Markov Chains, Eigenvalues, and Coupling

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by

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Summary. This is an expository paper which presents certain basic ideas related to non-asymptotic rates of convergence for Markov chains. In particular, we describe eigenvalue analysis, random walks on groups, coupling, and minorization conditions. Connections are made to modern areas of research, including analysis of card shuffling and analysis of stochastic algorithms used in statistics and computer science. Elements of linear algebra, probability theory, group theory, and measure theory are used, but efforts are made to keep the presentation elementary and accessible.

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1. Introduction.

Imagine 1000 lily-pads arranged in a circle, numbered 0 through 999. Suppose a frog begins on lily-pad number 0, and proceeds as follows. Each minute, she jumps either to the pad immediately to her right, or to the pad immediately to her left, or to the pad she's already on, each with probability 1/3. Thus, after one minute she is equally likely to be at pad 999, pad 0, or pad 1. After two minutes, she has probability 1/9 of being at pad 998 or pad 2, probability 2/9 of being at pad 999 or pad 1, and probability $3/9 = 1/3$ of being at pad 0.

It is intuitively clear that if we wait for a very large number of minutes, then our frog will have approximately equal probability of being at any of the 1000 pads. But how might we prove this assertion? More importantly, how long do we have to wait until this approximate equality of probabilities occurs? Is 1000 minutes enough? How about 10,000 minutes?

These questions are closely connected to an exciting area of modern mathematical research, the study of convergence rates for Markov chains. This research has applications to card shuffling (in which the arrangements of the cards have various probabilities) and to stochastic algorithms (in which a computer program follows a certain random procedure, and we must determine when various probabilities converge to their desired values). It involves such areas of mathematics as linear algebra, probability theory, group theory, measure theory, and graph theory.

In this paper, we present some of the basic results about convergence rates for finite (and infinite) Markov chains. We shall attempt to make connections to modern research, but at the same time to keep the presentation elementary and accessible. After the preliminary material, we shall present the basic connection between Markov chains and eigenvalues (Section 4). We shall then explore the subject of random walks on groups (Section 5), for which tremendous progress has been made, which includes our frog's travels and also includes most models of card-shuffling. Finally, we shall discuss coupling and minorization conditions (Section 6), which are robust techniques that have been used to study various stochastic algorithms.

Along the way, we shall prove that we would have to wait over 120,000 minutes (over two months!) for our frog to have approximately equal probability of being at any of the 1000 pads.

None of the results presented here are new. Connections and references to the relevant literature are given where possible.

2. The general problem.

Our frog-process above is an example of a (discrete-time) *Markov chain*. In general, a Markov chain consists of a (measurable) state space $\mathcal{X}$, an initial distribution (i.e. probability measure) μ_0 on $\mathcal{X}$, and a *transition kernel* $P(x, dy)$ which gives, for each point $x \in \mathcal{X}$, a distribution $P(x, \cdot)$ on $\mathcal{X}$ (which represents the probabilities of where the Markov chain will go one step after being at the point x). If $\mathcal{X}$ is a discrete space (e.g. a finite space), then the initial distribution can be specified by the non-negative real numbers $\mu_0(x)$ for $x \in \mathcal{X}$, where $\sum_x \mu_0(x) = 1$. Similarly, the transition kernel can be specified by the non-negative real numbers $P(x, y)$ for $x, y \in \mathcal{X}$, where $\sum_y P(x, y) = 1$ for each $x \in \mathcal{X}$.

In our frog example above, $\mathcal{X}$ consists of the integers $0, 1, 2, \ldots, 999$. Since the frog starts at the point 0 with probability 1, the initial distribution is specified by $\mu_0(0) = 1$, and $\mu_0(x) = 0$ for $x \neq 0$. Finally, the transition kernel is specified by $P(x, y) = 1/3$ if $x = y$ or x and y are adjacent in the circle, and $P(x, y) = 0$ otherwise.

Given the initial distribution μ_0 and transition kernel $P(x, dy)$, we can inductively define distributions μ_k on $\mathcal{X}$, representing the probabilities of where the Markov chain will be after k steps, by

$$\mu_k(A) \;=\; \int_{\mathcal{X}} P(x, A)\, \mu_{k-1}(dx), \qquad k = 1, 2, 3, \ldots .$$

On a discrete space, this can be written more directly as

$$\mu_k(y) \;=\; \sum_x P(x, y) \mu_{k-1}(x)\,.$$

If we write μ_k as a row-vector, and P as a matrix with $[P]_{xy} = P(x, y)$, then this can be written even more directly as

$$\mu_k \;=\; \mu_{k-1} P \;=\; \ldots \;=\; \mu_0 P^k\,.$$

There is nothing mysterious about these formulae. They simply say that to be at the point y at time k, we must have been at *some* point x at time $k-1$ (with probability $\mu_{k-1}(x)$), and then jumped from x to y on the next step (with probability $P(x, y)$).

Thus, in our frog example, we would have that $\mu_2(998) = \mu_2(2) = 1/9$, $\mu_2(999) = \mu_2(1) = 2/9$, and $\mu_2(0) = 1/3$.

Once we have defined μ_k for all non-negative integers k, we can ask about convergence properties. To be quantitative, we define the *total variation distance* between probability measures ν_1 and ν_2 by $\|\nu_1 - \nu_2\| := \sup_{A \subseteq \mathcal{X}} |\nu_1(A) - \nu_2(A)|$ (where the supremum is taken

over measurable subsets A). (For later reference, we mention two easily-verified facts. Firstly, if $\mathcal{X}$ is finite, then $\|\nu_1 - \nu_2\| = \frac{1}{2}\sum_x |\nu_1(x) - \nu_2(x)|$. Secondly, for any $\mathcal{X}$, we have $\|\nu_1 - \nu_2\| = \frac{1}{2} \sup_{\substack{f:\mathcal{X}\to\mathbf{C} \\ |f(x)|\le 1}} |E_{\nu_1}(f) - E_{\nu_2}(f)|$ where E stands for expected value). We may now state our

Fundamental Questions.

(A) Does there exist a probability distribution π on $\mathcal{X}$ such that $\|\mu_k - \pi\| \to 0$ as $k \to \infty$?

(B) If so, then given $\epsilon > 0$, how large should k be to ensure that $\|\mu_k - \pi\| \le \epsilon$?

Question (B) in particular represents a modern, "non-asymptotic" approach to Markov chains, as pioneered by David Aldous, Persi Diaconis, and others. Rather than simply asking yes/no questions about eventual convergence of Markov chains, researchers now often want *quantitative bounds* on the number of steps required until the chain has approximately converged. Into this category falls the now-famous result (Bayer and Diaconis, 1992) that seven ordinary shuffles are required to properly mix a deck of 52 cards. Similarly, much of the analysis of stochastic algorithms in computer science (see e.g. Jerrum and Sinclair, 1989), and of Markov chain Monte Carlo (MCMC*) techniques in statistics (see e.g. Gelfand and Smith, 1990; Tierney, 1994; Rosenthal, 1993b), asks the question, how long must the algorithm be run until it converges to the correct answer? This is a very active area of modern research.

3. The simplest non-trivial example.

To get a sense of what convergence properties a Markov chain can have, we consider what might** be called the "simplest non-trivial example". We consider the state space $\mathcal{X} = \{0, 1\}$ consisting of just two points! Setting $p = P(0, 1)$, and $q = P(1, 0)$, we may write P in matrix form as

$$P = \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix}.$$

(We leave p and q as arbitrary numbers between 0 and 1.) We further suppose that the initial distribution is given by $\mu_0(0) = 1$, $\mu_0(1) = 0$, meaning that we start in state 0 with probability 1.

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* In 1992, Jim Fill hosted a workshop about Markov chain Monte Carlo techniques, and observed that he was the MCMC MC!

** Raoul Bott says that a study of a new mathematical topic should always begin with the simplest non-trivial example! He also says that when reading a new math book, you should always begin in the middle, so that when you don't understand something you are able to search backwards for clarification!

This example is simple enough that we can solve for μ_k explicitly. It is verified by induction (see Hoel, Port, and Stone, 1972, Section 1.2) that (assuming $p+q>0$)

$$\mu_k(0) \;=\; \frac{q}{p+q} \;+\; \left(1-\frac{q}{p+q}\right)(1-p-q)^k\,.$$

It immediately follows that

$$\mu_k(1) \;=\; 1 \;-\; \mu_k(0) \;=\; \frac{p}{p+q} \;-\; \left(1-\frac{q}{p+q}\right)(1-p-q)^k\,.$$

(Naturally, if $p=q=0$, then $\mu_k(0)=1$ and $\mu_k(1)=0$ for all k.)

We wish to make a number of observations about this example, since they will generalize considerably. First, note that assuming $|1-p-q|<1$, we will indeed have convergence. Setting $\pi(0)=\frac{q}{p+q}$ and $\pi(1)=\frac{p}{p+q}$, we have that

$$\|\mu_k-\pi\| \;=\; \left(1-\frac{q}{p+q}\right)|1-p-q|^k\,,$$

which decreases exponentially quickly to 0, with rate governed by the quantity $1-p-q$.

Second, note that this limiting distribution π is a *stationary distribution* in the sense that $\pi P=\pi$, and thus corresponds to a left-eigenvector of the matrix P with eigenvalue 1. It is easily seen (by taking the limit $k\to\infty$ in the equation $\mu_k=\mu_{k-1}P$) that *any* limiting distribution π for any Markov chain must be stationary in this sense.

Third, note that the only time this convergence *fails* to take place is if $p=q=0$ or $p=q=1$. If $p=q=0$ the Markov chain is *decomposable*, meaning that the state space $\mathcal{X}$ can be partitioned into two non-empty subsets $\mathcal{X}_1$ and $\mathcal{X}_2$ such that $P(x,y)=0$ whenever x and y are not in the same subset. If $p=q=1$ the Markov chain is *periodic*, meaning that the state space $\mathcal{X}$ can be partitioned into non-empty subsets $\mathcal{X}_1,\ldots,\mathcal{X}_d$ (with $d\geq 2$) such that for $x\in\mathcal{X}_j$, $P(x,\mathcal{X}_{j+1})=1$ (where if $j=d$, then $j+1$ is taken to mean 1). The quantity d is the *period* of the Markov chain; in this example $d=2$. However, if our Markov chain is *indecomposable* and *aperiodic*, then it converges exponentially quickly. We shall see in the next section that all finite Markov chains follow this rule.

Fourth, it is easily computed that the *eigenvalues* of the matrix P are 1 and $1-p-q$. The eigenvalue 1, of course, corresponds to the eigenvector π. This computation suggests that the "non-trivial" eigenvalue $1-p-q$ is intimately connected with convergence of the chain. We shall develop this connection in the next section.

Fifth, and perhaps even more intriguing, we compute that the quantity β defined by

$$\beta \;:=\; \sum_y \min_x P(x,y)$$

satisfies $\beta = \min(p+q,\ 2-p-q)$, so that $1-\beta = |1-p-q|$ is the absolute value of the non-trivial eigenvalue as above. This suggests that the convergence of the chain might be related to the quantity $1-\beta$, with β defined as above; this relationship is explored in Section 6 via the method of "coupling".

Sixth, we compute that $\pi(0)P(0,1) = \pi(1)P(1,0)$. This is equivalent to saying that this chain is "reversible". Among other things, this guarantees that its eigenvalues will all be real. However, not all Markov chains have this property. This issue is discussed briefly in Section 7.

Finally, we consider the even more specialized case in which $p = q$. This corresponds to a *random walk* on the *group* $\mathbf{Z}/(2)$ of integers modulo 2, because we step in the "same manner" no matter where on $\mathcal{X}$ we are. Here the "step distribution" is given by $Q(0) = 1-p$, $Q(1) = p$ (corresponding to the group element that we will add (modulo 2), at each step, to our present position). We compute that $E_Q\left((-1)^x\right) = 1-p-q$, the eigenvalue of the matrix P! (Here $(-1)^x$ equals 1 when $x = 0$, and equals -1 when $x = 1$.) This suggests that for random walks on groups, the eigenvalues can be computed simply by taking certain expected values with respect to the step distribution $Q(\cdot)$. This is discussed further in Section 5.

4. The eigenvalue connection.

We let $\mathcal{X} = \{0, 1, \ldots, n-1\}$ be a finite state space, μ_0 an initial distribution on $\mathcal{X}$, and P be a transition kernel on $\mathcal{X}$. The fact that $\mu_k = \mu_0 P^k$ suggests that we need to control high powers of the transition matrix P. This in turn suggests that the eigenvalues of P will play an important role. We develop this idea here, drawing heavily on work of Diaconis and Shashahani (1981), Diaconis (1988), and Belsley (1993).

In studying these eigenvalues, we shall make use of the fact that P has the same eigenvalues whether it operates on vectors from the right-side or the left-side. We begin with

Fact 1. *Any stochastic matrix P has an eigenvalue equal to 1.*

Proof. Define the vector u by $u(x) = 1$ for all $x \in \mathcal{X}$, then it is easily verified that $Pu = u$. ∎

We now write the (generalized) eigenvalues of P (counted with algebraic multiplicity) as $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$. Without loss of generality we take $\lambda_0 = 1$. We further set $\lambda_* = \max\limits_{1 \le j \le n-1} |\lambda_j|$, the largest absolute value of the non-trivial eigenvalues of P.

Fact 2. *We have $\lambda_* \leq 1$. Furthermore, if $P(x,y) > 0$ for all $x, y \in \mathcal{X}$, then $\lambda_* < 1$.*

Proof. Suppose $Pv = \lambda v$. Choose an index x so that $|v(x)| \geq |v(y)|$ for all $y \in \mathcal{X}$. Then

$$|\lambda v(x)| = |(Pv)_x| = |\sum_y P(x,y)v(y)| \leq \sum_y |v(y)|P(x,y) \leq \sum_y |v(x)|P(x,y) = |v(x)|\,,$$

so that $|\lambda| \leq 1$. Hence $\lambda_* \leq 1$.

Now suppose $P(x,y) > 0$ for all x and y. It is then easily seen that the inequality above can only be equality if v is a constant vector, i.e. $v(0) = v(1) = \ldots = v(n-1)$. This shows that $\lambda_0 = 1$ is the only eigenvalue of absolute value 1 in this case. Hence if P is diagonalizable we are done.

If P is not diagonalizable, then we still need to prove that the eigenvalue $\lambda_0 = 1$ is not part of a larger Jordan block. If it were, then for some vector v we would have $Pv = v + u$, where $u = (1, 1, \ldots, 1)^t$ as in the proof of Fact 1. But then, choosing $x \in \mathcal{X}$ with $\Re e\, v(x) \geq \Re e\, v(y)$ for all $y \in \mathcal{X}$, we have that

$$1 + \Re e\, v(x) = \Re e\, (Pv)_x = \Re e \sum_y P(x,y)v(y) \leq \Re e \sum_y P(x,y)v(x) = \Re e\, v(x)\,,$$

a contradiction. ∎

The importance of eigenvalues for convergence properties comes from the following.

Fact 3. *Suppose P satisfies $\lambda_* < 1$. Then, there is a unique stationary distribution π on $\mathcal{X}$ and, given an initial distribution μ_0 and point $x \in \mathcal{X}$, there is a constant $C_x > 0$ such that*

$$|\mu_k(x) - \pi(x)| \;\leq\; C_x k^{J-1} (\lambda_*)^{k-J+1}\,.$$

where J is the size of the largest Jordan block of P. (It follows immediately that $\|\mu_k - \pi\| \leq Ck^{J-1}(\lambda_*)^{k-J+1}$, where $C = \frac{1}{2}\sum C_x$.) In particular, if P is diagonalizable (so that $J = 1$), then

$$|\mu_k(x) - \pi(x)| \;\leq\; \sum_{m=1}^{n-1} |a_m v_m(x)||\lambda_m|^k \;\leq\; \left(\sum_{m=1}^{n-1} |a_m v_m(x)|\right)(\lambda_*)^k\,,$$

where $v_0, \ldots, v_{n-1}$ are a basis of right-eigenvectors corresponding to $\lambda_0, \ldots, \lambda_{n-1}$ respectively, and where a_m are the (unique) complex coefficients satisfying

$$\mu_0 \;=\; a_0 v_0 + a_1 v_1 + \ldots + a_{n-1} v_{n-1}\,.$$

If the eigenvectors v_j are orthonormal in $L^2(\pi)$, i.e. if $\sum_x v_i(x)\overline{v_j(x)}\pi(x) = \delta_{ij}$, then we get the further bound

$$\sum_x |\mu_k(x) - \pi(x)|^2 \pi(x) \;=\; \sum_{m=1}^{n-1} |a_m|^2 \, |\lambda_m|^{2k} \;\leq\; \left(\sum_{m=1}^{n-1} |a_m|^2 \right) (\lambda_*)^k \,.$$

Proof. We begin by assuming that P is diagonalizable. Then, using that $\mu_k = \mu_0 P^k$, that $v_m P = \lambda_m v_m$, and that $\lambda_0 = 1$, we have that

$$\mu_k \;=\; a_0 v_0 + a_1 v_1 (\lambda_1)^k + \ldots + a_{n-1} v_{n-1} (\lambda_{n-1})^k \,.$$

Since $\lambda_* < 1$, we have $(\lambda_m)^k \to 0$ as $k \to \infty$ for $1 \leq m \leq n-1$, so that $\mu_k \to a_0 v_0$. It follows that $\pi = a_0 v_0$ must be a probability distribution. Hence in particular $a_0 = (\sum_y v_0(y))^{-1}$ so it does not depend on the choice of μ_0. Thus,

$$\mu_k(x) - \pi(x) \;=\; a_1 v_1(x) (\lambda_1)^k + \ldots + a_{n-1} v_{n-1}(x) (\lambda_{n-1})^k \,.$$

The stated bound on $|\mu_k(x) - \pi(x)|$ now follows from the triangle inequality. The expression for the $L^2(\pi)$ norm of $\mu_k - \pi$ follows immediately from orthonormality.

For non-diagonalizable P, we must allow some of the vectors v_m to be *generalized eigenvectors* in the sense that we may have $v_m P = \lambda_m v_m + \lambda_{m+1}$. The only difference from the previous argument is that now μ_k may contain some additional terms. If $v_j, v_{j+1}, \ldots, v_{j+\ell-1}$ form a Jordan block of size ℓ, corresponding to the value λ_m, then we may have to add to μ_k extra terms of the form $a_r v_s (\lambda_m)^{k_0}$, with $j \leq r < s \leq j + \ell - 1$ and $k_0 \geq k - \ell + 1$. Keeping track of these extra terms, and bounding their number by k^{J-1}, the stated conclusion follows. ∎

We illustrate these ideas with a concrete example.

Example.

Consider the Markov chain on the state space $\mathcal{X} = \{1, 2, 3, 4\}$, with transition probabilities

$$P \;=\; \begin{pmatrix} 0.4 & 0.2 & 0.3 & 0.1 \\ 0.4 & 0.4 & 0.2 & 0 \\ 0.6 & 0.2 & 0.1 & 0.1 \\ 0.7 & 0.1 & 0 & 0.2 \end{pmatrix}$$

Suppose the Markov chain starts in the state 1, so that $\mu_0 = (1, 0, 0, 0)$.

We compute numerically that the matrix P has eigenvalues $\lambda_0 = 1,\ \lambda_1 = 0.2618,\ \lambda_2 = 0.0382,\ \lambda_3 = -0.2$, with corresponding left-eigenvectors

$$v_0 = (0.4671, 0.2394, 0.2089, 0.0846)$$

$$v_1 = (-0.4263, 0, 0.4263, 0)$$

$$v_2 = (-0.0369, 0.2301, -0.5656, 0.3724)$$

$$v_3 = (-0.2752, 0.4854, 0.0898, -0.3)$$

In terms of these eigenvectors, the initial state $\mu_0 = (1, 0, 0, 0)$ can be written as

$$\mu_0 \;=\; v_0 - 1.031\, v_1 - 0.4518\, v_2 - 0.2791\, v_3\,.$$

Now, we have taken v_0 to be a probability vector, so we immediately have $\pi(\cdot) = v_0(\cdot)$. Also, by the eigenvector properties, we have for example that

$$\begin{aligned}\mu_k(3) \;&=\; v_0(3) - 1.031(\lambda_1)^k v_1(3) - 0.4518(\lambda_2)^k v_2(3) - 0.2791(\lambda_3)^k v_3(3)\\ &=\; (0.2089) - 1.031(0.2618)^k(0.4263)\\ &\qquad - 0.4518(0.0382)^k(-0.5656) - 0.2791(-0.2)^k(0.0898)\,.\end{aligned}$$

Thus, noting that $|(1.031)(0.4263) + (0.4518)(0.5656) + (0.2791)(0.0898)| < 0.8$, and that $\lambda_* = 0.2618$, we have that

$$|\mu_k(3) - \pi(3)| \;<\; 0.8\,(0.2618)^k\,,$$

from which we can deduce values of k which make $\mu_k(3)$ arbitrarily close to $\pi(3)$. Other points in the state space (besides 3) are handled similarly. ■

Fact 3 gives a nice picture of a Markov chain converging geometrically quickly to a unique stationary distribution π. However, many Markov chains will not satisfy the condition that $P(x, y) > 0$ for all x and y. This raises the question of necessary and sufficient conditions to have $\lambda_* < 1$. The answer is as follows.

Fact 4. *A finite Markov chain satisfies $\lambda_* < 1$ if and only if it is both indecomposable and aperiodic.*

Proof. If the Markov chain is decomposable, leaving the disjoint subspaces $\mathcal{X}_1$ and $\mathcal{X}_2$ invariant, define vectors u_1 and u_2 by $u_j(x) = 1$ if $x \in \mathcal{X}_j$, 0 otherwise. Then it is easily seen that $Pu_j = u_j$, for $j = 1, 2$, so that P has multiple eigenvalues 1, and $\lambda_* = 1$.

If the Markov chain is periodic, then there are subspaces $\mathcal{X}_1, \ldots, \mathcal{X}_d$ with $P(x, \mathcal{X}_{j+1}) = 1$ for $x \in \mathcal{X}_j$, $1 \leq j \leq d-1$, and $P(x, \mathcal{X}_1) = 1$ for $x \in \mathcal{X}_d$. Define the vector v by $v(x) = e^{2\pi ij/d}$ for $x \in \mathcal{X}_j$. Then it is easily verified that $Pv = e^{2\pi i/d}v$. Thus, $e^{2\pi i/d}$ is an eigenvalue of P, so that again $\lambda_* = 1$.

For the converse, assume the Markov chain is indecomposable and aperiodic. Assume first that the Markov chain contains no transient states, i.e. there is positive probability of getting from any point x to any other point y (in some finite number of steps). We shall argue that some power of P has all its entries positive, so that the result will follow from our previous Fact.

Fix $x \in \mathcal{X}$, and let $S_x = \{k \mid P^k(x,x) > 0\}$. Our assumptions imply that S_x is infinite and has gcd 1. The set S_x is also *additive,* in the sense that if $a, b \in S_x$ then $a + b \in S_x$. It is then a straightforward exercise to verify that there must be some $k_x > 0$ such that $k \in S_x$ for all $k \geq k_x$.

Find such k_x for each $x \in \mathcal{X}$, and set $k_0 = \left(\max_x \; k_x\right) + n$. We claim that $P^{k_0}(x,y) > 0$ for all $x, y \in \mathcal{X}$. Indeed, given x and y, by assumption there exists r_{xy} such that $P^{r_{xy}}(x,y) > 0$, and we may clearly take $r_{xy} \leq n$. But then $P^{k_0}(x,y) \geq P^{k_0 - r_{xy}}(x,x)P^{r_{xy}}(x,y) > 0$, as desired.

It remains only to consider transient elements of the Markov chain. Suppose $x \in \mathcal{X}$ is transient. Then there exists $y \in \mathcal{X}$ and $r > 0$ such that $P^r(x,y) = \epsilon > 0$, but $P^m(y,x) = 0$ for all $m \geq 0$. Set $T = \{j \in \mathcal{X} \mid P^m(j,x) > 0 \text{ for some } m \geq 0\}$, so $y \notin T$. It is then easily computed that

$$\sum_{j \in T} |(vP^r)_j| \;\leq\; \sum_{j \in T} |v(j)| \;-\; \epsilon\,|v(x)|\,.$$

It follows that if $vP = \lambda v$ with $|\lambda| = 1$, then we must have $v(x) = 0$, so that λ is an eigenvalue of the Markov chain restricted to $\mathcal{X} - \{x\}$. This reduces the problem to the previous case. ∎

We close by observing that this discussion has relied heavily on the fact that the state space $\mathcal{X}$ is *finite.* On infinite spaces, P is a linear operator, and the notion of eigenvalues must be replaced by the more general notion of *spectrum* of an operator. Conclusions about convergence are much more difficult in this case, but some progress has been made. See for example Schervish and Carlin (1992).

5. Random walks on groups.

There is a particular class of Markov chains for which the eigenvalues and eigenvectors are often immediately available, namely random walks on groups. Here $\mathcal{X}$ is a group (finite for most of the present discussion), and $Q(\cdot)$ is a probability distribution on $\mathcal{X}$ (to be referred to as the "step distribution"). The transition probabilities are then defined by $P(x,y) = Q(x^{-1}y)$; this has the interpretation that at each step we are multiplying our previous group element x on the right by a new group element, chosen according to the distribution $Q(\cdot)$; the probability that this brings us to y is the probability that we multiplied by the group element $x^{-1}y$.

Typically we take $\mu_0(id) = 1$. Then $\mu_1 = Q$, and $\mu_{k+1} = \mu_k * Q$, where $*$ stands for the *convolution* of measures.

These random walks on groups are much easier to analyze in terms of convergence to stationarity than are general Markov chains. The ideas presented here were pioneered by Diaconis and Shashahani (1981), and were greatly advanced by Diaconis (1988) and many others. This section draws heavily upon Chapter 3 of Diaconis (1988); in particular, many of our examples are taken from there. The interested reader is urged to consult this reference for a deeper treatment of this subject.

We begin with the elementary

Fact 5. *Any random walk P on a finite group $\mathcal{X}$ satisfies $\pi P = \pi$, where π is defined by $\pi(x) = 1/n$ for all $x \in \mathcal{X}$ (and where $n = |\mathcal{X}|$). In words, the uniform distribution is stationary for any random walk on any finite group.*

Proof. We have

$$(\pi P)_y \;=\; \sum_x \pi(x)P(x,y) \;=\; (1/n)\sum_x Q(x^{-1}y) \;=\; (1/n)\sum_z Q(z) \;=\; 1/n \;=\; \pi(y)\,,$$

as desired. ∎

We begin our investigation with the abelian case, in which there are very complete and satisfying results.

5.1. Finite abelian groups.

All finite abelian (i.e. commutative) groups $\mathcal{X}$ are of the form

$$\mathcal{X} \;=\; \mathbf{Z}/(n_1) \times \mathbf{Z}/(n_2) \times \ldots \times \mathbf{Z}/(n_r)\,,$$

a direct product of cyclic groups. That is, they consist of elements of the form $x = (x_1, \ldots, x_r)$, with the group operation being addition, done modulo n_j in coordinate j. A random walk on such $\mathcal{X}$ is defined in terms of a probability distribution $Q(\cdot)$ on $\mathcal{X}$. This induces transition probabilities defined by $P(x, y) = Q(y - x)$. (We write $y - x$ instead of $x^{-1}y$ here simply because we are writing the group operation using additive notation, as is standard for abelian groups.)

Example #1. Let $\mathcal{X} = \mathbf{Z}/(2)$, the two-element group, and set $Q(1) = p$, $Q(0) = 1 - p$. This corresponds exactly to our "simplest non-trivial example" with $q = p$.

Example #2. Frog's Walk. Let $\mathcal{X} = \mathbf{Z}/(n)$, the integers mod n, and set $Q(-1) = Q(0) = Q(1) = 1/3$. This corresponds to our frog's walk from the Introduction, in which there are n points arranged in a circle, and the frog either moves one step to the right, one step to the left, or stays where she is, each with probability 1/3.

Example #3. Bit flipping. Let $\mathcal{X} = (\mathbf{Z}/(2))^d$, a product of d copies of the two-element group. Set $Q(0) = Q(e_1) = \ldots = Q(e_r) = 1/(d+1)$, where e_r is the vector with a 1 in the r'th spot and 0 elsewhere. This corresponds to a "bit-flipping" random walk on binary d-tuples, where at each stage we do nothing (with probability $1/(d+1)$) or change one of the d coordinates (chosen uniformly) to its opposite value.

The usefulness of random walks on finite abelian groups comes from the fact that we can explicitly describe their eigenvalues and eigenvectors. To do this, we need to introduce *characters*. For $m = (m_1, \ldots, m_d) \in \mathcal{X}$, define

$$\chi_m(x) \;=\; e^{2\pi i[(m_1x_1/n_1)+\ldots+(m_dx_d/n_d)]}\,, \qquad x \in \mathcal{X}\,.$$

Thus, χ_m is a function from the state space $\mathcal{X}$ to the complex numbers. The following facts are easily verified.

1. $\chi_m(x + y) = \chi_m(x)\chi_m(y)$.
2. $\chi_m(0) = 1$. $|\chi_m(x)| = 1$. $\chi_m(-x) = \overline{\chi_m(x)}$.
3. $\langle \chi_m, \chi_j \rangle \;=\; \delta_{mj}$, where the inner product is defined by $\langle f, g \rangle = (1/n) \sum_x f(x)\overline{g(x)}$. In words, the characters are *orthonormal* in $L^2(\pi)$. In particular, they form a basis for all functions on $\mathcal{X}$.
4. $\sum_m \chi_m(x) \;=\; n\,\delta_{x0}$.

These properties imply the following key fact.

Fact 6. *For each $m \in \mathcal{X}$, we have*

$$\overline{\chi_m}\, P \;=\; \lambda_m\, \overline{\chi_m}\,,$$

where

$$\lambda_m \;=\; E_Q(\chi_m)\,.$$

In words, for each m, $\overline{\chi_m}$ is an eigenvector of P corresponding to the eigenvalue $E_Q(\chi_m)$.

Proof. We have

$$(\overline{\chi_m}\, P)_y \;=\; \sum_x \overline{\chi_m(x)}\, P(x,y) \;=\; \sum_x \chi_m(-x)\, Q(y-x) \;=\; \sum_z \chi_m(z-y)\, Q(z)$$

$$=\; \sum_z \chi_m(z)\chi_m(-y)\, Q(z) \;=\; E_Q(\chi_m)\, \overline{\chi_m(y)}\,,$$

as desired. ∎

This fact immediately gives us all of the eigenvalues of the random walk, which is a significant achievement. (For example, in the simplest non-trivial example with $q = p$, it correctly predicts the eigenvalue $E_Q\left((-1)^x\right) = 1 - 2p$.) Combining this with Fact 3, and recalling that the characters are orthonormal in $L^2(\pi)$, we have

Fact 7. *A random walk on a finite abelian group satisfies*

$$\|\mu_k - \pi\| \;\le\; \frac{1}{2}\sqrt{\sum_{m\neq 0} |\lambda_m|^{2k}} \;\le\; (\sqrt{n}/2)(\lambda_*)^k\,,$$

where $\lambda_m = E_Q(\chi_m)$.

Proof. We have from Fact 3 (since the χ_m are orthonormal) that

$$\sum_x |\mu_k(x) - \pi(x)|^2 \pi(x) \;=\; \sum_{m\neq 0} |a_m|^2\, |\lambda_m|^{2k}\,,$$

where $\lambda_m = E_Q(\chi_m)$ as in Fact 6. Recalling that $\pi(x) = 1/n = a_m$, this reduces to

$$\sum_x |\mu_k(x) - \pi(x)|^2 \;=\; (1/n) \sum_{m\neq 0} |\lambda_m|^{2k}\,.$$

The result now follows from

$$4\,\|\mu_k - \pi\|^2 = \left(\sum_x |\mu_k(x) - \pi(x)|\right)^2 \le n \sum_x |\mu_k(x) - \pi(x)|^2 \,,$$

by the Cauchy-Schwarz inequality. ∎

Let us now apply this bound to the second and third examples above. For the frog's walk, we have

$$\lambda_m \;=\; E_Q(\chi_m) \;=\; (1/3) + (2/3)\cos(2\pi m/n) \;.$$

It follows that $\lambda_* = (1/3) + (2/3)\cos(2\pi/n)$. Using just λ_* in our bound above, we have (assuming $n \ge 3$, and using that $\cos(x) \le 1 - x^2/4$ for $0 \le x \le \sqrt{6}$, and that $1 - x \le e^{-x}$ for any x) that

$$\|\mu_k - \pi\| \;\le\; (\sqrt{n}/2)(\lambda_*)^k \;\le\; (\sqrt{n}/2)e^{-\frac{2\pi^2}{3n^2}k} \,.$$

This bound is small if k is large compared to $n^2 \log n$. We can actually get rid of the $\log n$ term by using the stronger bound with all the eigenvalues:

$$\begin{aligned}
\|\mu_k - \pi\|^2 \;&\le\; \frac{1}{4}\sum_{m=1}^{n-1} (\lambda_m)^{2k} \\
&\le\; \sum_{m=1}^{\lceil \frac{n-1}{4} \rceil} e^{-\frac{4\pi^2 m^2}{3n^2}k} \\
&\le\; \sum_{m=1}^{\infty} e^{-\frac{4\pi^2 m}{3n^2}k} \\
&=\; \frac{e^{-\frac{4\pi^2}{3n^2}k}}{1 - e^{-\frac{4\pi^2}{3n^2}k}} \,.
\end{aligned}$$

This last expression is small if k is large compared to n^2.

One might wonder if the order n^2 can be reduced still further. In fact, it cannot. To see this, we produce a *lower bound* as follows. First note that

$$E_{\mu_k}(\chi_m) \;=\; (E_Q(\chi_m))^k \;.$$

(This is similar to the fact that the characteristic function of a sum of independent random variables is the product of the individual characteristic functions.) This statement can easily be proved by induction. It can also be seen directly by noting that the quantity on

the left is the eigenvalue of P^k corresponding to the eigenvector $\overline{\chi_m}$, and is thus the k'th power of the corresponding eigenvalue for P.

It is further seen directly (or from the fact that χ_m is orthonormal to $\chi_0 \equiv 1$) that $E_\pi(\chi_m) = 0$ for $m \neq 0$. It now follows from our third equivalent definition of variation distance that

$$\|\mu_k - \pi\| \;\geq\; \frac{1}{2}|E_{\mu_k}(\chi_1)| \;=\; \frac{1}{2}|E_Q(\chi_1)|^k \;=\; \frac{1}{2}|\frac{1}{3} + \frac{2}{3}\cos(\frac{2\pi}{n})|^k \,.$$

(We could have chosen any other character χ_m with $m \neq 0$ in place of χ_1.)

Taking n =1000 and k =10,000, this equals 0.438. Thus, our frog would have to take considerably more than 10,000 steps to have approximately equal chance of being at any of her 1000 lily pads. To make this less than 0.1, we need $k = 122,302$.

More generally, for $n \geq 5$ this lower bound implies that

$$\|\mu_k - \pi\| \;\geq\; \frac{1}{2}\left(1 - \frac{1}{3}\left(\frac{2\pi}{n}\right)^2\right)^k \;\geq\; \frac{1}{2}\left(1 - \frac{k}{3}\left(\frac{2\pi}{n}\right)^2\right) \,.$$

It is easily seen that this quantity will be far from 0 unless k is large compared to n^2. Thus, $O(n^2)$ iterations are, for large n, both necessary and sufficient to converge to uniformity for this process.

For the "bit-flipping" process, Example #3 above, we have $\chi_m(x) = (-1)^{m \cdot x}$, where $m \cdot x = m_1 x_1 + \ldots + m_d x_d$. It is easily computed that

$$\lambda_m \;=\; E_Q(\chi_m) \;=\; 1 - \frac{2N(m)}{d+1} \,,$$

where $N(m)$ stands for the number of 1's in the binary d-tuple m. Hence, $\lambda_* = 1 - \frac{2}{d+1}$. Using this directly, and recalling that $n = |\mathcal{X}| = 2^d$, we have

$$\|\mu_k - \pi\| \;\leq\; 2^{d-1}\left(1 - \frac{2}{d+1}\right)^k \;\leq\; 2^d e^{-2k/(d+1)} \,,$$

which is small provided k is large compared to d^2.

As in the previous example, we can do better by using all the eigenvalues. Indeed, there are $\binom{d}{j}$ choices for m which have $N(m) = j$. Hence, we have (cf. Diaconis, 1988,

Section 3C) that

$$\begin{aligned}
\|\mu_k - \pi\|^2 &\le \frac{1}{4}\sum_{j=1}^{d}\binom{d}{j}|1-\frac{2j}{d+1}|^{2k} \\
&\le \frac{1}{2}\sum_{j=1}^{\lceil\frac{d+1}{2}\rceil}\binom{d}{j}(1-\frac{2j}{d+1})^{2k} \\
&\le \frac{1}{2}\sum_{j=1}^{\infty}\frac{d^j}{j!}\,e^{-\frac{4j}{d+1}k} \\
&= \frac{1}{2}\left(e^{de^{-\frac{4k}{d+1}}}-1\right).
\end{aligned}$$

This last expression is small if k is of the form $\frac{1}{4}d\log d + Cd$ with C large. This result is in fact the "correct" answer. Indeed, it can be shown (Diaconis, 1988) that to first order in d, *precisely* $\frac{1}{4}d\log d$ iterations are required to get close to uniform. Such a sharp result as this, giving the number of iterations *exactly* to first order in the size of the group, is the essence of the "cut-off phenomenon"; see Diaconis and Shashahani (1981), Aldous and Diaconis (1987), Diaconis (1988), and Rosenthal (1994c).

5.2. Finite non-abelian groups.

For non-abelian groups, the situation is more complicated, but we can still make use of the "characters" of the group to find eigenvalues, at least under the additional assumption that our step distribution is "conjugate-invariant".

Let $\mathcal{X}$ be a finite, non-abelian group (such as the symmetric group S_ℓ, which corresponds to shuffling a deck of cards). Such a group has associated with it *irreducible representations* $\rho_0, \rho_1, \ldots, \rho_r$, where $\rho_m : \mathcal{X} \to M_{d_m}(\mathbf{C})$ is a function taking the group $\mathcal{X}$ into the set of $d_m \times d_m$ complex matrices, which is multiplicative in the sense that $\rho_m(xy) = \rho_m(x)\rho_m(y)$ and that $\rho_m(id) = I_{d_m}$. (Here the multiplication on the left is in the group, while the multiplication on the right is matrix multiplication.)

It is known that these irreducible representations satisfy $\sum_m (d_m)^2 = |\mathcal{X}|$, i.e. that there are as many "representation entries" as there are elements of the group. Furthermore we may assume that $\rho_m(x^{-1}) = \rho_m(x)^*$, the conjugate transpose of $\rho_m(x)$. (In words, we may assume the matrices $\rho_m(x)$ are unitary.) It is then true that these "representation entries" are *orthogonal* under the appropriate inner product.

The connection with the abelian case comes as follows. The *characters* of the group are given by $\chi_m = \operatorname{tr}\rho_m$, the trace of the matrix. For *abelian* groups, we have $d_m = 1$ for all m, so that the character and the representation are essentially the same; in that case,

the current situation reduces to the previous one. In general, we have that $\sum_m d_m \chi_m(s) = n\,\delta_{s,id}$; again, if $d_m = 1$ for all m, this reduces to the previous case. Also, once again, the characters are orthonormal in $L^2(\pi)$.

In this generality, one cannot obtain simple formulas for the eigenvalues of the transition kernel P. Indeed, the matrix for P need not even be diagonalizable. However, let us assume that the step distribution $Q(\cdot)$ is *conjugate-invariant,* in the sense that $Q(x^{-1}yx) = Q(y)$ for all $x, y \in \mathcal{X}$. That is easily seen to imply that $\rho_m(x^{-1})E_Q(\rho_m)\rho_m(x) = E_Q(\rho_m)$ for all m and for all $x \in \mathcal{X}$. In words, the matrix $E_Q(\rho_m)$ commutes with every matrix of the form $\rho_m(x)$, for $x \in \mathcal{X}$. A well-known result from group representation theory, Schur's Lemma, then implies that $E_Q(\chi_m)$ is a *scalar* matrix, i.e. a multiple of the identity. It follows by taking traces that

$$E_Q(\rho_m) \;=\; (E_Q(\chi_m)/d_m)\; I_{d_m}\;,$$

where I_{d_m} is the $d_m \times d_m$ identity matrix.

Under this "conjugate-invariant" assumption, we have

Fact 8. *Let P correspond to a conjugate-invariant random walk on a finite group $\mathcal{X}$ as above. For $0 \le m \le r$, and $1 \le i, j \le d_m$, we have*

$$\overline{\rho_{m(ij)}}\,P \;=\; (E_Q(\chi_m)/d_m)\,\overline{\rho_{m(ij)}}\,.$$

In words, the vector whose value at the point $x \in \mathcal{X}$ is the complex conjugate of the ij entry of the matrix $\rho_m(x)$, is an eigenvector for P, with eigenvalue $E_Q(\chi_m)/d_m$.

Proof. For $g \in \mathcal{X}$, we have

$$\begin{aligned}
\left(\overline{\rho_{m(ij)}}\,P\right)_g \;&=\; \sum_{x\in\mathcal{X}} \overline{\rho_{m(ij)}(x)}\,P(g,x) \\
&=\; \sum_{x\in\mathcal{X}} \overline{\rho_{m(ij)}(x)}\,Q(x^{-1}g) \\
&=\; \sum_{y\in\mathcal{X}} \overline{\rho_{m(ij)}(gy^{-1})}\,Q(y) \\
&=\; \sum_{y} Q(y) \sum_{z} \overline{\rho_{m(iz)}(g)\rho^*_{m(jz)}(y)} \\
&=\; \sum_{z} \overline{(\rho_m(g))_{iz}\;(E_Q(\rho_m)^*)_{jz}} \\
&=\; (E_Q(\chi_m)/d_m)\;\left(\overline{\rho_m(g)}\right)_{ij}\;,
\end{aligned}$$

where we have used that $E_Q(\rho_m)$ is diagonal, with diagonal entries $E_Q(\chi_m)/d_m$. ∎

It follows immediately that the eigenvalues of P are precisely $E_Q(\chi_m)/d_m$, each repeated $(d_m)^2$ times. It also follows that the vector $\overline{\chi_m}$ is an eigenvector with this same eigenvalue, which directly generalizes the abelian case. Furthermore, as mentioned above, the characters χ_m are again orthonormal in $L^2(\pi)$. By exact analogy with our discussion there, we have

Fact 9. *The variation distance to the uniform distribution π satisfies*

$$\|\mu_k - \pi\| \;\le\; \frac{1}{2}\sqrt{\sum_{m\neq 0}(d_m)^2|\lambda_m|^{2k}} \;\le\; (\sqrt{n}/2)(\lambda_*)^k\,,$$

with $n = |\mathcal{X}|$ and with $\lambda_m = E_Q(\chi_m)/d_m$.

Example: Random Transpositions. Consider the symmetric group S_ℓ, with step distribution given by $Q(id) = 1/\ell$, $Q((ij)) = 2/\ell^2$ for all $i \neq j$. This corresponds to shuffling a deck of cards by choosing a random card uniformly with the left hand, choosing a random card uniformly with the right hand, and interchanging their positions in the deck (and doing nothing if we happened to pick the same card with both hands). Bounds on the distance to stationarity then correspond to bounds on how long the deck of cards must be shuffled until it is well mixed.

This was the example that motivated Diaconis and Shashahani (1981) to develop the modern, quantitative study of random walks on groups. To do a careful analysis of this model requires detailed knowledge of the representation theory of the symmetric group, which is rather involved. We note here simply that χ_1 for the symmetric group is the function that assigns to each group element, one less than the number of points in $\{1, 2, \ldots, \ell\}$ that it leaves fixed. Thus, $\chi_1(id) = \ell - 1$, and $\chi_1((ij)) = \ell - 3$. Also, $d_1 = \ell - 1$. Hence, the eigenvalue corresponding to χ_1 is given by

$$\lambda_1 \;=\; E_Q(\chi_1)/d_1 \;=\; \frac{(1/\ell)(\ell-1) + (1-(1/\ell))(\ell-3)}{\ell-1} \;=\; 1 - \frac{2}{\ell} \;\le\; e^{-2/\ell}\,.$$

Now, it so happens (though we cannot prove it here) that for this random walk, $\lambda_* = \lambda_1$. Thus, using our bound developed above, we have that

$$\|\mu_k - \pi\| \;\le\; \sqrt{\ell!/2}(\lambda_*)^k \;\le\; e^{\ell\log\ell}e^{-2k/\ell}\,,$$

which is small if k is large compared to $\ell^2 \log \ell$. Diaconis and Shashahani (1981) did a much more careful analysis of this process, using all the eigenvalues, and proved that to first order in ℓ, $\frac{1}{2}\ell\log\ell$ steps were necessary and sufficient, again proving a cut-off phenomenon. ∎

A number of other random walks on finite groups have been considered and shown to exhibit a cut-off phenomenon, including Random Transvections (Hildebrand, 1992) and Rank-One Deformations (Belsley, 1993). Bayer and Diaconis (1992) analyzed ordinary "riffle" card shuffles on the symmetric group, and proved a cut-off phenomenon at $(3/2)\log_2 \ell$ iterations. In particular, for $\ell = 52$, they showed that about 7 such shuffles were required to get close to stationarity. This shuffle is *not* conjugate-invariant; thus, their methods were somewhat different from the above, and involved deriving exact expressions for μ_k for this random walk.

5.3. Compact Lie groups.

Similar analyses to the above have been carried out for conjugate-invariant random walks on (infinite) compact Lie groups, In Rosenthal (1994a), a process of "random rotations" on the orthogonal group $SO(n)$ was shown to converge to Haar measure with a cut-off at $\frac{1}{2}n\log n$. In Porod (1993), generalizations of a process of "random reflections" were shown to exhibit the cut-off phenomenon on all of the classical compact Lie groups (orthogonal, unitary, and symplectic). The basic method of proof in these examples is the same as for finite groups. However, here the number of eigenvalues is *infinite*, so there is the additional complication that bounds are required are infinite sums.

6. Coupling and minorization conditions.

There is another approach to bounding convergence of Markov chains, which does not use eigenvalues at all. Rather, it uses probabilistic ideas directly.

6.1. Coupling.

The basic idea of coupling is the following. Suppose we have two *random variables* X and Y, defined jointly on some space $\mathcal{X}$. If we write $\mathcal{L}(X)$ and $\mathcal{L}(Y)$ for their respective probability distributions, then we can write

$$\begin{aligned}
\|\mathcal{L}(X) - \mathcal{L}(Y)\| &= \sup_A |P(X \in A) - P(Y \in A)| \\
&= \sup_A |P(X \in A, X = Y) + P(X \in A, X \neq Y) \\
&\qquad - P(Y \in A, Y = X) - P(Y \in A, Y \neq X)| \\
&= \sup_A |P(X \in A, X \neq Y) - P(Y \in A, Y \neq X)| \\
&\leq P(X \neq Y)\,.
\end{aligned}$$

Thus, *the variation distance between the laws of two random variables is bounded by the probability that they are unequal.*

We shall make use of this fact as follows. Given a Markov chain P on a space $\mathcal{X}$, with initial distribution μ_0, suppose we can find a new Markov chain (X_k, Y_k) on $\mathcal{X} \times \mathcal{X}$ with

(i) $X_0 \sim \mu_0$;

(ii) $Y_0 \sim \pi$;

(iii) $P(X_{k+1} \in A \mid X_k) \;=\; P(X_k, A)$;

(iv) $P(Y_{k+1} \in A \mid Y_k) \;=\; P(Y_k, A)$.

(v) There is a random time T such that $X_k = Y_k$ for all $k \geq T$.

In words, the chain X_k starts in the distribution μ_0 and proceeds according to the transitions $P(\cdot, \cdot)$. The chain Y_k starts in the distribution π and proceeds according to the same transitions $P(\cdot, \cdot)$. However, the *joint* law of (X_k, Y_k) is arbitrary, except that after some time T (called the *coupling time*), the two processes become equal.

The benefit of the above "coupling" is as follows. Since X_k is updated from $P(\cdot, \cdot)$, we have $\mathcal{L}(X_k) = \mu_k$. Also, since Y_k is also updated from $P(\cdot, \cdot)$, and since the distribution π is stationary, we have $\mathcal{L}(Y_k) = \pi$ for all k. It follows that

$$\|\mu_k - \pi\| = \|\mathcal{L}(X_k) - \mathcal{L}(Y_k)\| \leq P(X_k \neq Y_k) \leq P(T > k)\,.$$

Thus, if we can find a coupling as above, we get an immediate bound on $\|\mu_k - \pi\|$ simply in terms of the tail probabilities of the coupling time T.

There is a huge literature on coupling, and it has a long history in Markov chain theory. See for example Aldous (1983), Lindvall (1992), and references therein. We shall here concentrate on a particularly simple and elegant use of coupling, related to minorization conditions.

6.2. Uniform minorization conditions.

Suppose a Markov chain satisfies an inequality of the form

$$P^{k_0}(x, A) \;\geq\; \beta\,\zeta(A)\,, \qquad x \in R, \quad A \subseteq \mathcal{X}$$

where k_0 is a positive integer, R is a subset of the state space $\mathcal{X}$, $\beta > 0$, and $\zeta(\cdot)$ is some probability distribution on $\mathcal{X}$.

Such an inequality is called a *minorization condition* for a Markov chain, and says that the transition probabilities from a set R all have common *overlap* of at least size β. Minorization conditions were developed by Athreya and Ney (1978), Nummelin (1984), and others. We shall see that they can help us define a coupling to get bounds on the chain's rate of convergence.

We consider here the *uniform* case in which $R = \mathcal{X}$, i.e. in which the minorization condition holds on the entire state space. (This is sometimes called the Doeblin condition.) We further assume for simplicity that $k_0 = 1$.

We shall now use this minorization condition to define a coupling. First define (X_k, Z_k) jointly as follows. Choose $X_0 \sim \mu_0$ and $Z_0 \sim \pi$ independently. Then, given X_k and Z_k, choose X_{k+1} and Z_{k+1} by flipping an independent coin that has probability β of coming up heads, and then

(a) If the coin is heads, choose a point $z \in \mathcal{X}$ distributed independently according to $\zeta(\cdot)$, and set $X_{k+1} = Z_{k+1} = z$.

(b) If the coin is tails, then choose X_{k+1} and Z_{k+1} independently with

$$P(X_{k+1} \in A) \;=\; \frac{P(X_k, A) - \beta\,\zeta(A)}{1-\beta}\,;$$

$$P(Z_{k+1} \in A) \;=\; \frac{P(Z_k, A) - \beta\,\zeta(A)}{1-\beta}\,.$$

These probabilities have been chosen precisely so that $P(X_{k+1} \in A \mid X_k) = P(X_k, A)$ (and similarly for Z_{k+1}). The point is, option (a) forces X_{k+1} to be equal to Z_{k+1}, and this chance of becoming equal is good for getting coupling bounds.

Let T be the first time the coin comes up heads. Then define Y_k by

$$Y_k \;=\; \begin{cases} Z_k, & k \le T\,; \\ X_k, & k > T \end{cases}\,.$$

Thus, Y_k is essentially the same as Z_k, except that after the Markov chains become equal at time T, they will *remain* equal forever.

The combined chain (X_k, Y_k) is now a coupling with coupling time T. Also, since we had probability β of choosing option (a) each time, we see that $P(T > k) = (1-\beta)^k$. Our above inequality immediately gives the following.

Fact 10. *Suppose a Markov chain satisfies $P(x, A) \ge \beta\,\zeta(A)$, for all $x \in \mathcal{X}$ and for all measurable subsets $A \subseteq \mathcal{X}$, for some probability distribution $\zeta(\cdot)$ on $\mathcal{X}$. Then given any initial distribution μ_0 and stationary distribution π, we have*

$$\|\mu_k - \pi\| \;\le\; (1-\beta)^k\,.$$

This fact goes back to Doob (1953), and been used in Roberts and Polson (1994), Rosenthal (1993a), and many other places. It is quite powerful. For example, it immediately generalizes our earlier result that, on a finite state space, if all entries are positive

then the chain converges geometrically quickly. In fact, now we require only that some column of the matrix be all positive (and furthermore we immediately obtain a quantitative bound on convergence in that case).

It is easily seen that, given a Markov chain $P(x, \cdot)$, the largest value of β that we can use as above should be given by

$$\beta \;=\; \int\limits_{\mathcal{X}} \inf_{x \in \mathcal{X}} P(x, dy)\,,$$

which on a discrete space reduces to

$$\beta \;=\; \sum_{y \in \mathcal{X}} \min_{x \in \mathcal{X}} P(x, y)\,.$$

In words, we may take β to be the sum of the minimum values of the entries in each column of P. We can then immediately conclude that $\|\mu_k - \pi\| \leq (1-\beta)^k$. Note that this was precisely our finding in the simplest non-trivial example of Section 3.

Example. Consider the Markov chain on $\mathcal{X} = \{1, 2, 3, 4, 5\}$ with transition kernel

$$P \;=\; \begin{pmatrix} 0.2 & 0.2 & 0.3 & 0.3 & 0 \\ 0.4 & 0 & 0.3 & 0.3 & 0 \\ 0.2 & 0.2 & 0.4 & 0.1 & 0.1 \\ 0.2 & 0.1 & 0.3 & 0.1 & 0.3 \\ 0.2 & 0 & 0.5 & 0.3 & 0 \end{pmatrix}$$

We see by inspection that the column minimums are $0.2, 0, 0.3, 0.1, 0$, respectively. Thus we may take $\beta = 0.6$, and immediately conclude that $\|\mu_k - \pi\| \leq (0.4)^k$. (Note that here $Q(1) = 1/3$, $Q(3) = 1/2$, and $Q(4) = 1/6$.) ∎

Example. Let $\mathcal{X} = [0, 1]$ (the interval from 0 to 1), and set

$$P(x, dy) \;=\; \frac{1 + x + y}{\frac{3}{2} + x}\; dy\,.$$

We see by inspection that $P(x, dy) \geq \frac{2}{3}\, dy$ for all x and y, so that we may take $\beta = \frac{2}{3}$ to conclude that $\|\mu_k - \pi\| \leq (1/3)^k$. We can do even better by finding the best β as above:

$$\beta \;=\; \int\limits_0^1 \left(\inf_{0 \leq x \leq 1} \frac{1 + x + y}{\frac{3}{2} + x} \right) dy \;=\; \int\limits_0^{\frac{1}{2}} \frac{2}{3}(1 + y) dy \;+\; \int\limits_{\frac{1}{2}}^1 \frac{2}{5}(2 + y) dy \;=\; \frac{29}{30}\,.$$

Hence, we actually have $\|\mu_k - \pi\| \leq (1/30)^k$. (Note that here $Q(\cdot)$ has density (with respect to dy) given by $\frac{30}{29}\,\frac{2}{3}(1+y)$ for $0 \leq y \leq \frac{1}{2}$, and by $\frac{30}{29}\,\frac{2}{5}(2+y)$ for $\frac{1}{2} < y \leq 1$.) ■

These two examples will probably convince the reader that the minorization method is sometimes very powerful. On the other hand, the best value of β above will often be 0; for example, this is certainly true for the Frog's Walk discussed in the introduction. One way to get around this difficulty is to replace P by P^{k_0} in the minorization condition, which requires replacing k by $[k/k_0]$ in the conclusion (see exercise 6). In principle this approach should usually work well, but in practice it may be very difficult to compute or estimate quantities related to P^{k_0}. See Rosenthal (1993a) for one attempt in this direction.

Another method is to restrict the values of x in the minorization condition to being in some subset $R \subseteq \mathcal{X}$, as we now discuss.

6.3. Minorization conditions on subsets.

Suppose that instead of the uniform minorization condition as above, we have a minorization condition which holds only on a subset $R \subseteq \mathcal{X}$. Then our above bound, which was based on coupling with probability β at each step, cannot be applied. Various other approaches have been used in this case. We very briefly outline them here.

If one allows the subset R to be arbitrarily large (in fact, to grow as a function of k), then it may be possible to bound the probability of escaping from R, and draw conclusions about $\|\mu_k - \pi\|$ in that way; see Rosenthal (1991).

In any case, each time our coupled process (X_k, Y_k) visits the subset $R \times R$, it has probability β of coupling. Using "drift conditions", it may be possible to bound the number of such returns to $R \times R$, and then use coupling as in the uniform case; see Rosenthal (1993b).

A related approach is presented in Meyn and Tweedie (1993), who use minorizations, drift conditions, splittings, and careful bounding to obtain bounds on $\|\mu_k - \pi\|$ directly, without introducing a second, coupled chain.

Instead of trying to bound $\|\mu_k - \pi\|$ directly, or use coupling, another approach is as follows. Consider a single Markov chain X_k, and each time it is in the subset R, with probability β update it according to $\zeta(\cdot)$. Call the times of such updatings *regeneration times*. Then, it is easily seen that the distribution of X_k depends only on the time since the last regeneration time. Thus, if these "times since the last regeneration" converge, then the original chain X_k must also converge. This is the essential idea behind convergence results in Athreya and Ney (1978), Nummelin (1984), Asmussen (1990), Mykland et al (1992), and elsewhere.

7. Other approaches.

There are many other methods of bounding convergence rates of Markov chains. We briefly mention some of them here.

For certain Markov chains including birth-death chains (i.e. Markov chains on the integers, which can move at most distance 1 on a given step), the eigenvalues and eigenvectors are related to the "orthogonal polynomials". Classically known results can be used to get good bounds on convergence rates. See Belsley (1993) and references therein.

Related to the coupling and minorization bounds presented herein is the method of strong stopping times (Aldous and Diaconis, 1986, 1987). Essentially, if the reference measure $\zeta(\cdot)$ in the minorization condition happens to be the stationary distribution $\pi(\cdot)$, then one can construct a random time τ such that the law of X_τ is precisely $\pi(\cdot)$, and such that X_τ is independent of τ. Such a time τ is a strong stopping time, and it is easily seen that $\|\mu_k - \pi\| \leq P(\tau > k)$. Another method of constructing strong stopping times is by constructing a dual Markov chain that keeps track of "how stationary" the Markov chain has become; see Diaconis and Fill (1990).

A different and very beautiful method of bounding convergence to certain specific distributions (e.g. normal, poisson) is the method of Stein (1971) and Chen (1975). This involves characterizing the distribution of interest through some "identity" that it satisfies, and then seeing to what extent the distribution μ_k approximately satisfies that identity. In certain cases the technique has been simplified to the point where it is very usable. See Arratia et al. (1989) and Barbour et al. (1992).

Finally, geometric arguments involving "paths" on graphs have recently been used to bound eigenvalues of Markov chains, with great success in certain examples; see Jerrum and Sinclair (1989) and Diaconis and Stroock (1991). Geometric approaches have also been used to allow different Markov chains to be "compared" to each other, so that known information about one Markov chain can be used to obtain information about related chains; see Diaconis and Saloff-Coste (1993).

Some of these approaches use *reversibility* of a Markov chain. A Markov chain is reversible if the identity $\pi(dx)P(x, dy) = \pi(dy)P(y, dx)$ holds for all $x, y \in \mathcal{X}$. This is equivalent to saying that, if the chain starts in the stationary distribution $\pi(\cdot)$, it has the same law whether time runs forwards or backwards. This immediately implies that P is a self-adjoint operator on $L^2(\pi)$. Such structure is exploited in Diaconis and Stroock (1991), Fill (1991), and elsewhere.

Most of the above work has been concerned primarily with convergence in total variation distance (or the related separation distance). There are of course many other notions

of distance between probability measures that could be used, such as relative entropy, etc. See Su (1994) for a start in this direction.

Naturally, these few words scarcely begin to cover the depth of work that has been applied to convergence questions. The reader is strongly encouraged to consult these and other references for further information.

EXERCISES

To further the reader's understanding, we provide here a number of exercises which expand upon the material presented herein.

1. For each of the following transition matrices, determine (with explanation!) whether $\lambda_* = 1$ or $\lambda_* < 1$.

(a)

$$P = \begin{pmatrix} 1/4 & 1/4 & 1/2 \\ 1/3 & 1/3 & 1/3 \\ 0.01 & 0.01 & 0.98 \end{pmatrix}$$

(b)

$$P = \begin{pmatrix} 1/4 & 1/4 & 1/2 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

(c)

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

2. Let $\mathcal{X} = \{0, 1, 2, 3\}$, and let

$$P = \begin{pmatrix} 0.2 & 0.4 & 0 & 0.4 \\ 0.4 & 0.2 & 0.4 & 0 \\ 0 & 0.4 & 0.2 & 0.4 \\ 0.4 & 0 & 0.4 & 0.2 \end{pmatrix} .$$

Let $\mu_0(0) = 1$ give the initial distribution. Find an exponentially decreasing bound on the variation distance $\|\mu_k - \pi\|$. (Hint: This is a random walk on a group!)

3. Repeat question 2 with P replaced by

$$P = \begin{pmatrix} 0.2 & 0.4 & 0 & 0.4 \\ 0.4 & 0.2 & 0.4 & 0 \\ 0.3 & 0.4 & 0.2 & 0.1 \\ 0.4 & 0 & 0.4 & 0.2 \end{pmatrix} .$$

(Hint: Use a uniform minorization condition!)

4. Let P be a transition matrix on a state space $\mathcal{X}$, with initial distribution μ_0 and stationary distribution π. Prove that the distance to stationarity is *weakly decreasing,* in the sense that for any $k \geq 0$,

$$\|\mu_{k+1} - \pi\|_{\text{var}} \;\leq\; \|\mu_k - \pi\|_{\text{var}} .$$

5. Let $\mathcal{X}_1$ and $\mathcal{X}_2$ be finite state spaces. Let μ_1 and ν_1 be probability distributions on $\mathcal{X}_1$, and let μ_2 and ν_2 be probability distributions on $\mathcal{X}_2$. Then $\mu_1 \times \mu_2$ is a probability distribution on $\mathcal{X}_1 \times \mathcal{X}_2$, defined by $\mu_1 \times \mu_2\ (x, y) = \mu_1(x)\mu_2(y)$ (and similarly for $\nu_1 \times \nu_2$).

Prove that

$$\|\mu_1 \times \mu_2 \;-\; \nu_1 \times \nu_2\|_{\text{var}} \;\leq\; \|\mu_1 - \nu_1\|_{\text{var}} \;+\; \|\mu_2 - \nu_2\|_{\text{var}} .$$

6. *Multi-step minorization conditions.* Suppose we are given that $P^{k_0}(x, \cdot) \geq \beta\zeta(\cdot)$ for all $x \in \mathcal{X}$, for some positive integer k_0. Prove that

$$\|\mu_k - \pi\| \;\leq\; (1 - \beta)^{[k/k_0]} ,$$

where $[k/k_0]$ means the greatest integer not exceeding k/k_0. (Hint: First prove it for k an integer multiple of k_0, and then use exercise 4.)

7. *Explicit $O(n^2)$ bounds.* Consider random walk on the state space $\mathcal{X} = \mathbf{Z}/(n)$, the integers mod n, with initial distribution given by $\mu_0(0) = 1$, and with step distribution given by $Q(0) = 0.9$, $Q(1) = 0.1$.

Find, with proof, *explicit* constants $A, B, \alpha, \beta, k_0, n_0 > 0$ (independent of n and k) such that

$$A\, e^{-\alpha k/n^2} \;\leq\; \|\mu_k - \pi\| \;\leq\; B\, e^{-\beta k/n^2} , \qquad \text{for all } \; n \geq n_0 \,,\; k \geq k_0\, n^2 .$$

In particular, this proves that this random walk takes $O(n^2)$ steps to converge.

8. *Numerical bounds on the circle.* Consider random walk on $\mathbf{Z}/(n)$, with $n = 100$. For each of the following step distributions $Q(\cdot)$, find (i) $P(99, x)$ for all $x \in \mathbf{Z}/(n)$, (ii) $|\lambda_m|$ for $0 \le m \le 99$ (simplified if possible), and (iii) λ_*. (Note: λ_m may be a complex number!) Finally, (iv) find a value of k so that $\|\mu_k - \pi\|_{\text{var}} \le e^{-20}$. (Warning: Don't forget to compute appropriate cosines in radians, not in degrees!)

(a) $Q(0) = Q(1) = 1/2$, with $Q(x) = 0$ otherwise.

(b) $Q(3) = Q(4) = 1/2$, with $Q(x) = 0$ otherwise.

(c) $Q(-3) = Q(3) = 1/4$, and $Q(0) = 1/2$, with $Q(x) = 0$ otherwise.

9. *Random walk with two-point support.* Consider again random walk on $\mathbf{Z}/(n)$, but with n arbitrary. Let $j \in \mathbf{Z}/(n)$ with $j \neq 0$, and define the step distribution by $Q(0) = Q(j) = 1/2$.

(a) Under what conditions on n and j will we have $\lambda_* = 1$?

(b) For what values of n can we be sure that $\lambda_* < 1$, for *any* non-zero value of j?

10. *Convergence of projections.* Let $\mathcal{X} = \mathbf{Z}/(80) \times \mathbf{Z}/(100)$ be the abelian group consisting of pairs (x, y) with $x \in \mathbf{Z}/(80)$ and $y \in \mathbf{Z}/(100)$, with addition defined coordinate-wise as usual. Let the step distribution $Q(\cdot)$ on $\mathcal{X}$ be defined by

$$Q(0,0) = 1/2; \qquad Q(1,1) = Q(-1,1) = Q(1,-1) = Q(-1,-1) = 1/8\,.$$

As usual, let $P\left((x_1, x_2), (y_1, y_2)\right) = Q(y_1 - x_1, y_2 - x_2)$, define μ_0 by $\mu_0(0,0) = 1$, and let $\mu_k = \mu_0 P^k$ be the distribution of the random walk after k steps.

Furthermore, let ν_k be the distribution of the <u>first coordinate</u> after k steps. Formally,

$$\nu_k(x_1) \;=\; \sum_{x_2 \in \mathbf{Z}/(100)} \mu_k(x_1, x_2)\,.$$

Let π be the uniform distribution on $\mathcal{X}$, and let π_1 be the uniform distribution on $\mathbf{Z}/(80)$. Prove or disprove each of the following assertions.

(a) $\|\mu_k - \pi\|_{\text{var}} \;\to\; 0 \quad \text{as} \quad k \to \infty.$

(b) $\|\nu_k - \pi_1\|_{\text{var}} \to 0$ as $k \to \infty$.

11. *Convergence in a constant number of steps.* Consider random walk on $\mathcal{X} = \mathbf{Z}/(n)$ with $\mu_0(0) = 1$. Let n be a multiple of 4, and set $Q(x) = 1/(1 + (n/2))$ for $x = -n/4, -(n/4) + 1, \ldots, -1, 0, 1, 2, \ldots, (n/4) - 1, n/4$, with $Q(x) = 0$ otherwise. In words, at each step the random walk jumps to one of its $(n/2) + 1$ nearest neighbors (including the point it's already on), each with equal probability.

Prove that there are constants $A, \alpha > 0$ (independent of n and k) such that

$$\|\mu_k - \pi\| \le Ae^{-\alpha k}, \qquad \text{for all } n, k.$$

In particular, this proves that this random walk converges in $O(1)$ steps, i.e. in a "constant" (bounded) number of steps. (This fact is generalized in Rosenthal (1994b).)

12. *Random walk on the chessboard, Part I.* Consider the group $\mathbf{Z}/(n) \times \mathbf{Z}/(m)$, thought of as an $n \times m$ rectangular grid, to be used as a "chessboard". (In this interpretation, we must allow the chesspieces to "wrap around", in the sense that a chesspiece at (say) the right edge of the board could jump off to the right and re-appear on the left.) For each of the following three step distributions, get upper and lower bounds on the distance to stationarity for the corresponding random walk. (For simplicity, in this exercise you may neglect lower-order terms as $n, m \to \infty$.)

(a) The factorable king moves: $Q(a, b) = 1/9$ for $a, b = -1, 0, 1$. (Hint: Write this random walk as a "product" of two simpler random walks, and use exercise 5.)

(b) The non-factorable king moves: $Q(0, 0) = 1/2$, $Q(a, b) = 1/16$ for $a, b = -1, 0, 1$, with $(a, b) \neq (0, 0)$.

(c) The knight moves: $Q(\pm 1, \pm 2) = Q(\pm 2, \pm 1) = Q(0, 0) = 1/9$.

13. *Random walk on a stick.* Let $\mathcal{X} = \{1, 2, \ldots, n\}$, thought of as n points in a line (not in a circle). Define the transition probabilities P by

$$P(x, x-1) = P(x, x) = P(x, x+1) = 1/3, \qquad 2 \le x \le n-1;$$

$$P(1, 1) = P(n, n) = 1/3; \qquad P(1, 2) = P(n, n-1) = 2/3.$$

In words, the Markov chain jumps left or right, or stays still, each with probability 1/3, *except at the endpoints.* At the endpoints, it stays still with probability 1/3 and

jumps back towards the center with probability 2/3. (This corresponds to having "reflecting barriers" at the endpoints.)

You are to bound the convergence of this Markov chain by *lifting* it to a random walk on the group $\mathbf{Z}/(2n-2) = \{1', 2', 3', \ldots, (2n-2)'\}$, as follows. Identify the point 1 with the point $1'$, and the point n with the point n'. For $2 \leq x \leq n-1$, identify the point x with the point x' <u>and</u> with the point $(2n-x)'$.

(a) Argue that our "usual" random walk on $\mathbf{Z}/(2n-2)$ (which at each step moves left, right, or not at all, each with probability 1/3) "projects" (whatever that means!) under this identification onto the Markov chain on $\mathcal{X}$.

(b) Use this "projection" to determine the stationary distribution π of our Markov chain on $\mathcal{X}$.

(c) Argue that the variation distance to stationarity of the Markov chain on $\mathcal{X}$ is bounded above by the corresponding variation distance on the "covering chain" on $\mathbf{Z}/(2n-2)$.

(d) Use this to derive upper bounds on the rate of convergence of the Markov chain to the stationary distribution π.

14. *Random walk on the chessboard, Part II.* Redo the analysis of the non-factorable king moves on a chessboard (exercise 12 (b)), but with the "wrap around" assumption replaced by reflecting barriers on all sides. In other words, if the king is at one edge of the chessboard, then the probabilities that would normally make it move off the edge are instead added on to the probability of moving to the "reflected" point the other way. (That is, the new probabilities are designed so they can "lift" to a random walk on $\mathbf{Z}/(2n-2) \times \mathbf{Z}/(2m-2)$, similar to the previous question.) For example, $P((0,2),(1,3)) = 2/16 = 1/8$, because the probability of moving to $(-1,3)$ is instead added on to the probability of moving to $(1,3)$. Also $P((0,0),(1,1)) = 4/16 = 1/4$.

For this new, "reflecting barriers" king on the $n \times m$ chessboard, get upper bounds on the rate of convergence to stationarity. (As in question 12, you may neglect lower-order terms as $n, m \to \infty$.)

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