

Lecture 9 - Canonical Paths

Friday, September 3

In the previous class we showed how to compare Dirichlet forms. The most important corollary of this was shown by Diaconis and Stroock [1] and Sinclair [2].

Corollary 9.1 (Canonical Paths). *Given a reversible Markov chain \mathcal{M} , to every pair of states $x \neq y \in \Omega$ associate a path from x to y along edges (“canonical paths”). Then*

$$1 - \lambda_2 \geq 1/\bar{\rho} \quad \text{where} \quad \bar{\rho} = \max_{(a,b) \in E} \frac{1}{\pi(a)P(a,b)} \sum_{\gamma_{xy} \ni (a,b)} \pi(x)\pi(y) |\gamma_{xy}|.$$

Proof. Consider the Markov chain \mathcal{M}' with stationary distribution $\pi' = \pi$ and transitions $P'(x,y) = \pi(y)$. It was shown last class that $1 - \lambda_2' = 1$. To every edge (x,y) in \mathcal{M}' associate the canonical path given in the problem. Then the comparison theorem applies and $\bar{A} = \bar{\rho}$. \square

This is correct for the walk on the uniform two-point space, as $\bar{\rho} = 1/2(1-\gamma)$ which implies $1 - \lambda_2 \geq 2(1-\gamma)$, the correct value.

As with the comparison case, the easiest way to find $\bar{\rho}$ is typically to use the bound

$$\bar{\rho} \leq \rho \ell \quad \text{where} \quad \rho = \max_{(a,b) \in E} \frac{1}{\pi(a)P(a,b)} \sum_{\gamma_{xy} \ni (a,b)} \pi(x)\pi(y)$$

where ℓ is again the length of the longest path. In most applications the stationary distribution is uniform $\pi = 1/|\Omega|$ and the transition probabilities are constant with $P(a,b) = 0$ or φ . Then $\rho = \frac{1}{|\Omega|\varphi} \max_{(a,b) \in E} |\{(x,y) \in \Omega \times \Omega : \gamma_{xy} \ni (a,b)\}|$ and it suffices to find which edge has the most paths through it.

Example 9.2 (Odd Cycle). Consider the simple random walk on a cycle C_n of odd length, as discussed before.

Given a pair of states $x, y \in [1 \dots n]$ a natural choice of path is to take the shortest route around the cycle. The longest path is of length $\frac{n-1}{2}$, the stationary distribution is uniform at $\pi = 1/n$, and the transitions are all 0 or $1/2$, so it suffices to know the number of paths through a single edge. To count the number of paths through an edge e suppose the edge is $e = (a-1, a)$ and observe that the paths with an endpoint at $a+i$ must have begun somewhere from $a+i - \frac{n-1}{2}$ to $a-1$, i.e. there are $a-1 - a+i + \frac{n-1}{2} + 1 = \frac{n-1}{2} - i$ such paths, for a total of

$$\# \text{ paths} = \sum_{i=0}^{(n-1)/2} \frac{n-1}{2} - i = \frac{(n-1)(n+1)}{8}.$$

Then

$$\bar{\rho} \leq \frac{n-1}{2} \frac{1}{n(1/2)} \frac{(n-1)(n+1)}{8} = \frac{(n-1)^2(n+1)}{8n} < \frac{n^2}{8}$$

and so

$$1 - \lambda_2 \geq \frac{1}{\bar{\rho}} \geq \frac{8}{n^2}.$$

Recall from Lecture 6 that $1 - \lambda_2 = 1 - \cos(2\pi/n) \approx \frac{2\pi^2}{n^2}$. The canonical path bound was of the correct order, and off by only a factor of $\frac{\pi^2}{4} \approx 2.5$.

It is not hard to compute $\bar{\rho}$ directly for this problem. It is $\bar{\rho} = \frac{1}{n(1/2)} \sum_{i=1}^{(n-1)/2} i^2 = \frac{(n-1)(n+1)}{12} < \frac{n^2}{12}$. The bound $1 - \lambda_2 \geq \frac{12}{n^2}$ is off by only a factor of $\frac{\pi^2}{6} \approx 1.6$.

Example 9.3 (Boolean cube). Consider again the lazy walk on the boolean cube 2^d . This can be considered as a walk on $\{0, 1\}^d$ with transitions given by choosing a coordinate uniformly at random and flipping it with probability $1/2$.

Canonical paths can be defined as follows. If $\vec{x} = (x_1, x_2, \dots, x_d)$ and $\vec{y} = (y_1, y_2, \dots, y_d)$ then match the coordinates one at a time, that is follow the path

$$(x_1, x_2, \dots, x_d) \rightarrow (y_1, x_2, \dots, x_d) \rightarrow (y_1, y_2, \dots, x_d) \rightarrow \dots \rightarrow (y_1, y_2, \dots, y_d)$$

Once again the transition probabilities are a constant $\varphi = 1/2d$, the stationary distribution $\pi = 1/|\Omega| = 2^{-d}$, and the paths have max length d . To count paths, suppose that coordinate i is being changed. Then the paths through this edge may have started at anything in coordinates 1 to $i-1$ (for 2^{i-1} choices), and may be going to anything in coordinates $i+1$ to d (for 2^{d-i} choices). In total 2^{d-1} paths may pass through any particular edge.

Therefore

$$\bar{\rho} \leq \ell \rho \leq d \frac{1}{2^d (1/2d)} 2^{d-1} = d^2$$

and so

$$1 - \lambda_2 \geq 1/d^2.$$

The actual value is $1 - \lambda_2 = 1/d$, so our bound is not too great.

Example 9.4 (Metropolis). As our final example consider the Metropolis method discussed earlier to generate from a distribution π . Recall that a different Markov chain \mathcal{M}' makes transitions, and then these are accepted with some probability, so that $P(x, y) = P'(x, y) \min\{1, \frac{\pi(y)}{\pi(x)}\}$.

This is a natural problem for comparison, to find $1 - \lambda_2$ in terms of the spectral gap $1 - \lambda'_2$ of the base chain \mathcal{M}' . The easiest choice of paths is that if (a, b) is an edge in E' then simply take the path $\gamma_{ab} = (a, b)$ in E to be exactly the same edge. Then

$$\begin{aligned} \bar{A} &= \max_{e=(a,b) \in E} \frac{\pi'(a)P'(a,b)}{\pi(a)P(a,b)} = \max_{e=(a,b) \in E} \frac{\pi'(a)P'(a,b)}{\pi(a)P'(a,b) \min\{1, \pi(b)/\pi(a)\}} \\ &= \max_{e=(a,b) \in E} \frac{\pi'(a)}{\min\{\pi(a), \pi(b)\}} = \left(\min_{a \in \Omega} \frac{\pi(a)}{1/|\Omega|} \right)^{-1} \end{aligned}$$

just measures how much smaller the Metropolis distribution may be compared to the uniform distribution of \mathcal{M}' . It follows that $\mathcal{E}(f, f) \geq \mathcal{E}'(f, f)/\bar{A}$.

To bound the spectral gap, observe that

$$\begin{aligned} \text{Var}_{\pi}(f) &= \frac{1}{2} \sum_{x,y \in \Omega} (f(x) - f(y))^2 \pi(x)\pi(y) \\ &\leq \left(\max_{a \in \Omega} \frac{\pi(a)}{1/|\Omega|} \right)^2 \frac{1}{2} \sum_{x,y \in \Omega} (f(x) - f(y))^2 \frac{1}{|\Omega|} \frac{1}{|\Omega|} \\ &= \left(\max_{a \in \Omega} \frac{\pi(a)}{1/|\Omega|} \right)^2 \text{Var}_{\pi'}(f) \end{aligned}$$

It follows that

$$1 - \lambda_2 = \sup_{f \neq \text{constant}} \frac{\mathcal{E}(f, f)}{\text{Var}_{\pi}(f)} \geq \frac{\min_{a \in \Omega} \frac{\pi(a)}{1/|\Omega|}}{\left(\max_{a \in \Omega} \frac{\pi(a)}{1/|\Omega|} \right)^2} (1 - \lambda'_2)$$

If Metropolis changes the distribution by at most a factor of k then the Markov chain slows by at most a factor of k^3 . Why does increasing $\pi(a)$ from uniform causes a much bigger penalty than decreasing $\pi(a)$?

Canonical paths is one of the most widely used methods for studying the mixing time of Markov chains. Numerous applications can be found in the literature. Week 7 of Eric Vigoda's notes covers Approximating the Permanent (one of the most important results in "rapid mixing"), while Sinclair's notes 13 to 17 cover various applications such as Monomer-Dimer systems.

References

- [1] P. Diaconis and D. Stroock. Geometric bounds for eigenvalues of markov chains. *The Annals of Applied Probability*, 1:36–61, 1991.
- [2] A. Sinclair. Improved bounds for mixing rates of markov chains and multicommodity flow. *Combinatorics, Probability and Computing*, 1(4):351–370, 1992.