Making Markov chains less lazy

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21 January 2013

Abstract

The mixing time of an ergodic, reversible Markov chain can be bounded in terms of the eigenvalues of the chain: specifically, the second-largest eigenvalue and the smallest eigenvalue. It has become standard to focus only on the second-largest eigenvalue, by making the Markov chain “lazy”. (A lazy chain does nothing at each step with probability at least $\frac{1}{2}$, and has only nonnegative eigenvalues.)

An alternative approach to bounding the smallest eigenvalue was given by Diaconis and Stroock [5, Proposition 2] and Diaconis and Saloff-Coste [4, p.702].

We give examples to show that using this approach it can be quite easy to obtain a bound on the smallest eigenvalue of a combinatorial Markov chain which is several orders of magnitude below the best-known bound on the second-largest eigenvalue.

1 Introduction

Let $\mathcal{M}$ be an ergodic, reversible Markov chain with finite state space $\Omega$ and transition matrix $P$. It is well known that the eigenvalues of $\mathcal{M}$ satisfy

$$1 = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{N-1} > -1,$$

where $N = |\Omega|$. We refer to $\lambda_{N-1}$ as the \textit{smallest eigenvalue} of $\mathcal{M}$.

The connection between the mixing time of a Markov chain and its eigenvalues is well-known (see [14, Proposition 1]):

$$\tau(\varepsilon) \leq (1 - \lambda_*)^{-1} \ln \frac{1}{\varepsilon \pi_{\min}}$$

(1)

where $\tau(\varepsilon)$ denotes the mixing time of the Markov chain, $\pi_{\min} = \min_{x \in \Omega} \pi(x)$ and

$$\lambda_* = \max\{\lambda_1, |\lambda_{N-1}|\}.$$
When studying the mixing time of a Markov chain $\mathcal{M}$ using (1), the approach which has become standard is to make the chain $\mathcal{M}$ lazy by replacing $P$ by $(I + P)/2$, where $I$ denotes the identity matrix. Then all eigenvalues of the lazy chain are nonnegative, and only the second-largest eigenvalue must be investigated.

A lazy chain can be implemented so that its expected running time is the same as the mixing time of the original chain. So the problem with lazy chains is not their efficiency. In our opinion, the main problem with lazy Markov chains is conceptual: in order to prove that a Markov chain is fast, we first slow it down. The device of using lazy Markov chains has been called “crude” [15, p. 110] and “unnatural” [10, Chapter 5].

In this note, we aim to advertise an approach for bounding the smallest eigenvalue of a Markov chain. This approach was first proposed by Diaconis and Stroock in 1991 [5, Proposition 2], and a modified version was presented by Diaconis and Saloff-Coste two years later [4, p.702] (restated as Lemma 1.1 below). The method of [4] has been applied in [4, 5, 7], but in the theoretical computer science community it has become common to work with lazy chains. We urge researchers to first try the approach of [4, 5] before choosing to work with a lazy version of their chain.

Finally we remark that in [8] the author wrongly claimed that their [8, Lemma 1.3] was new, when in fact it is precisely the result of [4, p.702]. We sincerely apologise for this error.

### 1.1 The method

See [10] for Markov chain definitions not given here. Write $\mathcal{G}$ for the underlying directed graph of the Markov chain $\mathcal{M}$, where $\mathcal{G} = (\Omega, \Gamma)$ and each directed edge $e \in \Gamma$ corresponds to a transition of $\mathcal{M}$. If $P(x, x) > 0$ then the edge $xx$ is called a self-loop at $x$. Define $Q(e) = Q(x, y) = \pi(x)P(x, y)$ for the edge $e = xy$. A walk in $\mathcal{G}$ is a sequence of states $x_0x_1\cdots x_\ell$ such that $P(x_j, x_{j+1}) > 0$ for $j = 0, \ldots, \ell - 1$. The walk is closed if $x_\ell = x_0$. If a walk has odd length then we call it an odd walk.

For each $x \in \Omega$ let $w_x$ be an odd walk from $x$ to $x$ in $\mathcal{G}$. (Such a walk exists for each $x$, since the Markov chain is aperiodic.) Define $\mathcal{W} = \{w_x : x \in \Omega\}$, a set of “canonical closed odd walks”. For each transition $e \in \Gamma$ and each $w \in \mathcal{W}$, let $r(e, w)$ denote the number of times that $e$ appears as a directed edge of $w$. We can assume that $r(e, w) \leq 2$ for all transitions $e$ (indeed, if $e$ is a self-loop then we can assume that $r(e, w) \leq 1$.) The congestion of $\mathcal{W}$, denoted by $\eta(\mathcal{W})$, is defined by

$$
\eta(\mathcal{W}) = \max_{e \in \Gamma} Q(e)^{-1} \sum_{x \in \Omega, e \in w_x} r(e, w_x) \pi(x) |w_x|.
$$

**Lemma 1.1.** [4, p.702] Suppose that $\mathcal{M}$ is a reversible, ergodic Markov chain with state space $\Omega$, and let $\mathcal{W}$ be a set of odd walks defined as above. Then

$$(1 + \lambda_{N-1})^{-1} \leq \frac{\eta(\mathcal{W})}{2}.$$
If \(|w_x| = 1\) for all \(x \in \Omega\) then the bound of Lemma 1.1 simplifies further to
\[
(1 + \lambda_{N-1})^{-1} \leq \frac{1}{2} \max_{x \in \Omega} P(x, x)^{-1}.
\]

**Remark 1.2.** Suppose that the graph underlying a Markov chain \(\mathcal{M}\) can be obtained from a connected bipartite graph by adding loops to an exponentially small proportion of states. For example, many instances of the knapsack chain [13] satisfy this property. Since every closed odd walk must traverse at least one of these self-loop edges, it is very difficult to define a set of canonical closed odd walks with low congestion. So Lemma 1.1 is unlikely to be easy to apply in this case.

## 2 Applications of the method

We illustrate the use of Lemma 1.1 by applying it to three combinatorial Markov chains. Our applications are all ergodic and reversible with uniform stationary distribution, and no edge will be used more than once in any walk \(w_x\) that we define. In this case the congestion can be simplified to
\[
\eta(W) = \max_{e \in \Gamma} P(e)^{-1} \sum_{x \in \Omega, e \in w_x} |w_x|,
\]
where \(P(e) = P(x, y) = P(y, x)\) for the transition \(e = xy\).

### 2.1 The switch chain for sampling regular graphs

Our first application is to the Markov chain for sampling regular graphs known as the switch chain. A transition of the chain is performed as follows: from the current state \(G\) (a \(d\)-regular graph on vertex set \([n]\)) choose an unordered pair of non-incident edges uniformly at random, let \(G'\) be the multigraph obtained from \(G\) by deleting these edges and inserting a perfect matching of their four endvertices, selected uniformly at random. If \(G'\) has no repeated edges then the new state is \(G'\), otherwise it is \(G\).

The lazy version of this chain was analysed by Cooper et al. [1, 2]. Clearly \(P(G, G) \geq \frac{1}{3}\) for every state \(G\) of this chain, so by (2) we immediately conclude that
\[
(1 + \lambda_{N-1})^{-1} \leq \frac{3}{2}.
\]
This is several orders of magnitude smaller than the best-known bound on \((1 - \lambda_1)^{-1}\), which is \(O(d^3 n^8)\) (see [2]).

### 2.2 Jerrum and Sinclair’s matchings chain

The next application is to the well-known Markov chain for sampling perfect and near-perfect matchings of a fixed graph \(G\). A transition of the chain is performed as follows: from the current state \(M\) (which is a perfect or near-perfect matching of \(G\)), choose an edge \(e \in E(G)\) uniformly at random. If \(M\) is a perfect matching and \(e \in M\) then
the new state is \( M - \{e\} \). If \( M \) is a near-perfect matching and both endvertices of \( e \) are unmatched in \( M \) then the new state is \( M \cup \{e\} \). If \( M \) is a near-perfect matching, and exactly one endvertex of \( e \) is unmatched in \( M \) then let \( e' \) be the edge of \( M \) which matches the other endvertex of \( e \): the new state is \( (M - \{e'\}) \cup \{e\} \). In all other cases the new state is \( M \).

The lazy version of this chain was analysed by Jerrum and Sinclair [11, 12]. If \( G \) itself is not a perfect matching then \( P(M, M) \geq \frac{1}{|E|} \) for all states \( M \) of the chain (that is, for all perfect or near-perfect matchings \( M \) of \( G \)). Therefore (2) implies that

\[
(1 + \lambda_{N-1})^{-1} \leq \frac{|E|}{2}.
\]

This bound is at least a factor \( n^2 \) smaller than the smallest-known bound on \( (1 - \lambda_1)^{-1} \), which is \( O(n|E|q(n)) \) for graphs \( G \) for which the ratio between the number of near-perfect and perfect matchings is \( q(n) \) (see [12]).

2.3 A heat-bath chain for sampling contingency tables

Our final application involves contingency tables. Let \( \mathbf{r} = (r_1, \ldots, r_m) \) and \( \mathbf{c} = (c_1, \ldots, c_n) \) be two vectors of positive integers with the same sum. A contingency table with row sums \( \mathbf{r} \) and column sums \( \mathbf{c} \) is an \( m \times n \) matrix \( X = (x_{i,j}) \) with nonnegative integer entries, such that \( \sum_{j=1}^{n} x_{i,j} = r_i \) for \( i = 1, \ldots, m \) and \( \sum_{i=1}^{m} x_{i,j} = c_j \) for \( j = 1, \ldots, n \). Let \( \Omega_{r,c} \) denote the set of all contingency tables with row sums \( \mathbf{r} \) and column sums \( \mathbf{c} \).

To avoid trivialities we assume throughout this section that \( \min\{m, n\} \geq 2 \).

Dyer and Greenhill [6] proposed a Markov chain for sampling contingency tables, which we will call the contingency chain. A transition of the chain is performed as follows: choose a \( 2 \times 2 \) subsquare of the current table uniformly at random, then replace this \( 2 \times 2 \) subsquare by a uniformly chosen \( 2 \times 2 \) nonnegative integer matrix with the same row and column sums.

The lazy contingency chain does nothing at each step with probability \( \frac{1}{2} \), and otherwise performs a transition as described above. Cryan et al. [3] analysed the lazy contingency chain for a constant number of rows. They proved that \( (1 - \lambda_1)^{-1} \leq n f(m) \) for \( m \)-rowed contingency tables with \( n \) columns, where \( m \) is constant and \( f(m) \) is an expression satisfying \( f(m) \geq 68m^4 \). We now analyse the smallest eigenvalue of the (non-lazy) contingency chain.

There is always a positive probability that the next state \( X' \) of the contingency chain is equal to the current state \( X \), since the heat-bath step may simply replace the chosen \( 2 \times 2 \) subsquare with its current contents. However, the minimum of \( P(X, X) \) over all states \( X \) depends on \( \mathbf{r} \) and \( \mathbf{c} \). (To see this, consider \( 2 \times 2 \) squares.) We prefer a bound which depends only on \( m \) and \( d \), and so we do not simply apply (2).

**Lemma 2.1.** Let \( \mathbf{r} = (r_1, \ldots, r_m) \) and \( \mathbf{c} = (c_1, \ldots, c_n) \) be vectors of positive integers with a common sum which satisfy

\[
r_1 \geq r_2 \geq \cdots \geq r_m \quad \text{and} \quad c_1 \geq c_2 \geq \cdots \geq c_n.
\]
Suppose that \( \min\{r_1, c_1\} \geq 2 \) and \( \max\{m, n\} \geq 3 \). The smallest eigenvalue of the contingency chain on \( \Omega_{r,c} \) satisfies

\[
(1 + \lambda_{N-1})^{-1} \leq 45 m^3 n^3.
\]

**Proof.** Write \([a] = \{1, 2, \ldots, a\} \) for \( a \in \mathbb{Z}^+ \). From \( X = (x_{i,j}) \in \Omega_{r,c} \), first suppose that there exists a 5-tuple \((i_1, i_2, i_3, j_1, j_2)\) such that

- \( i_1, i_2, i_3 \) are distinct elements of \([m]\),
- \( j_1, j_2 \) are distinct elements of \([n]\),
- \( x_{i_1,j_1}, x_{i_2,j_1}, x_{i_3,j_2} \) are all positive.

Then \((i_1, i_2, i_3, j_1, j_2)\) is called row-good for \( X \), and \( X \) is called row-good. If \( X \) is row-good, fix the lexicographically least 5-tuple \((i_1, i_2, i_3, j_1, j_2)\) which is row-good for \( X \) and consider the following sequence of three transitions on the \( 3 \times 2 \) subsquare defined by rows \( i_1, i_2, i_3 \) and columns \( j_1, j_2 \):

\[
\begin{pmatrix}
    y_{1,1} & y_{1,2} \\
    y_{2,1} & y_{2,2} \\
    y_{3,1} & y_{3,2}
\end{pmatrix} \Rightarrow \begin{pmatrix}
    y_{1,1} - 1 & y_{1,2} + 1 \\
    y_{2,1} & y_{2,2} \\
    y_{3,1} + 1 & y_{3,2} - 1
\end{pmatrix} \Rightarrow \begin{pmatrix}
    y_{1,1} & y_{1,2} \\
    y_{2,1} - 1 & y_{2,2} + 1 \\
    y_{3,1} + 1 & y_{3,2} - 1
\end{pmatrix} \Rightarrow \begin{pmatrix}
    y_{1,1} & y_{1,2} \\
    y_{2,1} & y_{2,2} \\
    y_{3,1} & y_{3,2}
\end{pmatrix}.
\]

(For notational convenience we have written \( y_{k,\ell} \) for \( x_{i_k,j_\ell} \) in the above.) Note that all intermediate matrices are nonnegative, due to the row-good property. This defines a walk \( w_X \) of length 3 from \( X \) to \( X \) in the graph underlying the contingency chain.

We can define 5-tuples \((i_1, i_2, j_1, j_2, j_3)\) which are column-good for \( X \) in the analogous way, and say that \( X \) is column-good if there is a 5-tuple which is column-good for \( X \). If \( X \) is column-good then taking the transpose of each matrix in the sequence of transitions above defines an odd walk \( w_X \) of length 3 from \( X \) to \( X \).

Finally, suppose that \( X \in \Omega_{r,c} \) is not row-good and is not column-good. Such an \( X \) is said to be bad. Then no row or column of \( X \) contains more than one positive entry. Since all row and column sums are positive, it follows that \( m = n \geq 3 \) and that every row and column contains exactly one positive entry. Let \((i_1, i_2, i_3, j_1, j_2, j_3)\) be the lexicographically-least 6-tuple such that

- \( i_1, i_2, i_3 \) are distinct elements of \([m]\),
- \( j_1, j_2, j_3 \) are distinct elements of \([n]\),
- \( x_{i_1,j_1} \geq 2 \), while \( x_{i_2,j_2} \) and \( x_{i_3,j_3} \) are positive.

(The conditions on \( r \) and \( c \) guarantee that such a 6-tuple exists.) Consider the following sequence of 5 transitions, performed on the \( 3 \times 3 \) subsquare defined by rows \( i_1, i_2, i_3 \) and
columns $j_1, j_2, j_3$:
\[
\begin{pmatrix}
y_{1,1} & 0 & 0 \\
0 & y_{2,2} & 0 \\
0 & 0 & y_{3,3}
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
y_{1,1} - 1 & 1 & 0 \\
1 & y_{2,2} - 1 & 0 \\
0 & 0 & y_{3,3}
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
y_{1,1} - 1 & 1 & 0 \\
1 & y_{2,2} - 1 & 1 \\
0 & 0 & y_{3,3} - 1
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
y_{1,1} - 1 & 1 & 0 \\
1 & y_{2,2} - 1 & 1 \\
0 & 0 & y_{3,3} - 1
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
y_{1,1} & 0 & 0 \\
0 & y_{2,2} & 0 \\
0 & 0 & y_{3,3}
\end{pmatrix}.
\]

This defines a walk $w_X$ of length 5 from $X$ to $X$ in the graph underlying the chain.

Now we must analyse the set $W = \{w_X : X \in \Omega_{r,e}\}$ of odd walks defined above. Let $e = (Z, Z')$ be a transition of the contingency chain. Then $Z$ and $Z'$ only differ in a $2 \times 2$ subsquare defined by rows $i, i'$ and columns $j, j'$.

First we seek row-good $X$ with $e \in w_X$. Let $i'' \not\in \{i, i'\}$ be another row index, and fix one of the 6 ways to arrange $(i, i', i'', j, j')$ as $(i_1, i_2, i_3, j_1, j_2)$. This gives enough information to uniquely identify a potential candidate for $X$. For example, if the transition $e$ involves rows $i_1$ and $i_3$ then $X = Z$, while if the transition $e$ involves rows $i_2$ and $i_3$ then $X = Z'$. If $e$ involves rows $i_1$ and $i_2$ then $e$ is the second transition in the sequence, and $X$ can be obtained from $Z$ by reversing the first transition in the sequence: namely, adding 1 to entries $(i_1, j_1)$ and $(i_3, j_2)$ and subtracting 1 from entries $(i_1, j_2)$ and $(i_3, j_1)$. If $X$ is a valid contingency table then $(i_1, i_2, i_3, j_1, j_2)$ is row-good for $X$. If it is the lexicographically least such 5-tuple for $X$ then $e \in w_X$. This identifies at most $12(m - 2)$ tables $X$ such that $e \in w_X$. (This is an overcount, but good enough for our purposes.)

By choosing a third column index $j'' \not\in \{j, j'\}$, an analogous argument shows that there are at most $12(n - 2)$ column-good tables $X$ with $e \in w_X$.

Finally, we seek bad tables $X$ such that $e \in w_X$. Choose a row index $i'' \not\in \{i, i'\}$ and a column index $j'' \not\in \{j, j'\}$, and fix one of the at most 36 ways to arrange $(i, i', i'', j, j', j'')$ as $(i_1, i_2, i_3, j_1, j_2, j_3)$. Now each transition in the sequence alters a different $2 \times 2$ subsquare except the first and fourth, which both alter rows $i_1, i_2$ and columns $j_1, j_2$. Hence, arguing as above, there are at most two choices for $X$, for each fixed 6-tuple. This gives at most $72(m - 2)(n - 2)$ bad tables $X$ such that $e \in w_X$.

Combining all this, we find that the congestion parameter $\eta(W)$ satisfies
\[
\eta(W) \leq \binom{m}{2} \binom{n}{2} (36(m - 2) + 36(n - 2) + 360(m - 2)(n - 2)) \leq 90 m^3 n^3,
\]
and applying Lemma 1.1 completes the proof. 

Again we observe that this bound on $(1 + \lambda_{N-1})^{-1}$ is several orders of magnitude lower than the best-known bound on the second-largest eigenvalue [3].

Remark 2.2. It has recently been shown [9] that the contingency chain described above has no negative eigenvalues. We include Lemma 2.1 here to illustrate an application of Lemma 1.1 involving walks of length greater than one.
References


