Iterative Algorithms in Tomography

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Abstract

The fundamental mathematical problem in tomographic image reconstruction is the solution, often approximate, of large systems of linear equations, which we denote here as $Ax = b$. The unknown entries of the vector x often represent intensity levels, of beam attenuation in transmission tomography, of radionuclide concentration in emission tomography, and so are naturally nonnegative. The entries of the vector b are typically counts of detected photons, the entries of the matrix A are lengths or probabilities, and so these quantities are also nonnegative. The size of these systems, typically thousands of equations and thousands of unknowns, preclude the use of Gauss elimination and necessitate iterative methods of solution. We survey a variety of such methods and present some open questions concerning their behavior.

The step sizes for iterative algorithms such as the Landweber method involve parameters that depend on the largest eigenvalue λ_{max} of the matrix $A^\dagger A$. Because of the size of A, calculating $A^\dagger A$, let alone finding its largest eigenvalue, is out of the question. Easily calculated upper bounds for λ_{max} are available that are particularly useful when A is sparse, that is, most of the entries of A are zero, which is typically the case in tomography. These bounds become tighter as the size of A increases.

1 Introduction

Image reconstruction from tomographic data is a fairly recent, and increasingly important, area of applied numerical linear algebra, particularly for medical diagnosis [36, 39, 47, 58, 59, 67, 68] . Fundamentally, the problem is to solve, at least approximately, a large system of linear equations, $Ax = b$. The vector x is large because it is usually a vectorization of a discrete approximation of a function of two or three continuous spatial variables. The size of the system necessitates the use of iterative solution methods [52]. Because the entries of x usually represent intensity levels, of beam attenuation in transmission tomography, and of radionuclide concentration in

emission tomography, we require x to be nonnegative; the physics of the situation may impose additional constraints on the entries of x. In practice, we often have prior knowledge about the function represented, in discrete form, by the vector x and we may wish to include this knowledge in the reconstruction. In tomography the entries of A and b are also nonnegative. Iterative algorithms tailored to find solutions to these special, constrained problems may out-perform general iterative solution methods [57]. To be medically useful in the clinic, the algorithms need to produce acceptable reconstructions early in the iterative process.

Exact solutions of $Ax = b$ may not exist, so we need appropriate measures of distance between vectors to obtain suitable approximate solutions. The entries of the vector b are data obtained by measurements, and so are noisy. Consequently, exact solutions of $Ax = b$, even when available, may be too noisy to be useful. Bayesian or penalized optimization algorithms are used to obtain reconstructions displaying the desired smoothness [31, 35, 37, 38, 53, 54].

Certain iterative algorithms require that we select a parameter that governs the size of the steps taken at each iteration. For the Landweber and projected Landweber methods [1], this parameter is dependent on the largest eigenvalue, λ_{max}, of the matrix $A^\dagger A$. Because the system is large, calculating $A^\dagger A$, let alone computing λ_{max}, is impractical. If we overestimate λ_{max}, the step lengths become too small and the algorithm is too slow to be practical; tight upper bounds for λ_{max} that can be obtained from A itself help to accelerate these algorithms. Upper bounds exist that are particularly useful for the common case in which A is sparse, that is, most of its entries are zero [13]. These upper bounds are shown to become tighter as the size of the system increases [18].

Our purpose here is to discuss various algorithms that are employed in tomographic image reconstruction, and to present several open questions concerning these algorithms.

2 Tomography

These days, the term *tomography* is used by lay people and practitioners alike to describe any sort of scan, from ultrasound to magnetic resonance. It has apparently lost its association with the idea of slicing, as in the expression *three-dimensional tomography*. In this paper we focus on two important modalities, transmission tomography and emission tomography. An x-ray CAT scan is an example of the first, a positron-emission (PET) scan is an example of the second. Although there is some flexibility

in the mathematical description of the image reconstruction problem posed by these methods, we shall concentrate here on the algebraic formulation of the problem. In this formulation, the problem is to solve, at least approximately, a large system of linear equations, $Ax = b$. What the entries of the matrix A and the vectors x and b represent will vary from one modality to another; for our purposes, the main point is simply that all of these entries are nonnegative.

In both modalities the vector x that we seek is a vectorization, that is, a one-dimensional encoding, of an unknown two- or three-dimensional discrete function. It is this transition from higher dimensions to a single dimension that causes x to be large. The quantity x_j, the j-th entry of the vector x, represents the value of the function at the *pixel* or *voxel* corresponding to the index j. The quantity b_i, the i-th entry of the vector b, is measured data, the discrete line integral of x along the i-th line segment, in the transmission case, and photon counts at the i-th detector in the emission case. The entries of the matrix A describe the relationship that holds between the various pixels and the various detectors, that is, they describe the scanning process whereby the information about the unknown function is translated into measured data. In the transmission case, the entries of A describe the geometric relationship between the patient and the scanner, as well as the paths taken by the beams. In the emission case, the entries of A are the probabilities of a photon being detected at the various detectors, given that it was emitted at a particular pixel. In both cases, there is a certain amount of simplification and guesswork that goes into the choice of these entries. In the emission case, the probabilities depend, in part, on the attenuation encountered as the photons pass from within the body to the exterior, and so will depend on the anatomy of the particular patient being scanned.

2.1 Transmission Tomography

When an x-ray beam travels along a line segment through the body it becomes progressively weakened by the material it encounters. By comparing the initial strength of the beam as it enters the body with its final strength as it exits the body, we can estimate the integral of the attenuation function, along that line segment. The data in transmission tomography are these line integrals, corresponding to thousands of lines along which the beams have been sent. The image reconstruction problem is to create a discrete approximation of the attenuation function. The inherently three-dimensional problem is usually solved one two-dimensional plane, or slice, at a time, hence the name *tomography* [39].

The beam attenuation at a given point in the body will depend on the material

present at that point; estimating and imaging the attenuation as a function of spatial location will give us a picture of the material within the body. A bone fracture will show up as a place where significant attenuation should be present, but is not.

The attenuation function is discretized, in the two-dimensional case, by imagining the body to consist of finitely many squares, or *pixels*, within which the function has a constant, but unknown, value. This value at the j-th pixel is denoted x_j. In the three-dimensional formulation, the body is viewed as consisting of finitely many cubes, or *voxels*. The beam is sent through the body along various lines and both initial and final beam strength is measured. From that data we can calculate a discrete line integral along each line. For $i = 1, ..., I$ we denote by L_i the i-th line segment through the body and by b_i its associated line integral. Denote by A_{ij} the length of the intersection of the j-th pixel with L_i; therefore, A_{ij} is nonnegative. Most of the pixels do not intersect line L_i, so A is quite sparse. Then the data value b_i can be described, at least approximately, as

$$b_i = \sum_{j=1}^{J} A_{ij} x_j. \tag{2.1}$$

Both I, the number of lines, and J, the number of pixels or voxels, are quite large, although they certainly need not be equal, and are typically unrelated.

The matrix A is large and rectangular. The system $Ax = b$ may or may not have exact solutions. We are always free to select J, the number of pixels, as large as we wish, limited only by computation costs. We may also have some choice as to the number I of lines, but within the constraints posed by the scanning machine and the desired duration and dosage of the scan. When the system is underdetermined ($J > I$), there may be infinitely many exact solutions; in such cases we usually impose constraints and prior knowledge to select an appropriate solution. As we mentioned earlier, noise in the data, as well as error in our model of the physics of the scanning procedure, may make an exact solution undesirable, anyway. When the system is overdetermined ($J < I$), we may seek a least-squares approximate solution, or some other approximate solution. We may have prior knowledge about the physics of the materials present in the body that can provide us with upper bounds for x_j, as well as information about body shape and structure that may tell where $x_j = 0$. Incorporating such information in the reconstruction algorithms can often lead to improved images [57].

2.2 Emission Tomography

In *single-photon emission tomography* (SPECT) and *positron emission tomography* (PET) the patient is injected with, or inhales, a chemical to which a radioactive substance has been attached [68]. The chemical is designed to become concentrated in the particular region of the body under study. Once there, the radioactivity results in photons that travel through the body and, at least some of the time, are detected by the scanner. The function of interest is the actual concentration of the radioactive material at each spatial location within the region of interest. Learning what the concentrations are will tell us about the functioning of the body at the various spatial locations. Tumors may take up the chemical (and its radioactive passenger) more avidly than normal tissue, or less avidly, perhaps. Malfunctioning portions of the brain may not receive the normal amount of the chemical and will, therefore, exhibit an abnormal amount of radioactivity.

As in the transmission tomography case, this nonnegative function is discretized and represented as the vector x. The quantity b_i, the i-th entry of the vector b, is the photon count at the i-th detector; in coincidence-detection PET a detection is actually a nearly simultaneous detection of a photon at two different detectors. The entry A_{ij} of the matrix A is the probability that a photon emitted at the j-th pixel or voxel will be detected at the i-th detector.

In the emission tomography case it is common to take a statistical view [51, 50, 62, 64, 67], in which the quantity x_j is the expected number of emissions at the j-th pixel during the scanning time, so that the expected count at the i-th detector is

$$E(b_i) = \sum_{j=1}^{J} A_{ij} x_j. \tag{2.2}$$

The system of equations $Ax = b$ is obtained by replacing the expected count, $E(b_i)$, with the actual count, b_i; obviously, an exact solution of the system is not needed in this case. As in the transmission case, we seek an approximate, and nonnegative, solution of $Ax = b$, where, once again, all the entries of the system are nonnegative.

3 Iterative Reconstruction

We turn now to several iterative algorithms for solving the system $Ax = b$. Some of these algorithms apply only to nonnegative systems, in which the entries of the matrix and the vectors are nonnegative, while others apply even to complex-valued systems. We shall use complex notation whenever permitted.

When the (possibly complex) I by J matrix A is large finding exact or approximate solutions of the system of linear equations $Ax = b$ is usually accomplished using iterative algorithms. When the system is overdetermined we can obtain a least-squares approximate solution, which is any vector $x = x_{LS}$ that minimizes the Euclidean distance squared between Ax and b; that is, x_{LS} minimizes

$$||Ax - b||^2 = \sum_{i=1}^{I} |(Ax)_i - b_i|^2, \tag{3.1}$$

where

$$(Ax)_i = \sum_{j=1}^{J} A_{ij} x_j, \tag{3.2}$$

for each i.

3.1 The Landweber Algorithm

The Landweber algorithm [49, 1], with the iterative step

$$x^{k+1} = x^k + \gamma A^\dagger (b - Ax^k), \tag{3.3}$$

converges to the least squares solution closest to the starting vector x^0, provided that $0 < \gamma < 2/\lambda_{max}$, where λ_{max} is the largest eigenvalue of the nonnegative-definite matrix $A^\dagger A$. Loosely speaking, the larger γ is, the faster the convergence. However, precisely because A is large, calculating the matrix $A^\dagger A$, not to mention finding its largest eigenvalue, can be prohibitively expensive. The matrix A is said to be sparse if most of its entries are zero. In [13] upper bounds for λ_{max} were obtained in terms of the degree of sparseness of the matrix A. Later in this paper we investigate the tightness of these bounds.

3.2 The Projected Landweber Algorithm

When we require a nonnegative approximate solution x for the real system $Ax = b$ we can use a modified version of the Landweber algorithm, called the projected Landweber algorithm [1], having the iterative step

$$x^{k+1} = (x^k + \gamma A^T (b - Ax^k))_+, \tag{3.4}$$

where, for any real vector a, we denote by $(a)_+$ the nonnegative vector whose entries are those of a, for those that are nonnegative, and are zero otherwise. The

projected Landweber algorithm converges to a vector that minimizes $||Ax - b||$ over all nonnegative vectors x, for the same values of γ.

Both the Landweber and projected Landweber algorithms are special cases of the CQ algorithm [13], which, in turn, is a special case of a much more general iterative fixed point algorithm, the Krasnoselskii/Mann (KM) method; a proof of the KM method is given in [14].

3.3 The Algebraic Reconstruction Technique

The algebraic reconstruction technique (ART) [36] applies to any system $Ax = b$ of linear equations. For each index value i let B_i be the subset of J-dimensional vectors given by

$$B_i = \{x | (Ax)_i = b_i\}. \tag{3.5}$$

Given any vector z the vector in B_i closest to z, in the sense of the Euclidean distance, has the entries

$$x_j = z_j + \overline{A_{ij}}(b_i - (Az)_i) / \sum_{m=1}^{J} |A_{im}|^2. \tag{3.6}$$

The ART is the following: begin with an arbitrary vector x^0; for each nonnegative integer k, having found x^k, let $i = k(\mathrm{mod}\, I) + 1$ and let x^{k+1} be the vector in B_i closest to x^k. We can use Equation (3.6) to write

$$x_j^{k+1} = x_j^k + \overline{A_{ij}}(b_i - (Ax^k)_i) / \sum_{m=1}^{J} |A_{im}|^2. \tag{3.7}$$

When the system $Ax = b$ has exact solutions the ART converges to the solution closest to x^0. How fast the algorithm converges will depend on the ordering of the equations and on whether or not we use relaxation. Relaxed ART has the iterative step

$$x_j^{k+1} = x_j^k + \gamma\overline{A_{ij}}(b_i - (Ax^k)_i) / \sum_{m=1}^{J} |A_{im}|^2, \tag{3.8}$$

where $\gamma \in (0, 2)$. In selecting the equation ordering, the important thing is to avoid particularly bad orderings, in which the hyperplanes B_i and B_{i+1} are nearly parallel.

When there are no exact solutions, the ART does not converge to a single vector; for each fixed i the subsequence $\{x^{nI+i},\, n = 0, 1, ...\}$ converges to a vector z^i and the collection $\{z^i \,|i = 1, ..., I\}$ is called the *limit cycle* [66, 32, 16]. The limit cycle will

vary with the ordering of the equations, and contains more than one vector unless an exact solution exists. There are several open questions about the limit cycle.

Open Question 1: For a fixed ordering, does the limit cycle depend on the initial vector x^0? If so, how?

Open Question 2: If there is a unique least-squares solution, where is it, in relation to the vectors of the limit cycle? Can it be calculated easily, from the vectors of the limit cycle?

There is a partial answer to the second question. In [7] (see also [16]) it was shown that if the system $Ax = b$ has no exact solution, and if $I = J + 1$, then the vectors of the limit cycle lie on a sphere in J-dimensional space having the least-squares solution at its center. This is not generally true, however.

Open Question 3: In both the consistent and inconsistent cases, the sequence $\{x^k\}$ of ART iterates is bounded [66, 32, 7, 16]. The proof is easy in the consistent case. Is there an easy proof for the inconsistent case?

Dax [29] has demonstrated interesting connections between the ART, applied to $Ax = b$, and the Gauss-Seidel method, applied to the system $AA^\dagger z = b$.

3.4 Nonnegatively Constrained ART

If we are seeking a nonnegative solution for the real system $Ax = b$, we can modify the ART by replacing the x^{k+1} given by Equation (3.7) with $(x^{k+1})_+$. This version of ART will converge to a nonnegative solution, whenever one exists, but will produce a limit cycle otherwise.

3.5 The Multiplicative ART (MART)

Closely related to the ART is the multiplicative ART (MART) [36]. The MART, which can be applied only to nonnegative systems, also uses one equation only at each step of the iteration. The MART begins with a positive vector x^0. Having found x^k for nonnegative integer k, we let $i = k(\mathrm{mod}\, I) + 1$ and define x^{k+1} by

$$x_j^{k+1} = x_j^k \left(\frac{b_i}{(Ax^k)_i}\right)^{m_i^{-1} A_{ij}}, \tag{3.9}$$

where $m_i = \max\{A_{ij} \,|j = 1, 2, ..., J\}$. When $Ax = b$ has nonnegative solutions, MART converges to such a solution. As with ART, the speed of convergence is greatly affected by the ordering of the equations, converging most slowly when consecutive equations correspond to nearly parallel hyperplanes.

Open Question 4: When there are no nonnegative solutions, MART does not converge to a single vector, but, like ART, is always observed to produce a limit cycle of vectors. Unlike ART, there is no proof of the existence of a limit cycle for MART.

3.6 The Simultaneous MART (SMART)

There is a simultaneous version of MART, called the SMART [21, 28, 63]. As with MART, the SMART begins with a positive vector x^0. Having calculated x^k, we calculate x^{k+1} using

$$\log x_j^{k+1} = \log x_j^k + s_j^{-1} \sum_{i=1}^{I} A_{ij} \log \frac{b_i}{(Ax^k)_i}, \tag{3.10}$$

where $s_j = \sum_{i=1}^{I} A_{ij} > 0$.

When $Ax = b$ has no nonnegative solutions, the SMART converges to an approximate solution in the sense of cross-entropy, or Kullback-Leibler distance [3, 16]. For positive numbers u and v, the Kullback-Leibler distance [48] from u to v is

$$KL(u, v) = u \log \frac{u}{v} + v - u. \tag{3.11}$$

We also define $KL(0, 0) = 0$, $KL(0, v) = v$ and $KL(u, 0) = +\infty$. The KL distance is extended to nonnegative vectors component-wise, so that for nonnegative vectors x and z we have

$$KL(x, z) = \sum_{j=1}^{J} KL(x_j, z_j). \tag{3.12}$$

Clearly, $KL(x, z) \geq 0$ and $KL(x, z) = 0$ if and only if $x = z$.

When there are nonnegative solutions of $Ax = b$, both MART and SMART converge to the nonnegative solution minimizing the Kullback-Leibler distance $KL(x, x^0)$; if x^0 is the vector whose entries are all one, then the solution minimizes the Shannon entropy, $SE(x)$, given by

$$SE(x) = \sum_{j=1}^{J} x_j \log x_j - x_j. \tag{3.13}$$

One advantage that SMART has over MART is that, if the nonnegative system $Ax = b$ has no nonnegative solutions, the SMART converges to the nonnegative minimizer of the function $KL(Ax, b)$ for which $KL(x, x^0)$ is minimized. One disadvantage of SMART, compared to MART, is that it is slow.

3.7 Expectation Maximization Maximum Likelihood (EMML)

For nonnegative systems $Ax = b$ in which the column sums of A and the entries of b are positive, the expectation maximization maximum likelihood (EMML) method produces a nonnegative solution of $Ax = b$, whenever one exists [3, 4, 15, 25, 55, 64, 50, 67, 51] . If not, the EMML converges to a nonnegative approximate solution that minimizes the function $KL(b, Ax)$ [3, 5, 15, 25, 67]. The EMML begins with a positive vector x^0. The iterative step of the EMML method is

$$x_j^{k+1} = s_j^{-1} x_j^k \sum_{i=1}^{I} A_{ij} \frac{b_i}{(Ax^k)_i}, \tag{3.14}$$

for $s_j = \sum_{i=1}^{I} A_{ij} > 0$.

The EMML algorithm can also be viewed as a method for maximizing the likelihood function, when the data b_i are instances of independent Poisson random variables with mean value $(Ax)_i$; here the entries of x are the parameters to be estimated.

An open question about the EMML algorithm is the following:

Open Question 5: How does the EMML limit depend on the starting vector x^0? In particular, when there are nonnegative exact solutions of $Ax = b$, which one does the EMML produce and how does it depend on x^0?

3.8 The Rescaled Block-Iterative EMML (RBI-EMML)

One drawback to the use of the EMML in practice is that it is slow; this is typical behavior for simultaneous algorithms, which use all the equations at each step of the iteration. The *ordered-subset* version of the EMML (OSEM) [44] often produces images of similar quality in a fraction of the time. The OSEM is a block-iterative method, in the sense that only some of the equations are used at each step of the iteration. Unfortunately, the OSEM usually fails to converge, even when there are exact nonnegative solutions of the system $Ax = b$. The rescaled block-iterative EMML (RBI-EMML) is a corrected version of OSEM that does converge whenever there are nonnegative solutions [6, 8, 15].

We begin by selecting subsets S_n, $n = 1, ..., N$ whose union is the set of equation indices $\{i = 1, ..., I\}$; the S_n need not be disjoint. Having found iterate x^k, set $n = k(\mathrm{mod}\, N) + 1$; the OSEM iterative step is then

$$x_j^{k+1} = s_{nj}^{-1} x_j^k \sum_{i \in S_n} A_{ij} \frac{b_i}{(Ax^k)_i}, \tag{3.15}$$

for $s_{nj} = \sum_{i \in S_n} A_{ij} > 0$. Notice that the OSEM iterative step mimics that of EMML, except that each summation is over only i in the current subset, S_n. It has been

shown that the OSEM converges to a nonnegative solution of $Ax = b$, when such exact solutions exist, provided that the sums s_{nj} are independent of n, for each j; this is the so-called *subset-balanced* condition and is quite restrictive. Without this condition, the OSEM can produce a limit cycle, even when there are nonnegative exact solutions of $Ax = b$, and when there are no such solutions, the vectors of its limit cycle are typically farther apart than the level of noise in the data would seem to indicate. The problem with OSEM is that there should be a second term on the right side of Equation (3.15).

The RBI-EMML algorithm has the following iterative step:

$$x_j^{k+1} = x_j^k(1 - m_n^{-1}s_j^{-1}s_{nj}) + x_j^k m_n^{-1}s_j^{-1}\sum_{i\in S_n} A_{ij}\frac{b_i}{(Ax^k)_i}, \tag{3.16}$$

where

$$m_n = \max\{s_{nj}/s_j \,|j = 1, ..., J\}. \tag{3.17}$$

For any choice of subsets S_n, and any starting vector $x^0 > 0$, the RBI-EMML converges to a nonnegative solution whenever one exists. If subset-balance holds, then the RBI-EMML reduces to the OSEM method. The acceleration, compared to the EMML, is roughly on the order of N, the number of subsets. As with the ART, the composition of the subsets, as well as their ordering, can affect the rate of convergence. As with the EMML, there are several open questions.

Open Question 6: When there are nonnegative solutions of $Ax = b$, how does the solution given by the RBI-EMML depend on the starting vector x^0 and on the choice and ordering of the subsets?

Open Question 7: When there are no nonnegative solutions of $Ax = b$ does the RBI-EMML produce a limit cycle? This is always observed in actual calculations, but no proof is known.

Open Question 8: When there are no nonnegative solutions of $Ax = b$ how do the vectors of the RBI-EMML limit cycle relate to the approximate solution given by EMML?

3.9 The Rescaled Block-Iterative SMART (RBI-SMART)

The SMART algorithm also has a rescaled block-iterative version, the RBI-SMART [21, 6, 8, 15]. The iterative step of the RBI-SMART is

$$x_j^{k+1} = x_j^k \exp\Big(m_n^{-1}s_j^{-1}\sum_{i\in S_n} A_{ij}\frac{b_i}{(Ax^k)_i}\Big). \tag{3.18}$$

When $Ax = b$ has nonnegative solutions, the RBI-SMART converges to the same limit as MART and SMART, for all choices of subsets S_n.

Open Question 9: When $Ax = b$ has no nonnegative solutions, the RBI-SMART is always observed to produce a limit cycle, but no proof of this is known.

4 Feedback in Block-Iterative Reconstruction

When the nonnegative system $Ax = b$ has no nonnegative exact solutions, block-iterative methods such as MART, RBI-SMART, and RBI-EMML have always been observed to exhibit subsequential convergence to a limit cycle, although no proof of this is known. These algorithms approach their limit cycles much sooner than their simultaneous versions, SMART and EMML, approach their limits.

Open Question 10: Can we use the vectors of the limit cycle for MART or RBI-SMART (RBI-EMML) to calculate easily the limit of SMART (EMML)?

In this section we present a partial answer to this question, using a *feedback* method. More detail concerning the feedback method is in [17]. We assume throughout this section that the limit cycles always exist.

We assume that, for each fixed $n = 1, 2, ..., N$, the subsequence $\{x^{mN+n}, m = 0, 1, ...\}$ converges to a vector z^n and the collection $\{z^n | n = 1, ..., N\}$ is called the *limit cycle*; for convenience, we also define $z^0 = z^N$. The main property of the limit cycle is the following: if we restart the algorithm at z^0, the next iterate is z^1, followed by $z^2, ..., z^N$ again. The limit cycle will vary with the algorithm, with N, with the choice of subsets S_n, with ordering of the equations, and will contain more than one vector unless an exact nonnegative solution exists.

For each n and for each i in the subset S_n, let $c_i = (Az^{n-1})_i$, The vector c with entries c_i will now be viewed as *new data*, replacing the vector b, and the algorithm restarted at the original x^0. This is the feedback step. Once again, a limit cycle will be produced, another vector of *new data* will be generated, feedback will take place again, and the process will continue. What are we obtaining by this succession of feedback steps?

This feedback approach was considered originally in [7], where it was also applied to the ART. For the ART case it was shown there that the systems $Ax = b$ and $Ax = c$ have the same least-squares solutions, which suggests the possibility that the limit cycles generated by feedback might converge to the least-squares solution of the original system, $Ax = b$. Results along these lines were presented in [7]. The success with ART prompted us to ask the same questions about feedback applied to other

block-iterative algorithms; some partial results were obtained [7].

Open Question 11: When feedback is applied to the RBI-SMART algorithm do the limit cycles obtained converge to a nonnegative minimizer of the function

$$\sum_{n=1}^{N} m_n^{-1} \sum_{i \in S_n} KL((Ax)_i, b_i)?$$

If $J > I$, how should the feedback step deal with the zero entries in the vectors z^n?

Open Question 12: When feedback is applied to the RBI-EMML algorithm do the limit cycles obtained converge to a nonnegative minimizer of the function

$$\sum_{n=1}^{N} m_n^{-1} \sum_{i \in S_n} KL(b_i, (Ax)_i)?$$

If $J > I$, how should the feedback step deal with the zero entries in the vectors z^n?

5 Iterative Regularization in ART

It is often the case that the entries of the vector b in the system $Ax = b$ come from measurements, so are usually noisy. If the entries of b are noisy but the system $Ax = b$ remains consistent (which can easily happen in the underdetermined case, with $J > I$), the ART begun at $x^0 = 0$ converges to the solution having minimum norm, but this norm can be quite large. The resulting solution is probably useless. Instead of solving $Ax = b$, we *regularize* by minimizing, for example, the function

$$||Ax - b||^2 + \epsilon^2 ||x||^2, \tag{5.1}$$

for some small $\epsilon > 0$. The solution to this problem is the vector x for which

$$(A^\dagger A + \epsilon^2 I)x = A^\dagger b. \tag{5.2}$$

However, we do not want to have to calculate $A^\dagger A$, particularly when the matrix A is large.

We discuss two methods for using ART to obtain regularized solutions of $Ax = b$. The first one is presented in [16], while the second one is due to Eggermont, Herman, and Lent [33]. For notational convenience, we consider only real systems.

In our first method we use ART to solve the system of equations given in matrix form by

$$\begin{bmatrix} A^T & \epsilon I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0.$$

We begin with $u^0 = b$ and $v^0 = 0$. The lower component of the limit vector is then $v^\infty = -\epsilon\hat{x}$, where $\hat{x}$ minimizes the function in line (5.1).

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

$$[\, A \quad \epsilon I \,] \begin{bmatrix} x \\ v \end{bmatrix} = b.$$

We begin at $x^0 = 0$ and $v^0 = 0$. Then, the limit vector has for its upper component $x^\infty = \hat{x}$ as before. Also, $\epsilon v^\infty = b - A\hat{x}$.

Complicating our analysis for the case in which $Ax = b$ has no nonnegative solutions is the behavior of approximate solutions when nonnegativity is imposed, which is the subject of the next section.

6 Approximate Solutions and the Nonnegativity Constraint

For the real system $Ax = b$, consider the *nonnegatively constrained least-squares* problem of minimizing the function $||Ax - b||$, subject to the constraints $x_j \geq 0$ for all j; this is a nonnegatively constrained least-squares approximate solution. As noted previously, we can solve this problem using a slight modification of the ART. Although there may be multiple solutions $\hat{x}$, we know, at least, that $A\hat{x}$ is the same for all solutions.

According to the Karush-Kuhn-Tucker theorem [60], the vector $A\hat{x}$ must satisfy the condition

$$\sum_{i=1}^{I} A_{ij}((A\hat{x})_i - b_i) = 0 \tag{6.1}$$

for all j for which $\hat{x}_j > 0$ for some solution $\hat{x}$. Let S be the set of all indices j for which there exists a solution $\hat{x}$ with $\hat{x}_j > 0$. Then Equation (6.1) must hold for all j in S. Let Q be the matrix obtained from A by deleting those columns whose index j is not in S. Then $Q^T(A\hat{x} - b) = 0$. If Q has full rank and the cardinality of S is greater than or equal to I, then Q^T is one-to-one and $A\hat{x} = b$. We have proven the following result.

Theorem 6.1 *Suppose that A and every matrix Q obtained from A by deleting columns has full rank. Suppose there is no nonnegative solution of the system of equations $Ax = b$. Then there is a subset S of the set $\{i = 1, 2, ..., I\}$ with cardinality at most $I - 1$ such that, if $\hat{x}$ is any minimizer of $||Ax - b||$ subject to $x \geq 0$, then $\hat{x}_j = 0$ for j not in S. Therefore, $\hat{x}$ is unique.*

When $\hat{x}$ is a vectorized two-dimensional image and $J > I$, the presence of at most $I-1$ positive pixels makes the resulting image resemble stars in the sky; for that reason this theorem and the related result for the EMML algorithm ([3]) are sometimes called *night sky* theorems. The zero-valued pixels typically appear scattered throughout the image. This behavior occurs with all the algorithms discussed so far that impose nonnegativity, whenever the real system $Ax = b$ has no nonnegative solutions.

This result leads to the following open question:

Open Question 13: How does the set S defined above vary with the choice of algorithm, with the choice of x^0 for a given algorithm, and for the choice of subsets in the block-iterative algorithms?

We return now to an issue that arose in the discussion of the Landweber and projected Landweber algorithms, namely, obtaining a good upper bound for λ_{max}, the maximum eigenvalue of $A^\dagger A$.

7 An Upper Bound for the Maximum Eigenvalue of $A^\dagger A$

The upper bounds for λ_{max} we present here apply to any matrix A, but will be particularly helpful when A is sparse.

7.1 The Normalized Case

We assume now that the matrix A has been normalized so that each of its rows has Euclidean length one. Denote by s_j the number of nonzero entries in the jth column of A, and let s be the maximum of the s_j. Our first result is the following [13]:

Theorem 7.1 *For normalized A, λ_{max}, the largest eigenvalue of the matrix $A^\dagger A$, does not exceed s.*

Proof: For notational simplicity, we consider only the case of real matrices and vectors. Let $A^T Av = cv$ for some nonzero vector v. We show that $c \leq s$. We have $AA^T Av = cAv$ and so $w^T AA^T w = v^T A^T AA^T Av = cv^T A^T Av = cw^T w$, for $w = Av$. Then, with $e_{ij} = 1$ if $A_{ij} \neq 0$ and $e_{ij} = 0$ otherwise, we have

$$(\sum_{i=1}^{I} A_{ij} w_i)^2 = (\sum_{i=1}^{I} A_{ij} e_{ij} w_i)^2$$

$$\leq (\sum_{i=1}^{I} A_{ij}^2 w_i^2)(\sum_{i=1}^{I} e_{ij}^2) =$$

$$(\sum_{i=1}^{I} A_{ij}^2 w_i^2) s_j \leq (\sum_{i=1}^{I} A_{ij}^2 w_i^2) s.$$

Therefore,

$$w^T A A^T w = \sum_{j=1}^{J} (\sum_{i=1}^{I} A_{ij} w_i)^2 \leq \sum_{j=1}^{J} (\sum_{i=1}^{I} A_{ij}^2 w_i^2) s,$$

and

$$w^T A A^T w = c \sum_{i=1}^{I} w_i^2 = c \sum_{i=1}^{I} w_i^2 (\sum_{j=1}^{J} A_{ij}^2)$$

$$= c \sum_{i=1}^{I} \sum_{j=1}^{J} w_i^2 A_{ij}^2.$$

The result follows immediately. ∎

When A is normalized the trace of AA^T, that is, the sum of its diagonal entries, is M. Since the trace is also the sum of the eigenvalues of both AA^T and $A^T A$, we have $\lambda_{max} \leq M$. When A is sparse, s is much smaller than M, so provides a much tighter upper bound for λ_{max}.

7.2 The General Case

A similar upper bound for λ_{max} is given for the case in which A is not normalized.

Theorem 7.2 *For each $i = 1, ..., I$ let $\nu_i = \sum_{j=1}^{J} |A_{ij}|^2 > 0$. For each $j = 1, ..., J$, let $\sigma_j = \sum_{i=1}^{I} e_{ij} \nu_i$, where $e_{ij} = 1$ if $A_{ij} \neq 0$ and $e_{ij} = 0$ otherwise. Let σ denote the maximum of the σ_j. Then the eigenvalues of the matrix $A^\dagger A$ do not exceed σ.*

The proof of Theorem 7.2 is similar to that of Theorem 7.1; the details are in [13].

7.3 Upper Bounds for ϵ-Sparse Matrices

If A is not sparse, but most of its entries have magnitude not exceeding $\epsilon > 0$ we say that A is ϵ-sparse. We can extend the results for the sparse case to the ϵ-sparse case.

Given a matrix A, define the entries of the matrix B to be $B_{ij} = A_{ij}$ if $|A_{ij}| > \epsilon$, and $B_{ij} = 0$, otherwise. Let $C = A - B$; then $|C_{ij}| \leq \epsilon$, for all i and j. If A is ϵ-sparse, then B is sparse. The 2-norm of the matrix A, written $||A||$, is defined to be the square root of the largest eigenvalue of the matrix $A^\dagger A$, that is, $||A|| = \sqrt{\lambda_{max}}$. From Theorem 7.2 we know that $||B|| \leq \sigma$. The trace of the matrix $C^\dagger C$ does not exceed $IJ\epsilon^2$. Therefore

$$\sqrt{\lambda_{max}} = ||A|| = ||B + C|| \leq ||B|| + ||C|| \leq \sqrt{\sigma} + \sqrt{IJ}\epsilon, \tag{7.1}$$

so that

$$\lambda_{max} \leq \sigma + 2\sqrt{\sigma IJ}\epsilon + IJ\epsilon^2. \tag{7.2}$$

Simulation studies have shown that these upper bounds become tighter as the size of the matrix A increases. In hundreds of runs, with I and J in the hundreds, we found that the relative error of the upper bound was around one percent [18].

8 From General Systems to Nonnegative Systems

The EMML and SMART algorithms require that the matrix involved have nonnegative entries. Here, we show how to convert general linear systems to equivalent systems having this desired form.

Suppose that $Hc = d$ is an arbitrary (real) system of linear equations, with the matrix $H = [H_{ij}]$. Rescaling the equations if necessary, we may assume that for each j the column sum $\sum_i H_{ij}$ is nonzero; note that if a particular rescaling of one equation to make the first column sum nonzero causes another column sum to become zero, we simply choose a different rescaling. Since there are finitely many columns to worry about, we can always succeed in making all the column sums nonzero. Now redefine H and c as follows: replace H_{kj} with $G_{kj} = \frac{H_{kj}}{\sum_i H_{ij}}$ and c_j with $g_j = c_j \sum_i H_{ij}$; the product Hc is equal to Gg and the new matrix G has column sums equal to one. The system $Gg = d$ still holds, but now we know that $\sum_i d_i = d_+ = \sum_j g_j = g_+$. Let U be the matrix whose entries are all one, and let $t \geq 0$ be large enough so that $B = G + tU$ has all nonnegative entries. Then $Bg = Gg + (tg_+)1$, where 1 is the vector whose entries are all one. So, the new system of equations to solve is $Bg = d + (td_+)1 = y$.

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