, y)$*. Then* $\hat{x}$ *solves the primal problem, that is,* $\hat{x}$ *minimizes* $f(x)$*, over all* x *in* X*, and* $\hat{y}$ *solves the dual problem, that is,* $\hat{y}$ *maximizes* $g(y)$*, over all* y *in* Y*. In addition, we have*

$$g(y) \leq K(\hat{x}, \hat{y}) \leq f(x), \tag{10.23}$$

for all x *and* y*, so that the maximum value of* $g(y)$ *and the minimum value of* $f(x)$ *are both equal to* $K(\hat{x}, \hat{y})$*.*

10.4.3 A Duality Approach to Optimization

Suppose that our original problem is to minimize a function $f(x)$ over x in some set X. One approach is to find a second set Y and a function $K(x, y)$ of two variables for which Equation (10.17) holds, use Equation (10.19) to construct a second function $g(y)$, defined for y in Y, and then maximize $g(y)$. If a saddle point exists, then, according to the theorem, we have solved the original problem.

10.5 The Karush-Kuhn-Tucker Theorem

The Karush-Kuhn-Tucker Theorem gives necessary and sufficient conditions for a vector x^* to be a solution of a super-consistent problem (P).

10.5.1 The KKT Theorem: Saddle-Point Form

This form of the KKT Theorem does not require that the functions involved be differentiable. The *saddle-point* form of the Karush-Kuhn-Tucker (KKT) Theorem is the following.

Theorem 10.4 *Let (P) be super-consistent. Then* x^* *solves (P) if and only if there is a vector* λ^* *such that*

- **1)** $\lambda^* \geq 0$*;*
- **2)** $L(x^*, \lambda) \leq L(x^*, \lambda^*) \leq L(x, \lambda^*)$*, for all* x *and all* $\lambda \geq 0$*;*
- **3)** $\lambda_i^* g_i(x^*) = 0$*, for all* $i = 1, ..., I$*.*

Proof: Since (P) is super-consistent and x^* solves (P), we know from Theorem 10.2 that there is $\lambda^* \geq 0$ such that

$$f(x^*) = \inf_{x \in C} L(x, \lambda^*). \tag{10.24}$$

We do not yet know that $f(x^*) = L(x^*, \lambda^*)$, however. We do have

$$f(x^*) \leq L(x^*, \lambda^*) = f(x^*) + \langle \lambda^*, g(x^*) \rangle, \tag{10.25}$$

though, and since $\lambda^* \geq 0$ and $g(x^*) \leq 0$, we also have

$$f(x^*) + \langle \lambda^*, g(x^*) \rangle \leq f(x^*). \tag{10.26}$$

Now we can conclude that $f(x^*) = L(x^*, \lambda^*)$ and $\langle \lambda^*, g(x^*) \rangle = 0$. It follows that $\lambda_i^* g_i(x^*) = 0$, for all $i = 1, ..., I$. Since, for $\lambda \geq 0$,

$$L(x^*, \lambda^*) - L(x^*, \lambda) = \langle \lambda^* - \lambda, g(x^*) \rangle = \langle -\lambda, g(x^*) \rangle \geq 0, \tag{10.27}$$

we also have

$$L(x^*, \lambda) \leq L(x^*, \lambda^*), \tag{10.28}$$

for all $\lambda \geq 0$.

Conversely, suppose that x^* and λ^* satisfy the three conditions of the theorem. First, we show that x^* is feasible for (P), that is, $g(x^*) \leq 0$. Let i be fixed and take λ to have the same entries as λ^*, except that $\lambda_i = \lambda_i^* + 1$. then, $\lambda \geq 0$ and

$$0 \leq L(x^*, \lambda^*) - L(x^*, \lambda) = -g_i(x^*). \tag{10.29}$$

Also,

$$f(x^*) = L(x^*, 0) \leq L(x^*, \lambda^*) = f(x^*) + \langle \lambda^*, g(x^*) \rangle = f(x^*), \tag{10.30}$$

so

$$f(x^*) = L(x^*, \lambda^*) \leq L(x, \lambda^*). \tag{10.31}$$

But we also have

$$L(x^*, \lambda^*) \leq \inf_{x \in C} \Big(f(x) + \langle \lambda^*, g(x) \rangle \Big) \leq \inf_{x \in C, g(x) \leq 0} f(x) = MP(0). \tag{10.32}$$

We conclude that $f(x^*) = MP(0)$, and since x^* is feasible for (P), x^* solves (P). ∎

Condition **3)** is called *complementary slackness*. If $g_i(x^*) = 0$, we say that the ith constraint is *binding*.

10.5.2 The KKT Theorem- The Gradient Form

Now we assume that the functions $f(x)$ and $g_i(x)$ are differentiable.

Theorem 10.5 *Let (P) be super-consistent. Then x^* solves (P) if and only if there is a vector λ^* such that*

- **1)** $\lambda^* \geq 0$*;*
- **2)** $\lambda_i^* g_i(x^*) = 0$*, for all* $i = 1, ..., I$*;*
- **3)** $\nabla f(x^*) + \sum_{i=1}^{I} \lambda_i^* \nabla g_i(x^*) = 0$.

The proof is similar to the previous one and we omit it. The interested reader should consult [136], p. 185.

10.6 On Existence of Lagrange Multipliers

As we saw previously, if (P) is super-consistent, then $z = 0$ is in the interior of the domain of the function $MP(z)$, and so the sub-differential of $MP(z)$ is non-empty at $z = 0$. The sub-gradient d was shown to be non-positive and we defined the sensitivity vector, or the vector of Lagrange multipliers, to be $\lambda^* = -d$. Theorem 10.5 tells us that if (P) is super-consistent and x^* solves (P), then the vector $\nabla f(x^*)$ is a non-negative linear combination of the vectors $-\nabla g_i(x^*)$. This sounds like the assertion in Farkas' Lemma.

For any point x, define the set

$$B = \{i | g_i(x) = 0\},$$

and

$$Z(x) = \{z | z^T \nabla g_i(x) \leq 0,\ i \in B(x), \text{ and } z^T \nabla f(x) < 0\}.$$

If $Z(x)$ is empty, then

$$z^T(-\nabla g_i(x)) \geq 0$$

for $i \in B(x)$ implies

$$\nabla f(x) \geq 0,$$

which, by Farkas' Lemma, implies that $\nabla f(x)$ is a non-negative linear combination of the vectors $-\nabla g_i(x)$ for $i \in B(x)$. The objective, then, is to find some condition which, if it holds at the solution x^*, will imply that $Z(x^*)$ is empty; first-order necessary conditions are of this sort. It will then follow that there are non-negative Lagrange multipliers for which

$$\nabla f(x^*) + \sum_{i=1}^{I} \lambda_i^* \nabla g_i(x^*) = 0;$$

for i not in $B(x^*)$ we let $\lambda_i^* = 0$. For more discussion of this issue, see Fiacco and McCormick [89]

10.7 The Problem of Equality Constraints

We consider now what happens when some of the constraints are equalities.

10.7.1 The Problem

Let f and g_i, $i = 1, ..., I$, be differentiable functions defined on R^J. We consider the following problem: minimize $f(x)$, subject to the constraints

$$\begin{cases} g_i(x) \leq 0, \text{ for } i = 1, ..., K; \\ g_i(x) = 0, \text{ for } i = K+1, ..., I. \end{cases} \tag{10.33}$$

If $1 \leq K < I$, the constraints are said to be mixed. If $K = I$, there are only inequality constraints, so, for convex $f(x)$ and $g_i(x)$, the problem is (P), given by (10.1). If $K < I$, we cannot convert it to a CP problem by rewriting the equality constraints as $g_i(x) \leq 0$ and $-g_i(x) \leq 0$, since then we would lose the convexity property of the constraint functions. Nevertheless, a version of the KKT Theorem holds for such problems.

Definition 10.3 *The* feasible set *for this problem is the set F of all x satisfying the constraints.*

Definition 10.4 *The problem is said to be* consistent *if F is not empty.*

Definition 10.5 *Let $\mathcal{I}(x)$ be the set of all indices $1 \leq i \leq I$ for which $g_i(x) = 0$. The point x is* regular *if the set of gradients $\{\nabla g_i(x) | i \in \mathcal{I}(x)\}$ is linearly independent.*

10.7.2 The KKT Theorem for Mixed Constraints

The following version of the KKT Theorem provides a necessary condition for a regular point x^* to be a local constrained minimizer.

Theorem 10.6 *Let x^* be a regular point for the problem in (10.33). If x^* is a local constrained minimizer of $f(x)$, then there is a vector λ^* such that*

- **1)** $\lambda_i^* \geq 0$, *for* $i = 1, ..., K$;
- **2)** $\lambda_i^* g_i(x^*) = 0$, *for* $i = 1, ..., K$;
- **3)** $\nabla f(x^*) + \sum_{i=1}^{I} \lambda_i^* \nabla g_i(x^*) = 0$.

Note that, if there are some equality constraints, then the vector λ need not be non-negative.

10.7.3 The KKT Theorem for LP

Consider the LP problem (PS): minimize $z = c^T x$, subject to $Ax = b$ and $x \geq 0$. We let

$$z = f(x) = c^T x,$$
$$g_i(x) = b_i - (Ax)_i,$$

for $i = 1, ..., I$, and

$$g_i(x) = -x_j,$$

for $i = I+1, ..., I+J$ and $j = i - I$. We assume that $I < J$ and that the I by J matrix A has rank I. Then, since $\nabla g_i(x)$ is a^i, the ith column of A^T, the vectors $\{\nabla g_i(x) \,|i = 1, ..., I\}$ are linearly independent and every $x > 0$ is a regular point.

Suppose that a regular point x^* solves (PS). Let λ^* be the vector in R^{I+J} whose existence is guaranteed by Theorem 10.6. Denote by y^* the vector in R^I whose entries are the first I entries of λ^*, and r the non-negative vector in R^J whose entries are the last J entries of λ^*. Then, applying Theorem 10.6, we have $r^T x^* = 0$, $Ax^* = b$, and

$$c - \sum_{i=1}^{I} \lambda_i^* a^i + \sum_{j=1}^{J} r_j(-\delta_j) = 0,$$

or,

$$c - A^T y^* = r \geq 0,$$

where δ_j is the column vector whose jth entry is one and the rest are zero.

The KKT Theorem for this problem is then the following.

Theorem 10.7 *Let A have full rank I. The regular point x^* solves (PS) if and only if there are vectors y^* in R^I and $r \geq 0$ in R^J such that*

- **1)** $Ax^* = b$;
- **2)** $r = c - A^T y^*$;
- **3)** $r^T x^* = 0$.

Then y^* solves (DS).

The first condition in the theorem is *primal feasibility*, the second one is *dual feasibility*, and the third is *complementary slackness*. The first two conditions tell us that x^* is feasible for (PS) and y^* is feasible for (DS). Combining these two conditions with complementary slackness, we can write

$$z^* = c^T x^* = (A^T y^* + r)^T x^* = (A^T y^*)^T x^* + r^T x^* = (y^*)^T b = w^*,$$

so $z^* = w^*$ and there is no duality gap. Invoking Corollary 5.3 to the Weak Duality Theorem, we conclude that x^* and y^* solve their respective problems.

10.7.4 The Lagrangian Fallacy

As Kalman notes in [109], it is quite common, when discussing the use of Lagrange multipliers in optimization, to say, incorrectly, that the problem of minimizing $f(x)$, subject to $g(x) = 0$, has been converted into the problem of finding a local minimum of the Lagrangian function $L(x, \lambda)$, as a function of (x, λ). The following example, taken from [109], shows that this interpretation is false.

Minimize the function $f(x, y) = x^2 + y^2$, subject to $g(x, y) = xy - 1 = 0$. Using a Lagrange multiplier λ, and the Lagrangian

$$L(x, y, \lambda) = x^2 + y^2 + \lambda(xy - 1) = (x - y)^2 + \lambda(xy - 1) + 2xy,$$

we find that

$$2x + \lambda y = 0,$$

$$2y + \lambda x = 0,$$

and

$$xy - 1 = 0.$$

It follows that $x = 1$, $y = 1$, $\lambda = -2$, and $L(1, 1, -2) = 2$. Now let us move away from the point $(1, 1, -2)$ along the line $(x, x, -2 + t)$, so that the Lagrangian takes on the values

$$L(x, x, -2 + t) = (x - x)^2 + (-2 + t)(x^2 - 1) + 2x^2 = 2 + t(x^2 - 1).$$

For small positive values of t, the Lagrangian takes on values greater than 2, while, for small negative values of t, its values are smaller than 2.

10.8 Two Examples

We illustrate the use of the gradient form of the KKT Theorem with two examples that appeared in the paper of Driscoll and Fox [79].

10.8.1 A Linear Programming Problem

Minimize $f(x_1, x_2) = 3x_1 + 2x_2$, subject to the constraints $2x_1 + x_2 \geq 100$, $x_1 + x_2 \geq 80$, $x_1 \geq 0$ and $x_2 \geq 0$. We define

$$g_1(x_1, x_2) = 100 - 2x_1 - x_2 \leq 0, \tag{10.34}$$

$$g_2(x_1, x_2) = 80 - x_1 - x_2, \tag{10.35}$$

$$g_3(x_1, x_2) = -x_1, \tag{10.36}$$

and

$$g_4(x_1, x_2) = -x_2. \tag{10.37}$$

The Lagrangian is then

$$L(x, \lambda) = 3x_1 + 2x_2 + \lambda_1(100 - 2x_1 - x_2)$$

$$+\lambda_2(80 - x_1 - x_2) - \lambda_3 x_1 - \lambda_4 x_2. \tag{10.38}$$

From the KKT Theorem, we know that if there is a solution x^*, then there is $\lambda^* \geq 0$ with

$$f(x^*) = L(x^*, \lambda^*) \leq L(x, \lambda^*),$$

for all x. For notational simplicity, we write λ in place of λ^*.

Taking the partial derivatives of $L(x, \lambda)$ with respect to the variables x_1 and x_2, we get

$$3 - 2\lambda_1 - \lambda_2 - \lambda_3 = 0, \tag{10.39}$$

and

$$2 - \lambda_1 - \lambda_2 - \lambda_4 = 0. \tag{10.40}$$

The complementary slackness conditions are

$$\lambda_1 = 0 \ , \text{ if } 2x_1 + x_2 \neq 100, \tag{10.41}$$

$$\lambda_2 = 0 \ , \text{ if } x_1 + x_2 \neq 80, \tag{10.42}$$

$$\lambda_3 = 0 \ , \text{ if } x_1 \neq 0, \tag{10.43}$$

and

$$\lambda_4 = 0 \ , \text{ if } x_2 \neq 0. \tag{10.44}$$

A little thought reveals that precisely two of the four constraints must be binding. Examining the six cases, we find that the only case satisfying all the conditions of the KKT Theorem is $\lambda_3 = \lambda_4 = 0$. The minimum occurs at $x_1 = 20$ and $x_2 = 60$ and the minimum value is $f(20, 60) = 180$.

We can use these results to illustrate Theorem 10.2. The sensitivity vector is $\lambda^* = (1, 1, 0, 0)$ and the Lagrangian function at λ^* is

$$L(x, \lambda^*) = 3x_1 + 2x_2 + 1(100 - 2x_1 - x_2). \tag{10.45}$$

In this case, we find that $L(x, \lambda^*) = 180$, for all x.

10.8.2 A Nonlinear Convex Programming Problem

Minimize the function

$$f(x_1, x_2) = (x_1 - 14)^2 + (x_2 - 11)^2,$$

subject to

$$g_1(x_1, x_2) = (x_1 - 11)^2 + (x_2 - 13)^2 - 49 \leq 0,$$

and

$$g_2(x_1, x_2) = x_1 + x_2 - 19 \leq 0.$$

The Lagrangian is then

$$L(x, \lambda) = (x_1 - 14)^2 + (x_2 - 11)^2 +$$

$$\lambda_1\Big((x_1 - 11)^2 + (x_2 - 13)^2 - 49\Big) + \lambda_2\Big(x_1 + x_2 - 19\Big). \tag{10.46}$$

Again, we write λ in place of λ^*. Setting the partial derivatives, with respect to x_1 and x_2, to zero, we get the KKT equations

$$2x_1 - 28 + 2\lambda_1 x_1 - 22\lambda_1 + \lambda_2 = 0, \tag{10.47}$$

and

$$2x_2 - 22 + 2\lambda_1 x_2 - 26\lambda_1 + \lambda_2 = 0. \tag{10.48}$$

The complementary slackness conditions are

$$\lambda_1 = 0\,, \quad \text{if } (x_1 - 11)^2 + (x_2 - 13)^2 \neq 49, \tag{10.49}$$

and

$$\lambda_2 = 0\,, \quad \text{if } x_1 + x_2 \neq 19. \tag{10.50}$$

There are four cases to consider. First, if neither constraint is binding, the KKT equations have solution $x_1 = 14$ and $x_2 = 11$, which is not feasible. If only the first constraint is binding, we obtain two solutions, neither feasible. If only the second constraint is binding, we obtain $x_1^* = 11$, $x_2^* = 8$, and $\lambda_2 = 6$. This is the optimal solution. If both constraints are binding, we obtain, with a bit of calculation, two solutions, neither feasible. The minimum value is $f(11, 8) = 18$, and the sensitivity vector is $\lambda^* = (0, 6)$. Using these results, we once again illustrate Theorem 10.2.

The Lagrangian function at λ^* is

$$L(x, \lambda^*) = (x_1 - 14)^2 + (x_2 - 11)^2 + 6(x_1 + x_2 - 19). \tag{10.51}$$

Setting to zero the first partial derivatives of $L(x, \lambda^*)$, we get

$$0 = 2(x_1 - 14) + 6,$$

and

$$0 = 2(x_2 - 11) + 6,$$

so that $x_1^* = 11$ and $x_2^* = 8$. Note that Theorem 10.2 only guarantees that 18 is the infimum of the function $L(x, \lambda^*)$. It does not say that this smallest value must occur at $x = x^*$ or even occurs anywhere; that is, it does not say that $L(x^*, \lambda^*) \leq L(x, \lambda^*)$. This stronger result comes from the KKT Theorem.

10.9 The Dual Problem

The *dual problem* (DP) corresponding to (P) is

$$\text{maximize } h(\lambda) = \inf_{x \in C} L(x, \lambda), \text{ for } \lambda \geq 0. \quad \text{(DP)} \tag{10.52}$$

Let

$$MD = \sup_{\lambda \geq 0} h(\lambda). \tag{10.53}$$

A vector $\lambda \geq 0$ is feasible for (DP) if $h(\lambda) > -\infty$. Then (DP) is consistent if there are feasible λ. Recall that Theorem 10.2 tells us that if a sensitivity vector $\lambda^* \geq 0$ exists, then $h(\lambda^*) = MP$.

10.9.1 When is $MP = MD$?

We have the following theorem.

Theorem 10.8 *Assume that (P) is super-consistent, so that there is a sensitivity vector $\lambda^* \geq 0$, and that MP is finite. Then*

- **1)** *$MP = MD$;*
- **2)** *$MD = h(\lambda^*)$, so the supremum in Equation (10.53) is attained at λ^*;*
- **3)** *if the infimum in the definition of MP is attained at x^*, then $\langle \lambda^*, g(x^*) \rangle = 0$;*
- **4)** *such an x^* also minimizes $L(x, \lambda^*)$ over $x \in C$.*

Proof: For all $\lambda \geq 0$ we have

$$h(\lambda) = \inf_{x \in C} L(x, \lambda) \leq \inf_{x \in C, g(x) \leq 0} L(x, \lambda) \leq \inf_{x \in C, g(x) \leq 0} f(x) = MP.$$

Therefore, $MD \leq MP$. But we also know that

$$MP = h(\lambda^*) \leq MD,$$

so $MP = MD$, and the supremum in the definition of MD is attained at λ^*. From

$$f(x^*) = MP = \inf_{x \in C} L(x, \lambda^*) \leq \inf_{x \in C, g(x) \leq 0} L(x, \lambda^*)$$

$$\leq L(x^*, \lambda^*) \leq f(x^*),$$

it follows that $\langle \lambda^*, g(x^*) \rangle = 0$. ∎

10.9.2 The Primal-Dual Method

From Theorem 10.8 we see that one approach to solving (P) is to solve (DP) for λ^* and then minimize $L(x, \lambda^*)$ over $x \in C$. This is useful only if solving (DP) is simpler than solving (P) directly. Each evaluation of $h(\lambda)$ involves minimizing $L(x, \lambda)$ over $x \in C$. Once we have found λ^*, we find x^* by minimizing $L(x, \lambda^*)$ over $x \in C$. The advantage is that all the minimizations are over all $x \in C$, not over just the feasible vectors.

10.9.3 An Example

Let $f(x) = \frac{1}{2}||x||_2^2$. The primary problem is to minimize $f(x)$ over all x for which $Ax \geq b$. Then $g_i = b_i - (Ax)_i$, for $i = 1, ..., I$, and the set C is all of R^J. The Lagrangian is then

$$L(x, \lambda) = \frac{1}{2}||x||_2^2 - \lambda^T Ax + \lambda^T b. \tag{10.54}$$

The infimum over x occurs when $x = A^T \lambda$ and so

$$h(\lambda) = \lambda^T b - \frac{1}{2}||A^T \lambda||_2^2. \tag{10.55}$$

For any x satisfying $Ax \geq b$ and any $\lambda \geq 0$ we have $h(\lambda) \leq f(x)$. If x^* is the unique solution of the primal problem and λ^* any solution of the dual problem, we have $f(x^*) = h(\lambda^*)$. The point here is that the constraints in the dual problem are easier to implement in an iterative algorithm, so solving the dual problem is the simpler task.

10.9.4 An Iterative Algorithm for the Dual Problem

In [119] Lent and Censor present the following sequential iterative algorithm for solving the dual problem above. At each step only one entry of the current λ is altered.

Algorithm 10.1 (Lent-Censor) *Let a_i denote the i-th row of the matrix A. Having calculated x^k and $\lambda^k > 0$, let $i = k(\mathrm{mod}\, I) + 1$. Then let*

$$\theta = (b_i - (a_i)^T x^k)/a_i^T a_i, \tag{10.56}$$

$$\delta = \max\{-\lambda_i^k, \omega\theta\}, \tag{10.57}$$

and set

$$\lambda_i^{k+1} = \lambda_i^k + \delta, \tag{10.58}$$

and

$$x^{k+1} = x^k + \delta a_i. \tag{10.59}$$

10.10 Minimum One-Norm Solutions

When the system of linear equations $Ax = b$ is under-determined, it is common practice to seek a solution that also minimizes some objective function. For example, the *minimum two-norm solution* is the vector x satisfying $Ax = b$ for which the (square of the) two-norm,

$$||x||_2^2 = \sum_{j=1}^{J} x_j^2,$$

is minimized. Alternatively, we may seek the *minimum one-norm solution*, for which the one-norm,

$$||x||_1 = \sum_{j=1}^{J} |x_j|,$$

is minimized.

If the vector x is required to be non-negative, then the one-norm is simply the sum of the entries, and minimizing the one-norm subject to $Ax = b$ becomes a linear programming problem. This is the situation in applications involving image reconstruction.

In *compressed sampling* [77] one seeks a solution of $Ax = b$ having relatively few non-zero entries. The vector x here is not assumed to be non-negative, and the solution is found by minimizing the one-norm, subject to the constraints $Ax = b$. The one-norm is not a linear functional of x, but the problem can still be converted into a linear programming problem.

10.10.1 Reformulation as an LP Problem

The entries of x need not be non-negative, so the problem is not yet a linear programming problem. Let

$$B = [\, A \quad -A \,],$$

and consider the linear programming problem of minimizing the function

$$c^T z = \sum_{j=1}^{2J} z_j,$$

subject to the constraints $z \geq 0$, and $Bz = b$. Let z^* be the solution. We write

$$z^* = \begin{bmatrix} u^* \\ v^* \end{bmatrix}.$$

Then $x^* = u^* - v^*$ minimizes the one-norm, subject to $Ax = b$. To see why this is true, select any x with $Ax = b$. Write $u_j = x_j$, if $x_j \geq 0$, and $u_j = 0$, otherwise. Let $v_j = u_j - x_j$, so that $x = u - v$. Then let

$$z = \begin{bmatrix} u \\ v \end{bmatrix}.$$

Then $b = Ax = Bz$, and $c^T z = \|x\|_1$. Consequently,

$$\|x^*\|_1 = c^T z^* \leq c^T z = \|x\|_1,$$

and x^* must be a minimum one-norm solution.

10.10.2 Image Reconstruction

In image reconstruction from limited linear-functional data, the vector x is non-negative and arises as a vectorization of a two-dimensional image. The data we have pertaining to x is linear and takes the form $Ax = b$, for some matrix A and vector b. Typically, the problem is under-determined, since the number of entries of x is the number of pixels in the image, which we can make as large as we wish. The problem then is to select, from among all the feasible images, one particular one that has a good chance of being near the correct image. One approach is to take the solution of $Ax = b$ having the minimum Euclidean norm, $||x||_2$. Algorithms such as the projected ART and projected Landweber iterative methods can be used to find such solutions.

Another approach is to find the non-negative solution of $Ax = b$ for which the one-norm,

$$||x||_1 = \sum_{j=1}^{J} |x_j|,$$

is minimized [77]. Since the x_j are to be non-negative, the problem becomes the following: minimize

$$f(x) = \sum_{j=1}^{J} x_j,$$

subject to

$$g_i(x) = (Ax)_i - b_i = 0,$$

for $i = 1, ..., I$, and

$$g_i(x) = -x_{i-I} \leq 0,$$

for $i = I + 1, ..., I + J$.

When the system $Ax = b$ is under-determined, the minimum one-norm solution tends to be sparser than the minimum two-norm solution. A simple example will illustrate this point.

Consider the equation $x + 2y = 1$. The minimum two-norm solution is $(0.2, 0.4)$, with two-norm $\frac{\sqrt{5}}{5}$, which is about 0.4472, but one-norm equal to 0.6. The solution $(0, 0.5)$ has two-norm and one-norm equal to 0.5, and the solution $(1.0, 0)$ has two-norm and one-norm equal to 1.0. Therefore, the minimum one-norm solution is $(0, 0.5)$, not $(0.2, 0.4)$.

We can write the one-norm of the vector x as

$$||x||_1 = \sum_{j=1}^{J} \frac{|x_j|^2}{|x_j|}.$$

The PDFT approach to image reconstruction [45] selects the solution of $Ax = b$ that minimizes the weighted two-norm

$$||x||_w^2 = \sum_{j=1}^{J} \frac{|x_j|^2}{p_j} = \sum_{j=1}^{J} |x_j|^2 w_j,$$

where $p_j > 0$ is a prior estimate of the non-negative image x to be reconstructed, and $w_j = p_j^{-1}$. To the extent that p_j accurately models the main features of x, such as which x_j are nearly zero and which are not, the two approaches should give similar reconstructions. The PDFT can be implemented using the ART algorithm (see [145, 146, 147]. For more discussion of one-norm minimization, see the chapter on compressed sensing.

10.11 Exercises

10.1 *Prove Theorem 10.3.*

10.2 *Apply the gradient form of the KKT Theorem to minimize the function* $f(x, y) = (x + 1)^2 + y^2$ *over all* $x \geq 0$ *and* $y \geq 0$.

10.3 ([89]) *Consider the following problem : minimize the function*

$$f(x, y) = |x - 2| + |y - 2|,$$

subject to

$$g(x, y) = y^2 - x \leq 0,$$

and

$$h(x, y) = x^2 + y^2 - 1 = 0.$$

Illustrate this problem graphically, showing lines of constant value of f and the feasible region of points satisfying the constraints. Where is the solution of the problem? Where is the solution, if the equality constraint is removed? Where is the solution, if both constraints are removed?

10.4 ([136], Ex. 5.2.9 (a)) *Minimize the function*

$$f(x, y) = \sqrt{x^2 + y^2},$$

subject to

$$x + y \leq 0.$$

Show that the function $MP(z)$ is not differentiable at $z = 0$.

10.5 ([136], Ex. 5.2.9 (b)) *Minimize the function*

$$f(x, y) = -2x - y,$$

subject to

$$x + y \leq 1,$$

$$0 \leq x \leq 1,$$

and

$$y \geq 0.$$

Again, show that the function $MP(z)$ is not differentiable at $z = 0$.

10.6 (Duffin; [136], Ex. 5.2.9 (c)) *Minimize the function*

$$f(x, y) = e^{-y},$$

subject to

$$\sqrt{x^2 + y^2} - x \leq 0.$$

Show that the function $MP(z)$ is not continuous at $z = 0$.

10.7 *Apply the theory of convex programming to the primal Quadratic Programming Problem (QP), which is to minimize the function*

$$f(x) = \frac{1}{2} x^T Q x,$$

subject to

$$a^T x \leq c,$$

where a and c are given vectors in R^J.

10.8 *Use Theorem 10.6 to prove that any real N by N symmetric matrix has N mutually orthonormal eigenvectors.*

10.12 Course Homework

Do Exercises 10.1, 10.2, and 10.3.

Chapter 11

Iterative Optimization

11.1 Chapter Summary

Now we begin our discussion of iterative methods for solving optimization problems. Topics include the role of the gradient operator, the Newton-Raphson (NR) method, and various computationally simpler variants of the NR method.

11.2 The Need for Iterative Methods

We know from beginning calculus that, if we want to optimize a differentiable function $g(x)$ of a single real variable x, we begin by finding the places where the derivative is zero, $g'(x) = 0$. Similarly, if we want to optimize a differentiable function $g(x)$ of a real vector variable x, we begin by finding the places where the gradient is zero, $\nabla g(x) = 0$. Generally, though, this is not the end of the story, for we still have to solve an equation for the optimal x. Unless we are fortunate, solving this equation algebraically may be computationally expensive, or may even be impossible, and we will need to turn to iterative methods. This suggests that we might use iterative methods to minimize $g(x)$ directly, and not solve an equation.

For example, suppose we wish to solve the over-determined system of linear equations $Ax = b$, but we don't know if the system has solutions. In that case, we may wish to minimize the function

$$g(x) = \frac{1}{2}\|Ax - b\|_2^2,$$

to get a least-squares solution. We know from linear algebra that if the matrix $A^T A$ is invertible, then the unique minimizer of $g(x)$ is given by

$$x^* = (A^T A)^{-1} A^T b.$$

In many applications, the number of equations and the number of unknowns may be quite large, making it expensive even to calculate the entries of the matrix A^TA. In such cases, we can find x^* using an iterative method such as Landweber's Algorithm, which has the iterative step

$$x^{k+1} = x^k + \gamma A^T(b - Ax^k).$$

The sequence $\{x^k\}$ converges to x^* for any value of γ in the interval $(0, 2/\lambda_{max})$, where λ_{max} is the largest eigenvalue of the matrix A^TA.

11.3 Optimizing Functions of a Single Real Variable

Suppose $g : R \to R$ is differentiable and attains its minimum value. We want to minimize the function $g(x)$. Solving $g'(x) = 0$ to find the optimal $x = x^*$ may not be easy, so we may turn to an iterative algorithm for finding roots of $g'(x)$, or one that minimizes $g(x)$ directly. In the latter case, we may consider an iterative procedure

$$x^{k+1} = x^k - \gamma_k g'(x^k), \tag{11.1}$$

for some sequence $\{\gamma_k\}$ of positive numbers. Such iterative procedures are called *descent algorithms* because, if $g'(x^k) > 0$, then we want to move to the left of x^k, while, if $g'(x^k) < 0$, we want to move to the right.

We shall be particularly interested in algorithms in which $\gamma_k = \gamma$ for all k. We denote by T the operator

$$Tx = x - \gamma g'(x). \tag{11.2}$$

Then, using $g'(x^*) = 0$, we find that

$$|x^* - x^{k+1}| = |Tx^* - Tx^k|. \tag{11.3}$$

11.3.1 Iteration and Operators

The iterative methods we shall consider involve the calculation of a sequence $\{x^k\}$ of vectors in R^J, according to the formula $x^{k+1} = Tx^k$, where T is some function $T : R^J \to R^J$; such functions are called *operators* on R^J. The operator $Tx = x - g'(x)$ above is an operator on R.

Definition 11.1 *An operator T on R^J is* continuous *at x in the interior of its domain if*

$$\lim_{z \to x} \|Tz - Tx\| = 0.$$

All the operators we shall consider are continuous.

The sequences generated by iterative methods can then be written $\{T^k x^0\}$, where $x = x^0$ is the starting point for the iteration and T^k means apply the operator T k times. If the sequence $\{x^k\}$ converges to a limit vector $\hat{x}$ in the domain of T, then, taking the limit, as $k \to +\infty$, on both sides of

$$x^{k+1} = Tx^k,$$

and using the continuity of the operator T, we have

$$\hat{x} = T\hat{x},$$

that is, the limit vector $\hat{x}$ is a *fixed point* of T.

Definition 11.2 *A vector x in the domain of the operator T is a* fixed point *of T if $T\hat{x} = \hat{x}$. The set of all fixed points of T is denoted* $\mathrm{Fix}(T)$.

We have several concerns, when we use iterative methods:

- Does the operator T have any fixed points?
- Does the sequence $\{T^k x_0\}$ converge?
- Does convergence depend on the choice of x^0?
- When the sequence $\{T^k x^0\}$ converges, is the limit a solution to our problem?
- How fast does the sequence $\{T^k x^0\}$ converge?
- How difficult is it to perform a single step, going from x^k to x^{k+1}?
- How does the limit depend on the starting vector x^0?

To answer these questions, we will need to learn about the properties of the particular operator T being used. We begin our study of iterative optimization algorithms with the gradient descent methods, particularly as they apply to convex functions.

11.4 Gradient Operators

Suppose that $g(x)$ is convex and the function $f(x) = g'(x)$ is L-Lipschitz. If $g(x)$ is twice differentiable, this would be the case if

$$0 \leq g''(x) \leq L, \tag{11.4}$$

for all x. If γ is in the interval $(0, \frac{2}{L})$, then the operator $Tx = x - \gamma g'(x)$ is an averaged operator; from the KM Theorem 17.2, we know that the

iterative sequence $\{T^k x^0\}$ converges to a minimizer of $g(x)$, whenever a minimizer exists.

If $g(x)$ is convex and $f(x) = g'(x)$ is L-Lipschitz, then $\frac{1}{L}g'(x)$ is nonexpansive, so that, by Theorem 8.12 $\frac{1}{L}g'(x)$ is fne and $g'(x)$ is $\frac{1}{L}$-ism. Then, as we shall see later, the operator

$$Tx = x - \gamma g'(x) \tag{11.5}$$

is av whenever $0 < \gamma < \frac{2}{L}$, and so the iterative sequence $x^{k+1} = Tx^k = x^k - \gamma g'(x^k)$ converges to a minimizer of $g(x)$, whenever minimizers exist.

In the next section we extend these results to functions of several variables.

11.5 Optimizing Functions of Several Real Variables

Suppose $g : R^J \to R$ is differentiable and attains its minimum value. We want to minimize the function $g(x)$. Solving $\nabla g(x) = 0$ to find the optimal $x = x^*$ may not be easy, so we may turn to an iterative algorithm for finding roots of $\nabla g(x)$, or one that minimizes $g(x)$ directly. From Cauchy's Inequality, we know that the directional derivative of $g(x)$, at $x = a$, and in the direction of the vector unit vector d, satisfies

$$|g'(a;d)| = |\langle \nabla g(a), d\rangle| \leq \|\nabla g(a)\|_2 \, \|d\|_2,$$

and that $g'(a;d)$ attains its most positive value when the direction d is a positive multiple of $\nabla g(a)$. This suggests *steepest descent* optimization.

Steepest descent iterative optimization makes use of the fact that the direction of greatest increase of $g(x)$ away from $x = x^k$ is in the direction $d = \nabla g(x^k)$. Therefore, we select as the next vector in the iterative sequence

$$x^{k+1} = x^k - \gamma_k \nabla g(x^k), \tag{11.6}$$

for some $\gamma_k > 0$. Ideally, we would choose γ_k so that

$$g(x^k + \gamma_k \nabla g(x^k)) \leq g(x^k + \alpha \nabla g(x^k)),$$

for all α; that is, we would proceed away from x^k, in the direction of $-\nabla g(x^k)$, stopping just as $g(x)$ begins to increase. Then we call this point x^{k+1} and repeat the process. In practice, finding the optimal γ_k is not a simple matter. Instead, one can try a few values of α and accept the best of these few, or one can try to find a constant value γ of the parameter having the property that the iterative step

$$x^{k+1} = x^k - \gamma \nabla g(x^k)$$

leads to a convergent sequence. It is this latter approach that we shall consider here.

We denote by T the operator

$$Tx = x - \gamma \nabla g(x). \tag{11.7}$$

Then, using $\nabla g(x^*) = 0$, we find that

$$\|x^* - x^{k+1}\|_2 = \|Tx^* - Tx^k\|_2. \tag{11.8}$$

We would like to know if there are choices for γ that imply convergence of the iterative sequence. As in the case of functions of a single variable, for functions $g(x)$ that are *convex*, the answer is yes.

If $g(x)$ is convex and $f(x) = \nabla g(x)$ is L-Lipschitz, then $\frac{1}{L}\nabla g(x)$ is non-expansive, Then, as we shall see later, for $\gamma > 0$, the operator

$$Tx = x - \gamma \nabla g(x) \tag{11.9}$$

is *averaged*, whenever $0 < \gamma < \frac{2}{L}$. It follows from the KM Theorem 17.2 that the iterative sequence $x^{k+1} = Tx^k = x^k - \gamma \nabla g(x^k)$ converges to a minimizer of $g(x)$, whenever minimizers exist.

For example, the function $g(x) = \frac{1}{2}\|Ax - b\|_2^2$ is convex and its gradient is

$$f(x) = \nabla g(x) = A^T(Ax - b).$$

A steepest descent algorithm for minimizing $g(x)$ then has the iterative step

$$x^{k+1} = x^k - \gamma_k A^T(Ax^k - b),$$

where the parameter γ_k should be selected so that

$$g(x^{k+1}) < g(x^k).$$

The linear operator that transforms each vector x into A^TAx has the property that

$$\|A^TAx - A^TAy\|_2 \leq \lambda_{max}\|x - y\|_2,$$

where λ_{max} is the largest eigenvalue of the matrix A^TA; this operator is then L-Lipschitz, for $L = \lambda_{max}$. Consequently, the operator that transforms x into $\frac{1}{L}A^TAx$ is non-expansive.

11.6 The Newton-Raphson Approach

The Newton-Raphson approach to minimizing a real-valued function $f : R^J \to R$ involves finding x^* such that $\nabla f(x^*) = 0$.

11.6.1 Functions of a Single Variable

We begin with the problem of finding a root of a function $g : R \to R$. If x^0 is not a root, compute the line tangent to the graph of g at $x = x^0$ and let x^1 be the point at which this line intersects the horizontal axis; that is,

$$x^1 = x^0 - g(x^0)/g'(x^0). \tag{11.10}$$

Continuing in this fashion, we have

$$x^{k+1} = x^k - g(x^k)/g'(x^k). \tag{11.11}$$

This is the *Newton-Raphson algorithm* for finding roots. Convergence, when it occurs, is usually more rapid than gradient descent, but requires that x^0 be sufficiently close to the solution.

Now suppose that $f : R \to R$ is a real-valued function that we wish to minimize by solving $f'(x) = 0$. Letting $g(x) = f'(x)$ and applying the Newton-Raphson algorithm to $g(x)$ gives the iterative step

$$x^{k+1} = x^k - f'(x^k)/f''(x^k). \tag{11.12}$$

This is the Newton-Raphson optimization algorithm. Now we extend these results to functions of several variables.

11.6.2 Functions of Several Variables

The Newton-Raphson algorithm for finding roots of functions $g : R^J \to R^J$ has the iterative step

$$x^{k+1} = x^k - [\mathcal{J}(g)(x^k)]^{-1} g(x^k), \tag{11.13}$$

where $\mathcal{J}(g)(x)$ is the Jacobian matrix of first partial derivatives, $\frac{\partial g_m}{\partial x_j}(x^k)$, for $g(x) = (g_1(x), ..., g_J(x))^T$.

To minimize a function $f : R^J \to R$, we let $g(x) = \nabla f(x)$ and find a root of g. Then the Newton-Raphson iterative step becomes

$$x^{k+1} = x^k - [\nabla^2 f(x^k)]^{-1} \nabla f(x^k), \tag{11.14}$$

where $\nabla^2 f(x) = \mathcal{J}(g)(x)$ is the Hessian matrix of second partial derivatives of f.

The quadratic approximation to $f(x)$ around the point x^k is

$$f(x) \approx f(x^k) + \langle \nabla f(x^k), x - x^k \rangle + \frac{1}{2}(x - x^k)^T \nabla^2 f(x^k)(x - x^k).$$

The right side of this equation attains its minimum value when

$$0 = \nabla f(x^k) + \nabla^2 f(x^k)(x - x^k),$$

that is, when $x = x^{k+1}$ as given by Equation (11.14).

If $f(x)$ is a quadratic function, that is,

$$f(x) = x^T Q x + x^T b + c,$$

for constant invertible matrix Q and constant vectors b and c, then the Newton-Raphson iteration converges to the answer in one step. Therefore, if $f(x)$ is close to quadratic, the convergence should be reasonably rapid. This leads to the notion of *self-concordant functions*, for which the third derivative of $f(x)$ is small, relative to the second derivative [129].

11.7 Approximate Newton-Raphson Methods

To implement the NR method in this case, at each step of the iteration we need to solve a system of equations involving the Hessian matrix for f. There are many iterative procedures designed to retain much of the advantages of the NR method, but without the use of the Hessian matrix, or, indeed, without the use of the gradient. These methods are discussed in most texts on numerical methods [129]. We sketch briefly some of these approaches.

11.7.1 Avoiding the Hessian Matrix

Quasi-Newton methods, designed to avoid having to calculate the Hessian matrix, are often used instead of the Newton-Raphson algorithm. The iterative step of the quasi-Newton methods is

$$x^{k+1} = x^k - B_k^{-1} \nabla f(x^k), \tag{11.15}$$

where the matrix B_k is an approximation of $\nabla^2 f(x^k)$ that is easier to compute.

In the case of $g : R \to R$, the second derivative of $g(x)$ is approximately

$$g''(x^k) \approx \frac{g'(x^k) - g'(x^{k-1})}{x^k - x^{k-1}}. \tag{11.16}$$

This suggests that, for the case of functions of several variables, the matrix B_k should be selected so that

$$B_k(x^k - x^{k-1}) = \nabla f(x^k) - \nabla f(x^{k-1}). \tag{11.17}$$

In addition to satisfying Equation (11.17), the matrix B_k should also be symmetric and positive-definite. Finally, we should be able to obtain B_{k+1} relatively easily from B_k.

The BFGS Method

The Broyden, Fletcher, Goldfarb, and Shanno (BFGS) method uses the rank-two update formula

$$B_{k+1} = B_k - \frac{(B_k s^k)(B_k s^k)^T}{(s^k)^T B_k s^k} + \frac{y^k (y^k)^T}{(y^k)^T s^k}, \tag{11.18}$$

with

$$s^k = x^{k+1} - x^k, \tag{11.19}$$

and

$$y^k = \nabla f(x^{k+1}) - \nabla f(x^k). \tag{11.20}$$

The Broyden Class

A general class of update methods, known as the Broyden class, uses the update formula

$$B_{k+1} = B_k - \frac{(B_k s^k)(B_k s^k)^T}{(s^k)^T B_k s^k} + \frac{y^k (y^k)^T}{(y^k)^T s^k} + \phi((s^k)^T B_k s^k) u^k (u^k)^T, \tag{11.21}$$

with ϕ a scalar and

$$u^k = \frac{y^k}{(y^k)^T s^k} - \frac{B_k s^k}{(s^k)^T B_k s^k}. \tag{11.22}$$

When $\phi = 0$ we get the BFGS method, while the choice of $\phi = 1$ gives the Davidon, Fletcher, and Powell (DFP) method.

Note that for the updates in the Broyden class, the matrix B_{k+1} has the form

$$B_{k+1} = B_k + x^k (x^k)^T + z^k (z^k)^T,$$

for certain vectors x^k and z^k. Therefore, using the Sherman-Morrison-Woodbury Identity (see Exercise 11.40), the inverse of B_{k+1} can be obtained easily from the inverse of B_k.

11.7.2 Avoiding the Gradient

Quasi-Newton methods use an approximation of the Hessian matrix that is simpler to calculate, but still employ the gradient at each step. For functions $g : R \to R$, the derivative can be approximated by a *finite difference*, that is,

$$g'(x^k) \approx \frac{g(x^k) - g(x^{k-1})}{x^k - x^{k-1}}. \tag{11.23}$$

In the case of functions of several variables, the gradient vector can be approximated by using a finite-difference approximation for each of the first partial derivatives.

11.8 Derivative-Free Methods

In many important applications, calculating values of the function to be optimized is expensive and calculating gradients impractical. In such cases, it is common to use *direct-search methods*. Generally, these are iterative methods that are easy to program, do not employ derivatives or their approximations, require relatively few function evaluations, and are useful even when the measurements are noisy.

11.8.1 Multi-directional Search Algorithms

Methods such as the *multi-directional search* algorithms begin with the values of the function $f(x)$ at $J+1$ points, where x is in R^J, and then use these values to move to a new set of points. These points are chosen to describe a simplex pattern in R^J, that is, they do not all lie on a single hyperplane in R^J. For that reason, these methods are sometimes called *simplex* methods, although they are unrelated to Dantzig's method of the same name. The Nelder-Mead algorithm [130, 114, 124] is one such simplex algorithm.

11.8.2 The Nelder-Mead Algorithm

For simplicity, we follow McKinnon [124] and describe the Nelder-Mead (NM) algorithm only for the case of $J = 2$. The NM algorithm begins with the choice of vertices:

ORDER: obtain b, s, and w, with

$$f(b) \leq f(s) \leq f(w).$$

Then take

$$m = \frac{1}{2}(b + s).$$

Let the *search line* be

$$L(\rho) = m + \rho(m - w),$$

and

$$r = L(1) = 2m - w.$$

- **{if** $f(r) < f(b)$**}** let $e = L(2)$. If $f(e) < f(b)$ *accept* e; otherwise *accept* r.
- **{if** $f(b) \leq f(r)$**}** then
  - **{if** $f(r) < f(s)$**}** *accept* r.

- **{if** $f(s) \leq f(r)$**}**
  - **{if** $f(r) < f(w)$**}** let $c = L(0.5)$
    - **{if** $f(c) \leq f(r)$**}** *accept* c;
    - **{if** $f(r) < f(c)$**}** go to SHRINK.
  - **{if** $f(w) \leq f(r)$**}** let $c = L(-0.5)$.
    - **{if** $f(c) < f(w)$**}** *accept* c; otherwise go to SHRINK.

Replace w with the *accepted* point and go to ORDER.
SHRINK: Replace s with $\frac{1}{2}(s + b)$ and w with $\frac{1}{2}(w + b)$; go to ORDER.

11.8.3 Comments on the Nelder-Mead Algorithm

Although the Nelder-Mead algorithm is quite popular in many areas of applications, relatively little of a theoretical nature is known. The interested reader is directed to the papers [114, 124], as well as to more recent work by Margaret Wright of NYU. A good treatment of the Nelder-Mead algorithm, along with a number of other derivative-free techniques, is the new book by Conn, Scheinberg and Vicente [70].

11.9 Rates of Convergence

In this section we illustrate the concept of *rate of convergence* [22] by considering the fixed-point iteration $x_{k+1} = g(x_k)$, for the twice continuously differentiable function $g : R \to R$. We suppose that $g(z) = z$ and we are interested in the distance $|x_k - z|$.

11.9.1 Basic Definitions

Definition 11.3 *Suppose the sequence* $\{x_k\}$ *converges to* z*. If there are positive constants* λ *and* α *such that*

$$\lim_{k \to \infty} \frac{|x_{k+1} - z|}{|x_k - z|^\alpha} = \lambda, \tag{11.24}$$

then $\{x_k\}$ *is said to converge to* z *with* order α *and* asymptotic error constant λ*. If* $\alpha = 1$*, the convergence is said to be* linear*; if* $\alpha = 2$*, the convergence is said to be* quadratic*.*

11.9.2 Illustrating Quadratic Convergence

According to the Mean Value Theorem,

$$g(x) = g(z) + g'(z)(x - z) + \frac{1}{2} g''(c)(x - z)^2, \tag{11.25}$$

for some c between x and z. Suppose now that $x_k \to z$ and, in addition, $g'(z) = 0$. Then we have

$$x_{k+1} = g(x_k) = z + \frac{1}{2}g''(c_k)(x_k - z)^2, \tag{11.26}$$

for some c_k between x_k and z. Therefore,

$$|x_{k+1} - z| = \frac{1}{2}|g''(c_k)|\,|x_k - z|^2, \tag{11.27}$$

and the convergence is quadratic, with $\lambda = |g''(z)|$.

11.9.3 Motivating the Newton-Raphson Method

Suppose that we are seeking a root z of the function $f : R \to R$. We define

$$g(x) = x - h(x)f(x), \tag{11.28}$$

for some function $h(x)$ to be determined. Then $f(z) = 0$ implies that $g(z) = z$. In order to have quadratic convergence of the iterative sequence $x_{k+1} = g(x_k)$, we want $g'(z) = 0$. From

$$g'(x) = 1 - h'(x)f(x) - h(x)f'(x), \tag{11.29}$$

it follows that we want

$$h(z) = 1/f'(z). \tag{11.30}$$

Therefore, we choose

$$h(x) = 1/f'(x), \tag{11.31}$$

so that

$$g(x) = x - f(x)/f'(x). \tag{11.32}$$

The iteration then takes the form

$$x_{k+1} = g(x_k) = x_k - f(x_k)/f'(x_k), \tag{11.33}$$

which is the Newton-Raphson iteration.

11.10 Feasible-Point Methods

We consider now the problem of minimizing the function $f(x) : R^J \to R$, subject to the equality constraints $Ax = b$, where A is an I by J real matrix, with rank I and $I < J$. The two methods we consider here are *feasible-point methods*, also called *interior-point methods*.

11.10.1 The Reduced Newton-Raphson Method

The first method we consider is a modification of the Newton-Raphson method, in which we begin with a feasible point and each NR step is projected into the null space of the matrix A, to maintain the condition $Ax = b$. The discussion here is taken from [129].

Let $\hat{x}$ be a *feasible point*, that is, $A\hat{x} = b$. Then $x = \hat{x} + p$ is also feasible if p is in the null space of A, that is, $Ap = 0$. Let Z be a $J - I$ by J matrix whose columns form a basis for the null space of A. We want $p = Zv$ for some v. The best v will be the one for which the function

$$\phi(v) = f(\hat{x} + Zv)$$

is minimized. We can apply to the function $\phi(v)$ the steepest descent method, or Newton-Raphson or any other minimization technique. The steepest descent method, applied to $\phi(v)$, is called the *reduced steepest descent method*; the Newton-Raphson method, applied to $\phi(v)$, is called the *reduced Newton-Raphson method*. The gradient of $\phi(v)$, also called the *reduced gradient*, is

$$\nabla\phi(v) = Z^T \nabla f(x),$$

and the Hessian matrix of $\phi(v)$, also called the *reduced Hessian matrix*, is

$$\nabla^2\phi(v) = Z^T \nabla^2 f(x) Z,$$

where $x = \hat{x} + Zv$, so algorithms to minimize $\phi(v)$ can be written in terms of the gradient and Hessian of f itself.

An Example

Consider the problem of minimizing the function

$$f(x) = \frac{1}{2}x_1^2 - \frac{1}{2}x_3^2 + 4x_1x_2 + 3x_1x_3 - 2x_2x_3,$$

subject to

$$x_1 - x_2 - x_3 = -1.$$

Let $\hat{x} = [1, 1, 1]^T$. Then the matrix A is $A = [1, -1, -1]$ and the vector b is $b = [-1]$. Let the matrix Z be

$$Z = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{11.34}$$

The reduced gradient at $\hat{x}$ is then

$$Z^T \nabla f(\hat{x}) = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 8 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 10 \\ 8 \end{bmatrix}, \tag{11.35}$$

and the reduced Hessian matrix at $\hat{x}$ is

$$Z^T \nabla^2 f(\hat{x}) Z = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 4 & 3 \\ 4 & 0 & -2 \\ 3 & -2 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 9 & 6 \\ 6 & 6 \end{bmatrix}. \quad (11.36)$$

Then the reduced Newton-Raphson equation yields

$$v = \begin{bmatrix} -2/3 \\ -2/3 \end{bmatrix}, \quad (11.37)$$

and the reduced Newton-Raphson direction is

$$p = Zv = \begin{bmatrix} -4/3 \\ -2/3 \\ -2/3 \end{bmatrix}. \quad (11.38)$$

Since the function $\phi(v)$ is quadratic, one reduced Newton-Raphson step suffices to obtain the solution, $x_* = [-1/3, 1/3, 1/3]^T$.

11.10.2 A Primal-Dual Approach

In this approach we begin with the Lagrangian,

$$L(x, \lambda) = f(x) + \lambda^T (b - Ax).$$

Setting to zero the x-gradient of $L(x, \lambda)$, we have to solve the equations

$$\nabla f(x) - A^T \lambda = 0$$

and

$$Ax = b.$$

We define the function $G(x, \lambda)$ taking values in R^2 to be

$$G(x, \lambda) = (\nabla f(x) - A^T \lambda, Ax - b).$$

We then apply the NR method to find a zero of the function G. The Jacobian matrix for G is

$$J_G(x, \lambda) = \begin{bmatrix} \nabla^2 f(x) & -A^T \\ A & 0 \end{bmatrix},$$

so one step of the NR method is

$$(x^{k+1}, \lambda^{k+1})^T = (x^k, \lambda^k)^T - J_G(x^k, \lambda^k)^{-1} G(x^k, \lambda^k). \quad (11.39)$$

Therefore

$$A(x^{k+1} - x^k) = b - Ax^k.$$

Consequently, each successive step of the Newton-Raphson iteration produces a feasible x^k.

11.11 Simulated Annealing

In this chapter we have focused on the minimization of convex functions. For such functions, a local minimum is necessarily a global one. For non-convex functions, this is not the case. For example, the function $f(x) = x^4 - 8x^3 + 20x^2 - 16.5x + 7$ has a local minimum around $x = 0.6$ and a global minimum around $x = 3.5$. The descent methods we have discussed can get caught at a local minimum that is not global, since we insist on always taking a step that reduces $f(x)$. The *simulated annealing algorithm* [1, 126], also called the *Metropolis algorithm*, is sometimes able to avoid being trapped at a local minimum by permitting an occasional step that increases $f(x)$. The name comes from the analogy with the physical problem of lowering the energy of a solid by first raising the temperature, to bring the particles into a disorganized state, and then gradually reducing the temperature, so that a more organized state is achieved.

Suppose we have calculated x^k. We now generate a random direction and a small random step length. If the new vector $x^k + \Delta x$ makes $f(x)$ smaller, we accept the vector as x^{k+1}. If not, then we accept this vector, with probability

$$Prob(\text{accept}) = \exp\Big(\frac{f(x^k) - f(x^k + \Delta x)}{c_k}\Big),$$

where $c_k > 0$, known as the *temperature*, is chosen by the user. As the iteration proceeds, the temperature c_k is gradually reduced, making it easier to accept increases in $f(x)$ early in the process, but harder later. How to select the temperatures is an art, not a science.

11.12 Exercises

11.1 *Apply the Newton-Raphson method to obtain an iterative procedure for finding $\sqrt{a}$, for any positive a. For which x^0 does the method converge? There are two answers, of course; how does the choice of x^0 determine which square root becomes the limit?*

11.2 *Apply the Newton-Raphson method to obtain an iterative procedure for finding $a^{1/3}$, for any real a. For which x^0 does the method converge?*

11.3 *Extend the Newton-Raphson method to complex variables. Redo the previous exercises for the case of complex a. For the complex case, a has two square roots and three cube roots. How does the choice of x^0 affect the limit? Warning: The case of the cube root is not as simple as it may appear.*

11.4 (The Sherman-Morrison-Woodbury Identity) *Let A be an invertible matrix. Show that, if $\omega = 1 + v^T A^{-1} u \neq 0$, then $A + uv^T$ is invertible and*

$$(A + uv^T)^{-1} = A^{-1} - \frac{1}{\omega} A^{-1} u v^T A^{-1}. \tag{11.40}$$

11.5 *Use the reduced Newton-Raphson method to minimize the function $\frac{1}{2} x^T Q x$, subject to $Ax = b$, where*

$$Q = \begin{bmatrix} 0 & -13 & -6 & -3 \\ -13 & 23 & -9 & 3 \\ -6 & -9 & -12 & 1 \\ -3 & 3 & 1 & -1 \end{bmatrix},$$

$$A = \begin{bmatrix} 2 & 1 & 2 & 1 \\ 1 & 1 & 3 & -1 \end{bmatrix},$$

and

$$b = \begin{bmatrix} 3 \\ 2 \end{bmatrix}.$$

Start with

$$x^0 = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}.$$

11.6 *Use the reduced steepest descent method with an exact line search to solve the problem in the previous exercise.*

11.13 Course Homework

Do Exercises 11.1, 11.2, 11.4, 11.5, and 11.6.

Chapter 12

Quadratic Programming

12.1 Chapter Summary

The *quadratic-programming* problem (QP) is to minimize a quadratic function, subject to inequality constraints and, often, the nonnegativity of the variables. Using the Karush-Kuhn-Tucker Theorem 10.6 for mixed constraints and introducing slack variables, this problem can be reformulated as a linear programming problem and solved by Wolfe's Algorithm [136], a variant of the simplex method. In the case of general constrained optimization, the Newton-Raphson method for finding a stationary point of the Lagrangian can be viewed as solving a sequence of quadratic programming problems. This leads to *sequential quadratic programming* [129].

12.2 The Quadratic-Programming Problem

The primal QP problem is to minimize the quadratic function

$$f(x) = a + x^T c + \frac{1}{2} x^T Q x, \tag{12.1}$$

subject to the constraints

$$Ax \leq b, \tag{12.2}$$

and $x_j \geq 0$, for $j = 1, ..., J$. Here a, b, and c are given, Q is a given J by J positive-definite matrix with entries Q_{ij}, and A is an I by J matrix with rank I and entries A_{ij}. To allow for some equality constraints, we say that

$$(Ax)_i \leq b_i, \tag{12.3}$$

for $i = 1, ..., K$, and

$$(Ax)_i = b_i, \tag{12.4}$$

for $i = K+1, ..., I$.

We incorporate the nonnegativity constraints $x_j \geq 0$ by requiring

$$-x_j \leq 0, \tag{12.5}$$

for $j = 1, ..., J$. Applying the KKT Theorem 10.6 to this problem, we find that if a regular point x^* is a solution, then there are vectors μ^* and ν^* such that

- **1)** $\mu_i^* \geq 0$, for $i = 1, ..., K$;
- **2)** $\nu_j^* \geq 0$, for $j = 1, ..., J$;
- **3)** $c + Qx^* + A^T\mu^* - v^* = 0$;
- **4)** $\mu_i^*((Ax^*)_i - b_i) = 0$, for $i = 1, ..., I$;
- **5)** $x_j^*\nu_j^* = 0$, for $j = 1, ..., J$.

One way to solve this problem is to reformulate it as a linear-programming problem. To that end, we introduce slack variables x_{J+i}, $i = 1, ..., K$, and write the problem as

$$\sum_{j=1}^{J} A_{ij}x_j + x_{J+i} = b_i, \tag{12.6}$$

for $i = 1, ..., K$,

$$\sum_{j=1}^{J} A_{ij}x_j = b_i, \tag{12.7}$$

for $i = K+1, ..., I$,

$$\sum_{j=1}^{J} Q_{mj}x_j + \sum_{i=1}^{I} A_{im}\mu_i - \nu_m = -c_m, \tag{12.8}$$

for $m = 1, ..., J$,

$$\mu_i x_{J+i} = 0, \tag{12.9}$$

for $i = 1, ..., K$, and

$$x_j\nu_j = 0, \tag{12.10}$$

for $j = 1, ..., J$. The objective now is to formulate the problem as a primal linear-programming problem in standard form.

The variables x_j and ν_j, for $j = 1, ..., J$, and μ_i and x_{J+i}, for $i = 1, ..., K$, must be nonnegative; the variables μ_i are unrestricted, for $i = K+1, ..., I$, so for these variables we write

$$\mu_i = \mu_i^+ - \mu_i^-, \tag{12.11}$$

and require that both μ_i^+ and μ_i^- be nonnegative. Finally, we need a linear functional to minimize.

We rewrite Equation (12.6) as

$$\sum_{j=1}^{J} A_{ij}x_j + x_{J+i} + y_i = b_i, \tag{12.12}$$

for $i = 1, ..., K$, Equation (12.7) as

$$\sum_{j=1}^{J} A_{ij}x_j + y_i = b_i, \tag{12.13}$$

for $i = K+1, ..., I$, and Equation (12.8) as

$$\sum_{j=1}^{J} Q_{mj}x_j + \sum_{i=1}^{I} A_{im}\mu_i - \nu_m + y_{I+m} = -c_m, \tag{12.14}$$

for $m = 1, ..., J$. In order for all the equations to hold, each of the y_i must be zero. The linear programming problem is therefore to minimize the linear functional

$$y_1 + ... + y_{I+J}, \tag{12.15}$$

over nonnegative y_i, subject to the equality constraints in the equations (12.12), (12.13), and (12.14). Any solution to the original problem must be a basic feasible solution to this primal linear-programming problem. Wolfe's Algorithm [136] is a modification of the simplex method that guarantees the complementary slackness conditions; that is, we never have μ_i and x_{J+i} positive basic variables at the same time, nor x_j and ν_j.

12.3 An Example

The following example is taken from [136]. Minimize the function

$$f(x_1, x_2) = x_1^2 - x_1x_2 + 2x_2^2 - x_1 - x_2,$$

subject to the constraints

$$x_1 - x_2 \geq 3,$$

and

$$x_1 + x_2 = 4.$$

We introduce the slack variable x_3 and then minimize

$$y_1 + y_2 + y_3 + y_4,$$

subject to $y_i \geq 0$, for $i = 1, ..., 4$, and the equality constraints

$$x_1 - x_2 - x_3 + y_1 = 3,$$

$$x_1 + x_2 + y_2 = 4,$$

$$2x_1 - x_2 - \mu_1 + \mu_2^+ - \mu_2^- - \nu_1 + y_3 = 1,$$

and

$$-x_1 + 4x_2 + \mu_1 + \mu_2^+ - \mu_2^- - \nu_2 + y_4 = 1.$$

This problem is then solved using the simplex algorithm, modified according to Wolfe's Algorithm.

12.4 Quadratic Programming with Equality Constraints

We turn now to the particular case of QP in which all the constraints are equations. The problem is, therefore, to minimize

$$f(x) = a + x^T c + \frac{1}{2} x^T Q x, \tag{12.16}$$

subject to the constraints

$$Ax = b. \tag{12.17}$$

The KKT Theorem then tells us that there is λ^* so that $\nabla L(x^*, \lambda^*) = 0$ for the solution vector x^*. Therefore, we have

$$Qx^* + A^T \lambda^* = -c,$$

and

$$Ax^* = b.$$

Such quadratic programming problems arise in sequential quadratic programming.

12.5 Sequential Quadratic Programming

Consider once again the CP problem of minimizing the convex function $f(x)$, subject to $g_i(x) = 0$, for $i = 1, ..., I$. The Lagrangian is

$$L(x, \lambda) = f(x) + \sum_{i=1}^{I} \lambda_i g_i(x). \tag{12.18}$$

We assume that a sensitivity vector λ^* exists, so that x^* solves our problem if and only if (x^*, λ^*) satisfies

$$\nabla L(x^*, \lambda^*) = 0. \tag{12.19}$$

The problem can then be formulated as finding a zero of the function

$$G(x, \lambda) = \nabla L(x, \lambda),$$

and the Newton-Raphson iterative algorithm can be applied.

One step of the Newton-Raphson algorithm has the form

$$\begin{pmatrix} x^{k+1} \\ \lambda^{k+1} \end{pmatrix} = \begin{pmatrix} x^k \\ \lambda^k \end{pmatrix} + \begin{pmatrix} p^k \\ v^k \end{pmatrix}, \tag{12.20}$$

where

$$\begin{bmatrix} \nabla^2_{xx} L(x^k, \lambda^k) & \nabla g(x^k) \\ \nabla g(x^k)^T & 0 \end{bmatrix} \begin{pmatrix} p^k \\ v^k \end{pmatrix} = \begin{pmatrix} -\nabla_x L(x^k, \lambda^k) \\ -g(x^k) \end{pmatrix}. \tag{12.21}$$

The incremental vector $\begin{pmatrix} p^k \\ v^k \end{pmatrix}$ obtained by solving this system is also the solution to the quadratic-programming problem of minimizing the function

$$\frac{1}{2} p^T \nabla^2_{xx} L(x^k, \lambda^k) p + p^T \nabla_x L(x^k, \lambda^k), \tag{12.22}$$

subject to the constraint

$$\nabla g(x^k)^T p + g(x^k) = 0. \tag{12.23}$$

Therefore, the Newton-Raphson algorithm for the original minimization problem can be implemented as a sequence of quadratic programs, each solved by the methods discussed previously. In practice, variants of this approach that employ approximations for the first and second partial derivatives are often used.

Chapter 13

Solving Systems of Linear Equations

13.1 Chapter Summary

Optimization plays an important role in solving systems of linear equations. In many applications the linear system is under-determined, meaning that there are multiple, indeed, infinitely many, solutions to the system. It is natural, then, to seek a solution that is optimal, in some sense. When the system involves measured data, as is often the case, there may be no exact solution, or an exact solution to the system may be too noisy. Then, an approximate solution, or a solution to a related, *regularized*, system is sought. In this chapter, we discuss briefly both of these situations, focusing on iterative algorithms that have been designed for such problems. For a more in-depth analysis of these problems, see [50].

13.2 Arbitrary Systems of Linear Equations

We begin by considering systems of the form $Ax = b$, where A is an M by N matrix, b an M by 1 vector, both with real or complex entries, and x is the real or complex N by 1 solution vector being sought. If the system has solutions, if there are no additional constraints being imposed on x, and if M and N are not too large, standard non-iterative methods, such as Gauss elimination, can be used to find a solution. When one or more of these conditions is not met, iterative methods are usually needed.

13.2.1 Landweber's Method

Landweber's iterative method [115] has the following iterative step: for $k = 0, 1, ...$ let

$$x^{k+1} = x^k + \gamma A^\dagger (b - Ax^k), \tag{13.1}$$

where $A^\dagger$ denotes the conjugate transpose of the matrix A. If the parameter γ is chosen to lie within the interval $(0, 2/L)$, where L is the largest eigenvalue of the matrix $A^\dagger A$, then the sequence $\{x^k\}$ converges to the solution of $Ax = b$ for which $\|x - x^0\|$ is minimized, provided that solutions exist. If not, the sequence $\{x^k\}$ converges to a *least-squares* solution: the limit is the minimizer of the function $\|b - Ax\|$ for which $\|x - x^0\|$ is minimized.

A least-squares solution of $Ax = b$ is an exact solution of the system

$$A^\dagger Ax = A^\dagger b.$$

One advantage to using Landweber's algorithm is that we do not have to use the matrix $A^\dagger A$, which can be time-consuming to calculate when M and N are large. As discussed in [50], reasonable estimates of L can also be obtained without knowing $A^\dagger A$.

13.2.2 The Projected Landweber Method

Suppose that C is a non-empty, closed and convex subset of R^N, and we want to find an exact or approximate solution of $Ax = b$ within C. The *projected Landweber algorithm* has the following iterative step:

$$x^{k+1} = P_C\Big(x^k + \gamma A^\dagger (b - Ax^k)\Big), \tag{13.2}$$

where $P_C x$ denotes the orthogonal projection of x onto C. If the parameter γ is chosen to lie within the interval $(0, 2/L)$, the sequence $\{x^k\}$ converges to an x in C that solves $Ax = b$, provided that solutions exist in C. If not, the sequence $\{x^k\}$ converges to a minimizer, over x in C, of the function $\|b - Ax\|$, if such a minimizer exists.

13.2.3 The Split-Feasibility Problem

Suppose now that C and Q are non-empty, closed and convex subsets of R^N and R^M, respectively, and we want x in C for which Ax is in Q; this is the *split-feasibility problem* (SFP) [57]. The CQ algorithm [42, 43] has the following iterative step:

$$x^{k+1} = P_C\Big(x^k - \gamma A^\dagger (I - P_Q) Ax^k\Big). \tag{13.3}$$

For γ in the interval $(0, 2/L)$, the CQ algorithm converges to a solution of the SFP, when solutions exist. If not, it converges to a minimizer, over x in C, of the function $\|P_Q Ax - Ax\|$, provided such minimizers exist. Both the Landweber and projected Landweber methods are special cases of the CQ algorithm.

Extensions of the CQ algorithm have been applied recently to problems in intensity-modulated radiation therapy [55, 59].

13.2.4 The Algebraic Reconstruction Technique

The algorithms presented previously in this chapter are *simultaneous* methods, meaning that all the equations of the system are used at each step of the iteration. Such methods tend to converge slowly, which presents a major problem for large systems. The *algebraic reconstruction technique* (ART) is a *row-action* method, meaning that only a single equation is used at each step of the iteration. The ART has the following iterative step: for $k = 0, 1, ...$ and $m = k(\mathrm{mod}\, M) + 1$, let

$$x_n^{k+1} = x_n^k + \overline{A_{mn}}(b_m - (Ax^k)_m)/\sum_{j=1}^{N} |A_{mj}|^2. \tag{13.4}$$

We can describe the ART geometrically as follows: once we have x^k and m, the vector x^{k+1} is the orthogonal projection of x^k onto the hyperplane H_m given by

$$H_m = \{x|(Ax)_m = b_m\}.$$

The Landweber algorithm can be similarly described: the vector x^{k+1} is a weighted sum of the orthogonal projections of x^k onto each of the hyperplanes H_m, for all m.

In the consistent case, when the system $Ax = b$ has solutions, the ART converges to the solution for which $\|x - x^0\|$ is minimized. Unlike the simultaneous methods, when no solution exists, the ART sequence $\{x^k\}$ does not converge to a single vector, but subsequences do converge to members of a *limit cycle* consisting of (typically) M distinct vectors. Generally speaking, the ART will converge, in the consistent case, faster than the Landweber method, especially if the equations are selected in a random order [103].

13.2.5 Double ART

Because the ART is significantly faster to converge than the Landweber method in the consistent case, we would like to be able to use the ART in the inconsistent case, as well, to get a least-squares solution. To avoid the limit-cycle behavior of ART in this case, we can use *double ART* (DART).

We know from basic linear algebra that the vector b can be written as

$$b = A\hat{x} + \hat{w},$$

where $\hat{x}$ minimizes the function $\|b - Ax\|$ and $w = \hat{w}$ minimizes the function $\|b - w\|$, subject to $A^\dagger w = 0$. Said another way, $A\hat{x}$ is the orthogonal projection of b onto the range of A and $\hat{w}$ is the orthogonal projection of b onto the null space of $A^\dagger$.

In DART we apply the ART algorithm twice, first to the consistent linear system $A^\dagger w = 0$, with $w^0 = b$, so that the limit is $\hat{w}$, and then to the consistent system $Ax = b - \hat{w}$. The result is the minimizer of $\|b - Ax\|$ for which $\|x - x^0\|$ is minimized.

13.3 Regularization

In many applications in which systems of linear equations must be solved, the entries of the vector b are measured data and $Ax = b$ is a model that attempts to describe, in a somewhat simplified way, how b depends on the unknown vector x. The statistical noise in the measured data introduces one type of error, while the approximate nature of the model itself introduces another. Because the model is simplified, but the data b is noisy, an exact solution x itself usually ends up noisy. Also, it is common for the system to be *ill-conditioned*, that is, for small changes in b to lead to large changes in the exact solution x. This happens when the ratio of the largest to smallest eigenvalues of the matrix $A^\dagger A$ is large. In such cases even a minimum-norm solution of $Ax = b$ can have a large norm. Consequently, we often do not want an exact solution of $Ax = b$, even when such solutions exist. Instead, we *regularize* the problem.

13.3.1 Norm-Constrained Least-Squares

One way to regularize the problem is to minimize not $\|b - Ax\|_2$, but, say,

$$f(x) = \|b - Ax\|_2^2 + \epsilon^2 \|x\|_2^2, \tag{13.5}$$

for some small $\epsilon > 0$. Now we are still trying to make $\|b - Ax\|_2$ small, but managing to keep $\|x\|_2$ from becoming too large in the process. This leads to a *norm-constrained least-squares* solution.

The minimizer of $f(x)$ is the unique solution $\hat{x}_\epsilon$ of the system

$$(A^\dagger A + \epsilon^2 I)x = A^\dagger b. \tag{13.6}$$

When M and N are large, we need ways to solve this system without having to deal with the matrix $A^\dagger A + \epsilon^2 I$. The Landweber method allowed us to avoid $A^\dagger A$ in calculating the least-squares solution. Is there a similar method to use now? Yes, there is.

13.3.2 Regularizing Landweber's Algorithm

Our goal is to minimize the function $f(x)$ in Equation (13.5). Notice that this is equivalent to minimizing the function

$$F(x) = ||Bx - c||_2^2, \tag{13.7}$$

for

$$B = \begin{bmatrix} A \\ \epsilon I \end{bmatrix}, \tag{13.8}$$

and

$$c = \begin{bmatrix} b \\ 0 \end{bmatrix}, \tag{13.9}$$

where 0 denotes a column vector with all entries equal to zero. The Landweber iteration for the problem $Bx = c$ is

$$x^{k+1} = x^k + \alpha B^\dagger (c - Bx^k), \tag{13.10}$$

for $0 < \alpha < 2/\rho(B^\dagger B)$, where $\rho(B^\dagger B)$ is the largest eigenvalue, or the spectral radius, of $B^\dagger B$. Equation (13.10) can be written as

$$x^{k+1} = (1 - \alpha\epsilon^2)x^k + \alpha A^\dagger (b - Ax^k). \tag{13.11}$$

We see from Equation (13.11) that the Landweber algorithm for solving the regularized least-squares problem amounts to a relaxed version of the Landweber algorithm applied to the original least squares problem.

13.3.3 Regularizing the ART

We would like to get the regularized solution $\hat{x}_\epsilon$ by taking advantage of the faster convergence of the ART. Fortunately, there are ways to find $\hat{x}_\epsilon$, using only the matrix A and the ART algorithm. We discuss two methods for using ART to obtain regularized solutions of $Ax = b$. The first one is presented in [45], while the second one is due to Eggermont, Herman, and Lent [84].

In our first method we use ART to solve the system of equations given in matrix form by

$$[\, A^\dagger \quad \epsilon I \,] \begin{bmatrix} u \\ v \end{bmatrix} = 0. \tag{13.12}$$

We begin with $u^0 = b$ and $v^0 = 0$. Then, the lower component of the limit vector is $v^\infty = -\epsilon\hat{x}_\epsilon$.

The method of Eggermont *et al.* is similar. In their method we use ART to solve the system of equations given in matrix form by

$$[\, A \quad \epsilon I \,] \begin{bmatrix} x \\ v \end{bmatrix} = b. \tag{13.13}$$

We begin at $x^0 = 0$ and $v^0 = 0$. Then, the limit vector has for its upper component $x^\infty = \hat{x}_\epsilon$, and $\epsilon v^\infty = b - A\hat{x}_\epsilon$.

13.4 Non-Negative Systems of Linear Equations

We turn now to non-negative systems of linear equations, which we shall denote by $y = Px$, with the understanding that P is an I by J matrix with non-negative entries P_{ij}, such that, for each j, the column sum

$$s_j = \sum_{i=1}^{I} P_{ij}$$

is positive, y is an I by 1 vector with positive entries y_i, and we seek a solution x with non-negative entries x_j. We say that the system is *consistent* whenever such non-negative solutions exist. Denote by $\mathcal{X}$ the set of all non-negative x for which the vector Px has only positive entries. In what follows, all vectors x will lie in $\mathcal{X}$ and the initial vector x^0 will always be positive.

13.4.1 The Multiplicative ART

Both the algebraic reconstruction technique (ART) and the *multiplicative algebraic reconstruction technique* (MART) were introduced by Gordon, Bender and Herman [98] as two iterative methods for discrete image reconstruction in transmission tomography. It was noticed somewhat later that the ART is a special case of Kaczmarz's algorithm [108].

Both methods are what are called *row-action* methods, meaning that each step of the iteration uses only a single equation from the system. The MART is limited to non-negative systems for which non-negative solutions are sought. In the under-determined case, both algorithms find the solution closest to the starting vector, in the two-norm or weighted two-norm sense for ART, and in the cross-entropy sense for MART, so both algorithms can be viewed as solving optimization problems. We consider two different versions of the MART.

MART I

The iterative step of the first version of MART, which we call MART I, is the following: for $k = 0, 1, ...$, and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \Big(\frac{y_i}{(Px^k)_i} \Big)^{P_{ij}/m_i},$$

for $j = 1, ..., J$, where the parameter m_i is defined to be

$$m_i = \max\{P_{ij} | j = 1, ..., J\}.$$

The MART I algorithm converges, in the consistent case, to the non-negative solution for which the KL distance $KL(x, x^0)$ is minimized.

MART II

The iterative step of the second version of MART, which we shall call MART II, is the following: for $k = 0, 1, ...$, and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \Big(\frac{y_i}{(Px^k)_i} \Big)^{P_{ij}/s_j n_i},$$

for $j = 1, ..., J$, where the parameter n_i is defined to be

$$n_i = \max\{P_{ij} s_j^{-1} | j = 1, ..., J\}.$$

The MART II algorithm converges, in the consistent case, to the non-negative solution for which the KL distance

$$\sum_{j=1}^{J} s_j KL(x_j, x_j^0)$$

is minimized. Just as the Landweber method is a simultaneous cousin of the row-action ART, there is a simultaneous cousin of the MART, called, not surprisingly, the *simultaneous MART* (SMART).

13.4.2 The Simultaneous MART

The SMART minimizes the cross-entropy, or Kullback-Leibler distance, $f(x) = KL(Px, y)$, over nonnegative vectors x [72, 64, 142, 31].

Having found the vector x^k, the next vector in the SMART sequence is x^{k+1}, with entries given by

$$x_j^{k+1} = x_j^k \exp\Big(s_j^{-1} \sum_{i=1}^{I} P_{ij} \log\Big(\frac{y_i}{(Px^k)_i} \Big) \Big). \tag{13.14}$$

As with MART II, when there are non-negative solutions of $y = Px$, the SMART converges to the solution for which the KL distance

$$\sum_{j=1}^{J} s_j KL(x_j, x_j^0)$$

is minimized.

13.4.3 The EMML Iteration

The *expectation maximization maximum likelihood* algorithm (EMML) minimizes the function $f(x) = KL(y, Px)$, over nonnegative vectors x [143, 116, 155, 117, 31]. Having found the vector x^k, the next vector in the EMML sequence is x^{k+1}, with entries given by

$$x_j^{k+1} = x_j^k s_j^{-1} \Big(\sum_{i=1}^{I} P_{ij} \Big(\frac{y_i}{(Px^k)_i} \Big) \Big). \tag{13.15}$$

The iterative step of the EMML is closely related to that of the SMART, except that the exponentiation and logarithm are missing. When there are non-negative solutions of the system $y = Px$, the EMML converges to a non-negative solution, but no further information about this solution is known. Both the SMART and the EMML are slow to converge, particularly when the system is large.

13.4.4 Alternating Minimization

In [31] the SMART and the EMML were derived using the following *alternating minimization* approach.

For each $x \in \mathcal{X}$, let $r(x)$ and $q(x)$ be the I by J arrays with entries

$$r(x)_{ij} = x_j P_{ij} y_i / (Px)_i, \tag{13.16}$$

and

$$q(x)_{ij} = x_j P_{ij}. \tag{13.17}$$

In the iterative step of the SMART we get x^{k+1} by minimizing the function

$$KL(q(x), r(x^k)) = \sum_{i=1}^{I} \sum_{j=1}^{J} KL(q(x)_{ij}, r(x^k)_{ij})$$

over $x \geq 0$. Note that $KL(Px, y) = KL(q(x), r(x))$. Similarly, the iterative step of the EMML is to minimize the function $KL(r(x^k), q(x))$ to get $x = x^{k+1}$. Note that $KL(y, Px) = KL(r(x), q(x))$.

13.4.5 The Row-Action Variant of EMML

When there are non-negative solutions of $y = Px$, the MART converges faster than the SMART, and to the same solution. The SMART involves exponentiation and a logarithm, and the MART a non-integral power, both of which complicate their calculation. The EMML is considerably simpler in this respect, but, like SMART, converges slowly. We would like to have a row-action variant of the EMML that converges faster than the EMML in the consistent case, but is easier to calculate than the MART. The EM-MART is such an algorithm. As with the MART, we distinguish two versions, EM-MART I and EM-MART II. When the system $y = Px$ has non-negative solutions, both EM-MART I and EM-MART II converge to non-negative solutions, but nothing further is known about these solutions. To motivate these algorithms, we rewrite the MART algorithms as follows:

MART I

The iterative step of MART I can be written as follows: for $k = 0, 1, ...$, and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \exp\Big(\Big(\frac{P_{ij}}{m_i}\Big)\log\Big(\frac{y_i}{(Px^k)_i}\Big)\Big),$$

or, equivalently, as

$$\log x_j^{k+1} = \Big(1 - \frac{P_{ij}}{m_i}\Big)\log x_j^k + \Big(\frac{P_{ij}}{m_i}\Big)\log\Big(x_j^k \frac{y_i}{(Px^k)_i}\Big). \tag{13.18}$$

MART II

Similarly, the iterative step of MART II can be written as follows: for $k = 0, 1, ...$, and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = x_j^k \exp\Big(\Big(\frac{P_{ij}}{s_j n_i}\Big)\log\Big(\frac{y_i}{(Px^k)_i}\Big)\Big),$$

or, equivalently, as

$$\log x_j^{k+1} = \Big(1 - \frac{P_{ij}}{s_j n_i}\Big)\log x_j^k + \Big(\frac{P_{ij}}{s_j n_i}\Big)\log\Big(x_j^k \frac{y_i}{(Px^k)_i}\Big). \tag{13.19}$$

We obtain the EM-MART I and EM-MART II simply by removing the logarithms in Equations (13.18) and (13.19), respectively.

EM-MART I

The iterative step of EM-MART I is as follows: for $k = 0, 1, ...$, and $i = k(\mathrm{mod}\, I) + 1$, let

$$x_j^{k+1} = \Big(1 - \frac{P_{ij}}{m_i}\Big)x_j^k + \Big(\frac{P_{ij}}{m_i}\Big)\Big(x_j^k \frac{y_i}{(Px^k)_i}\Big). \tag{13.20}$$

EM-MART II

The iterative step of EM-MART II is as follows:

$$x_j^{k+1} = \Big(1 - \frac{P_{ij}}{s_j n_i}\Big)x_j^k + \Big(\frac{P_{ij}}{s_j n_i}\Big)\Big(x_j^k \frac{y_i}{(Px^k)_i}\Big). \tag{13.21}$$

13.5 Regularized SMART and EMML

As with the Landweber algorithm, there are situations that arise in practice in which, because of noisy measurements, the exact or approximate solutions of $y = Px$ provided by the SMART and EMML algorithms are not suitable. In such cases, we need to regularize the SMART and the EMML, which is usually done by including a penalty function.

13.5.1 Regularized SMART

As we have seen, the iterative step of the SMART is obtained by minimizing the function $KL(q(x), r(x^k))$ over non-negative x, and the limit of the SMART minimizes $KL(Px, y)$. We can regularize by minimizing

$$KL(Px, y) + KL(x, p),$$

where the vector p with positive entries p_j is a prior estimate of the solution. To obtain x^{k+1} from x^k, we minimize

$$KL(q(x), r(x^k)) + \sum_{j=1}^{J} \delta_j KL(x_j, p_j).$$

There are many penalty functions we could use here, but the one we have chosen permits the minimizing x^{k+1} to be obtained in closed form.

The iterative step of the regularized SMART is as follows:

$$\log x_j^{k+1} = \frac{\delta_j}{\delta_j + s_j} \log p_j + \frac{1}{\delta_j + s_j} x_j^k \sum_{i=1}^{I} P_{ij} \log\Big(\frac{y_i}{(Px^k)_i}\Big). \tag{13.22}$$

13.5.2 Regularized EMML

As we have seen, the iterative step of the EMML is obtained by minimizing the function $KL(r(x^k), q(x))$ over non-negative x, and the limit of the EMML minimizes $KL(y, Px)$. We can regularize by minimizing

$$KL(y, Px) + KL(p, x).$$

To obtain x^{k+1} from x^k, we minimize

$$KL(r(x^k), q(x)) + \sum_{j=1}^{J} \delta_j KL(p_j, x_j).$$

Again, there are many penalty functions we could use here, but the one we have chosen permits the minimizing x^{k+1} to be obtained in closed form.

The iterative step of the regularized EMML is as follows:

$$x_j^{k+1} = \frac{\delta_j}{\delta_j + s_j} p_j + \frac{1}{\delta_j + s_j} x_j^k \sum_{i=1}^{I} P_{ij} \Big(\frac{y_i}{(Px^k)_i} \Big). \tag{13.23}$$

13.6 Block-Iterative Methods

The algorithms we have considered in this chapter are either simultaneous algorithms or row-action ones. There are also *block-iterative* variants of MART and ART, in which some, but not all, equations of the system are used at each step. The subsets of equations used at a single step are called *blocks*. Generally speaking, the smaller the blocks, the faster the convergence, in the consistent case. On the other hand, it may be inconvenient, given the architecture of the computer, to deal with only a single equation at each step. By using blocks, we can achieve a compromise between speed of convergence and compatibility with the architecture of the computer. These block-iterative methods are discussed in detail in [50].

13.7 Exercises

13.1 *Show that the two algorithms associated with Equations (13.12) and (13.13), respectively, do actually perform as claimed.*

Chapter 14

Sequential Unconstrained Minimization Algorithms

14.1 Chapter Summary

In this chapter we consider an approach to optimization in which the original problem is replaced by a series of simpler problems. This approach can be particularly effective for constrained optimization. Suppose, for example, that we want to minimize $f(x)$, subject to the constraint that x lie within a set C. At the kth step of the iteration we minimize the function $G_k(x) = f(x) + g_k(x)$, with no additional restrictions on x, to get the vector x^k, where the functions $g_k(x)$ are related to the set C in some way. In practice, minimizing $G_k(x)$ may require iteration, but we will not deal with that issue here. In the best case, the sequence $\{x^k\}$ will converge to the solution to the original problem.

14.2 Introduction

In many inverse problems, we have measured data pertaining to the object x, which may be, for example, a vectorized image, as well as prior information about x, such as that its entries are nonnegative. Tomographic imaging is a good example. We want to find an estimate of x that is (more or less) consistent with the data, as well as conforming to the prior constraints. The measured data and prior information are usually not sufficient to determine a unique x and some form of optimization is performed. For example, we may seek the image x for which the entropy is maximized, or a minimum-norm least-squares solution.

There are many well-known methods for minimizing a function $f : R^J \rightarrow R$; we can use the Newton-Raphson algorithm or any of its sev-

eral approximations, or nonlinear conjugate-gradient algorithms, such as the Fletcher-Reeves, Polak-Ribiere, or Hestenes-Stiefel methods. When the problem is to minimize the function $f(x)$, subject to constraints on the variable x, the problem becomes much more difficult. For such constrained minimization, we can employ *sequential unconstrained minimization algorithms* [89].

We assume that $f : R^J \to (-\infty, +\infty]$ is a continuous function. Our objective is to minimize $f(x)$ over x in some given closed nonempty set C. At the kth step of a sequential unconstrained minimization algorithm we minimize a function $G_k(x)$ to get the vector x^k. We shall assume throughout that a global minimizer x^k exists for each k. The existence of these minimizers can be established, once additional conditions, such as convexity, are placed on the functions $G_k(x)$; see, for example, Fiacco and McCormick [89], p.95. We shall consider briefly the issue of computing the x^k.

In the best case, the sequence $\{x^k\}$ converges to a constrained minimizer of the original objective function $f(x)$. Obviously, the functions $G_k(x)$ must involve both the function $f(x)$ and the set C. Those methods for which each x^k is *feasible*, that is, each x^k is in C, are called *interior-point* methods, while those for which only the limit of the sequence is in C are called *exterior-point* methods. Barrier-function algorithms are typically interior-point methods, while penalty-function algorithms are exterior-point methods. The purpose of this chapter is to present a fairly broad class of sequential unconstrained minimization algorithms, which we call SUMMA [47]. The SUMMA include both barrier- and penalty-function algorithms, as well as proximity-function methods of Teboulle [151] and Censor and Zenios [65, 66], and the simultaneous multiplicative algebraic reconstruction technique (SMART)[31, 44, 45, 46].

14.3 SUMMA

The sequential unconstrained minimization algorithms (SUMMA) we present here use functions of the form

$$G_k(x) = f(x) + g_k(x), \tag{14.1}$$

with the auxiliary functions $g_k(x)$ chosen so that

$$0 \leq g_{k+1}(x) \leq G_k(x) - G_k(x^k), \tag{14.2}$$

for $k = 1, 2, ...$ We assume throughout that there exists $\hat{x}$ minimizing the function $f(x)$ over x in C. Our main results are that the sequence $\{f(x^k)\}$ is monotonically decreasing to $f(\hat{x})$, and, subject to certain conditions on the function $f(x)$, the sequence $\{x^k\}$ converges to a feasible x^* with $f(x^*) = f(\hat{x})$.

We begin with a brief review of several types of sequential unconstrained minimization methods, including those mentioned previously. Then we state and prove the convergence results for the SUMMA. Finally, we show that each of these methods reviewed previously is a particular case of the SUMMA.

14.4 Barrier-Function Methods (I)

Let $b(x) : R^J \rightarrow (-\infty, +\infty]$ be continuous, with effective domain the set

$$D = \{x | \, b(x) < +\infty\}.$$

The goal is to minimize the objective function $f(x)$, over x in the closed set $C = \overline{D}$, the closure of D. In the barrier-function method, we minimize

$$f(x) + \frac{1}{k} b(x) \tag{14.3}$$

over x in D to get x^k. Each x^k lies within D, so the method is an interior-point algorithm. If the sequence $\{x^k\}$ converges, the limit vector x^* will be in C and $f(x^*) = f(\hat{x})$.

Barrier functions typically have the property that $b(x) \rightarrow +\infty$ as x approaches the boundary of D, so not only is x^k prevented from leaving D, it is discouraged from approaching the boundary.

14.4.1 Examples of Barrier Functions

Consider the convex programming (CP) problem of minimizing the convex function $f : R^J \rightarrow R$, subject to $g_i(x) \leq 0$, where each $g_i : R^J \rightarrow R$ is convex, for $i = 1, ..., I$. Let $D = \{x | g_i(x) < 0, i = 1, ..., I\}$; then D is open. We consider two barrier functions appropriate for this problem.

The Logarithmic Barrier Function

A suitable barrier function is the *logarithmic barrier function*

$$b(x) = \Big(- \sum_{i=1}^{I} \log(-g_i(x)) \Big). \tag{14.4}$$

The function $-\log(-g_i(x))$ is defined only for those x in D, and is positive for $g_i(x) > -1$. If $g_i(x)$ is near zero, then so is $-g_i(x)$ and $b(x)$ will be large.

The Inverse Barrier Function

Another suitable barrier function is the *inverse barrier function*

$$b(x) = \sum_{i=1}^{I} \frac{-1}{g_i(x)}, \tag{14.5}$$

defined for those x in D.

In both examples, when k is small, the minimization pays more attention to $b(x)$, and less to $f(x)$, forcing the $g_i(x)$ to be large negative numbers. But, as k grows larger, more attention is paid to minimizing $f(x)$ and the $g_i(x)$ are allowed to be smaller negative numbers. By letting $k \to \infty$, we obtain an iterative method for solving the constrained minimization problem.

An Illustration

We minimize the function $f(u, v) = u^2 + v^2$, subject to the constraint that $u + v \geq 1$. The constraint is then written $g(u, v) = 1 - (u + v) \leq 0$. We use the logarithmic barrier. The vector $x^k = (u_k, v_k)$ minimizing the function

$$G_k(x) = u^2 + v^2 - \frac{1}{k} \log(u + v - 1)$$

has entries

$$u_k = v_k = \frac{1}{4} + \frac{1}{4}\sqrt{1 + \frac{4}{k}}.$$

Notice that $u_k + v_k > 1$, so each x^k satisfies the constraint. As $k \to +\infty$, x^k converges to $(\frac{1}{2}, \frac{1}{2})$, which is the solution to the original problem.

14.5 Penalty-Function Methods (I)

Instead of minimizing a function $f(x)$ over x in R^J, we sometimes want to minimize a *penalized* version, $f(x) + p(x)$. As with barrier-function methods, the new function $f(x) + p(x)$ may be the function we really want to minimize, and we still need to find a method for doing this. In other cases, it is $f(x)$ that we wish to minimize, and the inclusion of the term $p(x)$ occurs only in the iterative steps of the algorithm. As we shall see, under conditions to be specified later, the penalty-function method can be used to minimize a continuous function $f(x)$ over the nonempty set of minimizers of another continuous function $p(x)$.

14.5.1 Imposing Constraints

When we add a barrier function to $f(x)$ we restrict the domain. When the barrier function is used in a sequential unconstrained minimization algorithm, the vector x^k that minimizes the function $f(x) + \frac{1}{k}b(x)$ lies in the effective domain D of $b(x)$, and we prove that, under certain conditions, the sequence $\{x^k\}$ converges to a minimizer of the function $f(x)$ over the closure of D. The constraint of lying within the set $\overline{D}$ is satisfied at every step of the algorithm; for that reason such algorithms are called interior-point methods. Constraints may also be imposed using a penalty function. In this case, violations of the constraints are discouraged, but not forbidden. When a penalty function is used in a sequential unconstrained minimization algorithm, the x^k need not satisfy the constraints; only the limit vector need be feasible.

14.5.2 Examples of Penalty Functions

Consider the CP problem. We wish to minimize the convex function $f(x)$ over all x for which the convex functions $g_i(x) \leq 0$, for $i = 1, ..., I$.

The Absolute-Value Penalty Function

We let $g_i^+(x) = \max\{g_i(x), 0\}$, and

$$p(x) = \sum_{i=1}^{I} g_i^+(x). \tag{14.6}$$

This is the *Absolute-Value* penalty function; it penalizes violations of the constraints $g_i(x) \leq 0$, but does not forbid such violations. Then, for $k = 1, 2, ...$, we minimize

$$f(x) + kp(x), \tag{14.7}$$

to get x^k. As $k \to +\infty$, the penalty function becomes more heavily weighted, so that, in the limit, the constraints $g_i(x) \leq 0$ should hold. Because only the limit vector satisfies the constraints, and the x^k are allowed to violate them, such a method is called an *exterior-point* method.

The Courant-Beltrami Penalty Function

The *Courant-Beltrami* penalty-function method is similar, but uses

$$p(x) = \sum_{i=1}^{I} [g_i^+(x)]^2. \tag{14.8}$$

The Quadratic-Loss Penalty Function

Penalty methods can also be used with equality constraints. Consider the problem of minimizing the convex function $f(x)$, subject to the constraints $g_i(x) = 0$, $i = 1, ..., I$. The *quadratic-loss* penalty function is

$$p(x) = \frac{1}{2}\sum_{i=1}^{I}(g_i(x))^2. \tag{14.9}$$

The inclusion of a penalty term can serve purposes other than to impose constraints on the location of the limit vector. In image processing, it is often desirable to obtain a reconstructed image that is locally smooth, but with well defined edges. Penalty functions that favor such images can then be used in the iterative reconstruction [93]. We survey several instances in which we would want to use a penalized objective function.

Regularized Least-Squares

Suppose we want to solve the system of equations $Ax = b$. The problem may have no exact solution, precisely one solution, or there may be infinitely many solutions. If we minimize the function

$$f(x) = \frac{1}{2}\|Ax - b\|_2^2,$$

we get a *least-squares* solution, generally, and an exact solution, whenever exact solutions exist. When the matrix A is ill-conditioned, small changes in the vector b can lead to large changes in the solution. When the vector b comes from measured data, the entries of b may include measurement errors, so that an exact solution of $Ax = b$ may be undesirable, even when such exact solutions exist; exact solutions may correspond to x with unacceptably large norm, for example. In such cases, we may, instead, wish to minimize a function such as

$$\frac{1}{2}\|Ax - b\|_2^2 + \frac{\epsilon}{2}\|x - z\|_2^2, \tag{14.10}$$

for some vector z. If $z = 0$, the minimizing vector x_ϵ is then a *norm-constrained* least-squares solution. We then say that the least-squares problem has been *regularized*. In the limit, as $\epsilon \to 0$, these regularized solutions x_ϵ converge to the least-squares solution closest to z.

Suppose the system $Ax = b$ has infinitely many exact solutions. Our problem is to select one. Let us select z that incorporates features of the desired solution, to the extent that we know them *a priori*. Then, as $\epsilon \to 0$, the vectors x_ϵ converge to the exact solution closest to z. For example, taking $z = 0$ leads to the *minimum-norm solution*.

Minimizing Cross-Entropy

In image processing, it is common to encounter systems $Px = y$ in which all the terms are non-negative. In such cases, it may be desirable to solve the system $Px = y$, approximately, perhaps, by minimizing the *cross-entropy* or *Kullback-Leibler distance*

$$KL(y, Px) = \sum_{i=1}^{I} \Big(y_i \log \frac{y_i}{(Px)_i} + (Px)_i - y_i \Big), \tag{14.11}$$

over vectors $x \geq 0$. When the vector y is noisy, the resulting solution, viewed as an image, can be unacceptable. It is wise, therefore, to add a penalty term, such as $p(x) = \epsilon KL(z, x)$, where $z > 0$ is a prior estimate of the desired x [116, 155, 117, 31].

A similar problem involves minimizing the function $KL(Px, y)$. Once again, noisy results can be avoided by including a penalty term, such as $p(x) = \epsilon KL(x, z)$ [31].

The Lagrangian in Convex Programming

When there is a sensitivity vector λ for the CP problem, minimizing $f(x)$ is equivalent to minimizing the Lagrangian,

$$f(x) + \sum_{i=1}^{I} \lambda_i g_i(x) = f(x) + p(x); \tag{14.12}$$

in this case, the addition of the second term, $p(x)$, serves to incorporate the constraints $g_i(x) \leq 0$ in the function to be minimized, turning a constrained minimization problem into an unconstrained one. The problem of minimizing the Lagrangian still remains, though. We may have to solve that problem using an iterative algorithm.

Moreau's Proximity-Function Method

The Moreau envelope of the function f is the function

$$m_f(z) = \inf_x \Big\{ f(x) + \frac{1}{2}\|x - z\|_2^2 \Big\}, \tag{14.13}$$

which is also the *infimal convolution* of the functions $f(x)$ and $\frac{1}{2}\|x\|_2^2$. It can be shown that the infimum is uniquely attained at the point denoted $x = \text{prox}_f z$ (see [140]). In similar fashion, we can define $m_{f^*} z$ and $\text{prox}_{f^*} z$, where $f^*(z)$ denotes the function conjugate to f.

Proposition 14.1 *The infimum of $m_f(z)$, over all z, is the same as the infimum of $f(x)$, over all x.*

Proof: We have

$$\inf_z m_f(z) = \inf_z \inf_x \{f(x) + \frac{1}{2}\|x - z|_2^2\}$$

$$= \inf_x \inf_z \{f(x) + \frac{1}{2}\|x - z|_2^2\} = \inf_x \{f(x) + \frac{1}{2} \inf_z \|x - z\|_2^2\} = \inf_x f(x).$$

∎

The minimizers of $m_f(z)$ and $f(x)$ are the same, as well. Therefore, one way to use Moreau's method is to replace the original problem of minimizing the possibly non-smooth function $f(x)$ with the problem of minimizing the smooth function $m_f(z)$. Another way is to convert Moreau's method into a sequential minimization algorithm, replacing z with x^{k-1} and minimizing with respect to x to get x^k. As we shall see, this leads to the proximal minimization algorithm to be discussed below.

14.5.3 The Roles Penalty Functions Play

From the examples just surveyed, we can distinguish several distinct roles that penalty functions can play.

Impose Constraints

The first role is to penalize violations of constraints, as part of sequential minimization, or even to turn a constrained minimization into an equivalent unconstrained one: the Absolute-Value and Courant-Beltrami penalty functions penalize violations of the constraints $g_i(x) \leq 0$, while Quadratic-Loss penalty function penalizes violations of the constraints $g_i(x) = 0$. The augmented objective functions $f(x) + kp(x)$ now become part of a sequential unconstrained minimization method. It is sometimes possible for $f(x)$ and $f(x) + p(x)$ to have the same minimizers, or for constrained minimizers of $f(x)$ to be the same as unconstrained minimizers of $f(x) + p(x)$, as happens with the Lagrangian in the CP problem.

Regularization

The second role is regularization: in the least-squares problem, the main purpose for adding the norm-squared penalty function in Equation (14.10) is to reduce sensitivity to noise in the entries of the vector b. Also, regularization will usually turn a problem with multiple solutions into one with a unique solution.

Incorporate Prior Information

The third role is to incorporate prior information: when $Ax = b$ is underdetermined, using the penalty function $\epsilon\|x - z\|_2^2$ and letting $\epsilon \to 0$ encourages the solution to be close to the prior estimate z.

Simplify Calculations

A fourth role that penalty functions can play is to simplify calculation: in the case of cross-entropy minimization, adding the penalty functions $KL(z, x)$ and $KL(x, z)$ to the objective functions $KL(y, Px)$ and $KL(Px, y)$, respectively, regularizes the minimization problem. But, as we shall see later, the SMART algorithm minimizes $KL(Px, y)$ by using a sequential approach, in which each minimizer x^k can be calculated in closed form.

Sequential Unconstrained Minimization

More generally, a fifth role for penalty functions is as part of sequential minimization. Here the goal is to replace one computationally difficult minimization with a sequence of simpler ones. Clearly, one reason for the difficulty can be that the original problem is constrained, and the sequential approach uses a series of unconstrained minimizations, penalizing violations of the constraints through the penalty function. However, there are other instances in which the sequential approach serves to simplify the calculations, not to remove constraints, but, perhaps, to replace a nondifferentiable objective function with a differentiable one, or a sequence of differentiable ones, as in Moreau's method.

14.6 Proximity-Function Minimization (I)

Let $f : R^J \to (-\infty, +\infty]$ be closed, proper, convex and differentiable. Let h be a closed proper convex function, with effective domain D, that is differentiable on the nonempty open convex set int D. Assume that $f(x)$ is finite on $C = \overline{D}$ and attains its minimum value on C at $\hat{x}$. The corresponding *Bregman distance* $D_h(x, z)$ is defined for x in D and z in int D by

$$D_h(x, z) = h(x) - h(z) - \langle \nabla h(z), x - z \rangle. \tag{14.14}$$

Note that $D_h(x, z) \geq 0$ always. If h is essentially strictly convex, then $D_h(x, z) = 0$ implies that $x = z$. Our objective is to minimize $f(x)$ over x in $C = \overline{D}$.

14.6.1 Proximal Minimization Algorithm

At the kth step of the *proximal minimization algorithm* (PMA) [39], we minimize the function

$$G_k(x) = f(x) + D_h(x, x^{k-1}), \tag{14.15}$$

to get x^k. The function

$$g_k(x) = D_h(x, x^{k-1}) \tag{14.16}$$

is nonnegative and $g_k(x^{k-1}) = 0$. We assume that each x^k lies in int D.

14.6.2 The Method of Auslander and Teboulle

In [6] Auslander and Teboulle consider an iterative method similar to the PMA, in which, at the kth step, one minimizes the function

$$F_k(x) = f(x) + d(x, x^{k-1}) \tag{14.17}$$

to get x^k. Their distance $d(x, y)$ is not assumed to be a Bregman distance. Instead, they assume that the distance d has an associated *induced proximal distance* $H(a, b) \geq 0$, finite for a and b in D, with $H(a, a) = 0$ and

$$\langle \nabla_1 d(b, a), c - b \rangle \leq H(c, a) - H(c, b), \tag{14.18}$$

for all c in D. The notation $\nabla_1 d(x, y)$ denotes the gradient with respect to the vector variable x.

If $d = D_h$, that is, if d is a Bregman distance, then from the equation

$$\langle \nabla_1 d(b, a), c - b \rangle = D_h(c, a) - D_h(c, b) - D_h(b, a) \tag{14.19}$$

we see that D_h has $H = D_h$ for its associated induced proximal distance, so D_h is *self-proximal*, in the terminology of [6].

14.7 The Simultaneous MART (SMART) (I)

Our next example is the simultaneous multiplicative algebraic reconstruction technique (SMART). For $a > 0$ and $b > 0$, the Kullback-Leibler distance, $KL(a, b)$, is defined as

$$KL(a, b) = a \log \frac{a}{b} + b - a. \tag{14.20}$$

In addition, $KL(0, 0) = 0$, $KL(a, 0) = +\infty$ and $KL(0, b) = b$. The KL distance is then extended to nonnegative vectors coordinate-wise.

14.7.1 The SMART Iteration

The SMART minimizes the function $f(x) = KL(Px, y)$, over nonnegative vectors x. Here y is a vector with positive entries, and P is a matrix with nonnegative entries, such that $s_j = \sum_{i=1}^{I} P_{ij} > 0$. Denote by $\mathcal{X}$ the set of all nonnegative x for which the vector Px has only positive entries.

Having found the vector x^{k-1}, the next vector in the SMART sequence is x^k, with entries given by

$$x_j^k = x_j^{k-1} \exp s_j^{-1} \Big(\sum_{i=1}^{I} P_{ij} \log(y_i/(Px^{k-1})_i) \Big). \tag{14.21}$$

14.7.2 The EMML Iteration

The EMML algorithm minimizes the function $f(x) = KL(y, Px)$, over nonnegative vectors x. Having found the vector x^{k-1}, the next vector in the EMML sequence is x^k, with entries given by

$$x_j^k = x_j^{k-1} s_j^{-1} \Big(\sum_{i=1}^{I} P_{ij} (y_i/(Px^{k-1})_i) \Big). \tag{14.22}$$

14.7.3 The EMML and the SMART as Alternating Minimization

In [31] the SMART was derived using the following alternating minimization approach.

For each $x \in \mathcal{X}$, let $r(x)$ and $q(x)$ be the I by J arrays with entries

$$r(x)_{ij} = x_j P_{ij} y_i / (Px)_i, \tag{14.23}$$

and

$$q(x)_{ij} = x_j P_{ij}. \tag{14.24}$$

In the iterative step of the SMART we get x^k by minimizing the function

$$KL(q(x), r(x^{k-1})) = \sum_{i=1}^{I} \sum_{j=1}^{J} KL(q(x)_{ij}, r(x^{k-1})_{ij})$$

over $x \geq 0$. Note that $KL(Px, y) = KL(q(x), r(x))$.

Similarly, the iterative step of the EMML is to minimize the function $KL(r(x^{k-1}), q(x))$ to get $x = x^k$. Note that $KL(y, Px) = KL(q(x), r(x))$.

Now we establish the basic results for the SUMMA.

14.8 Convergence Theorems for SUMMA

At the kth step of the SUMMA we minimize the function $G_k(x)$ to get x^k. In practice, of course, this minimization may need to be performed iteratively; we shall not address this issue here, and shall assume that x^k can be computed. We make the following additional assumptions.

Assumption 1: The functions $g_k(x)$ are finite-valued and continuous on a set D in R^J, with $C = \overline{D}$.

Assumption 2: There is $\hat{x}$ in C with $f(\hat{x}) \leq f(x)$, for all x in C.

Assumption 3: The functions $g_k(x)$ satisfy the inequality in (14.2); that is,

$$0 \leq g_k(x) \leq G_{k-1}(x) - G_{k-1}(x^{k-1}),$$

for $k = 2, 3, ...$ Consequently,

$$g_k(x^{k-1}) = 0.$$

Assumption 4: There is a real number α with

$$\alpha \leq f(x),$$

for all x in R^J.

Assumption 5: Each x^k is in D.

Using these assumptions, we can conclude several things about the sequence $\{x^k\}$.

Proposition 14.2 *The sequence $\{f(x^k)\}$ is decreasing, and the sequence $\{g_k(x^k)\}$ converges to zero.*

Proof: We have

$$f(x^{k+1}) + g_{k+1}(x^{k+1}) = G_{k+1}(x^{k+1}) \leq G_{k+1}(x^k) = f(x^k) + g_{k+1}(x^k) = f(x^k).$$

Therefore,

$$f(x^k) - f(x^{k+1}) \geq g_{k+1}(x^{k+1}) \geq 0.$$

Since the sequence $\{f(x^k)\}$ is decreasing and bounded below by α, the difference sequence must converge to zero. Therefore, the sequence $\{g_k(x^k)\}$ converges to zero. ∎

Theorem 14.1 *The sequence $\{f(x^k)\}$ converges to $f(\hat{x})$.*

Proof: Suppose that there is $\delta > 0$ with

$$f(x^k) \geq f(\hat{x}) + \delta,$$

for all k. Since $\hat{x}$ is in C, there is z in D with

$$f(x^k) \geq f(z) + \frac{\delta}{2},$$

for all k. From

$$g_{k+1}(z) \leq G_k(z) - G_k(x^k),$$

we have

$$g_k(z) - g_{k+1}(z) \geq f(x^k) + g_k(x^k) - f(z) \geq f(x^k) - f(z) \geq \frac{\delta}{2} > 0.$$

This says that the nonnegative sequence $\{g_k(z)\}$ is decreasing, but that successive differences remain bounded away from zero, which cannot happen. ∎

Definition 14.1 *A real-valued function $p(x)$ on R^J has* bounded level sets *if, for all real γ, the level set $\{x|p(x) \leq \gamma\}$ is bounded.*

Theorem 14.2 *Let the restriction of $f(x)$ to x in C have bounded level sets. Then the sequence $\{x^k\}$ is bounded, and $f(x^*) = f(\hat{x})$, for any cluster point x^*. If $\hat{x}$ is unique, $x^* = \hat{x}$ and $\{x^k\} \to \hat{x}$.*

Proof: From the previous theorem we have $f(x^*) = f(\hat{x})$, for all cluster points x^*. But, by uniqueness, $x^* = \hat{x}$, and so $\{x^k\} \to \hat{x}$. ∎

Corollary 14.1 *Let $f(x)$ be closed, proper and convex. If $\hat{x}$ is unique, the sequence $\{x^k\}$ converges to $\hat{x}$.*

Proof: Let $\iota_C(x)$ be the indicator function of the set C, that is, $\iota_C(x) = 0$, for all x in C, and $\iota_C(x) = +\infty$, otherwise. Then the function $g(x) = f(x) + \iota_C(x)$ is closed, proper and convex. If $\hat{x}$ is unique, then we have

$$\{x|f(x) + \iota_C(x) \leq f(\hat{x})\} = \{\hat{x}\}.$$

Therefore, one of the level sets of $g(x)$ is bounded and nonempty. It follows from Corollary 8.7.1 of [140] that every level set of $g(x)$ is bounded, so that the sequence $\{x^k\}$ is bounded. ∎

If $\hat{x}$ is not unique, we may still be able to prove convergence of the sequence $\{x^k\}$, for particular cases of SUMMA, as we shall see shortly.

14.9 Barrier-Function Methods (II)

We return now to the barrier-function methods, to show that they are particular cases of the SUMMA. The iterative step of the barrier-function method can be formulated as follows: minimize

$$f(x) + [(k-1)f(x) + b(x)] \tag{14.25}$$

to get x^k. Since, for $k = 2, 3, ...$, the function

$$(k-1)f(x) + b(x) \tag{14.26}$$

is minimized by x^{k-1}, the function

$$g_k(x) = (k-1)f(x) + b(x) - (k-1)f(x^{k-1}) - b(x^{k-1}) \tag{14.27}$$

is nonnegative, and x^k minimizes the function

$$G_k(x) = f(x) + g_k(x). \tag{14.28}$$

From

$$G_k(x) = f(x) + (k-1)f(x) + b(x) - f(x^{k-1}) - (k-1)f(x^{k-1}) - b(x^{k-1}),$$

it follows that

$$G_k(x) - G_k(x^k) = kf(x) + b(x) - kf(x^k) - b(x^k) = g_{k+1}(x),$$

so that $g_{k+1}(x)$ satisfies the condition in (14.2). This shows that the barrier-function method is a particular case of SUMMA.

The goal is to minimize the objective function $f(x)$, over x in the closed set $C = \overline{D}$, the closure of D. In the barrier-function method, we minimize

$$f(x) + \frac{1}{k}b(x) \tag{14.29}$$

over x in D to get x^k. Each x^k lies within D, so the method is an interior-point algorithm. If the sequence $\{x^k\}$ converges, the limit vector x^* will be in C and $f(x^*) = f(\hat{x})$.

From the results for SUMMA, we conclude that $\{f(x^k)\}$ is decreasing to $f(\hat{x})$, and that $\{g_k(x^k)\}$ converges to zero. From the nonnegativity of $g_k(x^k)$ we have that

$$(k-1)(f(x^k) - f(x^{k-1})) \geq b(x^{k-1}) - b(x^k).$$

Since the sequence $\{f(x^k)\}$ is decreasing, the sequence $\{b(x^k)\}$ must be increasing, but might not be bounded above.

If $\hat{x}$ is unique, and $f(x)$ has bounded level sets, then it follows, from our discussion of SUMMA, that $\{x^k\} \rightarrow \hat{x}$. Suppose now that $\hat{x}$ is not known to be unique, but can be chosen in D, so that $G_k(\hat{x})$ is finite for each k. From

$$f(\hat{x}) + \frac{1}{k}b(\hat{x}) \geq f(x^k) + \frac{1}{k}b(x^k)$$

we have

$$\frac{1}{k}\Big(b(\hat{x}) - b(x^k)\Big) \geq f(x^k) - f(\hat{x}) \geq 0,$$

so that

$$b(\hat{x}) - b(x^k) \geq 0,$$

for all k. If either f or b has bounded level sets, then the sequence $\{x^k\}$ is bounded and has a cluster point, x^* in C. It follows that $b(x^*) \leq b(\hat{x}) < +\infty$, so that x^* is in D. If we assume that $f(x)$ is convex and $b(x)$ is strictly convex on D, then we can show that x^* is unique in D, so that $x^* = \hat{x}$ and $\{x^k\} \rightarrow \hat{x}$.

To see this, assume, to the contrary, that there are two distinct cluster points x^* and x^{**} in D, with

$$\{x^{k_n}\} \rightarrow x^*,$$

and

$$\{x^{j_n}\} \rightarrow x^{**}.$$

Without loss of generality, we assume that

$$0 < k_n < j_n < k_{n+1},$$

for all n, so that

$$b(x^{k_n}) \leq b(x^{j_n}) \leq b(x^{k_{n+1}}).$$

Therefore,

$$b(x^*) = b(x^{**}) \leq b(\hat{x}).$$

From the strict convexity of $b(x)$ on the set D, and the convexity of $f(x)$, we conclude that, for $0 < \lambda < 1$ and $y = (1-\lambda)x^* + \lambda x^{**}$, we have $b(y) < b(x^*)$ and $f(y) \leq f(x^*)$. But, we must then have $f(y) = f(x^*)$. There must then be some k_n such that

$$G_{k_n}(y) = f(y) + \frac{1}{k_n}b(y) < f(x_{k_n}) + \frac{1}{k_n}b(x_{k_n}) = G_{k_n}(x^{k_n}).$$

But, this is a contradiction. ∎

The following theorem summarizes what we have shown with regard to the barrier-function method.

Theorem 14.3 *Let $f : R^J \to (-\infty, +\infty]$ be a continuous function. Let $b(x) : R^J \to (0, +\infty]$ be a continuous function, with effective domain the nonempty set D. Let $\hat{x}$ minimize $f(x)$ over all x in $C = \overline{D}$. For each positive integer k, let x^k minimize the function $f(x) + \frac{1}{k}b(x)$. Then the sequence $\{f(x^k)\}$ is monotonically decreasing to the limit $f(\hat{x})$, and the sequence $\{b(x^k)\}$ is increasing. If $\hat{x}$ is unique, and $f(x)$ has bounded level sets, then the sequence $\{x^k\}$ converges to $\hat{x}$. In particular, if $\hat{x}$ can be chosen in D, if either $f(x)$ or $b(x)$ has bounded level sets, if $f(x)$ is convex and if $b(x)$ is strictly convex on D, then $\hat{x}$ is unique in D and $\{x^k\}$ converges to $\hat{x}$.*

Each step of the barrier method requires the minimization of the function $f(x) + \frac{1}{k}b(x)$. In practice, this must also be performed iteratively, with, say, the Newton-Raphson algorithm. It is important, therefore, that barrier functions be selected so that relatively few Newton-Raphson steps are needed to produce acceptable solutions to the main problem. For more on these issues see Renegar [139] and Nesterov and Nemirovski [131].

14.10 Penalty-Function Methods (II)

Let M be the non-empty closed set of all x for which the continuous function $p(x)$ attains its minimum value; this value need not be zero. Now we consider the problem of minimizing a continuous function $f(x) : R^J \to (-\infty, +\infty]$ over the closed set M. We assume that the constrained minimum of $f(x)$ is attained at some vector $\hat{x}$ in M. We also assume that the function $p(x)$ has bounded level sets.

For $k = 1, 2, ...$, let x^k be a minimizer of the function $f(x) + kp(x)$. As we shall see, we can formulate this penalty-function algorithm as a barrier-function iteration.

14.10.1 Penalty-Function Methods as Barrier-Function Methods

In order to relate penalty-function methods to barrier-function methods, we note that minimizing $f(x)+kp(x)$ is equivalent to minimizing $p(x)+\frac{1}{k}f(x)$. This is the form of the barrier-function iteration, with $p(x)$ now in the role previously played by $f(x)$, and $f(x)$ now in the role previously played by $b(x)$. We are not concerned here with the effective domain of $f(x)$.

Now our Assumption 2 simply says that there is a vector $\hat{x}$ at which $p(x)$ attains its minimum; so M is not empty. From our discussion of barrier-function methods, we know that the sequence $\{p(x^k)\}$ is decreasing to a limit $\hat{p} \geq p(\hat{x})$ and the sequence $\{f(x^k)\}$ is increasing. Since $p(x)$ has bounded level sets, the sequence $\{x^k\}$ is bounded; let x^* be an arbitrary

cluster point. We then have $p(x^*) = \hat{p}$. It may seem odd that we are trying to minimize $f(x)$ over the set M using a sequence $\{x^k\}$ with $\{f(x^k)\}$ increasing, but remember that these x^k are not in M.

We now show that $f(x^*) = f(\hat{x})$. This does not follow from our previous discussion of barrier-function methods.

Let $s(x) = p(x) - p(\hat{x})$, so that $s(x) \geq 0$ and $s(\hat{x}) = 0$. For each k, let

$$T_k(x) = f(x) + ks(x) = f(x) + kp(x) - kp(\hat{x}).$$

Then x^k minimizes $T_k(x)$.

Lemma 14.1 *The sequence $\{T_k(x^k)\}$ is increasing to some limit $\gamma \leq f(\hat{x})$.*

Proof: Because the penalty function $s(x)$ is nonnegative, we have

$$T_k(x^k) \leq T_k(x^{k+1}) \leq T_k(x^{k+1}) + s(x^{k+1}) = T_{k+1}(x^{k+1}).$$

We also have

$$f(\hat{x}) = f(\hat{x}) + ks(\hat{x}) = T_k(\hat{x}) \geq T_k(x^k),$$

for all k. ∎

Lemma 14.2 *For all cluster points x^* of $\{x^k\}$ we have $s(x^*) = 0$, so that $p(x^*) = p(\hat{x})$ and x^* is in M.*

Proof: For each k we have

$$\alpha + ks(x^k) \leq f(x^k) + ks(x^k) = T_k(x^k) \leq f(\hat{x}),$$

so that

$$0 \leq ks(x^k) \leq f(\hat{x}) - \alpha,$$

for all k. It follows that $\{s(x^k)\}$ converges to zero. By the continuity of $s(x)$, we conclude that $s(x^*) = 0$, so x^* is in M. ∎

Lemma 14.3 *For all cluster points x^* of the sequence $\{x^k\}$ we have $f(x^*) = f(\hat{x})$, so x^* minimizes $f(x)$ over x in M.*

Proof: Let $\{x^{k_n}\} \to x^*$. We have

$$f(x^*) = f(x^*) + s(x^*) = \lim_{n \to +\infty} \left(f(x^{k_n}) + s(x^{k_n}) \right)$$

$$\leq \lim_{n \to +\infty} \left(f(x^{k_n}) + k_n s(x^{k_n}) \right) \leq f(\hat{x}).$$

Since x^* is in M, it follows that $f(x^*) = f(\hat{x})$. ∎

To assert that the sequence $\{x^k\}$ itself converges, we would need to make additional assumptions. For example, if the minimizer of $f(x)$ over x in M is unique, then the sequence $\{x^k\}$ has $\hat{x}$ for its only cluster point, so must converge to $\hat{x}$.

The following theorem summarizes what we have shown with regard to penalty-function methods.

Theorem 14.4 *Let $f : R^J \rightarrow (-\infty, +\infty]$ be a continuous function. Let $p(x) : R^J \rightarrow R$ be a continuous function, with bounded level sets, and M the set of all $\tilde{x}$ such that $p(\tilde{x}) \leq p(x)$ for all x in R^J. Let $\hat{x}$ in M minimize $f(\tilde{x})$ over all $\tilde{x}$ in M. For each positive integer k, let x^k minimize the function $f(x) + kp(x)$. Then the sequence $\{f(x^k)\}$ is monotonically increasing to the limit $f(\hat{x})$, and the sequence $\{p(x^k)\}$ is decreasing to $p(\hat{x})$. If $\hat{x}$ is unique, which happens, for example, if $f(x)$ is strictly convex on M, then the sequence $\{x^k\}$ converges to $\hat{x}$.*

14.11 The Proximal Minimization Algorithm (II)

We show now that Assumption 3 holds, so that the PMA is a particular case of the SUMMA. We remind the reader that $f(x)$ is now assumed to be convex and differentiable, so that the Bregman distance $D_f(x, z)$ is defined and nonnegative, for all x in D and z in int$D$.

Lemma 14.4 *For each k we have*

$$G_k(x) = G_k(x^k) + D_f(x, x^k) + D_h(x, x^k). \tag{14.30}$$

Proof: Since x^k minimizes $G_k(x)$ within the set D, we have

$$0 = \nabla f(x^k) + \nabla h(x^k) - \nabla h(x^{k-1}). \tag{14.31}$$

Then

$$G_k(x) - G_k(x^k) = f(x) - f(x^k) + h(x) - h(x^k) - \langle \nabla h(x^{k-1}), x - x^k \rangle.$$

Now substitute, using Equation (14.31), and use the definition of Bregman distances. ∎

It follows from Lemma 14.4 that

$$G_k(x) - G_k(x^k) = g_{k+1}(x) + D_f(x, x^k),$$

so Assumption 3 holds.

From the discussion of the SUMMA we know that $\{f(x^k)\}$ is monotonically decreasing to $f(\hat{x})$. As we noted previously, if the sequence $\{x^k\}$ is bounded, and $\hat{x}$ is unique, we can conclude that $\{x^k\} \rightarrow \hat{x}$.

Suppose that $\hat{x}$ is not known to be unique, but can be chosen in D; this will be the case, of course, whenever D is closed. Then $G_k(\hat{x})$ is finite for each k. From the definition of $G_k(x)$ we have

$$G_k(\hat{x}) = f(\hat{x}) + D_h(\hat{x}, x^{k-1}). \tag{14.32}$$

From Equation (14.30) we have

$$G_k(\hat{x}) = G_k(x^k) + D_f(\hat{x}, x^k) + D_h(\hat{x}, x^k), \tag{14.33}$$

so that

$$G_k(\hat{x}) = f(x^k) + D_h(x^k, x^{k-1}) + D_f(\hat{x}, x^k) + D_h(\hat{x}, x^k). \tag{14.34}$$

Therefore,

$$\begin{gathered} D_h(\hat{x}, x^{k-1}) - D_h(\hat{x}, x^k) = \\ f(x^k) - f(\hat{x}) + D_h(x^k, x^{k-1}) + D_f(\hat{x}, x^k). \end{gathered} \tag{14.35}$$

It follows that the sequence $\{D_h(\hat{x}, x^k)\}$ is decreasing and that the sequence $\{D_f(\hat{x}, x^k)\}$ converges to 0. If either the function $f(x)$ or the function $D_h(\hat{x}, \cdot)$ has bounded level sets, then the sequence $\{x^k\}$ is bounded, has cluster points x^* in C, and $f(x^*) = f(\hat{x})$, for every x^*. We now show that $\hat{x}$ in D implies that x^* is also in D, whenever h is a Bregman -Legendre function.

Let x^* be an arbitrary cluster point, with $\{x^{k_n}\} \to x^*$. If $\hat{x}$ is not in int D, then, by Property B2 of Bregman-Legendre functions, we know that

$$D_h(x^*, x^{k_n}) \to 0,$$

so x^* is in D. Then the sequence $\{D_h(x^*, x^k)\}$ is decreasing. Since a subsequence converges to zero, we have $\{D_h(x^*, x^k)\} \to 0$. From Property R5, we conclude that $\{x^k\} \to x^*$.

If $\hat{x}$ is in int D, but x^* is not, then $\{D_h(\hat{x}, x^k)\} \to +\infty$, by Property R2. But, this is a contradiction; therefore x^* is in D. Once again, we conclude that $\{x^k\} \to x^*$.

Now we summarize our results for the PMA. Let $f : R^J \to (-\infty, +\infty]$ be closed, proper, convex and differentiable. Let h be a closed proper convex function, with effective domain D, that is differentiable on the nonempty open convex set int D. Assume that $f(x)$ is finite on $C = \overline{D}$ and attains its minimum value on C at $\hat{x}$. For each positive integer k, let x^k minimize the function $f(x) + D_h(x, x^{k-1})$. Assume that each x^k is in the interior of D.

Theorem 14.5 *If the restriction of $f(x)$ to x in C has bounded level sets and $\hat{x}$ is unique, and then the sequence $\{x^k\}$ converges to $\hat{x}$.*

Theorem 14.6 *If $h(x)$ is a Bregman-Legendre function and $\hat{x}$ can be chosen in D, then $\{x^k\} \to x^*$, x^* in D, with $f(x^*) = f(\hat{x})$.*

14.11.1 The Method of Auslander and Teboulle

The method of Auslander and Teboulle described in a previous section seems not to be a particular case of SUMMA. However, we can adapt the proof of Theorem 14.1 to prove the analogous result for their method. Once again, we assume that $f(\hat{x}) \leq f(x)$, for all x in C.

Theorem 14.7 *For $k = 2, 3, ...$, let x^k minimize the function*

$$F_k(x) = f(x) + d(x, x^{k-1}).$$

If the distance d has an induced proximal distance H, then $\{f(x^k)\} \to f(\hat{x})$.

Proof: First, we show that the sequence $\{f(x^k)\}$ is decreasing. We have

$$f(x^{k-1}) = F_k(x^{k-1}) \geq F_k(x^k) = f(x^k) + d(x^k, x^{k-1}),$$

from which we conclude that the sequence $\{f(x^k)\}$ is decreasing and the sequence $\{d(x^k, x^{k-1})\}$ converges to zero.

Now suppose that

$$f(x^k) \geq f(\hat{x}) + \delta,$$

for some $\delta > 0$ and all k. Since $\hat{x}$ is in C, there is z in D with

$$f(x^k) \geq f(z) + \frac{\delta}{2},$$

for all k. Since x^k minimizes $F_k(x)$, it follows that

$$0 = \nabla f(x^k) + \nabla_1 d(x^k, x^{k-1}).$$

Using the convexity of the function $f(x)$ and the fact that H is an induced proximal distance, we have

$$0 < \frac{\delta}{2} \leq f(x^k) - f(z) \leq \langle -\nabla f(x^k), z - x^k \rangle =$$

$$\langle \nabla_1 d(x^k, x^{k-1}), z - x^k \rangle \leq H(z, x^{k-1}) - H(z, x^k).$$

Therefore, the nonnegative sequence $\{H(z, x^k)\}$ is decreasing, but its successive differences remain bounded below by $\frac{\delta}{2}$, which is a contradiction. ∎

It is interesting to note that the Auslander-Teboulle approach places a restriction on the function $d(x, y)$, the existence of the induced proximal distance H, that is unrelated to the objective function $f(x)$, but this condition is helpful only for convex $f(x)$. In contrast, the SUMMA approach requires that

$$0 \leq g_{k+1}(x) \leq G_k(x) - G_k(x^k),$$

which involves the $f(x)$ being minimized, but does not require that this $f(x)$ be convex.

14.12 The Simultaneous MART (II)

It follows from the identities established in [31] that the SMART can also be formulated as a particular case of the SUMMA.

14.12.1 The SMART as a Case of SUMMA

We show now that the SMART is a particular case of the SUMMA. The following lemma is helpful in that regard.

Lemma 14.5 *For any non-negative vectors x and z, with $z_+ = \sum_{j=1}^J z_j > 0$, we have*

$$KL(x, z) = KL(x_+, z_+) + KL(x, \frac{x_+}{z_+} z). \tag{14.36}$$

For notational convenience, we assume, for the remainder of this chapter, that $s_j = 1$ for all j. From the identities established for the SMART in [31], we know that the iterative step of SMART can be expressed as follows: minimize the function

$$G_k(x) = KL(Px, y) + KL(x, x^{k-1}) - KL(Px, Px^{k-1}) \tag{14.37}$$

to get x^k. According to Lemma 14.5, the quantity

$$g_k(x) = KL(x, x^{k-1}) - KL(Px, Px^{k-1})$$

is nonnegative, since $s_j = 1$. The $g_k(x)$ are defined for all nonnegative x; that is, the set D is the closed nonnegative orthant in R^J. Each x^k is a positive vector.

It was shown in [31] that

$$G_k(x) = G_k(x^k) + KL(x, x^k), \tag{14.38}$$

from which it follows immediately that Assumption 3 holds for the SMART.

Because the SMART is a particular case of the SUMMA, we know that the sequence $\{f(x^k)\}$ is monotonically decreasing to $f(\hat{x})$. It was shown in [31] that if $y = Px$ has no nonnegative solution and the matrix P and every submatrix obtained from P by removing columns has full rank, then $\hat{x}$ is unique; in that case, the sequence $\{x^k\}$ converges to $\hat{x}$. As we shall see, the SMART sequence always converges to a nonnegative minimizer of $f(x)$. To establish this, we reformulate the SMART as a particular case of the PMA.

14.12.2 The SMART as a Case of the PMA

We take $F(x)$ to be the function

$$F(x) = \sum_{j=1}^{J} x_j \log x_j. \tag{14.39}$$

Then

$$D_F(x, z) = KL(x, z). \tag{14.40}$$

For nonnegative x and z in $\mathcal{X}$, we have

$$D_f(x, z) = KL(Px, Pz). \tag{14.41}$$

Lemma 14.6 $D_F(x, z) \geq D_f(x, z)$.

Proof: We have

$$\begin{aligned} D_F(x, z) &\geq \sum_{j=1}^{J} KL(x_j, z_j) \geq \sum_{j=1}^{J} \sum_{i=1}^{I} KL(P_{ij}x_j, P_{ij}z_j) \\ &\geq \sum_{i=1}^{I} KL((Px)_i, (Pz)_i) = KL(Px, Pz). \end{aligned} \tag{14.42}$$

∎

Then we let $h(x) = F(x) - f(x)$; then $D_h(x, z) \geq 0$ for nonnegative x and z in $\mathcal{X}$. The iterative step of the SMART is to minimize the function

$$f(x) + D_h(x, x^{k-1}). \tag{14.43}$$

So the SMART is a particular case of the PMA.

The function $h(x) = F(x) - f(x)$ is finite on D the nonnegative orthant of R^J, and differentiable on the interior, so $C = D$ is closed in this example. Consequently, $\hat{x}$ is necessarily in D. From our earlier discussion of the PMA, we can conclude that the sequence $\{D_h(\hat{x}, x^k)\}$ is decreasing and the sequence $\{D_f(\hat{x}, x^k)\} \to 0$. Since the function $KL(\hat{x}, \cdot)$ has bounded level sets, the sequence $\{x^k\}$ is bounded, and $f(x^*) = f(\hat{x})$, for every cluster point. Therefore, the sequence $\{D_h(x^*, x^k)\}$ is decreasing. Since a subsequence converges to zero, the entire sequence converges to zero. The convergence of $\{x^k\}$ to x^* follows from basic properties of the KL distance.

From the fact that $\{D_f(\hat{x}, x^k)\} \to 0$, we conclude that $P\hat{x} = Px^*$. Equation (14.35) now tells us that the difference $D_h(\hat{x}, x^{k-1}) - D_h(\hat{x}, x^k)$ depends on only on $P\hat{x}$, and not directly on $\hat{x}$. Therefore, the difference $D_h(\hat{x}, x^0) - D_h(\hat{x}, x^*)$ also depends only on $P\hat{x}$ and not directly on $\hat{x}$. Minimizing $D_h(\hat{x}, x^0)$ over nonnegative minimizers $\hat{x}$ of $f(x)$ is therefore

equivalent to minimizing $D_h(\hat{x}, x^*)$ over the same vectors. But the solution to the latter problem is obviously $\hat{x} = x^*$. Thus we have shown that the limit of the SMART is the nonnegative minimizer of $KL(Px, y)$ for which the distance $KL(x, x^0)$ is minimized.

The following theorem summarizes the situation with regard to the SMART.

Theorem 14.8 *In the consistent case the SMART converges to the unique nonnegative solution of $y = Px$ for which the distance $\sum_{j=1}^{J} s_j KL(x_j, x_j^0)$ is minimized. In the inconsistent case it converges to the unique nonnegative minimizer of the distance $KL(Px, y)$ for which $\sum_{j=1}^{J} s_j KL(x_j, x_j^0)$ is minimized; if P and every matrix derived from P by deleting columns has full rank then there is a unique nonnegative minimizer of $KL(Px, y)$ and at most $I - 1$ of its entries are nonzero.*

14.12.3 The EMML Algorithm

The *expectation maximization maximum likelihood* (EMML) algorithm minimizes the function $f(x) = KL(y, Px)$ over x in $\mathcal{X}$. In [45] the EMML algorithm and the SMART are developed in tandem to reveal how closely related these two methods are. There, the EMML algorithm is derived using alternating minimization, in which the vector x^k is the one for which the function $KL(r(x^{k-1}), q(x))$ is minimized. When we try to put the EMML into the framework of SUMMA, we find that x^k minimizes the function

$$G_k(x) = f(x) + KL(r(x^{k-1}), r(x)), \tag{14.44}$$

over all positive vectors x. However, the functions

$$g_k(x) = KL(r(x^{k-1}), r(x)) \tag{14.45}$$

appear not to satisfy the condition in (14.2). It does not appear to be true that the EMML is a particular case of SUMMA, even though it is true that $\{f(x^k)\}$ does converge monotonically to $f(\hat{x})$ and $\{x^k\}$ does converge to a nonnegative minimizer of $f(x)$. The obvious conjecture is that the EMML is an example of a wider class of sequential unconstrained minimization algorithms for which a nice theory of convergence still holds.

In the next section we present a variant of the SMART, designed to incorporate bounds on the entries of the vector x.

14.13 Minimizing $KL(Px, y)$ with upper and lower bounds on the vector x

Let $a_j < b_j$, for each j. Let $\mathcal{X}_{ab}$ be the set of all vectors x such that $a_j \leq x_j \leq b_j$, for each j. Now, we seek to minimize $f(x) = KL(Px, y)$,

over all vectors x in $\mathcal{X} \cap \mathcal{X}_{ab}$. We let

$$F(x) = \sum_{j=1}^{J} \Big((x_j - a_j) \log(x_j - a_j) + (b_j - x_j) \log(b_j - x_j) \Big). \quad (14.46)$$

Then we have

$$D_F(x, z) = \sum_{j=1}^{J} \Big(KL(x_j - a_j, z_j - a_j) + KL(b_j - x_j, b_j - z_j) \Big), \quad (14.47)$$

and, as before,

$$D_f(x, z) = KL(Px, Pz). \quad (14.48)$$

Lemma 14.7 *For any $c > 0$, with $a \geq c$ and $b \geq c$, we have $KL(a - c, b - c) \geq KL(a, b)$.*

Proof: Let $g(c) = KL(a - c, b - c)$ and differentiate with respect to c, to obtain

$$g'(c) = \frac{a - c}{b - c} - 1 - \log(\frac{a - c}{b - c}) \geq 0. \quad (14.49)$$

We see then that the function $g(c)$ is increasing with c. ∎

As a corollary of Lemma 14.7, we have

Lemma 14.8 *Let $a = (a_1, ..., a_J)^T$, and x and z in $\mathcal{X}$ with $(Px)_i \geq (Pa)_i$, $(Pz)_i \geq (Pa)_i$, for each i. Then $KL(Px, Pz) \leq KL(Px - Pa, Pz - Pa)$.*

Lemma 14.9 *$D_F(x, z) \geq D_f(x, z)$.*

Proof: We can easily show that

$$D_F(x, z) \geq KL(Px - Pa, Pz - Pa) + KL(Pb - Px, Pb - Pz),$$

along the lines used previously. Then, from Lemma 14.8, we have

$$KL(Px - Pa, Pz - Pa) \geq KL(Px, Pz) = D_f(x, z).$$

∎

Once again, we let $h(x) = F(x) - f(x)$, which is finite on the closed convex set $\mathcal{X} \cap \mathcal{X}_{ab}$. At the kth step of this algorithm we minimize the function

$$f(x) + D_h(x, x^{k-1}) \quad (14.50)$$

to get x^k.

Solving for x_j^k, we obtain

$$x_j^{k+1} = \alpha_j^k a_j + (1 - \alpha_j^k) b_j, \tag{14.51}$$

where

$$(\alpha_j^k)^{-1} = 1 + \Big(\frac{x_j^{k-1} - a_j}{b_j - x_j^{k-1}}\Big) \exp\Big(\sum_{i=1}^{I} P_{ij} \log(y_i/(Px^{k-1})_i)\Big). \tag{14.52}$$

Since the restriction of $f(x)$ to $\mathcal{X} \cap \mathcal{X}_{ab}$ has bounded level sets, the sequence $\{x^k\}$ is bounded and has cluster points. If $\hat{x}$ is unique, then $\{x^k\} \to \hat{x}$.

This algorithm is closely related to those presented in [37].

14.14 Computation

As we noted previously, we do not address computational issues in any detail in this chapter. Nevertheless, it cannot be ignored that both Equation (14.21) for the SMART and Equations (14.51) and (14.52) for the generalized SMART provide easily calculated iterates, in contrast to other examples of SUMMA. At the same time, showing that these two algorithms are particular cases of SUMMA requires the introduction of functions $G_k(x)$ that appear to be quite ad hoc. The purpose of this section is to motivate these choices of $G_k(x)$ and to indicate how other analogous computationally tractable SUMMA iterative schemes may be derived.

14.14.1 Landweber's Algorithm

Suppose that A is a real I by J matrix and we wish to obtain a least-squares solution $\hat{x}$ of $Ax = b$ by minimizing the function

$$f(x) = \frac{1}{2}\|Ax - b\|^2.$$

We know that

$$(A^T A)\hat{x} = A^T b, \tag{14.53}$$

so, in a sense, the problem is solved. However, in many applications, the dimensions I and J are quite large, perhaps in the tens of thousands, as in some image reconstruction problems. Solving Equation (14.53), and even calculating $A^T A$, can be prohibitively expensive. In such cases, we turn to iterative methods, not necessarily to incorporate constraints on x, but to facilitate calculation. Landweber's algorithm is one such iterative method for calculating a least-squares solution.

The iterative step of Landweber's algorithm is

$$x^k = x^{k-1} - \gamma A^T(Ax^{k-1} - b). \tag{14.54}$$

The sequence $\{x^k\}$ converges to the least-squares solution closest to x^0, for any choice of γ in the interval $(0, 2/\rho(A^TA))$, where $\rho(A^TA)$, the spectral radius of A^TA, is its largest eigenvalue; this is a consequence of the Krasnoselskii-Mann Theorem 17.2.

It is easy to verify that the x^k given by Equation (14.54) is the minimizer of the function

$$G_k(x) = \frac{1}{2}\|Ax - b\|^2 + \frac{1}{2\gamma}\|x - x^{k-1}\|^2 - \frac{1}{2}\|Ax - Ax^{k-1}\|^2, \tag{14.55}$$

that, for γ in the interval $(0, 1/\rho(A^TA))$, the iteration in Equation (14.54) is a particular case of SUMMA, and

$$G_k(x) - G_k(x^k) = \frac{1}{2\gamma}\|x - x^k\|^2.$$

The similarity between the $G_k(x)$ in Equation (14.55) and that in Equation (14.37) is not accidental and both are particular cases of a more general iterative scheme involving proximal minimization.

14.14.2 Extending the PMA

The proximal minimization algorithm (PMA) requires us to minimize the function $G_k(x)$ given by Equation (14.15) to get x^k. How x^k may be calculated was not addressed previously. Suppose, instead of minimizing $G_k(x)$ in Equation (14.15), we minimize

$$G_k(x) = f(x) + D_h(x, x^{k-1}) - D_f(x, x^{k-1}), \tag{14.56}$$

with the understanding that $f(x)$ is convex and

$$D_h(x, z) - D_f(x, z) \geq 0,$$

for all appropriate x and z. The next iterate x^k satisfies the equation

$$0 = \nabla h(x^k) - \nabla h(x^{k-1}) + \nabla f(x^{k-1}), \tag{14.57}$$

so that

$$\nabla h(x^k) = \nabla h(x^{k-1}) - \nabla f(x^{k-1}). \tag{14.58}$$

This iterative scheme is the *interior-point algorithm* (IPA) presented in [39]. If the function $h(x)$ is chosen carefully, then we can solve for x^k easily. The

Landweber algorithm, the SMART, and the generalized SMART are all particular cases of this IPA.

Using Lemma 14.4, we can show that

$$G_k(x) - G_k(x^k) = \frac{1}{2\gamma} D_h(x, x^k), \tag{14.59}$$

for all appropriate x, so that the IPA is a particular case of SUMMA. We consider now several other examples.

If we let $h(x) = \frac{1}{2\gamma}\|x\|^2$ in Equation (14.56), the iteration becomes

$$x^k = x^{k-1} - \gamma \nabla f(x^{k-1}). \tag{14.60}$$

If, for example, the operator ∇f is L-Lipschitz continuous, that is,

$$\|\nabla f(x) - \nabla f(z)\| \leq L\|x - z\|,$$

then, for any γ in the interval $(0, 1/2L)$, we have

$$\frac{1}{2\gamma}\|x - z\|^2 \geq L\|x - z\|^2 \geq \langle \nabla f(x) - \nabla f(z), x - z\rangle$$

$$= D_f(x, z) + D_f(z, x) \geq D_f(x, z).$$

Therefore, this iteration is a particular case of SUMMA. It should be noted that, in this case, the Krasnoselskii-Mann Theorem gives convergence for any γ in the interval $(0, 2/L)$.

Finally, we consider what happens if we replace the Euclidean norm with that induced by the local geometry derived from f itself. More specifically, let us take

$$h(x) = \frac{1}{2} x^T \nabla^2 f(x^{k-1}) x,$$

so that

$$D_h(x, x^{k-1}) = \frac{1}{2}(x - x^{k-1})^T \nabla^2 f(x^{k-1})(x - x^{k-1}).$$

Then the IPA iterate x^k becomes

$$x^k = x^{k-1} - \nabla^2 f(x^{k-1})^{-1} \nabla f(x^{k-1}), \tag{14.61}$$

which is the Newton-Raphson iteration. Using the SUMMA framework to study the Newton-Raphson method is work in progress.

Algorithms such as Landweber's and SMART can be slow to converge. It is known that convergence can often be accelerated using incremental gradient (partial gradient, block-iterative, ordered-subset) methods. Using the SUMMA framework to study such incremental gradient methods as the algebraic reconstruction technique (ART), its multiplicative version (MART), and other block-iterative methods is also the subject of on-going work.

14.15 Connections with Karmarkar's Method

As related by Margaret Wright in [157], a revolution in mathematical programming took place around 1984. In that year Narenda Karmarkar discovered the first efficient polynomial-time algorithm for the linear programming problem [110]. Khachian's earlier polynomial-time algorithm for LP was too slow and conventional wisdom prior to 1984 was that the simplex method was "the only game in town" . It was known that, for certain peculiar LP problems, the complexity of the simplex method grew exponentially with the size of the problem, and obtaining a polynomial-time method for LP had been a goal for quite a while. However, for most problems, the popular simplex method was more than adequate. Soon after Karmarkar's result was made known, others discovered that there was a close connection between this method and earlier barrier-function approaches in nonlinear programming [94]. This discovery not only revived barrier-function methods, but established a link between linear and nonlinear programming, two areas that had historically been treated separately.

The primary LP problem in standard form is to minimize $c^T x$, subject to the conditions $Ax = b$ and $x \geq 0$. The barrier-function approach is to use a logarithmic barrier to enforce the condition $x \geq 0$, and then to use the primal-dual approach of Equation (11.39) to maintain the condition $Ax = b$. The function to be minimized, subject to $Ax = b$, is then

$$c^T x - \mu \sum_{j=1}^{J} \log x_j,$$

where $\mu > 0$ is the *barrier parameter*. When this minimization is performed using the primal-dual method described by Equation (11.39), and the NR iteration is begun at a feasible x^0, each subsequent x^k satisfies $Ax^k = b$. The limit of the NR iteration is x_μ. Under reasonable conditions, x_μ will converge to the solution of the LP problem, as $\mu \to 0$. This interior-point approach to solving the LP problem is essentially equivalent to Karmarkar's approach.

14.16 Exercises

14.1 *Prove Lemma 14.5.*

14.2 ([129], Ex. 16.1) *Use the logarithmic barrier method to minimize the function*

$$f(x, y) = x - 2y,$$

subject to the constraints

$$1 + x - y^2 \geq 0,$$

and

$$y \geq 0.$$

14.3 ([129], Ex. 16.5) *Use the quadratic-loss penalty method to minimize the function*

$$f(x, y) = -xy,$$

subject to the equality constraint

$$x + 2y - 4 = 0.$$

14.17 Course Homework

Do all the exercises in this chapter.

Chapter 15

Likelihood Maximization

15.1 Chapter Summary

A fundamental problem in statistics is the estimation of underlying population parameters from measured data. A popular method for such estimation is likelihood maximization (ML). In a number of applications, such as image processing in remote sensing, the problem is reformulated as a statistical parameter estimation problem in order to make use of likelihood maximization methods.

15.2 Statistical Parameter Estimation

An important topic in statistics is the estimation of a population parameter from sampled data. For example, political pollsters want to estimate the percentage of voters who favor a particular candidate. They can't ask everyone, so they sample the population and estimate the percentage from the answers they receive from a relative few. Bottlers of soft drinks want to know if their process of sealing the bottles is effective. Obviously, they can't open every bottle to check the process. They open a few bottles, selected randomly according to some testing scheme, and make their assessment of the effectiveness of the overall process after opening a few bottles. As we shall see, optimization plays an important role in the estimation of parameters from data.

15.3 Maximizing the Likelihood Function

Suppose that $\mathbf{Y}$ is a random vector whose probability density function (pdf) $f(\mathbf{y};\mathbf{x})$ is a function of the vector variable $\mathbf{y}$ and is a member of a family of pdf parametrized by the vector variable $\mathbf{x}$. Our data is one instance of

$\mathbf{Y}$; that is, one particular value of the variable $\mathbf{y}$, which we also denote by $\mathbf{y}$. We want to estimate the correct value of the variable $\mathbf{x}$, which we shall also denote by $\mathbf{x}$. This notation is standard and the dual use of the symbols $\mathbf{y}$ and $\mathbf{x}$ should not cause confusion. Given the particular $\mathbf{y}$ we can estimate the correct $\mathbf{x}$ by viewing $f(\mathbf{y};\mathbf{x})$ as a function of the second variable, with the first variable held fixed. This function of the parameters only is called the *likelihood function*. A *maximum likelihood* (ML) estimate of the parameter vector $\mathbf{x}$ is any value of the second variable for which the function is maximized. We consider several examples.

15.3.1 Example 1: Estimating a Gaussian Mean

Let $Y_1, ..., Y_I$ be I independent Gaussian (or normal) random variables with known variance $\sigma^2 = 1$ and unknown common mean μ. Let $\mathbf{Y} = (Y_1, ..., Y_I)^T$. The parameter x we wish to estimate is the mean $x = \mu$. Then, the random vector $\mathbf{Y}$ has the pdf

$$f(\mathbf{y}; x) = (2\pi)^{-I/2} \exp(-\frac{1}{2}\sum_{i=1}^{I}(y_i - x)^2).$$

Holding $\mathbf{y}$ fixed and maximizing over x is equivalent to minimizing

$$\sum_{i=1}^{I}(y_i - x)^2$$

as a function of x. The ML estimate is the arithmetic mean of the data,

$$x_{ML} = \frac{1}{I}\sum_{i=1}^{I} y_i.$$

Notice that $E(\mathbf{Y})$, the expected value of $\mathbf{Y}$, is the vector $\mathbf{x}$ all of whose entries are $x = \mu$. The ML estimate is the least squares solution of the overdetermined system of equations $\mathbf{y} = E(\mathbf{Y})$; that is,

$$y_i = x$$

for $i = 1, ..., I$.

The least-squares solution of a system of equations $A\mathbf{x} = \mathbf{b}$ is the vector that minimizes the Euclidean distance between $A\mathbf{x}$ and $\mathbf{b}$; that is, it minimizes the Euclidean norm of their difference, $||A\mathbf{x} - \mathbf{b}||$, where, for any two vectors $\mathbf{a}$ and $\mathbf{b}$ we define

$$||\mathbf{a} - \mathbf{b}||^2 = \sum_{i=1}^{I}(a_i - b_i)^2.$$

As we shall see in the next example, another important measure of distance is the *Kullback-Leibler* (KL) distance between two nonnegative vectors $\mathbf{c}$ and $\mathbf{d}$, given by

$$KL(\mathbf{c},\mathbf{d}) = \sum_{i=1}^{I} c_i \log(c_i/d_i) + d_i - c_i.$$

15.3.2 Example 2: Estimating a Poisson Mean

Let $Y_1,...,Y_I$ be I independent Poisson random variables with unknown common mean λ, which is the parameter x we wish to estimate. Let $\mathbf{Y} = (Y_1,...,Y_I)^T$. Then, the probability function of $\mathbf{Y}$ is

$$f(\mathbf{y};x) = \prod_{i=1}^{I} \exp(-x)x^{y_i}/(y_i)!.$$

Holding $\mathbf{y}$ fixed and maximizing this likelihood function over positive values of x is equivalent to minimizing the Kullback-Leibler distance between the nonnegative vector $\mathbf{y}$ and the vector $\mathbf{x}$ whose entries are all equal to x, given by

$$KL(\mathbf{y},\mathbf{x}) = \sum_{i=1}^{I} y_i \log(y_i/x) + x - y_i.$$

The ML estimator is easily seen to be the arithmetic mean of the data,

$$x_{ML} = \frac{1}{I}\sum_{i=1}^{I} y_i.$$

The vector $\mathbf{x}$ is again $E(\mathbf{Y})$, so the ML estimate is once again obtained by finding an approximate solution of the overdetermined system of equations $\mathbf{y} = E(\mathbf{Y})$. In the previous example the approximation was in the least squares sense, whereas here it is in the minimum KL sense; the ML estimate is the arithmetic mean in both cases because the parameter to be estimated is one-dimensional.

15.3.3 Example 3: Estimating a Uniform Mean

Suppose now that $Y_1,...,Y_I$ are independent random variables uniformly distributed over the interval $[0,2x]$. The parameter to be determined is their common mean, x. The random vector $\mathbf{Y} = (Y_1,...,Y_I)^T$ has the pdf

$$f(\mathbf{y};x) = x^{-I}, \text{for } 2x \geq m,$$

$$f(\mathbf{y};x) = 0\,, \text{otherwise}\,,$$

where m is the maximum of the y_i. For fixed vector $\mathbf{y}$ the ML estimate of x is $m/2$. The expected value of $\mathbf{Y}$ is $E(\mathbf{Y}) = \mathbf{x}$ whose entries are all equal to x. In this case the ML estimator is not obtained by finding an approximate solution to the overdetermined system $\mathbf{y} = E(\mathbf{Y})$.

Since we can always write

$$\mathbf{y} = E(\mathbf{Y}) + (\mathbf{y} - E(\mathbf{Y})),$$

we can model $\mathbf{y}$ as the sum of $E(\mathbf{Y})$ and mean-zero error or noise. Since $f(\mathbf{y}; \mathbf{x})$ depends on $\mathbf{x}$, so does $E(\mathbf{Y})$. Therefore, it makes some sense to consider estimating our parameter vector $\mathbf{x}$ using an approximate solution for the system of equations

$$\mathbf{y} = E(\mathbf{Y}).$$

As the first two examples (as well as many others) illustrate, this is what the ML approach often amounts to, while the third example shows that this is not always the case, however. Still to be determined, though, is the metric with respect to which the approximation is to be performed. As the Gaussian and Poisson examples showed, the ML formalism can provide that metric. In those overly simple cases it did not seem to matter which metric we used, but it does matter.

15.3.4 Example 4: Image Restoration

A standard model for image restoration is the following:

$$\mathbf{y} = A\mathbf{x} + \mathbf{z},$$

where $\mathbf{y}$ is the blurred image, A is an I by J matrix describing the linear imaging system, $\mathbf{x}$ is the desired vectorized restored image, and $\mathbf{z}$ is (possibly correlated) mean-zero additive Gaussian noise. The noise covariance matrix is $Q = E(\mathbf{z}\mathbf{z}^T)$. Then $E(\mathbf{Y}) = A\mathbf{x}$, and the pdf is

$$f(\mathbf{y}; \mathbf{x}) = c \exp(-(\mathbf{y} - A\mathbf{x})^T Q^{-1} (\mathbf{y} - A\mathbf{x})),$$

where c is a constant that does not involve $\mathbf{x}$. Holding $\mathbf{y}$ fixed and maximizing $f(\mathbf{y}; \mathbf{x})$ with respect to $\mathbf{x}$ is equivalent to minimizing

$$(\mathbf{y} - A\mathbf{x})^T Q^{-1} (\mathbf{y} - A\mathbf{x}).$$

Therefore, the ML solution is obtained by finding a weighted least squares approximate solution of the over-determined linear system $\mathbf{y} = E(\mathbf{Y})$, with the weights coming from the matrix Q^{-1}. When the noise terms are uncorrelated and have the same variance, this reduces to the least squares solution.

15.3.5 Example 5: Poisson Sums

The model of sums of independent Poisson random variables is commonly used in emission tomography and elsewhere. Let P be an I by J matrix with nonnegative entries, and let $\mathbf{x} = (x_1, ..., x_J)^T$ be a vector of nonnegative parameters. Let $Y_1, ..., Y_I$ be independent Poisson random variables with positive means

$$E(Y_i) = \sum_{j=1}^{J} P_{ij} x_j = (P\mathbf{x})_i.$$

The probability function for the random vector $\mathbf{Y}$ is then

$$f(\mathbf{y}; \mathbf{x}) = c \prod_{i=1}^{I} \exp(-(P\mathbf{x})_i)((P\mathbf{x})_i)^{y_i},$$

where c is a constant not involving $\mathbf{x}$. Maximizing this function of $\mathbf{x}$ for fixed $\mathbf{y}$ is equivalent to minimizing the KL distance $KL(\mathbf{y}, P\mathbf{x})$ over nonnegative $\mathbf{x}$. The expected value of the random vector $\mathbf{Y}$ is $E(\mathbf{Y}) = P\mathbf{x}$ and once again we see that the ML estimate is a nonnegative approximate solution of the system of (linear) equations $\mathbf{y} = E(\mathbf{Y})$, with the approximation in the KL sense. The system $\mathbf{y} = P\mathbf{x}$ may not be over-determined; there may even be exact solutions. But we require in addition that $\mathbf{x} \geq 0$ and there need not be a nonnegative solution to $\mathbf{y} = P\mathbf{x}$. We see from this example that constrained optimization plays a role in solving our problems.

15.3.6 Example 6: Finite Mixtures of Probability Vectors

We say that a discrete random variable W taking values in the set $\{i = 1, ..., I\}$ is a *finite mixture of probability vectors* if there are probability vectors f_j and numbers $x_j > 0$, for $j = 1, ..., J$, such that the probability vector for W is

$$f(i) = \text{Prob}(W = i) = \sum_{j=1}^{J} x_j f_j(i). \tag{15.1}$$

We require, of course, that $\sum_{j=1}^{J} x_j = 1$.

The data are N realizations of the random variable W, denoted w_n, for $n = 1, ..., N$ and the incomplete data is the vector $y = (w_1, ..., w_N)$. The column vector $x = (x_1, ..., x_J)^T$ is the parameter vector of mixture probabilities to be estimated. The likelihood function is

$$L(x) = \prod_{n=1}^{N} \Big(x_1 f_1(w_n) + ... + x_J f_J(w_n) \Big),$$

which can be written as

$$L(x) = \prod_{i=1}^{I} \Big(x_1 f_1(i) + ... + x_J f_J(i) \Big)^{n_i},$$

where n_i is the cardinality of the set $\{n | \, i_n = i\}$. Then the log likelihood function is

$$LL(x) = \sum_{i=1}^{I} n_i \log \Big(x_1 f_1(i) + ... + x_J f_J(i) \Big).$$

With u the column vector with entries $u_i = n_i/N$, and P the matrix with entries $P_{ij} = f_j(i)$, we see that

$$\sum_{i=1}^{I} (Px)_i = \sum_{i=1}^{I} \Big(\sum_{j=1}^{J} P_{ij} x_j \Big) = \sum_{j=1}^{J} \Big(\sum_{i=1}^{I} P_{ij} \Big) = \sum_{j=1}^{J} x_j = 1,$$

so maximizing $LL(x)$ over non-negative vectors x with $\sum_{j=1}^{J} x_j = 1$ is equivalent to minimizing the KL distance $KL(u, Px)$ over the same vectors. The restriction that the entries of x sum to one turns out to be redundant, as we show now.

From the gradient form of the Karush-Kuhn-Tucker Theorem in optimization, we know that, for any $\hat{x}$ that is a non-negative minimizer of $KL(u, Px)$, we have

$$\sum_{i=1}^{I} P_{ij} \Big(1 - \frac{u_i}{(P\hat{x})_i} \Big) \geq 0,$$

and

$$\sum_{i=1}^{I} P_{ij} \Big(1 - \frac{u_i}{(P\hat{x})_i} \Big) = 0,$$

for all j such that $\hat{x}_j > 0$. Consequently, we can say that

$$s_j \hat{x}_j = \hat{x}_j \sum_{i=1}^{I} P_{ij} \Big(\frac{u_i}{(P\hat{x})_i} \Big),$$

for all j. Since, in the mixture problem, we have $s_j = \sum_{i=1}^{I} P_{ij} = 1$ for each j, it follows that

$$\sum_{j=1}^{J} \hat{x}_j = \sum_{i=1}^{I} \Big(\sum_{j=1}^{J} \hat{x}_j P_{ij} \Big) \frac{u_i}{(P\hat{x})_i} = \sum_{i=1}^{I} u_i = 1.$$

So we know now that any non-negative minimizer of $KL(u, Px)$ will be a probability vector that maximizes $LL(x)$. Since the EMML algorithm minimizes $KL(u, Px)$, when u_i replaces y_i, it can be used to find the maximum-likelihood estimate of the mixture probabilities.

If the set of values that W can take on is infinite, say $\{i = 1, 2, ...\}$, then the f_j are infinite probability sequences. The same analysis applies to this infinite case, and again we have $s_j = 1$. The iterative scheme is given by Equation (14.22), but with an apparently infinite summation; since only finitely many of the u_i are non-zero, the summation is actually only finite.

15.3.7 Example 7: Finite Mixtures of Probability Density Functions

For finite mixtures of probability density functions the problem is a bit more complicated. A variant of the EMML algorithm still solves the problem, but this is not so obvious.

Suppose now that W is a random variable with probability density function $f(w)$ given by

$$f(w) = \sum_{j=1}^{J} x_j f_j(w), \tag{15.2}$$

where the $f_j(w)$ are known pdf's and the mixing proportions x_j are unknown. Our data is $w_1, ..., w_N$, that is, N independent realizations of the random variable W, and $y = (w_1, ..., w_N)$ is the incomplete data. With x the column vector with entries x_j, we have the likelihood function

$$L(x) = \prod_{n=1}^{N} (\sum_{j=1}^{J} x_j f_j(w_n)),$$

and the log likelihood function

$$LL(x) = \sum_{n=1}^{N} \log(\sum_{j=1}^{J} x_j f_j(w_n)).$$

We want to estimate the vector x by maximizing $LL(x)$, subject to $x_j \geq 0$ and $x_+ = \sum_{j=1}^{J} x_j = 1$.

Let $P_{nj} = f_j(z_n)$, and $s_j = \sum_{n=1}^{N} P_{nj}$. Then

$$LL(x) = \sum_{n=1}^{N} \log(Px)_n.$$

With $u_n = \frac{1}{N}$ for each n, we have that maximizing $LL(x)$, subject to $x_j \geq 0$ and $x_+ = 1$, is equivalent to minimizing

$$KL(u, Px) - \sum_{n=1}^{N} (Px)_n, \tag{15.3}$$

subject to the same constraints. Since the non-negative minimizer of the function

$$F(x) = KL(u, Px) + \sum_{j=1}^{J} (1 - s_j) x_j \tag{15.4}$$

satisfies $x_+ = 1$, it follows that minimizing $F(x)$ subject to $x_j \geq 0$ and $x_+ = 1$ is equivalent to minimizing $F(x)$, subject only to $x_j \geq 0$.

The following theorem is found in [40]:

Theorem 15.1 *Let y be any positive vector and*

$$G(x) = KL(y, Px) + \sum_{j=1}^{J} \beta_j KL(\gamma_j, x_j).$$

If $s_j + \beta_j > 0$, $\alpha_j = s_j(s_j + \beta_j)^{-1}$, and $\beta_j \gamma_j \geq 0$ for each j, then the iterative sequence generated by

$$x_j^{k+1} = \alpha_j s_j^{-1} x_j^k \Big(\sum_{n=1}^{N} P_{nj} \frac{y_n}{(Px^k)_n} \Big) + (1 - \alpha_j)\gamma_j$$

converges to a non-negative minimizer of $G(x)$.

With $y_n = u_n = \frac{1}{N}$, $\gamma_j = 0$, and $\beta_j = 1 - s_j$, it follows that the iterative sequence generated by

$$x_j^{k+1} = x_j^k \frac{1}{N} \sum_{n=1}^{N} P_{nj} \frac{1}{(Px^k)_n} \tag{15.5}$$

converges to the maximum-likelihood estimate of the mixing proportions x_j. This is the EM iteration presented in McLachlan and Krishnan [125], Equations (1.36) and (1.37).

15.4 Alternative Approaches

The ML approach is not always the best approach. As we have seen, the ML estimate is often found by solving, at least approximately, the system of equations $\mathbf{y} = E(\mathbf{Y})$. Since noise is always present, this system of equations

is rarely a correct statement of the situation. It is possible to overfit the mean to the noisy data, in which case the resulting $\mathbf{x}$ can be useless. In such cases Bayesian methods and maximum *a posteriori* estimation, as well as other forms of regularization techniques and penalty function techniques, can help. Other approaches involve stopping iterative algorithms prior to convergence.

In most applications the data is limited and it is helpful to include prior information about the parameter vector $\mathbf{x}$ to be estimated. In the Poisson mixture problem the vector $\mathbf{x}$ must have nonnegative entries. In certain applications, such as transmission tomography, we might have upper bounds on suitable values of the entries of $\mathbf{x}$.

From a mathematical standpoint we are interested in the convergence of iterative algorithms, while in many applications we want usable estimates in a reasonable amount of time, often obtained by running an iterative algorithm for only a few iterations. Algorithms designed to minimize the same cost function can behave quite differently during the early iterations. Iterative algorithms, such as block-iterative or incremental methods, that can provide decent answers quickly will be important.

Chapter 16

Calculus of Variations

16.1 Chapter Summary

Up to now, we have been concerned with maximizing or minimizing real-valued functions of one or several variables, possibly subject to constraints. In this chapter, we consider another type of optimization problem, maximizing or minimizing *a function of functions*. The functions themselves we shall denote by simply $y = y(x)$, instead of the more common notation $y = f(x)$, and the function of functions will be denoted $J(y)$; in the calculus of variations, such functions of functions are called *functionals*. We then want to optimize $J(y)$ over a class of *admissible* functions $y(x)$. We shall focus on the case in which x is a single real variable, although there are situations in which the functions y are functions of several variables.

16.2 Overview

When we attempt to minimize a function $g(x_1, ..., x_N)$, we consider what happens to g when we perturb the values x_n to $x_n + \Delta x_n$. In order for $\mathbf{x} = (x_1, ..., x_N)$ to minimize g, it is necessary that

$$g(x_1 + \Delta x_1, ..., x_N + \Delta x_N) \geq g(x_1, ..., x_N),$$

for all perturbations $\Delta x_1, ..., \Delta x_N$. For differentiable g, this means that the gradient of g at $\mathbf{x}$ must be zero. In the calculus of variations, when we attempt to minimize $J(y)$, we need to consider what happens when we perturb the function y to a nearby *admissible* function, denoted $y + \Delta y$. In order for y to minimize $J(y)$, we need

$$J(y + \Delta y) \geq J(y),$$

for all Δy that make $y + \Delta y$ admissible. We end up with something analogous to a first derivative of J, which is then set to zero. The result is a differential equation, called the *Euler-Lagrange Equation*, which must be satisfied by the minimizing y.

16.3 Some Examples

In this section we present some of the more famous examples of problems from the calculus of variations.

16.3.1 The Shortest Distance

Among all the functions $y = y(x)$, defined for x in the interval $[0, 1]$, with $y(0) = 0$ and $y(1) = 1$, the straight-line function $y(x) = x$ has the shortest length. Assuming the functions are differentiable, the formula for the length of such curves is

$$J(y) = \int_0^1 \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\, dx. \tag{16.1}$$

Therefore, we can say that the function $y(x) = x$ minimizes $J(y)$, over all such functions.

In this example, the functional $J(y)$ involves only the first derivative of $y = y(x)$ and has the form

$$J(y) = \int f(x, y(x), y'(x))dx, \tag{16.2}$$

where $f = f(u, v, w)$ is the function of three variables

$$f(u, v, w) = \sqrt{1 + w^2}. \tag{16.3}$$

In general, the functional $J(y)$ can come from almost any function $f(u, v, w)$. In fact, if higher derivatives of $y(x)$ are involved, the function f can be a function of more than three variables. In this chapter we shall confine our discussion to problems involving only the first derivative of $y(x)$.

16.3.2 The Brachistochrone Problem

Consider a frictionless wire connecting the two points $A = (0, 0)$ and $B = (1, 1)$; for convenience, the positive y-axis is downward. A metal ball rolls from point A to point B under the influence of gravity. What shape should the wire take in order to make the travel time of the ball the smallest? This famous problem, known as the *Brachistochrone Problem*, was posed in 1696

by Johann Bernoulli. This event is viewed as marking the beginning of the calculus of variations.

The velocity of the ball along the curve is $v = \frac{ds}{dt}$, where s denotes the arc-length. Therefore,

$$dt = \frac{ds}{v} = \frac{1}{v}\sqrt{1 + \left(\frac{dy}{dx}\right)^2}dx.$$

Because the ball is falling under the influence of gravity only, the velocity it attains after falling from $(0,0)$ to (x,y) is the same as it would have attained had it fallen y units vertically; only the travel times are different. This is because the loss of potential energy is the same either way. The velocity attained after a vertical free fall of y units is $\sqrt{2gy}$. Therefore, we have

$$dt = \frac{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}dx}{\sqrt{2gy}}.$$

The travel time from A to B is therefore

$$J(y) = \frac{1}{\sqrt{2g}}\int_0^1 \sqrt{1 + \left(\frac{dy}{dx}\right)^2}\frac{1}{\sqrt{y}}dx. \tag{16.4}$$

For this example, the function $f(u,v,w)$ is

$$f(u,v,w) = \frac{\sqrt{1+w^2}}{\sqrt{v}}. \tag{16.5}$$

16.3.3 Minimal Surface Area

Given a function $y = y(x)$ with $y(0) = 1$ and $y(1) = 0$, we imagine revolving this curve around the x-axis, to generate a surface of revolution. The functional $J(y)$ that we wish to minimize now is the surface area. Therefore, we have

$$J(y) = \int_0^1 y\sqrt{1 + y'(x)^2}dx. \tag{16.6}$$

Now the function $f(u,v,w)$ is

$$f(u,v,w) = v\sqrt{1+w^2}. \tag{16.7}$$

16.3.4 The Maximum Area

Among all curves of length L connecting the points $(0,0)$ and $(1,0)$, find the one for which the area A of the region bounded by the curve and the

x-axis is maximized. The length of the curve is given by

$$L = \int_0^1 \sqrt{1 + y'(x)^2} dx, \tag{16.8}$$

and the area, assuming that $y(x) \geq 0$ for all x, is

$$A = \int_0^1 y(x) dx. \tag{16.9}$$

This problem is different from the previous ones, in that we seek to optimize a functional, subject to a second functional being held fixed. Such problems are called *problems with constraints*.

16.3.5 Maximizing Burg Entropy

The *Burg entropy* of a positive-valued function $y(x)$ on $[-\pi, \pi]$ is

$$BE(y) = \int_{-\pi}^{\pi} \log\Big(y(x)\Big) dx. \tag{16.10}$$

An important problem in signal processing is to maximize $BE(y)$, subject to

$$r_n = \int_{-\pi}^{\pi} y(x) e^{-inx} dx, \tag{16.11}$$

for $|n| \leq N$. The r_n are values of the Fourier transform of the function $y(x)$.

16.4 Comments on Notation

The functionals $J(y)$ that we shall consider in this chapter have the form

$$J(y) = \int f(x, y(x), y'(x)) dx, \tag{16.12}$$

where $f = f(u, v, w)$ is some function of three real variables. It is common practice, in the calculus of variations literature, to speak of $f = f(x, y, y')$, rather than $f(u, v, w)$. Unfortunately, this leads to potentially confusing notation, such as when $\frac{\partial f}{\partial u}$ is written as $\frac{\partial f}{\partial x}$, which is not the same thing as the total derivative of $f(x, y(x), y'(x))$,

$$\frac{d}{dx} f(x, y(x), y'(x)) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} y'(x) + \frac{\partial f}{\partial y'} y''(x). \tag{16.13}$$

Using the notation of this chapter, Equation (16.13) becomes

$$\frac{d}{dx}f(x,y(x),y'(x)) = \frac{\partial f}{\partial u}(x,y(x),y'(x))+$$

$$\frac{\partial f}{\partial v}(x,y(x),y'(x))y'(x) + \frac{\partial f}{\partial w}(x,y(x),y'(x))y''(x). \tag{16.14}$$

The common notation forces us to view $f(x,y,y')$ both as a function of three unrelated variables, x, y, and y', and as $f(x,y(x),y'(x))$, a function of the single variable x.

For example, suppose that

$$f(u,v,w) = u^2 + v^3 + \sin w,$$

and

$$y(x) = 7x^2.$$

Then

$$f(x,y(x),y'(x)) = x^2 + (7x^2)^3 + \sin(14x), \tag{16.15}$$

$$\frac{\partial f}{\partial x}(x,y(x),y'(x)) = 2x, \tag{16.16}$$

and

$$\frac{d}{dx}f(x,y(x),y'(x)) = \frac{d}{dx}\Big(x^2 + (7x^2)^3 + \sin(14x)\Big)$$

$$= 2x + 3(7x^2)^2(14x) + 14\cos(14x). \tag{16.17}$$

16.5 The Euler-Lagrange Equation

In the problems we shall consider in this chapter, admissible functions are differentiable, with $y(x_1) = y_1$ and $y(x_2) = y_2$; that is, the graphs of the admissible functions pass through the end points (x_1,y_1) and (x_2,y_2). If $y = y(x)$ is one such function and $\eta(x)$ is a differentiable function with $\eta(x_1) = 0$ and $\eta(x_2) = 0$, then $y(x) + \epsilon\eta(x)$ is admissible, for all values of ϵ. For fixed admissible function $y = y(x)$, we define

$$J(\epsilon) = J(y(x) + \epsilon\eta(x)), \tag{16.18}$$

and force $J'(\epsilon) = 0$ at $\epsilon = 0$. The tricky part is calculating $J'(\epsilon)$.

Since $J(y(x) + \epsilon\eta(x))$ has the form

$$J(y(x) + \epsilon\eta(x)) = \int_{x_1}^{x_2} f(x, y(x) + \epsilon\eta(x), y'(x) + \epsilon\eta'(x))dx, \tag{16.19}$$

we obtain $J'(\epsilon)$ by differentiating under the integral sign.

Omitting the arguments, we have

$$J'(\epsilon) = \int_{x_1}^{x_2} \frac{\partial f}{\partial v}\eta + \frac{\partial f}{\partial w}\eta' dx. \tag{16.20}$$

Using integration by parts and $\eta(x_1) = \eta(x_2) = 0$, we have

$$\int_{x_1}^{x_2} \frac{\partial f}{\partial w}\eta' dx = -\int_{x_1}^{x_2} \frac{d}{dx}(\frac{\partial f}{\partial w})\eta dx. \tag{16.21}$$

Therefore, we have

$$J'(\epsilon) = \int_{x_1}^{x_2} \Big(\frac{\partial f}{\partial v} - \frac{d}{dx}(\frac{\partial f}{\partial w})\Big)\eta dx. \tag{16.22}$$

In order for $y = y(x)$ to be the optimal function, this integral must be zero for every appropriate choice of $\eta(x)$, when $\epsilon = 0$. It can be shown without too much trouble that this forces

$$\frac{\partial f}{\partial v} - \frac{d}{dx}(\frac{\partial f}{\partial w}) = 0. \tag{16.23}$$

Equation (16.23) is the *Euler-Lagrange Equation*.

For clarity, let us rewrite that Euler-Lagrange Equation using the arguments of the functions involved. Equation (16.23) is then

$$\frac{\partial f}{\partial v}(x, y(x), y'(x)) - \frac{d}{dx}\Big(\frac{\partial f}{\partial w}(x, y(x), y'(x))\Big) = 0. \tag{16.24}$$

16.6 Special Cases of the Euler-Lagrange Equation

The Euler-Lagrange Equation simplifies in certain special cases.

16.6.1 If f is independent of v

If the function $f(u, v, w)$ is independent of the variable v then the Euler-Lagrange Equation (16.24) becomes

$$\frac{\partial f}{\partial w}(x, y(x), y'(x)) = c, \tag{16.25}$$

for some constant c. If, in addition, the function $f(u, v, w)$ is a function of w alone, then so is $\frac{\partial f}{\partial w}$, from which we conclude from the Euler-Lagrange Equation that $y'(x)$ is constant.

16.6.2 If f is independent of u

Note that we can write

$$\frac{d}{dx}f(x,y(x),y'(x)) = \frac{\partial f}{\partial u}(x,y(x),y'(x))$$

$$+\frac{\partial f}{\partial v}(x,y(x),y'(x))y'(x) + \frac{\partial f}{\partial w}(x,y(x),y'(x))y''(x). \tag{16.26}$$

We also have

$$\frac{d}{dx}\Big(y'(x)\frac{\partial f}{\partial w}(x,y(x),y'(x))\Big) =$$

$$y'(x)\frac{d}{dx}\Big(\frac{\partial f}{\partial w}(x,y(x),y'(x))\Big) + y''(x)\frac{\partial f}{\partial w}(x,y(x),y'(x)). \tag{16.27}$$

Subtracting Equation (16.27) from Equation (16.26), we get

$$\frac{d}{dx}\Big(f(x,y(x),y'(x)) - y'(x)\frac{\partial f}{\partial w}(x,y(x),y'(x))\Big) =$$

$$\frac{\partial f}{\partial u}(x,y(x),y'(x)) + y'(x)\Big(\frac{\partial f}{\partial v} - \frac{d}{dx}\frac{\partial f}{\partial w}\Big)(x,y(x),y'(x)). \tag{16.28}$$

Now, using the Euler-Lagrange Equation, we see that Equation (16.28) reduces to

$$\frac{d}{dx}\Big(f(x,y(x),y'(x)) - y'(x)\frac{\partial f}{\partial w}(x,y(x),y'(x))\Big) = \frac{\partial f}{\partial u}(x,y(x),y'(x)). \tag{16.29}$$

If it is the case that $\frac{\partial f}{\partial u} = 0$, then equation (16.29) leads to

$$f(x,y(x),y'(x)) - y'(x)\frac{\partial f}{\partial w}(x,y(x),y'(x)) = c, \tag{16.30}$$

for some constant c.

16.7 Using the Euler-Lagrange Equation

We derive and solve the Euler-Lagrange Equation for each of the examples presented previously.

16.7.1 The Shortest Distance

In this case, we have

$$f(u, v, w) = \sqrt{1 + w^2}, \tag{16.31}$$

so that

$$\frac{\partial f}{\partial v} = 0,$$

and

$$\frac{\partial f}{\partial u} = 0.$$

We conclude that $y'(x)$ is constant, so $y(x)$ is a straight line.

16.7.2 The Brachistochrone Problem

Equation (16.5) tells us that

$$f(u, v, w) = \frac{\sqrt{1 + w^2}}{\sqrt{v}}. \tag{16.32}$$

Then, since

$$\frac{\partial f}{\partial u} = 0,$$

and

$$\frac{\partial f}{\partial w} = \frac{w}{\sqrt{1 + w^2}\sqrt{v}},$$

Equation (16.30) tells us that

$$\frac{\sqrt{1 + y'(x)^2}}{\sqrt{y(x)}} - y'(x)\frac{y'(x)}{\sqrt{1 + y'(x)^2}\sqrt{y(x)}} = c. \tag{16.33}$$

Equivalently, we have

$$\sqrt{y(x)}\sqrt{1 + y'(x)^2} = \sqrt{a}. \tag{16.34}$$

Solving for $y'(x)$, we get

$$y'(x) = \sqrt{\frac{a - y(x)}{y(x)}}. \tag{16.35}$$

Separating variables and integrating, using the substitution

$$y = a\sin^2\theta = \frac{a}{2}(1 - \cos 2\theta),$$

we obtain

$$x = 2a \int \sin^2 \theta d\theta = \frac{a}{2}(2\theta - \sin 2\theta) + k. \tag{16.36}$$

From this, we learn that the minimizing curve is a *cycloid*, that is, the path a point on a circle traces as the circle rolls.

There is an interesting connection, discussed by Simmons in [148] , between the brachistochrone problem and the refraction of light rays. Imagine a ray of light passing from the point $A = (0, a)$, with $a > 0$, to the point $B = (c, b)$, with $c > 0$ and $b < 0$. Suppose that the speed of light is v_1 above the x-axis, and $v_2 < v_1$ below the x-axis. The path consists of two straight lines, meeting at the point $(0, x)$. The total time for the journey is then

$$T(x) = \frac{\sqrt{a^2 + x^2}}{v_1} + \frac{\sqrt{b^2 + (c - x)^2}}{v_2}.$$

Fermat's Principle of Least Time says that the (apparent) path taken by the light ray will be the one for which x minimizes $T(x)$. From calculus, it follows that

$$\frac{x}{v_1\sqrt{a^2 + x^2}} = \frac{c - x}{v_2\sqrt{b^2 + (c - x)^2}},$$

and from geometry, we get *Snell's Law*:

$$\frac{\sin \alpha_1}{v_1} = \frac{\sin \alpha_2}{v_2},$$

where α_1 and α_2 denote the angles between the upper and lower parts of the path and the vertical, respectively.

Imagine now a stratified medium consisting of many horizontal layers, each with its own speed of light. The path taken by the light would be such that $\frac{\sin \alpha}{v}$ remains constant as the ray passes from one layer to the next. In the limit of infinitely many infinitely thin layers, the path taken by the light would satisfy the equation $\frac{\sin \alpha}{v} = \text{constant}$, with

$$\sin \alpha = \frac{1}{\sqrt{1 + y'(x)^2}}.$$

As we have already seen, the velocity attained by the rolling ball is $v = \sqrt{2gy}$, so the equation to be satisfied by the path $y(x)$ is

$$\sqrt{2gy(x)}\sqrt{1 + y'(x)^2} = \text{constant},$$

which is what we obtained from the Euler-Lagrange Equation.

16.7.3 Minimizing the Surface Area

For the problem of minimizing the surface area of a surface of revolution, the function $f(u, v, w)$ is

$$f(u, v, w) = v\sqrt{1 + w^2}. \tag{16.37}$$

Once again, $\frac{\partial f}{\partial u} = 0$, so we have

$$\frac{y(x)y'(x)^2}{\sqrt{1 + y'(x)^2}} - y(x)\sqrt{1 + y'(x)^2} = c. \tag{16.38}$$

It follows that

$$y(x) = b \cosh \frac{x - a}{b}, \tag{16.39}$$

for appropriate a and b.

It is important to note that being a solution of the Euler-Lagrange Equation is a necessary condition for a differentiable function to be a solution to the original optimization problem, but it is not a sufficient condition. The optimal solution may not be a differentiable one, or there may be no optimal solution. In the case of minimum surface area, there may not be any function of the form in Equation (16.39) passing through the two given end points; see Chapter IV of Bliss [14] for details.

16.8 Problems with Constraints

We turn now to the problem of optimizing one functional, subject to a second functional being held constant. The basic technique is similar to ordinary optimization subject to constraints: we use Lagrange multipliers. We begin with a classic example.

16.8.1 The Isoperimetric Problem

A classic problem in the calculus of variations is the *Isoperimetric Problem*: find the curve of a fixed length that encloses the largest area. For concreteness, suppose the curve connects the two points $(0, 0)$ and $(1, 0)$ and is the graph of a function $y(x)$. The problem then is to maximize the area integral

$$\int_0^1 y(x)dx, \tag{16.40}$$

subject to the perimeter being held fixed, that is,

$$\int_0^1 \sqrt{1 + y'(x)^2}dx = P. \tag{16.41}$$

With

$$f(x, y(x), y'(x)) = y(x) + \lambda\sqrt{1 + y'(x)^2},$$

the Euler-Lagrange Equation becomes

$$\frac{d}{dx}\Big(\frac{\lambda y'(x)}{\sqrt{1 + y'(x)^2}}\Big) - 1 = 0, \tag{16.42}$$

or

$$\frac{y'(x)}{\sqrt{1 + y'(x)^2}} = \frac{x - a}{\lambda}. \tag{16.43}$$

Using the substitution $t = \frac{x-a}{\lambda}$ and integrating, we find that

$$(x - a)^2 + (y - b)^2 = \lambda^2, \tag{16.44}$$

which is the equation of a circle. So the optimal function $y(x)$ is a portion of a circle.

What happens if the assigned perimeter P is greater than $\frac{\pi}{2}$, the length of the semicircle connecting $(0, 0)$ and $(1, 0)$? In this case, the desired curve is not the graph of a function of x, but a parameterized curve of the form $(x(t), y(t))$, for, say, t in the interval $[0, 1]$. Now we have one independent variable, t, but two dependent ones, x and y. We need a generalization of the Euler-Lagrange Equation to the multivariate case.

16.8.2 Burg Entropy

According to the Euler-Lagrange Equation for this case, we have

$$\frac{1}{y(x)} + \sum_{n=-N}^{N} \lambda_n e^{-ixn}, \tag{16.45}$$

or

$$y(x) = 1/\sum_{n=-N}^{N} a_n e^{inx}. \tag{16.46}$$

The *spectral factorization* theorem [135] tells us that if the denominator is positive for all x, then it can be written as

$$\sum_{n=-N}^{N} a_n e^{inx} = |\sum_{m=0}^{N} b_m e^{imx}|^2. \tag{16.47}$$

With a bit more work (see [45]), it can be shown that the desired coefficients b_m are the solution to the system of equations

$$\sum_{m=0}^{N} r_{m-k} b_m = 0, \tag{16.48}$$

for $k = 1, 2, ..., N$ and

$$\sum_{m=0}^{N} r_m b_m = 1. \tag{16.49}$$

16.9 The Multivariate Case

Suppose that the integral to be optimized is

$$J(x, y) = \int_a^b f(t, x(t), x'(t), y(t), y'(t))dt, \tag{16.50}$$

where $f(u, v, w, s, r)$ is a real-valued function of five variables. In such cases, the Euler-Lagrange Equation is replaced by the two equations

$$\begin{aligned} \frac{d}{dt}\Big(\frac{\partial f}{\partial w}\Big) - \frac{\partial f}{\partial v} = 0, \\ \frac{d}{dx}\Big(\frac{\partial f}{\partial r}\Big) - \frac{\partial f}{\partial s} = 0. \end{aligned} \tag{16.51}$$

We apply this now to the problem of maximum area for a fixed perimeter.

We know from Green's Theorem in two dimensions that the area A enclosed by a curve C is given by the integral

$$A = \frac{1}{2}\oint_C (xdy - ydx) = \frac{1}{2}\int_0^1 (x(t)y'(t) - y(t)x'(t))dt. \tag{16.52}$$

The perimeter P of the curve is

$$P = \int_0^1 \sqrt{x'(t)^2 + y'(t)^2}dt. \tag{16.53}$$

So the problem is to maximize the integral in Equation (16.52), subject to the integral in Equation (16.53) being held constant.

The problem is solved by using a Lagrange multiplier. We write

$$J(x, y) = \int_0^1 \Big(x(t)y'(t) - y(t)x'(t) + \lambda\sqrt{x'(t)^2 + y'(t)^2}\Big)dt. \tag{16.54}$$

The generalized Euler-Lagrange Equations are

$$\frac{d}{dt}\Big(\frac{1}{2}x(t) + \frac{\lambda y'(t)}{\sqrt{x'(t)^2 + y'(t)^2}}\Big) + \frac{1}{2}x'(t) = 0, \tag{16.55}$$

and

$$\frac{d}{dt}\Big(-\frac{1}{2}y(t) + \frac{\lambda x'(t)}{\sqrt{x'(t)^2 + y'(t)^2}}\Big) - \frac{1}{2}y'(t) = 0. \tag{16.56}$$

It follows that

$$y(t) + \frac{\lambda x'(t)}{\sqrt{x'(t)^2 + y'(t)^2}} = c, \tag{16.57}$$

and

$$x(t) + \frac{\lambda y'(t)}{\sqrt{x'(t)^2 + y'(t)^2}} = d. \tag{16.58}$$

Therefore,

$$(x - d)^2 + (y - c)^2 = \lambda^2. \tag{16.59}$$

The optimal curve is then a portion of a circle.

16.10 Finite Constraints

Suppose that we want to minimize the functional

$$J(y) = \int_a^b f(x, y(x), y'(x))dx,$$

subject to the constraint

$$g(x, y(x)) = 0.$$

Such a problem is said to be one of *finite constraints*. In this section we illustrate this type of problem by considering the geodesic problem.

16.10.1 The Geodesic Problem

The space curve $(x(t), y(t), z(t))$, defined for $a \leq t \leq b$, lies on the surface described by $G(x, y, z) = 0$ if $G(x(t), y(t), z(t)) = 0$ for all t in $[a, b]$. The *geodesic problem* is to find the curve of shortest length lying on the surface and connecting points $A = (a_1, a_2, a_3)$ and $B = (b_1, b_2, b_3)$. The functional to be minimized is the arc length

$$J = \int_a^b \sqrt{\dot{x}^2 + \dot{y}^2 + \dot{z}^2}dt, \tag{16.60}$$

where $\dot{x} = \frac{dx}{dt}$.

We assume that the equation $G(x, y, z) = 0$ can be rewritten as

$$z = g(x, y),$$

that is, we assume that we can solve for the variable z, and that the function g has continuous second partial derivatives. We may not be able to do this

for the entire surface, as the equation of a sphere $G(x, y, z) = x^2 + y^2 + z^2 - r^2 = 0$ illustrates, but we can usually solve for z, or one of the other variables, on part of the surface, as, for example, on the upper or lower hemisphere.

We then have

$$\dot{z} = g_x\dot{x} + g_y\dot{y} = g_x(x(t), y(t))\dot{x}(t) + g_y(x(t), y(t))\dot{y}(t), \tag{16.61}$$

where $g_x = \frac{\partial g}{\partial x}$.

Lemma 16.1 *We have*

$$\frac{\partial \dot{z}}{\partial x} = \frac{d}{dt}(g_x).$$

Proof: From Equation (16.61) we have

$$\frac{\partial \dot{z}}{\partial x} = \frac{\partial}{\partial x}(g_x\dot{x} + g_y\dot{y}) = g_{xx}\dot{x} + g_{yx}\dot{y}.$$

We also have

$$\frac{d}{dt}(g_x) = \frac{d}{dt}(g_x(x(t), y(t)) = g_{xx}\dot{x} + g_{xy}\dot{y}.$$

Since $g_{xy} = g_{yx}$, the assertion of the lemma follows. ∎

From the Lemma we have both

$$\frac{\partial \dot{z}}{\partial x} = \frac{d}{dt}(g_x), \tag{16.62}$$

and

$$\frac{\partial \dot{z}}{\partial y} = \frac{d}{dt}(g_y). \tag{16.63}$$

Substituting for z in Equation (16.60), we see that the problem is now to minimize the functional

$$J = \int_a^b \sqrt{\dot{x}^2 + \dot{y}^2 + (g_x\dot{x} + g_y\dot{y})^2}dt, \tag{16.64}$$

which we write as

$$J = \int_a^b F(x, \dot{x}, y, \dot{y})dt. \tag{16.65}$$

The Euler-Lagrange Equations are then

$$\frac{\partial F}{\partial x} - \frac{d}{dt}(\frac{\partial F}{\partial \dot{x}}) = 0, \tag{16.66}$$

and

$$\frac{\partial F}{\partial y} - \frac{d}{dt}(\frac{\partial F}{\partial \dot{y}}) = 0. \tag{16.67}$$

Using

$$\begin{aligned}\frac{\partial F}{\partial x} &= \frac{\partial f}{\partial \dot{z}} \frac{\partial (g_x \dot{x} + g_y \dot{y})}{\partial x} \\ &= \frac{\partial f}{\partial \dot{z}} \frac{\partial}{\partial x}(\frac{dg}{dt}) = \frac{\partial f}{\partial \dot{z}} \frac{\partial \dot{z}}{\partial x}\end{aligned}$$

and

$$\frac{\partial F}{\partial y} = \frac{\partial f}{\partial \dot{z}} \frac{\partial \dot{z}}{\partial y},$$

we can rewrite the Euler-Lagrange Equations as

$$\frac{d}{dt}(\frac{\partial f}{\partial \dot{x}}) + g_x \frac{d}{dt}(\frac{\partial f}{\partial \dot{z}}) = 0, \tag{16.68}$$

and

$$\frac{d}{dt}(\frac{\partial f}{\partial \dot{y}}) + g_y \frac{d}{dt}(\frac{\partial f}{\partial \dot{z}}) = 0. \tag{16.69}$$

To see why this is the case, we reason as follows. First

$$\begin{aligned}\frac{\partial F}{\partial \dot{x}} &= \frac{\partial f}{\partial \dot{x}} + \frac{\partial f}{\partial \dot{z}} \frac{\partial \dot{z}}{\partial \dot{x}} \\ &= \frac{\partial f}{\partial \dot{x}} + \frac{\partial f}{\partial \dot{z}} g_x,\end{aligned}$$

so that

$$\begin{aligned}\frac{d}{dt}(\frac{\partial F}{\partial \dot{x}}) &= \frac{d}{dt}(\frac{\partial f}{\partial \dot{x}}) + \frac{d}{dt}(\frac{\partial f}{\partial \dot{z}} g_x) \\ &= \frac{d}{dt}(\frac{\partial f}{\partial \dot{x}}) + \frac{d}{dt}(\frac{\partial f}{\partial \dot{z}}) g_x + \frac{\partial f}{\partial \dot{z}} \frac{d}{dt}(g_x) \\ &= \frac{d}{dt}(\frac{\partial f}{\partial \dot{x}}) + \frac{d}{dt}(\frac{\partial f}{\partial \dot{z}}) g_x + \frac{\partial f}{\partial \dot{z}} \frac{\partial \dot{z}}{\partial \dot{x}}.\end{aligned}$$

Let the function $\lambda(t)$ be defined by

$$\frac{d}{dt}(\frac{\partial f}{\partial \dot{z}}) = \lambda(t) G_z,$$

and note that

$$g_x = -\frac{G_x}{G_z},$$

and

$$g_y = -\frac{G_y}{G_z}.$$

Then the Euler-Lagrange Equations become

$$\frac{d}{dt}(\frac{\partial f}{\partial \dot{x}}) = \lambda(t)G_x, \tag{16.70}$$

and

$$\frac{d}{dt}(\frac{\partial f}{\partial \dot{y}}) = \lambda(t)G_y. \tag{16.71}$$

Eliminating $\lambda(t)$ and extending the result to include z as well, we have

$$\frac{\frac{d}{dt}(\frac{\partial f}{\partial \dot{x}})}{G_x} = \frac{\frac{d}{dt}(\frac{\partial f}{\partial \dot{y}})}{G_y} = \frac{\frac{d}{dt}(\frac{\partial f}{\partial \dot{z}})}{G_z}. \tag{16.72}$$

Notice that we could obtain the same result by calculating the Euler-Lagrange Equation for the functional

$$\int_a^b f(\dot{x}, \dot{y}, \dot{z}) + \lambda(t)G(x(t), y(t), z(t))dt. \tag{16.73}$$

16.10.2 An Example

Let the surface be a sphere, with equation

$$0 = G(x, y, z) = x^2 + y^2 + z^2 - r^2.$$

Then Equation (16.72) becomes

$$\frac{f\ddot{x} - \dot{x}\dot{f}}{2xf^2} = \frac{f\ddot{y} - \dot{y}\dot{f}}{2yf^2} = \frac{f\ddot{z} - \dot{z}\dot{f}}{2zf^2}.$$

We can rewrite these equations as

$$\frac{\ddot{x}y - x\ddot{y}}{\dot{x}y - x\dot{y}} = \frac{y\ddot{z} - z\ddot{y}}{y\dot{z} - z\dot{y}} = \frac{\dot{f}}{f}.$$

The numerators are the derivatives, with respect to t, of the denominators, which leads to

$$\log|x\dot{y} - y\dot{x}| = \log|y\dot{z} - z\dot{y}| + c_1.$$

Therefore,

$$x\dot{y} - y\dot{x} = c_1(y\dot{z} - z\dot{y}).$$

Rewriting, we obtain

$$\frac{\dot{x} + c_1\dot{z}}{x + c_1 z} = \frac{\dot{y}}{y},$$

or

$$x + c_1 z = c_2 y,$$

which is a plane through the origin. The geodesics on the sphere are great circles, that is, the intersection of the sphere with a plane through the origin.

16.11 Exercises

16.1 *Suppose that the cycloid in the brachistochrone problem connects the starting point* $(0,0)$ *with the point* $(\pi a, -2a)$*, where* $a > 0$*. Show that the time required for the ball to reach the point* $(\pi a, -2a)$ *is* $\pi\sqrt{\frac{a}{g}}$*.*

16.2 *Show that, for the situation in the previous exercise, the time required for the ball to reach* $(\pi a, -2a)$ *is again* $\pi\sqrt{\frac{a}{g}}$*, if the ball begins rolling at any intermediate point along the cycloid. This is the tautochrone property of the cycloid.*

Chapter 17

Operators

17.1 Chapter Summary

In a broad sense, all iterative algorithms generate a sequence $\{x^k\}$ of vectors. The sequence may converge for any starting vector x^0, or may converge only if the x^0 is sufficiently close to a solution. The limit, when it exists, may depend on x^0, and may, or may not, solve the original problem. Convergence to the limit may be slow and the algorithm may need to be accelerated. The algorithm may involve measured data. The limit may be sensitive to noise in the data and the algorithm may need to be regularized to lessen this sensitivity. The algorithm may be quite general, applying to all problems in a broad class, or it may be tailored to the problem at hand. Each step of the algorithm may be costly, but only a few steps generally needed to produce a suitable approximate answer, or, each step may be easily performed, but many such steps needed. Although convergence of an algorithm is important, theoretically, sometimes in practice only a few iterative steps are used. In this chapter we consider several classes of operators that play important roles in optimization.

17.2 Operators

For most of the iterative algorithms we shall consider, the iterative step is

$$x^{k+1} = Tx^k, \tag{17.1}$$

for some operator T. If T is a continuous operator (and it usually is), and the sequence $\{T^k x^0\}$ converges to $\hat{x}$, then $T\hat{x} = \hat{x}$, that is, $\hat{x}$ is a *fixed point* of the operator T. We denote by $\text{Fix}(T)$ the set of fixed points of T. The convergence of the iterative sequence $\{T^k x^0\}$ will depend on the properties of the operator T.

Our approach here will be to identify several classes of operators for which the iterative sequence is known to converge, to examine the convergence theorems that apply to each class, to describe several applied problems that can be solved by iterative means, to present iterative algorithms for solving these problems, and to establish that the operator involved in each of these algorithms is a member of one of the designated classes.

17.3 Strict Contractions

The strict contraction operators are perhaps the best known class of operators associated with iterative algorithms.

Definition 17.1 *An operator T on R^J is* Lipschitz continuous*, with respect to a vector norm $||\cdot||$, or L-Lipschitz, if there is a positive constant L such that*

$$||Tx - Ty|| \leq L||x - y||, \tag{17.2}$$

for all x and y in R^J.

Definition 17.2 *An operator T on R^J is a* strict contraction *(sc), with respect to a vector norm $||\cdot||$, if there is $r \in (0, 1)$ such that*

$$||Tx - Ty|| \leq r||x - y||, \tag{17.3}$$

for all vectors x and y.

For strict contractions, we have the Banach-Picard Theorem [82]:

Theorem 17.1 *Let T be sc. Then, there is a unique fixed point of T and, for any starting vector x^0, the sequence $\{T^k x^0\}$ converges to the fixed point.*

The key step in the proof is to show that $\{x^k\}$ is a Cauchy sequence, therefore, it has a limit.

Definition 17.3 *An operator T is called an* affine linear operator *if T has the form $Tx = Bx + d$, where B is a linear operator, and d is a fixed vector.*

Lemma 17.1 *Let T be an affine linear operator. Then T is a strict contraction if and only if $||B||$, the induced matrix norm of B, is less than one.*

Definition 17.4 *The* spectral radius *of a square matrix B, written $\rho(B)$, is the maximum of $|\lambda|$, over all eigenvalues λ of B.*

Since $\rho(B) \leq ||B||$ for every norm on B induced by a vector norm, B is sc implies that $\rho(B) < 1$. When B is Hermitian, the matrix norm of B induced by the Euclidean vector norm is $||B||_2 = \rho(B)$, so if $\rho(B) < 1$, then B is sc with respect to the Euclidean norm.

When B is not Hermitian, it is not as easy to determine if the affine operator T is sc with respect to a given norm. Instead, we often tailor the norm to the operator T. Suppose that B is a diagonalizable matrix, that is, there is a basis for R^J consisting of eigenvectors of B. Let $\{u^1, ..., u^J\}$ be such a basis, and let $Bu^j = \lambda_j u^j$, for each $j = 1, ..., J$. For each x in R^J, there are unique coefficients a_j so that

$$x = \sum_{j=1}^{J} a_j u^j. \tag{17.4}$$

Then let

$$||x|| = \sum_{j=1}^{J} |a_j|. \tag{17.5}$$

Lemma 17.2 *The expression $||\cdot||$ in Equation (17.5) defines a norm on R^J. If $\rho(B) < 1$, then the affine operator T is sc, with respect to this norm.*

It is known that, for any square matrix B and any $\epsilon > 0$, there is a vector norm for which the induced matrix norm satisfies $||B|| \leq \rho(B) + \epsilon$. Therefore, if B is an arbitrary square matrix with $\rho(B) < 1$, there is a vector norm with respect to which B is sc.

In many of the applications of interest to us, there will be multiple fixed points of T. Therefore, T will not be sc for any vector norm, and the Banach-Picard fixed-point theorem will not apply. We need to consider other classes of operators. These classes of operators will emerge as we investigate the properties of orthogonal projection operators.

17.4 Two Useful Identities

The identities in the next two lemmas relate an arbitrary operator T to its complement, $G = I - T$, where I denotes the identity operator. These identities will allow us to transform properties of T into properties of G that may be easier to work with. A simple calculation is all that is needed to establish the following lemma.

Lemma 17.3 *Let T be an arbitrary operator T on R^J and $G = I - T$. Then*

$$||x - y||_2^2 - ||Tx - Ty||_2^2 = 2(\langle Gx - Gy, x - y\rangle) - ||Gx - Gy||_2^2. \tag{17.6}$$

Lemma 17.4 *Let T be an arbitrary operator T on R^J and $G = I - T$. Then*

$$\langle Tx - Ty, x - y\rangle - ||Tx - Ty||_2^2 =$$

$$\langle Gx - Gy, x - y\rangle - ||Gx - Gy||_2^2. \tag{17.7}$$

Proof: Use the previous lemma. ∎

17.5 Orthogonal Projection Operators

If C is a closed, non-empty convex set in R^J, and x is any vector, then, as we have seen, there is a unique point $P_C x$ in C closest to x, in the sense of the Euclidean distance. This point is called the orthogonal projection of x onto C. If C is a subspace, then we can get an explicit description of $P_C x$ in terms of x; for general convex sets C, however, we will not be able to express $P_C x$ explicitly, and certain approximations will be needed. Orthogonal projection operators are central to our discussion, and, in this overview, we focus on problems involving convex sets, algorithms involving orthogonal projection onto convex sets, and classes of operators derived from properties of orthogonal projection operators.

17.5.1 Properties of the Operator P_C

Although we usually do not have an explicit expression for $P_C x$, we can, however, characterize $P_C x$ as the unique member of C for which

$$\langle P_C x - x, c - P_C x\rangle \geq 0, \tag{17.8}$$

for all c in C; see Proposition 4.4.

P_C is Non-expansive

Recall that an operator T is non-expansive (ne), with respect to a given norm, if, for all x and y, we have

$$||Tx - Ty|| \leq ||x - y||. \tag{17.9}$$

Lemma 17.5 *The orthogonal projection operator $T = P_C$ is non-expansive, with respect to the Euclidean norm, that is,*

$$||P_C x - P_C y||_2 \leq ||x - y||_2, \tag{17.10}$$

for all x and y.

Proof: Use Inequality (17.8) to get

$$\langle P_C y - P_C x, P_C x - x \rangle \geq 0, \tag{17.11}$$

and

$$\langle P_C x - P_C y, P_C y - y \rangle \geq 0. \tag{17.12}$$

Add the two inequalities to obtain

$$\langle P_C x - P_C y, x - y \rangle \geq ||P_C x - P_C y||_2^2, \tag{17.13}$$

and use the Cauchy Inequality. ∎

Because the operator P_C has multiple fixed points, P_C cannot be a strict contraction, unless the set C is a singleton set.

P_C is Firmly Non-expansive

Definition 17.5 *An operator T is said to be* firmly non-expansive *(fne) if*

$$\langle Tx - Ty, x - y \rangle \geq ||Tx - Ty||_2^2, \tag{17.14}$$

for all x and y in R^J.

Lemma 17.6 *An operator T is fne if and only if $G = I - T$ is fne.*

Proof: Use the identity in Equation (17.7). ∎

From Equation (17.13), we see that the operator $T = P_C$ is not simply ne, but fne, as well. A good source for more material on these topics is the book by Goebel and Reich [95].

The Search for Other Properties of P_C

The class of non-expansive operators is too large for our purposes; the operator $Tx = -x$ is non-expansive, but the sequence $\{T^k x^0\}$ does not converge, in general, even though a fixed point, $x = 0$, exists. The class of firmly non-expansive operators is too small for our purposes. Although the convergence of the iterative sequence $\{T^k x^0\}$ to a fixed point does hold for firmly non-expansive T, whenever fixed points exist, the product of two or more fne operators need not be fne; that is, the class of fne operators is not *closed to finite products*. This poses a problem, since, as we shall see, products of orthogonal projection operators arise in several of the algorithms we wish to consider. We need a class of operators smaller than the ne ones, but larger than the fne ones, closed to finite products, and for which the sequence of iterates $\{T^k x^0\}$ will converge, for any x^0, whenever fixed points exist. The class we shall consider is the class of *averaged* operators.

17.6 Averaged Operators

The term 'averaged operator' appears in the work of Baillon, Bruck and Reich [20, 8]. There are several ways to define averaged operators. One way is in terms of the complement operator.

Definition 17.6 *An operator G on R^J is called* ν-inverse strongly monotone *(ν-ism)[96] (also called co-coercive in [68]) if there is $\nu > 0$ such that*

$$\langle Gx - Gy, x - y\rangle \geq \nu||Gx - Gy||_2^2. \tag{17.15}$$

Lemma 17.7 *An operator T is ne if and only if its complement $G = I - T$ is $\frac{1}{2}$-ism, and T is fne if and only if G is 1-ism, and if and only if G is fne. Also, T is ne if and only if $F = (I + T)/2$ is fne. If G is ν-ism and $\gamma > 0$ then the operator γG is $\frac{\nu}{\gamma}$-ism.*

Definition 17.7 *An operator T is called averaged (av) if $G = I - T$ is ν-ism for some $\nu > \frac{1}{2}$. If G is $\frac{1}{2\alpha}$-ism, for some $\alpha \in (0, 1)$, then we say that T is α-av.*

It follows that every av operator is ne, with respect to the Euclidean norm, and every fne operator is av.

The averaged operators are sometimes defined in a different, but equivalent, way, using the following characterization of av operators.

Lemma 17.8 *An operator T is av if and only if, for some operator N that is non-expansive in the Euclidean norm, and $\alpha \in (0, 1)$, we have*

$$T = (1 - \alpha)I + \alpha N.$$

Consequently, the operator T is av if and only if, for some α in $(0, 1)$, the operator

$$N = \frac{1}{\alpha}T - \frac{1 - \alpha}{\alpha}I = I - \frac{1}{\alpha}(I - T) = I - \frac{1}{\alpha}G$$

is non-expansive.

Proof: We assume first that there is $\alpha \in (0, 1)$ and ne operator N such that $T = (1 - \alpha)I + \alpha N$, and so $G = I - T = \alpha(I - N)$. Since N is ne, $I - N$ is $\frac{1}{2}$-ism and $G = \alpha(I - N)$ is $\frac{1}{2\alpha}$-ism. Conversely, assume that G is ν-ism for some $\nu > \frac{1}{2}$. Let $\alpha = \frac{1}{2\nu}$ and write $T = (1 - \alpha)I + \alpha N$ for $N = I - \frac{1}{\alpha}G$. Since $I - N = \frac{1}{\alpha}G$, $I - N$ is $\alpha\nu$-ism. Consequently $I - N$ is $\frac{1}{2}$-ism and N is ne. ∎

An averaged operator is easily constructed from a given ne operator N by taking a convex combination of N and the identity I. The beauty of the class of av operators is that it contains many operators, such as P_C, that

are not originally defined in this way. As we shall show in an appendix, finite products of averaged operators are again averaged, so the product of finitely many orthogonal projections is av.

Proposition 17.1 *An operator F is firmly non-expansive if and only if $F = \frac{1}{2}(I + N)$, for some non-expansive operator N.*

17.6.1 Gradient Operators

Another type of operator that is averaged can be derived from gradient operators.

Definition 17.8 *An operator T on R^J is* monotone *if*

$$\langle Tx - Ty, x - y\rangle \geq 0, \tag{17.16}$$

for all x and y.

Firmly non-expansive operators on R^J are monotone operators. Let $g(x) : R^J \to R$ be a differentiable convex function and $f(x) = \nabla g(x)$ its gradient. The operator ∇g is also monotone. If ∇g is non-expansive, then, according to Theorem 8.12, ∇g is fne . If, for some $L > 0$, ∇g is L-Lipschitz, for the 2-norm, that is,

$$||\nabla g(x) - \nabla g(y)||_2 \leq L||x - y||_2, \tag{17.17}$$

for all x and y, then $\frac{1}{L}\nabla g$ is ne, therefore fne, and the operator $T = I - \gamma\nabla g$ is av, for $0 < \gamma < \frac{2}{L}$.

17.6.2 The Krasnoselskii-Mann Theorem

For any operator T that is averaged, convergence of the sequence $\{T^k x^0\}$ to a fixed point of T, whenever fixed points of T exist, is guaranteed by the Krasnoselskii-Mann (KM) Theorem [121]:

Theorem 17.2 *Let T be averaged. Then the sequence $\{T^k x^0\}$ converges to a fixed point of T, whenever Fix(T) is non-empty.*

Proof: Let z be a fixed point of non-expansive operator N and let $\alpha \in (0, 1)$. Let $T = (1 - \alpha)I + \alpha N$, so the iterative step becomes

$$x^{k+1} = Tx^k = (1 - \alpha)x^k + \alpha N x^k. \tag{17.18}$$

The identity in Equation (17.6) is the key to proving Theorem 17.2.

Using $Tz = z$ and $(I - T)z = 0$ and setting $G = I - T$ we have

$$||z - x^k||_2^2 - ||Tz - x^{k+1}||_2^2 = 2\langle Gz - Gx^k, z - x^k\rangle - ||Gz - Gx^k||_2^2.$$

(17.19)

Since, by Lemma 17.8, G is $\frac{1}{2\alpha}$-ism, we have

$$||z - x^k||_2^2 - ||z - x^{k+1}||_2^2 \geq (\frac{1}{\alpha} - 1)||x^k - x^{k+1}||_2^2. \tag{17.20}$$

Consequently the sequence $\{x^k\}$ is bounded, the sequence $\{||z - x^k||_2\}$ is decreasing and the sequence $\{||x^k - x^{k+1}||_2\}$ converges to zero. Let x^* be a cluster point of $\{x^k\}$. Then we have $Tx^* = x^*$, so we may use x^* in place of the arbitrary fixed point z. It follows then that the sequence $\{||x^* - x^k||_2\}$ is decreasing; since a subsequence converges to zero, the entire sequence converges to zero. The proof is complete. ∎

A version of the KM Theorem 17.2, with variable coefficients, appears in Reich's paper [137].

17.7 Affine Linear Operators

It may not always be easy to decide if a given operator is averaged. The class of affine linear operators provides an interesting illustration of the problem.

The affine operator $Tx = Bx + d$ will be ne, sc, fne, or av precisely when the linear operator given by multiplication by the matrix B is the same.

17.7.1 The Hermitian Case

As we shall see later, when B is Hermitian, we can determine if B belongs to these classes by examining its eigenvalues λ:

- B is non-expansive if and only if $-1 \leq \lambda \leq 1$, for all λ;
- B is averaged if and only if $-1 < \lambda \leq 1$, for all λ;
- B is a strict contraction if and only if $-1 < \lambda < 1$, for all λ;
- B is firmly non-expansive if and only if $0 \leq \lambda \leq 1$, for all λ.

Affine linear operators T that arise, for instance, in splitting methods for solving systems of linear equations, generally have non-Hermitian linear part B. Deciding if such operators belong to these classes is more difficult. Instead, we can ask if the operator is *paracontractive*, with respect to some norm.

17.8 Paracontractive Operators

By examining the properties of the orthogonal projection operators P_C, we were led to the useful class of averaged operators. The orthogonal projections also belong to another useful class, the paracontractions.

Definition 17.9 *An operator T is called* paracontractive *(pc), with respect to a given norm, if, for every fixed point y of T, we have*

$$||Tx - y|| < ||x - y||, \tag{17.21}$$

unless $Tx = x$.

Paracontractive operators are studied by Censor and Reich in [63].

Proposition 17.2 *The operators $T = P_C$ are paracontractive, with respect to the Euclidean norm.*

Proof: It follows from Cauchy's Inequality that

$$||P_C x - P_C y||_2 \leq ||x - y||_2,$$

with equality if and only if

$$P_C x - P_C y = \alpha(x - y),$$

for some scalar α with $|\alpha| = 1$. But, because

$$0 \leq \langle P_C x - P_C y, x - y \rangle = \alpha ||x - y||_2^2,$$

it follows that $\alpha = 1$, and so

$$P_C x - x = P_C y - y.$$

∎

When we ask if a given operator T is pc, we must specify the norm. We often construct the norm specifically for the operator involved, as we did earlier in our discussion of strict contractions, in Equation (17.5). To illustrate, we consider the case of affine operators.

17.8.1 Linear and Affine Paracontractions

Let the matrix B be diagonalizable and let the columns of V be an eigenvector basis. Then we have $V^{-1}BV = D$, where D is the diagonal matrix having the eigenvalues of B along its diagonal.

Lemma 17.9 *A square matrix B is diagonalizable if all its eigenvalues are distinct.*

Proof: Let B be J by J. Let λ_j be the eigenvalues of B, $Bx^j = \lambda_j x^j$, and $x^j \neq 0$, for $j = 1, ..., J$. Let x^m be the first eigenvector that is in the span of $\{x_j | j = 1, ..., m-1\}$. Then

$$x^m = a_1 x^1 + ...a_{m-1} x^{m-1}, \tag{17.22}$$

for some constants a_j that are not all zero. Multiply both sides by λ_m to get

$$\lambda_m x^m = a_1 \lambda_m x^1 + ...a_{m-1} \lambda_m x^{m-1}. \tag{17.23}$$

From

$$\lambda_m x^m = Ax^m = a_1 \lambda_1 x^1 + ...a_{m-1} \lambda_{m-1} x^{m-1}, \tag{17.24}$$

it follows that

$$a_1(\lambda_m - \lambda_1)x^1 + ... + a_{m-1}(\lambda_m - \lambda_{m-1})x^{m-1} = 0, \tag{17.25}$$

from which we can conclude that some x^n in $\{x^1, ..., x^{m-1}\}$ is in the span of the others. This is a contradiction. ∎

We see from this Lemma that almost all square matrices B are diagonalizable. Indeed, all Hermitian B are diagonalizable. If B has real entries, but is not symmetric, then the eigenvalues of B need not be real, and the eigenvectors of B can have non-real entries. Consequently, we must consider B as a linear operator on C^J, if we are to talk about diagonalizability. For example, consider the real matrix

$$B = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{17.26}$$

Its eigenvalues are $\lambda = i$ and $\lambda = -i$. The corresponding eigenvectors are $(1, i)^T$ and $(1, -i)^T$. The matrix B is then diagonalizable as an operator on C^2, but not as an operator on R^2.

Proposition 17.3 *Let T be an affine linear operator whose linear part B is diagonalizable, and $|\lambda| < 1$ for all eigenvalues λ of B that are not equal to one. Then the operator T is pc, with respect to the norm given by Equation (17.5).*

Proof: This is Exercise 17.8. ∎

We see from Proposition 17.3 that, for the case of affine operators T whose linear part is not Hermitian, instead of asking if T is av, we can ask if T is pc; since B will almost certainly be diagonalizable, we can answer this question by examining the eigenvalues of B.

Unlike the class of averaged operators, the class of paracontractive operators is not necessarily closed to finite products, unless those factor operators have a common fixed point.

17.8.2 The Elsner-Koltracht-Neumann Theorem

Our interest in paracontractions is due to the Elsner-Koltracht-Neumann (EKN) Theorem [85]:

Theorem 17.3 *Let T be pc with respect to some vector norm. If T has fixed points, then the sequence $\{T^k x^0\}$ converges to a fixed point of T, for all starting vectors x^0.*

We follow the development in [85].

Theorem 17.4 *Suppose that there is a vector norm on R^J, with respect to which each T_i is a pc operator, for $i = 1, ..., I$, and that $F = \cap_{i=1}^{I} \mathrm{Fix}(T_i)$ is not empty. For $k = 0, 1, ...$, let $i(k) = k(\mathrm{mod}\, I) + 1$, and $x^{k+1} = T_{i(k)} x^k$. The sequence $\{x^k\}$ converges to a member of F, for every starting vector x^0.*

Proof: Let $y \in F$. Then, for $k = 0, 1, ...$,

$$||x^{k+1} - y|| = ||T_{i(k)} x^k - y|| \leq ||x^k - y||, \tag{17.27}$$

so that the sequence $\{||x^k - y||\}$ is decreasing; let $d \geq 0$ be its limit. Since the sequence $\{x^k\}$ is bounded, we select an arbitrary cluster point, x^*. Then $d = ||x^* - y||$, from which we can conclude that

$$||T_i x^* - y|| = ||x^* - y||, \tag{17.28}$$

and $T_i x^* = x^*$, for $i = 1, ..., I$; therefore, $x^* \in F$. Replacing y, an arbitrary member of F, with x^*, we have that $||x^k - x^*||$ is decreasing. But, a subsequence converges to zero, so the whole sequence must converge to zero. This completes the proof. ∎

Corollary 17.1 *If T is pc with respect to some vector norm, and T has fixed points, then the iterative sequence $\{T^k x^0\}$ converges to a fixed point of T, for every starting vector x^0.*

Corollary 17.2 *If $T = T_I T_{I-1} \cdots T_2 T_1$, and $F = \cap_{i=1}^{I} \mathrm{Fix}\,(T_i)$ is not empty, then $F = \mathrm{Fix}\,(T)$.*

Proof: The sequence $x^{k+1} = T_{i(k)} x^k$ converges to a member of $\mathrm{Fix}\,(T)$, for every x^0. Select x^0 in F. ∎

Corollary 17.3 *The product T of two or more pc operators T_i, $i = 1, ..., I$ is again a pc operator, if $F = \cap_{i=1}^{I} \mathrm{Fix}\,(T_i)$ is not empty.*

Proof: Suppose that for $T = T_I T_{I-1} \cdots T_2 T_1$, and $y \in F = \mathrm{Fix}\,(T)$, we have

$$||Tx - y|| = ||x - y||. \tag{17.29}$$

Then, since

$$||T_I(T_{I-1} \cdots T_1)x - y|| \leq ||T_{I-1} \cdots T_1 x - y|| \leq ... \leq ||T_1 x - y|| \leq ||x - y||, \tag{17.30}$$

it follows that

$$||T_i x - y|| = ||x - y||, \tag{17.31}$$

and $T_i x = x$, for each i. Therefore, $Tx = x$. ∎

17.9 Exercises

17.1 *Show that a strict contraction can have at most one fixed point.*

17.2 *Let T be sc. Show that the sequence $\{T^k x_0\}$ is a Cauchy sequence. Hint: consider*

$$||x^k - x^{k+n}|| \leq ||x^k - x^{k+1}|| + ... + ||x^{k+n-1} - x^{k+n}||, \tag{17.32}$$

and use

$$||x^{k+m} - x^{k+m+1}|| \leq r^m ||x^k - x^{k+1}||. \tag{17.33}$$

Since $\{x^k\}$ is a Cauchy sequence, it has a limit, say $\hat{x}$. Let $e^k = \hat{x} - x^k$. Show that $\{e^k\} \to 0$, as $k \to +\infty$, so that $\{x^k\} \to \hat{x}$. Finally, show that $T\hat{x} = \hat{x}$.

17.3 *Suppose that we want to solve the equation*

$$x = \frac{1}{2} e^{-x}.$$

Let $Tx = \frac{1}{2} e^{-x}$ for x in R. Show that T is a strict contraction, when restricted to non-negative values of x, so that, provided we begin with $x^0 > 0$, the sequence $\{x^k = Tx^{k-1}\}$ converges to the unique solution of the equation. Hint: use the mean value theorem from calculus.

17.4 *Prove Lemma 17.2.*

17.5 *Show that, if the operator T is α-av and $1 > \beta > \alpha$, then T is β-av.*

17.6 *Prove Lemma 17.7.*

17.7 *Prove Proposition 17.1.*

17.8 *Prove Proposition 17.3.*

17.9 *Show that, if B is a linear av operator, then $|\lambda| < 1$ for all eigenvalues λ of B that are not equal to one.*

17.10 Course Homework

Do all the exercises in this chapter.

Chapter 18

Compressed Sensing

18.1 Chapter Summary

One area that has attracted much attention lately is *compressed sensing* or *compressed sampling* (CS) [77]. For applications such as medical imaging, CS may provide a means of reducing radiation dosage to the patient without sacrificing image quality. An important aspect of CS is finding sparse solutions of under-determined systems of linear equations, which can often be accomplished by one-norm minimization. Perhaps the best reference to date on CS is [21].

18.2 Compressed Sensing

The objective in CS is exploit sparseness to reconstruct a vector f in R^J from relatively few linear functional measurements [77].

Let $U = \{u^1, u^2, ..., u^J\}$ and $V = \{v^1, v^2, ..., v^J\}$ be two orthonormal bases for R^J, with all members of R^J represented as column vectors. For $i = 1, 2, ..., J$, let

$$\mu_i = \max_{1 \leq j \leq J} \{|\langle u^i, v^j \rangle|\}$$

and

$$\mu(U, V) = \max\{\mu_i \, | i = 1, ..., I\}.$$

We know from Cauchy's Inequality that

$$|\langle u^i, v^j \rangle| \leq 1,$$

and from Parseval's Equation

$$\sum_{j=1}^{J} |\langle u^i, v^j \rangle|^2 = ||u^i||^2 = 1.$$

Therefore, we have

$$\frac{1}{\sqrt{J}} \leq \mu(U,V) \leq 1.$$

The quantity $\mu(U,V)$ is the *coherence* measure of the two bases; the closer $\mu(U,V)$ is to the lower bound of $\frac{1}{\sqrt{J}}$, the more *incoherent* the two bases are.

Let f be a fixed member of R^J; we expand f in the V basis as

$$f = x_1 v^1 + x_2 v^2 + ... + x_J v^J.$$

We say that the coefficient vector $x = (x_1, ..., x_J)$ is s-sparse if s is the number of non-zero x_j.

If s is small, most of the x_j are zero, but since we do not know which ones these are, we would have to compute all the linear functional values

$$x_j = \langle f, v^j \rangle$$

to recover f exactly. In fact, the smaller s is, the harder it would be to learn anything from randomly selected x_j, since most would be zero. The idea in CS is to obtain measurements of f with members of a different orthonormal basis, which we call the U basis. If the members of U are very much like the members of V, then nothing is gained. But, if the members of U are quite unlike the members of V, then each inner product measurement

$$y_i = \langle f, u^i \rangle = f^T u^i$$

should tell us something about f. If the two bases are sufficiently incoherent, then relatively few y_i values should tell us quite a bit about f. Specifically, we have the following result due to Candès and Romberg [53]: suppose the coefficient vector x for representing f in the V basis is s-sparse. Select uniformly randomly $M \leq J$ members of the U basis and compute the measurements $y_i = \langle f, u^i \rangle$. Then, if M is sufficiently large, it is highly probable that $z = x$ also solves the problem of minimizing the one-norm

$$||z||_1 = |z_1| + |z_2| + ... + |z_J|,$$

subject to the conditions

$$y_i = \langle g, u^i \rangle = g^T u^i,$$

for those M randomly selected u^i, where

$$g = z_1 v^1 + z_2 v^2 + ... + z_J v^J.$$

The smaller $\mu(U,V)$ is, the smaller the M is permitted to be without reducing the probability of perfect reconstruction.

18.3 Sparse Solutions

Suppose that A is a real M by N matrix, with $M < N$, and that the linear system $Ax = b$ has infinitely many solutions. For any vector x, we define the *support* of x to be the subset S of $\{1, 2, ..., N\}$ consisting of those n for which the entries $x_n \neq 0$. For any under-determined system $Ax = b$, there will, of course, be at least one solution of minimum support, that is, for which $s = |S|$, the size of the support set S, is minimum. However, finding such a maximally sparse solution requires combinatorial optimization, and is known to be computationally difficult. It is important, therefore, to have a computationally tractable method for finding maximally sparse solutions.

18.3.1 Maximally Sparse Solutions

Consider the problem P_0: among all solutions x of the consistent system $b = Ax$, find one, call it $\hat{x}$, that is maximally sparse, that is, has the minimum number of non-zero entries. Obviously, there will be at least one such solution having minimal support, but finding one, however, is a combinatorial optimization problem and is generally NP-hard.

18.3.2 Minimum One-Norm Solutions

Instead, we can seek a *minimum one-norm* solution, that is, solve the problem P_1: minimize

$$||x||_1 = \sum_{n=1}^{N} |x_n|,$$

subject to $Ax = b$. Problem P_1 can be formulated as a linear programming problem, so is more easily solved. The big questions are: when does P_1 have a unique solution, and when is it $\hat{x}$? The problem P_1 will have a unique solution if and only if A is such that the one-norm satisfies

$$||\hat{x}||_1 < ||\hat{x} + v||_1,$$

for all non-zero v in the null space of A.

18.3.3 Why the One-Norm?

When a system of linear equations $Ax = b$ is under-determined, we can find the *minimum-two-norm solution* that minimizes the square of the two-norm,

$$||x||_2^2 = \sum_{n=1}^{N} x_n^2,$$

subject to $Ax = b$. One drawback to this approach is that the two-norm penalizes relatively large values of x_n much more than the smaller ones, so tends to provide non-sparse solutions. Alternatively, we may seek the solution for which the one-norm,

$$||x||_1 = \sum_{n=1}^{N} |x_n|,$$

is minimized. The one-norm still penalizes relatively large entries x_n more than the smaller ones, but much less than the two-norm does. As a result, it often happens that the minimum one-norm solution actually solves P_0 as well.

18.3.4 Comparison with the PDFT

The PDFT approach [25, 26] to solving the under-determined system $Ax = b$ is to select weights $w_n > 0$ and then to find the solution $\tilde{x}$ that minimizes the weighted two-norm given by

$$\sum_{n=1}^{N} |x_n|^2 w_n.$$

Our intention is to select weights w_n so that w_n^{-1} is reasonably close to $|\hat{x}_n|$; consider, therefore, what happens when $w_n^{-1} = |\hat{x}_n|$. We claim that $\tilde{x}$ is also a minimum-one-norm solution.

To see why this is true, note that, for any x, we have

$$\sum_{n=1}^{N} |x_n| = \sum_{n=1}^{N} \frac{|x_n|}{\sqrt{|\hat{x}_n|}} \sqrt{|\hat{x}_n|}$$

$$\leq \sqrt{\sum_{n=1}^{N} \frac{|x_n|^2}{|\hat{x}_n|}} \sqrt{\sum_{n=1}^{N} |\hat{x}_n|}.$$

Therefore,

$$\sum_{n=1}^{N} |\tilde{x}_n| \leq \sqrt{\sum_{n=1}^{N} \frac{|\tilde{x}_n|^2}{|\hat{x}_n|}} \sqrt{\sum_{n=1}^{N} |\hat{x}_n|}$$

$$\leq \sqrt{\sum_{n=1}^{N} \frac{|\hat{x}_n|^2}{|\hat{x}_n|}} \sqrt{\sum_{n=1}^{N} |\hat{x}_n|} = \sum_{n=1}^{N} |\hat{x}_n|.$$

Therefore, $\tilde{x}$ also minimizes the one-norm.

18.3.5 Iterative Reweighting

We want each weight w_n to be a good prior estimate of the reciprocal of $|\hat{x}_n|$. Because we do not yet know $\hat{x}$, we may take a sequential-optimization approach, beginning with weights $w_n^0 > 0$, finding the PDFT solution using these weights, then using this PDFT solution to get a (we hope!) a better choice for the weights, and so on. This sequential approach was successfully implemented in the early 1980's by Michael Fiddy and his students [90].

In [54], the same approach is taken, but with respect to the one-norm. Since the one-norm still penalizes larger values disproportionately, balance can be achieved by minimizing a weighted-one-norm, with weights close to the reciprocals of the $|\hat{x}_n|$. Again, not yet knowing $\hat{x}$, they employ a sequential approach, using the previous minimum-weighted-one-norm solution to obtain the new set of weights for the next minimization. At each step of the sequential procedure, the previous reconstruction is used to estimate the true support of the desired solution.

It is interesting to note that an on-going debate among users of the PDFT has been the nature of the prior weighting. Does w_n approximate $|x_n|$ or $|x_n|^2$? This is close to the issue treated in [54], the use of a weight in the minimum-one-norm approach.

It should be noted again that finding a sparse solution is not usually the goal in the use of the PDFT, but the use of the weights has much the same effect as using the one-norm to find sparse solutions: to the extent that the weights approximate the entries of $\hat{x}$, their use reduces the penalty associated with the larger entries of an estimated solution.

18.4 Why Sparseness?

One obvious reason for wanting sparse solutions of $Ax = b$ is that we have prior knowledge that the desired solution is sparse. Such a problem arises in signal analysis from Fourier-transform data. In other cases, such as in the reconstruction of locally constant signals, it is not the signal itself, but its discrete derivative, that is sparse.

18.4.1 Signal Analysis

Suppose that our signal $f(t)$ is known to consist of a small number of complex exponentials, so that $f(t)$ has the form

$$f(t) = \sum_{j=1}^{J} a_j e^{i\omega_j t},$$

for some small number of frequencies ω_j in the interval $[0, 2\pi)$. For $n = 0, 1, ..., N-1$, let $f_n = f(n)$, and let f be the N-vector with entries f_n;

we assume that J is much smaller than N. The discrete (vector) Fourier transform of f is the vector $\hat{f}$ having the entries

$$\hat{f}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} f_n e^{2\pi i k n/N},$$

for $k = 0, 1, ..., N-1$; we write $\hat{f} = Ef$, where E is the N by N matrix with entries $E_{kn} = \frac{1}{\sqrt{N}} e^{2\pi i k n/N}$. If N is large enough, we may safely assume that each of the ω_j is equal to one of the frequencies $2\pi i k$ and that the vector $\hat{f}$ is J-sparse. The question now is: How many values of $f(n)$ do we need to calculate in order to be sure that we can recapture $f(t)$ exactly? We have the following theorem [52]:

Theorem 18.1 *Let N be prime. Let S be any subset of $\{0, 1, ..., N-1\}$ with $|S| \geq 2J$. Then the vector $\hat{f}$ can be uniquely determined from the measurements f_n for n in S.*

We know that

$$f = E^\dagger \hat{f},$$

where $E^\dagger$ is the conjugate transpose of the matrix E. The point here is that, for any matrix R obtained from the identity matrix I by deleting $N - |S|$ rows, we can recover the vector $\hat{f}$ from the measurements Rf.

If N is not prime, then the assertion of the theorem may not hold, since we can have $n = 0 \bmod N$, without $n = 0$. However, the assertion remains valid for most sets of J frequencies and most subsets S of indices; therefore, with high probability, we can recover the vector $\hat{f}$ from Rf.

Note that the matrix E is *unitary*, that is, $E^\dagger E = I$, and, equivalently, the columns of E form an orthonormal basis for C^N. The data vector is

$$b = Rf = RE^\dagger \hat{f}.$$

In this example, the vector f is not sparse, but can be represented sparsely in a particular orthonormal basis, namely as $f = E^\dagger \hat{f}$, using a sparse vector $\hat{f}$ of coefficients. The *representing basis* then consists of the columns of the matrix $E^\dagger$. The measurements pertaining to the vector f are the values f_n, for n in S. Since f_n can be viewed as the inner product of f with δ^n, the nth column of the identity matrix I, that is,

$$f_n = \langle \delta^n, f \rangle,$$

the columns of I provide the so-called *sampling basis*. With $A = RE^\dagger$ and $x = \hat{f}$, we then have

$$Ax = b,$$

with the vector x sparse. It is important for what follows to note that the matrix A is random, in the sense that we choose which rows of I to use to form R.

18.4.2 Locally Constant Signals

Suppose now that the function $f(t)$ is locally constant, consisting of some number of horizontal lines. We discretize the function $f(t)$ to get the vector $f = (f(0), f(1), ..., f(N))^T$. The discrete derivative vector is $g = (g_1, g_2, ..., g_N)^T$, with

$$g_n = f(n) - f(n-1).$$

Since $f(t)$ is locally constant, the vector g is sparse. The data we will have will not typically be values $f(n)$. The goal will be to recover f from M linear functional values pertaining to f, where M is much smaller than N. We shall assume, from now on, that we have measured, or can estimate, the value $f(0)$.

Our M by 1 data vector d consists of measurements pertaining to the vector f:

$$d_m = \sum_{n=0}^{N} H_{mn} f_n,$$

for $m = 1, ..., M$, where the H_{mn} are known. We can then write

$$d_m = f(0)\Big(\sum_{n=0}^{N} H_{mn}\Big) + \sum_{k=1}^{N}\Big(\sum_{j=k}^{N} H_{mj}\Big) g_k.$$

Since $f(0)$ is known, we can write

$$b_m = d_m - f(0)\Big(\sum_{n=0}^{N} H_{mn}\Big) = \sum_{k=1}^{N} A_{mk} g_k,$$

where

$$A_{mk} = \sum_{j=k}^{N} H_{mj}.$$

The problem is then to find a sparse solution of $Ax = g$. As in the previous example, we often have the freedom to select the linear functions, that is, the values H_{mn}, so the matrix A can be viewed as random.

18.4.3 Tomographic Imaging

The reconstruction of tomographic images is an important aspect of medical diagnosis, and one that combines aspects of both of the previous examples. The data one obtains from the scanning process can often be interpreted as values of the Fourier transform of the desired image; this is precisely the case in magnetic-resonance imaging, and approximately true for x-ray transmission tomography, positron-emission tomography (PET)

and single-photon emission tomography (SPECT). The images one encounters in medical diagnosis are often approximately locally constant, so the associated array of discrete partial derivatives will be sparse. If this sparse derivative array can be recovered from relatively few Fourier-transform values, then the scanning time can be reduced.

We turn now to the more general problem of compressed sampling.

18.5 Compressed Sampling

Our goal is to recover the vector $f = (f_1, ..., f_N)^T$ from M linear functional values of f, where M is much less than N. In general, this is not possible without prior information about the vector f. In compressed sampling, the prior information concerns the sparseness of either f itself, or another vector linearly related to f.

Let U and V be unitary N by N matrices, so that the column vectors of both U and V form orthonormal bases for C^N. We shall refer to the bases associated with U and V as the *sampling basis* and the *representing basis*, respectively. The first objective is to find a unitary matrix V so that $f = Vx$, where x is sparse. Then we want to find a second unitary matrix U such that, when an M by N matrix R is obtained from U by deleting rows, the sparse vector x can be determined from the data $b = RVx = Ax$. Theorems in compressed sensing describe properties of the matrices U and V such that, when R is obtained from U by a random selection of the rows of U, the vector x will be uniquely determined, with high probability, as the unique solution that minimizes the one-norm.

Chapter 19

Bregman-Legendre Functions

19.1 Chapter Summary

In [11] Bauschke and Borwein show convincingly that the Bregman-Legendre functions provide the proper context for the discussion of Bregman projections onto closed convex sets. The summary here follows closely the discussion given in [11].

19.2 Essential Smoothness and Essential Strict Convexity

Following [140] we say that a closed proper convex function f is *essentially smooth* if int$D$ is not empty, f is differentiable on int$D$ and $x^n \in \text{int}D$, with $x^n \to x \in \text{bd}D$, implies that $||\nabla f(x^n)|| \to +\infty$. Here int$D$ and bd$D$ denote the interior and boundary of the set D. A closed proper convex function f is *essentially strictly convex* if f is strictly convex on every convex subset of dom ∂f.

The closed proper convex function f is essentially smooth if and only if the subdifferential $\partial f(x)$ is empty for $x \in \text{bd}D$ and is $\{\nabla f(x)\}$ for $x \in \text{int}D$ (so f is differentiable on int$D$) if and only if the function f^* is essentially strictly convex.

Definition 19.1 *A closed proper convex function f is said to be a* Legendre function *if it is both essentially smooth and essentialy strictly convex.*

So f is Legendre if and only if its conjugate function is Legendre, in which case the gradient operator ∇f is a topological isomorphism with

∇f^* as its inverse. The gradient operator ∇f maps int dom f onto int dom f^*. If int dom $f^* = R^J$ then the range of ∇f is R^J and the equation $\nabla f(x) = y$ can be solved for every $y \in R^J$. In order for int dom $f^* = R^J$ it is necessary and sufficient that the Legendre function f be *super-coercive*, that is,

$$\lim_{||x|| \to +\infty} \frac{f(x)}{||x||} = +\infty. \tag{19.1}$$

If the effective domain of f is bounded, then f is super-coercive and its gradient operator is a mapping onto the space R^J.

19.3 Bregman Projections onto Closed Convex Sets

Let f be a closed proper convex function that is differentiable on the nonempty set int$D$. The corresponding *Bregman distance* $D_f(x, z)$ is defined for $x \in R^J$ and $z \in \text{int}D$ by

$$D_f(x, z) = f(x) - f(z) - \langle \nabla f(z), x - z \rangle. \tag{19.2}$$

Note that $D_f(x, z) \geq 0$ always and that $D_f(x, z) = +\infty$ is possible. If f is essentially strictly convex then $D_f(x, z) = 0$ implies that $x = z$.

Let K be a nonempty closed convex set with $K \cap \text{int}D \neq \emptyset$. Pick $z \in \text{int}D$. The *Bregman projection* of z onto K, with respect to f, is

$$P_K^f(z) = \text{argmin}_{x \in K \cap D} D_f(x, z). \tag{19.3}$$

If f is essentially strictly convex, then $P_K^f(z)$ exists. If f is strictly convex on D then $P_K^f(z)$ is unique. If f is Legendre, then $P_K^f(z)$ is uniquely defined and is in int$D$; this last condition is sometimes called *zone consistency*.

Example: Let $J = 2$ and $f(x)$ be the function that is equal to one-half the norm squared on D, the nonnegative quadrant, $+\infty$ elsewhere. Let K be the set $K = \{(x_1, x_2) | x_1 + x_2 = 1\}$. The Bregman projection of $(2, 1)$ onto K is $(1, 0)$, which is not in int$D$. The function f is not essentially smooth, although it is essentially strictly convex. Its conjugate is the function f^* that is equal to one-half the norm squared on D and equal to zero elsewhere; it is essentially smooth, but not essentially strictly convex.

If f is Legendre, then $P_K^f(z)$ is the unique member of $K \cap \text{int}D$ satisfying the inequality

$$\langle \nabla f(P_K^f(z)) - \nabla f(z), P_K^f(z) - c \rangle \geq 0, \tag{19.4}$$

for all $c \in K$. From this we obtain the *Bregman Inequality*:

$$D_f(c, z) \geq D_f(c, P_K^f(z)) + D_f(P_K^f(z), z), \tag{19.5}$$

for all $c \in K$.

19.4 Bregman-Legendre Functions

Following Bauschke and Borwein [11], we say that a Legendre function f is a *Bregman-Legendre* function if the following properties hold:

B1: for x in D and any $a > 0$ the set $\{z|D_f(x,z) \leq a\}$ is bounded.
B2: if x is in D but not in int$D$, for each positive integer n, y^n is in int$D$ with $y^n \to y \in \text{bd}D$ and if $\{D_f(x,y^n)\}$ remains bounded, then $D_f(y,y^n) \to 0$, so that $y \in D$.
B3: if x^n and y^n are in int$D$, with $x^n \to x$ and $y^n \to y$, where x and y are in D but not in int$D$, and if $D_f(x^n,y^n) \to 0$ then $x = y$.

Bauschke and Borwein then prove that Bregman's SGP method converges to a member of K provided that one of the following holds: 1) f is Bregman-Legendre; 2) $K \cap \text{int}D \neq \emptyset$ and dom f^* is open; or 3) dom f and dom f^* are both open.

The Bregman functions form a class closely related to the Bregman-Legendre functions. For details see [23].

19.5 Useful Results about Bregman-Legendre Functions

The following results are proved in somewhat more generality in [11].
R1: If $y^n \in$ int dom f and $y^n \to y \in$ int dom f, then $D_f(y,y^n) \to 0$.
R2: If x and $y^n \in$ int dom f and $y^n \to y \in$ bd dom f, then $D_f(x,y^n) \to +\infty$.
R3: If $x^n \in D$, $x^n \to x \in D$, $y^n \in$ int D, $y^n \to y \in D$, $\{x,y\} \cap$ int $D \neq \emptyset$ and $D_f(x^n,y^n) \to 0$, then $x = y$ and $y \in$ int D.
R4: If x and y are in D, but are not in int D, $y^n \in$ int D, $y^n \to y$ and $D_f(x,y^n) \to 0$, then $x = y$.
As a consequence of these results we have the following.
R5: If $\{D_f(x,y^n)\} \to 0$, for $y^n \in$ int D and $x \in R^J$, then $\{y^n\} \to x$.

Proof of R5: Since $\{D_f(x,y^n)\}$ is eventually finite, we have $x \in D$. By Property B1 above it follows that the sequence $\{y^n\}$ is bounded; without loss of generality, we assume that $\{y^n\} \to y$, for some $y \in \overline{D}$. If x is in int D, then, by result R2 above, we know that y is also in int D. Applying result R3, with $x^n = x$, for all n, we conclude that $x = y$. If, on the other hand, x is in D, but not in int D, then y is in D, by result R2. There are two cases to consider: 1) y is in int D; 2) y is not in int D. In case 1) we have $D_f(x,y^n) \to D_f(x,y) = 0$, from which it follows that $x = y$. In case 2) we apply result R4 to conclude that $x = y$. ∎

Chapter 20

Constrained Linear Systems

20.1 Chapter Summary

The ART and its simultaneous and block-iterative versions are designed to solve general systems of linear equations $Ax = b$. The SMART, EMML, MART, EM-MART and related methods require that the entries of A be nonnegative, those of b positive and produce nonnegative x. In this chapter we present variations of the SMART and EMML that impose the constraints $u_j \leq x_j \leq v_j$, where the u_j and v_j are selected lower and upper bounds on the individual entries x_j. These algorithms were used in [127] as a method for including in transmission tomographic reconstruction spatially varying upper and lower bounds on the x-ray attenuation.

20.2 Modifying the KL distance

Simultaneous iterative algorithms employ all of the equations at each step of the iteration; block-iterative methods do not. For the latter methods we assume that the index set $\{i = 1, ..., I\}$ is the (not necessarily disjoint) union of the N sets or *blocks* B_n, $n = 1, ..., N$. We shall require that $s_{nj} = \sum_{i \in B_n} A_{ij} > 0$ for each n and each j. Block-iterative methods like ART and MART for which each block consists of precisely one element are called *row-action* or *sequential* methods.

The SMART, EMML, MART and EM-MART methods are based on the Kullback-Leibler distance between nonnegative vectors. To impose more general constraints on the entries of x we derive algorithms based on shifted KL distances, also called *Fermi-Dirac generalized entropies*.

For a fixed real vector u, the shifted KL distance $KL(x-u, z-u)$ is defined for vectors x and z having $x_j \geq u_j$ and $z_j \geq u_j$. Similarly, the shifted distance $KL(v-x, v-z)$ applies only to those vectors x and z for which $x_j \leq v_j$ and $z_j \leq v_j$. For $u_j \leq v_j$, the combined distance

$$KL(x-u, z-u) + KL(v-x, v-z)$$

is restricted to those x and z whose entries x_j and z_j lie in the interval $[u_j, v_j]$. Our objective is to mimic the derivation of the SMART and EMML methods, replacing KL distances with shifted KL distances, to obtain algorithms that enforce the constraints $u_j \leq x_j \leq v_j$, for each j. The algorithms that result are the ABMART and ABEMML block-iterative methods. These algorithms were originally presented in [37], in which the vectors u and v were called a and b, hence the names of the algorithms. Throughout this chapter we shall assume that the entries of the matrix A are nonnegative. We shall denote by B_n, $n = 1, ..., N$ a partition of the index set $\{i = 1, ..., I\}$ into blocks. For $k = 0, 1, ...$ let $n(k) = k(\mathrm{mod}\, N)+1$.

The projected Landweber algorithm can also be used to impose the restrictions $u_j \leq x_j \leq v_j$; however, the projection step in that algorithm is implemented by clipping, or setting equal to u_j or v_j values of x_j that would otherwise fall outside the desired range. The result is that the values u_j and v_j can occur more frequently than may be desired. One advantage of the AB methods is that the values u_j and v_j represent barriers that can only be reached in the limit and are never taken on at any step of the iteration.

20.3 The ABMART Algorithm

We assume that $(Au)_i \leq b_i \leq (Av)_i$ and seek a solution of $Ax = b$ with $u_j \leq x_j \leq v_j$, for each j. The algorithm begins with an initial vector x^0 satisfying $u_j \leq x_j^0 \leq v_j$, for each j. Having calculated x^k, we take

$$x_j^{k+1} = \alpha_j^k v_j + (1 - \alpha_j^k) u_j, \tag{20.1}$$

with $n = n(k)$,

$$\alpha_j^k = \frac{c_j^k \prod^n (d_i^k)^{A_{ij}}}{1 + c_j^k \prod^n (d_i^k)^{A_{ij}}}, \tag{20.2}$$

$$c_j^k = \frac{(x_j^k - u_j)}{(v_j - x_j^k)}, \tag{20.3}$$

and

$$d_j^k = \frac{(b_i - (Au)_i)((Av)_i - (Ax^k)_i)}{((Av)_i - b_i)((Ax^k)_i - (Au)_i)}, \tag{20.4}$$

where $\prod^n$ denotes the product over those indices i in $B_{n(k)}$. Notice that, at each step of the iteration, x_j^k is a convex combination of the endpoints u_j and v_j, so that x_j^k lies in the interval $[u_j, v_j]$.

We have the following theorem concerning the convergence of the AB-MART algorithm:

Theorem 20.1 *If there is a solution of the system $Ax = b$ that satisfies the constraints $u_j \leq x_j \leq v_j$ for each j, then, for any N and any choice of the blocks B_n, the ABMART sequence converges to that constrained solution of $Ax = b$ for which the Fermi-Dirac generalized entropic distance from x to x^0,*

$$KL(x - u, x^0 - u) + KL(v - x, v - x^0),$$

is minimized. If there is no constrained solution of $Ax = b$, then, for $N = 1$, the ABMART sequence converges to the minimizer of

$$KL(Ax - Au, b - Au) + KL(Av - Ax, Av - b)$$

for which

$$KL(x - u, x^0 - u) + KL(v - x, v - x^0)$$

is minimized.

The proof is in [37].

20.4 The ABEMML Algorithm

We make the same assumptions as in the previous section. The iterative step of the ABEMML algorithm is

$$x_j^{k+1} = \alpha_j^k v_j + (1 - \alpha_j^k) u_j, \tag{20.5}$$

where

$$\alpha_j^k = \gamma_j^k / d_j^k, \tag{20.6}$$

$$\gamma_j^k = (x_j^k - u_j) e_j^k, \tag{20.7}$$

$$\beta_j^k = (v_j - x_j^k) f_j^k, \tag{20.8}$$

$$d_j^k = \gamma_j^k + \beta_j^k, \tag{20.9}$$

$$e_j^k = \left(1 - \sum_{i \in B_n} A_{ij}\right) + \sum_{i \in B_n} A_{ij} \left(\frac{b_i - (Au)_i}{(Ax^k)_i - (Au)_i}\right), \tag{20.10}$$

and

$$f_j^k = \left(1 - \sum_{i \in B_n} A_{ij}\right) + \sum_{i \in B_n} A_{ij} \left(\frac{(Av)_i - b_i}{(Av)_i - (Ax^k)_i}\right). \tag{20.11}$$

We have the following theorem concerning the convergence of the ABEMML algorithm:

Theorem 20.2 *If there is a solution of the system $Ax = b$ that satisfies the constraints $u_j \leq x_j \leq v_j$ for each j, then, for any N and any choice of the blocks B_n, the ABEMML sequence converges to such a constrained solution of $Ax = b$. If there is no constrained solution of $Ax = b$, then, for $N = 1$, the ABMART sequence converges to a constrained minimizer of*

$$KL(Ax - Au, b - Au) + KL(Av - Ax, Av - b).$$

The proof is found in [37]. In contrast to the ABMART theorem, this is all we can say about the limits of the ABEMML sequences.

Open Question: How does the limit of the ABEMML iterative sequence depend, in the consistent case, on the choice of blocks, and, in general, on the choice of x^0?

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