

# A LOCAL LIMIT THEOREM FOR A FAMILY OF NON-REVERSIBLE MARKOV CHAINS

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ABSTRACT. By proving a local limit theorem for higher-order transitions, we determine the time required for *necklace chains* to be close to stationarity. Because necklace chains, built by arranging identical smaller Markov chains around a directed cycle, are not reversible, have little symmetry, do not have uniform stationary distributions, and can be nearly periodic, prior general bounds on rates of convergence of Markov chains either do not apply or give poor bounds. Necklace chains can serve as test cases for future techniques for bounding rates of convergence.

*Keywords:* Markov chains, rates of convergence, non-reversibility.

## 1. INTRODUCTION

Determining the rate of convergence to stationarity of finite ergodic Markov chains is a problem of both theoretical and practical interest, with applications to sampling and estimation problems. It is also a difficult problem. Over the last 20 years, many techniques have been developed for bounding convergence behavior; see Aldous and Fill [1], Behrends [2], or Lovász [11] for surveys. Coupling, strong stationary time, and finite Fourier analysis arguments all exploit chain symmetry. Second-largest eigenvalue techniques and inequalities inspired by differential geometry generally require reversibility; symmetrized versions of those bounds, due to Diaconis and Saloff-Coste [7] and Fill [9], can be applied to non-reversible chains, but only those with strong types of aperiodicity.

Despite this plethora of methods, the time required to be close to stationary has been determined precisely—with, say, a correct leading term constant—only for certain families of chains (Diaconis [5] gives a survey focussed on chains whose time to be near stationarity displays sharp cutoffs). The current work adds the family of *necklace chains* to the list. Necklace chains have little symmetry, have non-uniform stationary distributions, are not reversible, and can be nearly periodic (due to deterministic transitions). Thus existing general bounds on rate of convergence are

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difficult to apply to necklaces. We hope our results will allow necklace chains to serve as test cases for techniques for bounding rates of convergence, and we provide an example of this utility.

Necklaces are built from smaller chains. A *bead*  $B$  is a finite Markov chain with states  $\{0, 1, \dots, b\}$  such that

- The only absorbing state is  $b$ , and every state lies on some path from 0 to  $b$ .
- The set of possible first passage times from 0 to  $b$  has maximal span 1 (that is, there do not exist integers  $h > 1$  and  $a$  such that every possible value of the first passage time is congruent to  $a \pmod{h}$ ).

State 0 is the *entrance state* of  $B$  and state  $b$  is the *exit state*. The *closure*  $\overline{B}$  of the bead  $B$  has the same transitions as  $B$ , except that  $\overline{B}(b, 0) = 1$ . See Figure 1(a,b).

To construct  $P_r$ , a *necklace built with bead  $B$  and indicator vector  $r = (r_0, \dots, r_{n-1})$* , start with *link states*  $s_0, s_1, \dots, s_{n-1}$ .

- If  $r_i = 1$ , *there is a bead at position  $i$* : attach  $s_i$  and  $s_{i+1}$  via a bead isomorphic to  $B$  with states  $s_{i,0} = s_i, s_{i,1}, \dots, s_{i,b} = s_{i+1}$ . The *states in the bead at position  $i$*  are  $s_{i,0} = s_i, s_{i,1}, \dots, s_{i,b-1}$ . (We exclude the link state  $s_{i,b} = s_{i+1}$  from the  $i$ -th bead.)
- If  $r_i = 0$ , *there is not a bead at position  $i$* : attach  $s_i$  and  $s_{i+1}$  with a directed *link edge*, and set  $P_r(s_i, s_{i+1}) = 1$ .

Indices are taken mod  $n$ , so that  $r_{n-1}$  determines how  $s_{n-1}$  is connected to  $s_0$ . See Figure 1(c). Let  $R_i = \sum_{k=0}^{i-1} r_k$  and let  $m = R_n$  be the total number of beads. The Markov chain  $P_r$  is always irreducible; it is aperiodic as long as  $m \geq 1$ .

In a *family of necklace chains*  $\{P_{n,m}\} = \{P_{n,m} : n \in \mathbb{N}\}$ ,  $P_{n,m}$  has  $n$  link states, has  $m = m(n)$  beads ( $1 \leq m \leq n$ ), and has indicator vector  $r = r(n)$ . All other parameters of a family depend on  $n$ , although we generally suppress that dependence. We include  $m$  in the notation because it appears explicitly in our results.

Our main results are Theorem 1, which approximates the higher-order transitions of families of necklaces, and Theorem 2, which describes the asymptotics of their distance from stationarity. When rescaled appropriately, families of necklaces behave like random walk on the cycle  $\mathbb{Z}/n\mathbb{Z}$ . They converge gradually to stationarity and have no cutoffs. The time to be near stationarity depends only on the number of beads, not on their arrangement, and can range from  $O(|S|^2)$  to  $O(|S|^3)$ , where  $|S|$  is the size of the state space.

Let  $\phi(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$  be the standard normal density and let

$$\theta_\tau(x) = \sum_{j \in \mathbb{Z}} \frac{1}{\sqrt{\tau}} \phi\left(\frac{j+x}{\sqrt{\tau}}\right)$$

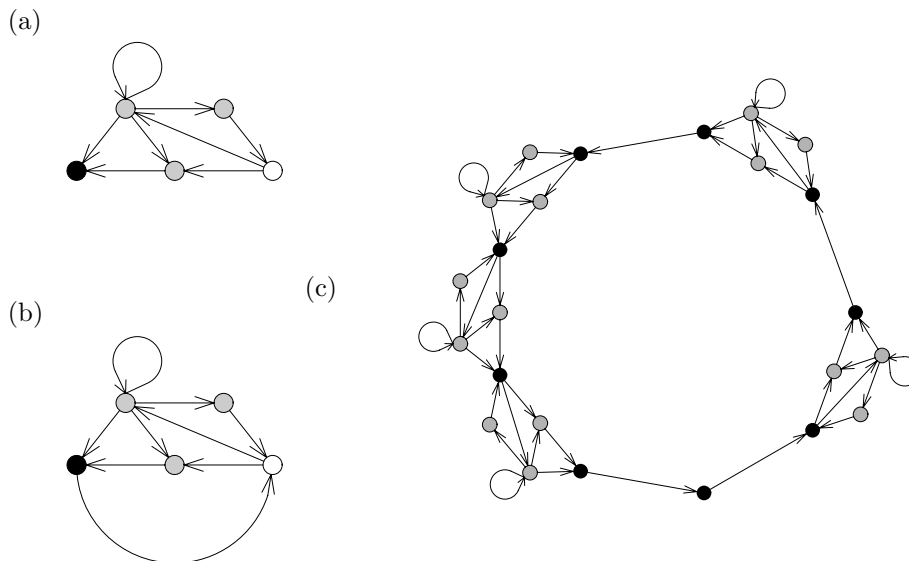


FIGURE 1. The underlying graphs of (a) a bead  $B$ , (b) its closure  $\bar{B}$ , and (c) a necklace chain built with  $B$ . Here,  $n = 9$ ,  $m = 5$ , and  $r = (1, 0, 1, 0, 1, 1, 1, 0, 0)$ . Entrance states are shown in white, while exit and link states are black.

be the density at time  $\tau$  of Brownian motion on the circle  $\mathbb{R}/\mathbb{Z}$  of unit circumference. We measure distance between distributions in *total variation*:

$$\|\pi(\cdot) - \pi'(\cdot)\|_{TV} = \sup_A |\pi(A) - \pi'(A)| = \frac{1}{2} \sum_s |\pi(s) - \pi'(s)|.$$

**Theorem 1.** *Let  $B$  be a bead with first passage time from entrance to exit of mean  $\mu$  and variance  $\sigma^2$ . Let  $\{P_{n,m}\}$  be a family of necklace chains built with bead  $B$ . Let  $\pi_{n,m}$  be the stationary distribution of  $P_{n,m}$ . Fix  $\tau > 0$  and let  $t = t(n)$  be a positive-integer-valued function such that*

$$t = \frac{\tau(n + (\mu - 1)m)^3}{\sigma^2 m} + O(n).$$

*For each  $n$ , let  $s$  be either  $s_0$  or a state in a bead at position  $n - 1$ , and let  $s'$  be either  $s_i$  or a state in a bead at position  $i$ . Then as  $n \rightarrow \infty$ ,*

$$P_{n,m}^t(s, s') = \pi_{n,m}(s') \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right).$$

**Theorem 2.** *Under the assumptions of Theorem 1, as  $n \rightarrow \infty$ ,*

$$\|P_{n,m}^t(s, \cdot) - \pi_{n,m}(\cdot)\|_{TV} \rightarrow \frac{1}{2} \int_{\mathbb{R}/\mathbb{Z}} |\theta_\tau(x) - 1| dx.$$

Section 2 collects for reference some standard facts and computes the stationary distributions and the higher-order transitions of necklace chains. In Section 3,

we prove Theorems 1 and 2. The argument applies a local central limit theorem due to Petrov, a classical large deviation bound, and Markov chain identities to the combinatorial expressions for the higher-order transitions. Section 4 examines several families of necklace chains, including one (with well-behaved multiplicative reversibilizations) for which a Nash inequality of Diaconis and Saloff-Coste [7] gives the correct rate of convergence, up to a constant factor.

## 2. PRELIMINARIES

First we state (for future reference) the specializations of two standard results on Markov chains to  $\overline{B}$ . See, for example, Aldous and Fill [1].

**Proposition 1.** *Let  $B$  be a bead, and let  $X$  be a random variable distributed as the first-passage time from 0 to  $b$  in  $B$  (or, equivalently,  $\overline{B}$ ). Then there exist a positive integer  $x_0$  and a constant  $0 < \epsilon < 1$  such that  $x \geq x_0$  implies  $\Pr(X > x) < \epsilon^x$ .*

**Proposition 2.** *Let  $B$  be a bead, let  $\pi$  be the stationary distribution of its closure  $\overline{B}$ , and let  $\mu$  be the expected first passage time from 0 to  $b$  in  $B$ . Then, for any state  $v \neq b$  of  $B$ ,*

$$\sum_{k \geq 0} B^k(0, v) = \pi(v)(\mu + 1).$$

*Proof.* This sum is the expected number of visits to state  $v$  when the chain  $B$  is started in 0 and run until hitting  $b$ . It is also equal to the expected number of visits to  $v$  made by the irreducible chain  $\overline{B}$  between visits to 0. By a standard result (see, e.g., Aldous and Fill [1, Chapter 2, Lemma 6]), this is

$$\pi(k)E_0T_0^+ = \pi(v)(\mu + 1),$$

where  $E_0T_0^+$  is the expected time to return to 0 in  $\overline{B}$ . □

We now compute the stationary distribution and higher-order transitions of necklace chains. Proposition 4, which expresses the higher-order transitions of  $P_{n,m}$  in terms of sums of i.i.d. random variables, is our central combinatorial argument.

**Proposition 3.** *Let  $P_{n,m}$  be a necklace chain with  $n$  link states and  $m$  beads of type  $B$ . Let  $\pi$  be the stationary distribution of  $\overline{B}$  and let  $\mu = E_0T_b$  in  $\overline{B}$ . Then the stationary distribution  $\pi_{n,m}$  of  $P_{n,m}$  is*

$$\pi_{n,m}(s) = \begin{cases} \frac{(\mu + 1)\pi(v)}{n + (\mu - 1)m} & \text{if } s = s_{i,v} \text{ is in a bead,} \\ \frac{1}{n + (\mu - 1)m} & \text{otherwise.} \end{cases}$$

*Proof.* The function

$$f(s) = \begin{cases} \pi(v) & \text{if } s = s_{i,v} \text{ is in a bead,} \\ \pi(b) & \text{otherwise} \end{cases}$$

satisfies  $\sum_{s'} P_{n,m}(s, s')f(s) = f(s')$ . Why? Non-backbone states are only accessible from other states in their own bead, so we are just verifying stationarity of  $\pi$  for  $\overline{B}$ . Backbone states not in beads receive and emit a steady flow of  $\pi(b)$ . Backbone states in beads receive  $\pi(b)$  (which in  $\overline{B}$  would come from the state  $b$ ) from what precedes them, whether bead or backbone state.

To normalize, note that  $\sum_s f(s) = (n-m)(1-\pi(b)) + m\pi(b)$ . Because  $\overline{B}(b, 0) = 1$ ,  $E_b T_b^+ = \mu + 1$  and  $\pi(b) = 1/(\mu + 1)$ .  $\square$

**Proposition 4.** *Let  $P_{n,m}$  be a necklace chain with  $n$  link states and  $m$  beads of type  $B$ . Let  $X_1, X_2, \dots$  be i.i.d. random variables distributed as the first passage time from 0 to  $b$  in the bead  $B$ , and set  $S_N = X_1 + X_2 + \dots + X_N$ . Then*

$$(1) \quad P_{n,m}^t(s_0, s) = \begin{cases} \sum_{j \geq 0} \Pr[S_{mj+R_i} = t - i + R_i - (n-m)j] & \text{when } s = s_i \text{ is not in a bead,} \\ \sum_{k \geq 0} B^k(0, v) \sum_{j \geq 0} \Pr[S_{mj+R_i} = t - k - i + R_i - (n-m)j] & \text{when } s = s_{i,v} \text{ is in a bead.} \end{cases}$$

When  $s_{n-1,w}$  is in a bead at position  $n-1$ ,

$$(2) \quad P_{n,m}^t(s_{n-1,w}, s) = \begin{cases} \sum_{k \geq 0} B^k(w, b) P_{n,m}^{t-k}(s_0, s) & \text{when } s \text{ is not in the bead at position } n-1, \\ \sum_{k \geq 0} B^k(w, b) P_{n,m}^{t-k}(s_0, s) + B^t(w, v) & \text{when } s = s_{n-1,v} \text{ is in the bead at position } n-1. \end{cases}$$

*Proof.* In the first case of (1),  $j$  counts the number of times the random walk has gone around the entire chain. By time  $t$ , the walk has gone through  $mj + R_i$  beads and  $(n-m)j + (i - R_i)$  deterministic steps. Thus it is at  $s_i$  exactly when  $S_{mj+R_i} + (n-m)j + (i - R_i) = t$ .

For the second case of (1), let  $x_t$  be the state occupied at time  $t$ , and consider a trajectory of length  $t$  from  $s_0$  to  $s_{i,v}$ . By the same reasoning as for the first case,

$$\begin{aligned} & \Pr[x_t = s_i \text{ and } x_{t-1} \text{ is not in the bead at position } i | x_0 = s_0] \\ &= \sum_{j \geq 0} \Pr[S_{mj+R(i)} = t - i + R(i) - (n - m)j]. \end{aligned}$$

Let  $t - k$  be the time of the last arrival at  $s_i = s_{i,0}$  from the  $i - 1$ -st bead before time  $t$ . In order to stay in the  $i$ -th bead until arriving at  $s_{i,v}$  at time  $t$ , we must avoid the state  $s_{i+1} = s_{i,b}$ .

For (2), note that when  $s$  is not in the bead at position  $n - 1$ , then we must pass through  $s_{n-1,b} = s_0$  on the way to  $s$ . When the target state is in the same bead, there are also paths that stay within a single bead.  $\square$

### 3. PROOFS OF LIMIT THEOREMS

The key to proving Theorem 1, and thus Theorem 2, is Lemma 1, an approximation of the sums appearing in Proposition 4. While the terms of this sum are simply probabilities of sums of i.i.d. random variables taking on particular values, each term is taken from a different distribution. We approximate the large terms with a local central limit theorem due to Petrov. The largest terms, which are very close to those taken from a single distribution, build a theta function. The rest of the terms are negligible—most are handled by the local central limit theorem, while a Chernoff-type large deviation bound covers those terms for which only a few random variables are added.

**Lemma 1.** *Let  $X_1, X_2, \dots$  be i.i.d. positive-integer-valued random variables with maximal span 1 such that for some  $\epsilon < 1$  and  $x_0, x \geq x_0$  implies  $\Pr[X_i > x] < \epsilon^x$ . Let  $\mu = \mathbb{E}[X_i]$ ,  $\sigma^2 = \text{Var}[X_i]$ , and  $S_N = X_1 + \dots + X_N$ .*

*Fix  $\tau > 0$ . Let  $m = m(n)$ ,  $r = r(n)$  and  $t = t(n)$  be positive-integer-valued functions such that  $1 \leq m \leq n$ ,  $0 \leq r \leq n$ , and*

$$t = t(n) = \frac{\tau(n + (\mu - 1)m)^3}{\sigma^2 m} + O(n).$$

*Then, as  $n \rightarrow \infty$  and uniformly in  $r$ ,*

$$\sum_{j \geq 0} \Pr[S_{mj+r} = t + r - (n - m)j] = \frac{1}{n + (\mu - 1)m} \theta_\tau \left( \frac{t - (\mu - 1)r}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right).$$

*Proof of Lemma 1.* First, we observe that the given conditions on  $n$ ,  $m$ , and  $t$  imply that

$$t = \Omega(n^2) \text{ and } t = O(n^3) \text{ as } n \rightarrow \infty$$

(both  $t = \Theta(n^2)$  and  $t = \Theta(n^3)$  are possible; consider  $m = n$  or  $m$  constant, respectively).

Next, we use the given bound on the tail of the distribution of the  $X_i$ 's to build a simple Chernoff-style large deviation bound (see Chernoff [4] or Chapter 2 of Janson, Łuczak, and Ruciński [10]). We can couple  $X_1$  to a shifted geometric random variable  $Y$  such that  $X_1 \leq Y$  always and

$$\Pr[Y \geq y + x_0] = \begin{cases} e^{-y} & \text{if } y \geq 0, \\ 1 & \text{otherwise.} \end{cases}$$

But then, for any  $c > E[Y] = x_0 + \frac{\epsilon}{1-\epsilon}$  (a restriction that suffices for the infimum calculation to go through and yield useful results),

$$\begin{aligned} \Pr[S_N = cN] &\leq \Pr[e^{tS_N} \geq e^{ctN}] \leq \left( \inf_{t>0} e^{-ct} \mathbb{E}[e^{tX_1}] \right)^N \leq \left( \inf_{t>0} e^{-ct} \mathbb{E}[e^{tY}] \right)^N \\ &= \left( \frac{(1-\epsilon)(c-x_0)^{x_0}}{\epsilon^{x_0}(c-x_0+1)^{x_0-1}} \left( \epsilon \left( 1 + \frac{1}{c-x_0} \right) \right)^c \right)^N. \end{aligned}$$

The first fraction inside the exponential above is a rational function of  $c$ ; the second decreases exponentially for  $c$  sufficiently large. Thus, there must exist a  $c_0 > E[Y]$  and a  $\delta > 0$  such that, for  $c \geq c_0$ ,

$$(3) \quad \Pr[S_N = cN] \leq e^{-\delta cN}.$$

We note that  $c_0 > E[Y]$  implies that  $c_0 > E[X_1] = \mu$ .

Because  $t+r-(n-m)j \geq c_0(mj+r)$  is equivalent to  $j \leq \frac{t-(c_0-1)r}{n+(c_0-1)m}$ , inequality (3) now implies

$$\begin{aligned} (4) \quad \sum_{j=0}^{\lfloor \frac{t-(c_0-1)r}{n+(c_0-1)m} \rfloor} \Pr[S_{mj+r} = t+r-(n-m)j] &\leq \sum_{j=0}^{\lfloor \frac{t-(c_0-1)r}{n+(c_0-1)m} \rfloor} e^{-\delta(t+r-(n-m)j)} \\ &\leq \left( \frac{t-(c_0-1)r}{n+(c_0-1)m} + 1 \right) e^{-\delta(t+r-(n-m)\left(\frac{t-(c_0-1)r}{n+(c_0-1)m}\right))} \\ &= O(n^2) e^{-\delta c_0\left(\frac{mt+nr}{n+(c_0-1)m}\right)} = O(n^2) e^{-\Omega(n)} = o\left(\frac{1}{n}\right). \end{aligned}$$

The given tail bound implies that the  $X_i$ 's have moments of all orders, so we may now apply a local central limit theorem for lattice random variables. We use a result of Petrov [12, Theorem 4], specialized to the lattice of integers: as  $N \rightarrow \infty$ ,

$$(5) \quad \sup_{k \in \mathbb{Z}} \left( 1 + \left| \frac{k - \mu N}{\sigma \sqrt{N}} \right|^3 \right) \left( \Pr[S_N = k] - \frac{1}{\sigma \sqrt{N}} \phi\left(\frac{k - \mu N}{\sigma \sqrt{N}}\right) \right) = o\left(\frac{1}{\sqrt{N}}\right).$$

(Petrov [12, Theorem 2] bounds the error left by an arbitrary number of terms in the Edgeworth asymptotic expansion of  $\Pr[S_N = a]$ ; see Esseen [8] for an earlier bound and a discussion. However, we need only the first term.)

Because the underlying random variables,  $X_i$ , are positive integers, all terms of our sum for which  $mj + r > t + r - (n - m)j$ , or equivalently  $j > \frac{t}{n}$ , are zero. Given the estimate of equation (4), we can restrict our attention to those terms for which  $\frac{t - (c_0 - 1)r}{n + (c_0 - 1)m} < j \leq \frac{t}{n}$ . On this range,

$$(6) \quad mj + r = \Theta(n^2).$$

Let

$$x_0 = \frac{t - (\mu - 1)r}{n + (\mu - 1)m}.$$

and

$$y_j = \frac{t + r - (n - m)j - \mu(mj + r)}{\sigma\sqrt{mj + r}} = \frac{(n + (\mu - 1)m)(x_0 - j)}{\sigma\sqrt{mj + r}}.$$

Because  $\frac{t - (c_0 - 1)r}{n + (c_0 - 1)m} < j \leq \frac{t}{n}$  implies  $y_j = \Theta(1) |x_0 - j|$ ,

$$(7) \quad \sum_{\frac{t - (c_0 - 1)r}{n + (c_0 - 1)m} < j \leq \frac{t}{n}} \frac{1}{1 + |y_j|^3} = \Theta(1).$$

Combining (5), (6), and (7) now yields

$$\begin{aligned} \sum_{\frac{t - (c_0 - 1)r}{n + (c_0 - 1)m} < j \leq \frac{t}{n}} \Pr[S_{mj+r} = t + r - (n - m)j] \\ = \sum_{\frac{t - (c_0 - 1)r}{n + (c_0 - 1)m} < j \leq \frac{t}{n}} \frac{1}{\sigma\sqrt{mj + r}} \phi(y_j) + o\left(\frac{1}{n}\right). \end{aligned}$$

We first consider the terms of the resulting sum for which  $|x_0 - j| < n^{1/4}$ . On this range,

$$(8) \quad \begin{aligned} \frac{1}{\sigma\sqrt{mj + r}} &= \frac{1}{\sigma\sqrt{\frac{\tau(n + (\mu - 1)m)^2}{\sigma^2} + \frac{nr}{n + (\mu - 1)m} - m(x_0 - j) + O(1)}} \\ &= \frac{1}{\sqrt{\tau}(n + (\mu - 1)m)\sqrt{1 + O\left(\frac{1}{n^{3/4}}\right)}} = \frac{1}{\sqrt{\tau}(n + (\mu - 1)m)} + O\left(\frac{1}{n^{7/4}}\right) \end{aligned}$$

and

$$(9) \quad y_j = \frac{(n + (\mu - 1)m)(x_0 - j)}{\sigma\sqrt{mj + r}} = \frac{x_0 - j}{\sqrt{\tau + O\left(\frac{1}{n^{3/4}}\right)}} = \frac{x_0 - j}{\sqrt{\tau}} + O\left(\frac{1}{\sqrt{n}}\right).$$

By (8), (9) and the boundedness of the derivative of  $\phi$ ,

$$\begin{aligned}
 \sum_{|x_0-j|<n^{1/4}} \frac{1}{\sigma\sqrt{mj+r}} \phi(y_j) &= \sum_{|x_0-j|<n^{1/4}} \left( \frac{1}{\sqrt{\tau}(n+(\mu-1)m)} + O\left(\frac{1}{n^{7/4}}\right) \right) \\
 &\quad \times \left( \phi\left(\frac{x_0-j}{\sqrt{\tau}}\right) + O\left(\frac{1}{\sqrt{n}}\right) \right) \\
 &= \frac{1}{\sqrt{\tau}(n+(\mu-1)m)} \sum_{|x_0-j|<n^{1/4}} \phi\left(\frac{x_0-j}{\sqrt{\tau}}\right) + O\left(\frac{1}{n^{5/4}}\right) \\
 &= \frac{\theta_\tau(x_0)}{n+(\mu-1)m} + o\left(\frac{1}{n}\right).
 \end{aligned}$$

The remaining terms are those for which  $\frac{t-(c_0-1)r}{n+(c_0-1)m} < j < x_0-n^{1/4}$  or  $x_0+n^{1/4} < j < \frac{t}{n}$ . Since there are only  $O(n^2)$  such terms, each of which is  $O(\phi(n^{1/4}))$ , their sum is certainly  $o(\frac{1}{n})$ .  $\square$

To complete the proof of Theorem 1 we need only check that transition probability factors weighting the inner sums in Proposition 4 give the correct stationary distribution factors in the final approximation.

*Proof of Theorem 1.* First, note that Proposition 1 legitimates applying Lemma 1 to sums arising from Proposition 4.

When  $s = s_0$  and  $s' = s_i$ , where  $s_i$  is not in a bead, applying Lemma 1 to the sum given by the first case of Proposition 4(1) and recalling Proposition 3 immediately yields the desired

$$P_{n,m}^t(s_0, s_i) = \pi_{n,m}(s_i) \theta_\tau \left( \frac{t-i-(\mu-1)R_i}{n+(\mu-1)m} \right) + o\left(\frac{1}{n}\right).$$

Next, we consider  $s' = s_{i,v}$ , a state in a bead at position  $i$ . Here, the second case of Proposition 4(1) applies. First we truncate to  $n^{1/3}$  terms; by the proof of Proposition 4(1), each truncated term is bounded by its first factor, so Proposition 1 ensures the error is small. Next we apply Lemma 1 to each term; Proposition 2 allows us to collect the errors. Then we use the upper bound on  $B^k(0, v)$  implied by Proposition 1 and the boundedness of both  $\theta_\tau$  and its derivative to approximate the theta function factor in the remaining terms by its value when  $k = 0$ , then de-truncate, still with small enough error. Finally, Propositions 2 and 3 evaluate

the remaining sum.

$$\begin{aligned}
P_{n,m}^t(s_0, s_{i,v}) &= \sum_{k \geq 0} B^k(0, v) \sum_{j \geq 0} \Pr[S_{mj+R_i} = t - k - i + R_i - (n - m)j] \\
&= \sum_{0 \leq k \leq n^{1/3}} B^k(0, v) \sum_{j \geq 0} \Pr[S_{mj+R_i} = t - k - i + R_i - (n - m)j] + o\left(\frac{1}{n}\right) \\
&= \sum_{0 \leq k \leq n^{1/3}} \frac{B^k(0, v)}{n + (\mu - 1)m} \theta_\tau \left( \frac{t - k - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right) \\
&= \sum_{0 \leq k \leq n^{1/3}} \frac{B^k(0, v)}{n + (\mu - 1)m} \left( \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + O\left(\frac{1}{n^{2/3}}\right) \right) + o\left(\frac{1}{n}\right) \\
&= \sum_{k \geq 0} \frac{B^k(0, v)}{n + (\mu - 1)m} \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right) \\
&= \pi_{n,m}(s_{i,v}) \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right).
\end{aligned}$$

We must still consider  $s = s_{n-1,w}$  (where  $w \neq b$ ), a state in a bead at position  $n - 1$ . The argument is very similar, except that now Proposition 4(2) applies. After truncating, we apply the immediately preceding computation to each term. This time, the weights sum as  $\sum_{k \geq 0} B^k(w, b) = 1$ , because the chain  $B$  started at  $w$  will eventually hit the absorbing state  $b$ . Proposition 1 covers the extra term in the second case of Proposition 4(2) (and is the reason for the error term in the first equality). From this point, the approximation, de-truncation, and summation run as above, yielding

$$\begin{aligned}
P_{n,m}^t(s_{n-1,w}, s') &= \sum_{k \geq 0} B^k(w, b) P_{n,m}^{t-k}(s_0, s') + o\left(\frac{1}{n}\right) \\
&= \sum_{0 \leq k \leq n^{1/3}} B^k(w, b) \left( \pi_{n,m}(s') \theta_\tau \left( \frac{t - k - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right) \right) + o\left(\frac{1}{n}\right) \\
&= \pi_{n,m}(s') \sum_{0 \leq k \leq n^{1/3}} B^k(w, b) \left( \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + O\left(\frac{1}{n^{2/3}}\right) \right) + o\left(\frac{1}{n}\right) \\
&= \pi_{n,m}(s') \sum_{k \geq 0} B^k(w, b) \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right) \\
&= \pi_{n,m}(s') \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o\left(\frac{1}{n}\right).
\end{aligned}$$

□

We now substitute Theorem 1 into the  $L^1$  expression for the total variation distance and collect terms to obtain a Riemann sum.

*Proof of Theorem 2.* Let  $f(x) = |\theta_\tau(x) - 1|$  and define  $z_0, z_1, \dots, z_{n-1} \in \mathbb{R}/\mathbb{Z}$  by

$$z_i = \begin{cases} \frac{-t}{n + (\mu - 1)m} & i = 0, \\ z_{i-1} + \frac{1 + (\mu - 1)r_i}{n + (\mu - 1)m} & 1 \leq i \leq n - 1. \end{cases}$$

The  $z_i$ 's cover the entire circle  $\mathbb{R}/\mathbb{Z}$  with spacing of  $O(\frac{1}{n})$ ; the size of the interval between  $z_{n-1}$  and  $z_0$  is determined by the presence or absence of a bead at position  $n - 1$ .

Without loss of generality, we may assume that  $s = s_0$  or  $s$  is in a bead at position  $n - 1$ . Then Theorem 1 implies

$$\begin{aligned} 2 \|P_{n,m}^t(s, \cdot) - \pi_{n,m}(\cdot)\|_{TV} &= \sum_{s'} |P_{n,m}^t(s, s') - \pi_{n,m}(s')| \\ &= \sum_{s'} \pi_{n,m}(s') \left| \theta_\tau \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o(1) - 1 \right| \\ &= \sum_{s'} \pi_{n,m}(s') f \left( \frac{t - i - (\mu - 1)R_i}{n + (\mu - 1)m} \right) + o(1). \end{aligned}$$

If  $s' = s_i$  is not in a bead, then  $\pi_{n,m}(s') = \frac{1}{n + (\mu - 1)m} = z_i - z_{i-1}$ . If there is a bead at position  $i$ , then Proposition 3,  $r_i = 1$ , and  $\pi(b) = \frac{1}{\mu + 1}$  imply that

$$\sum_{v=0}^{b-1} \pi_{n,m}(s_{i,v}) = \frac{(1 - \pi(b))(\mu + 1)}{n + (\mu - 1)m} = \frac{\mu}{n + (\mu - 1)m} = z_i - z_{i-1}.$$

Now group states by position and recall that  $f$  is an even function:

$$2 \|P_{n,m}^t(s, \cdot) - \pi_{n,m}(\cdot)\|_{TV} = \sum_{i=0}^{n-1} (z_i - z_{i-1}) f(z_i) + o(1) = \int_{\mathbb{R}/\mathbb{Z}} f(x) dx + o(1).$$

□

*Remark.* Let  $y_0^n, y_1^n, y_2^n, \dots$  be trajectory of  $P_n$ , and define, for  $s \in S$ ,

$$z_t^n(s) = \frac{i + (\mu - 1)R(i) - t}{n + (\mu - 1)m} \text{ whenever } s = s_i \text{ or } s \text{ is in a bead at position } i.$$

Then

$$Y^n(\tau) = z_{\lfloor \frac{(n + (\mu - 1)m)^3 \tau}{\sigma^2 m} \rfloor}^n \left( y_{\lfloor \frac{(n + (\mu - 1)m)^3 \tau}{\sigma^2 m} \rfloor}^n \right)$$

is a cadlag random function  $[0, 1] \rightarrow \mathbb{R}$ . Using a random-change-of-time argument parallel to Billingsley's proof of a functional limit theorem for the renewal process [3, pp. 148–50], it can be shown that the sequence  $Y^1, Y^2, \dots$  converges weakly to Brownian motion on the circle  $\mathbb{R}/\mathbb{Z}$ .

## 4. EXAMPLES

**Fixed number or fixed fraction of beads.** When  $m$  is constant,  $\{P_{n,m}\}$  converges to stationarity on a cubic time scale,

$$\frac{(n + (\mu - 1)m)^3}{\sigma^2 m} = \frac{1}{\sigma^2 m} (n^3) + O(n^2).$$

Now let  $m = \lfloor kn \rfloor$ , where  $0 < k \leq 1$ . Then  $\{P_{n,m}\}$  converges to stationarity on the quadratic time scale

$$\frac{(n + (\mu - 1)\lfloor kn \rfloor)^3}{\sigma^2 \lfloor kn \rfloor} = \frac{(k\mu - k + 1)^3}{\sigma^2 k} (n^2) + O(n).$$

**A simple bead I: rearranging beads.** Consider the bead  $B$  with state space  $\{0, 1\}$  and transition matrix  $\begin{pmatrix} p & q \\ 0 & 0 \end{pmatrix}$ . Then  $B^t(0, 1) = qp^{t-1}$ , so  $\mu = \frac{1}{q}$  and  $\sigma^2 = \frac{p}{q^2}$ . The closure  $\bar{B}$  has stationary distribution  $\pi(0) = \frac{1}{1+q}$ ,  $\pi(1) = \frac{q}{1+q}$ . Necklace chains built with  $B$  are just directed cycles, some of whose states have a hold probability of  $p$ . When  $\{P_{n,m}\}$  is a family of such chains, Proposition 3 implies

$$\pi_{n,m}(s) = \begin{cases} \frac{1}{qn+pm} & \text{if } s \text{ is in a bead,} \\ \frac{q}{qn+pm} & \text{otherwise,} \end{cases}$$

while Theorem 2 implies  $\{P_{n,m}\}$  converges to stationarity on a time scale of

$$(10) \quad \frac{(n + (\mu - 1)m)^3}{\sigma^2 m} = \frac{(qn + pm)^3}{pqm}.$$

Figure 2(a) shows the underlying graphs of two chains built with this bead: one alternates hold states with forced transitions, the other groups its holds together. Since they have the same number of beads, these chains should evolve at the same rate. Figure 2(b) shows the higher-order transition probabilities of these two chains at identical times (about .08 times the time scale of convergence). Notice the effects of the two-valued stationary distributions. Figure 2(c) shows the same weights respaced according to the points at which Theorem 1 evaluated  $\theta_c$ , so that the value of  $P_{n,m}^t(0, s)$  is attached to  $\frac{t-i-(\mu-1)R_i}{n+(\mu-1)m}$ . The two apparent ‘‘curves’’ correspond to the two values of the stationary distribution. Figure 2(d) normalizes the weight at  $\frac{t-i-(\mu-1)R_i}{n+(\mu-1)m}$  by  $\pi_{n,m}(s_i)$ . The convergence claimed in Theorem 1 is now clear.

**A simple bead II: optimizing convergence.** First, let  $m = n$ , so that  $\{P_{n,m}\}$  is a family of walks on  $\mathbb{Z}/n\mathbb{Z}$ . Many techniques for analyzing convergence apply, including Theorem 2: the time scale of convergence is  $n^2/pq$ , which is fastest when  $p = q = 1/2$ .

Now consider a family  $\{P_{n,m}\}$  with holds at  $\lfloor kn \rfloor$  states,  $0 < k < 1$ . One might expect that  $p = 1/2$  would optimize convergence again, since the variance per coin

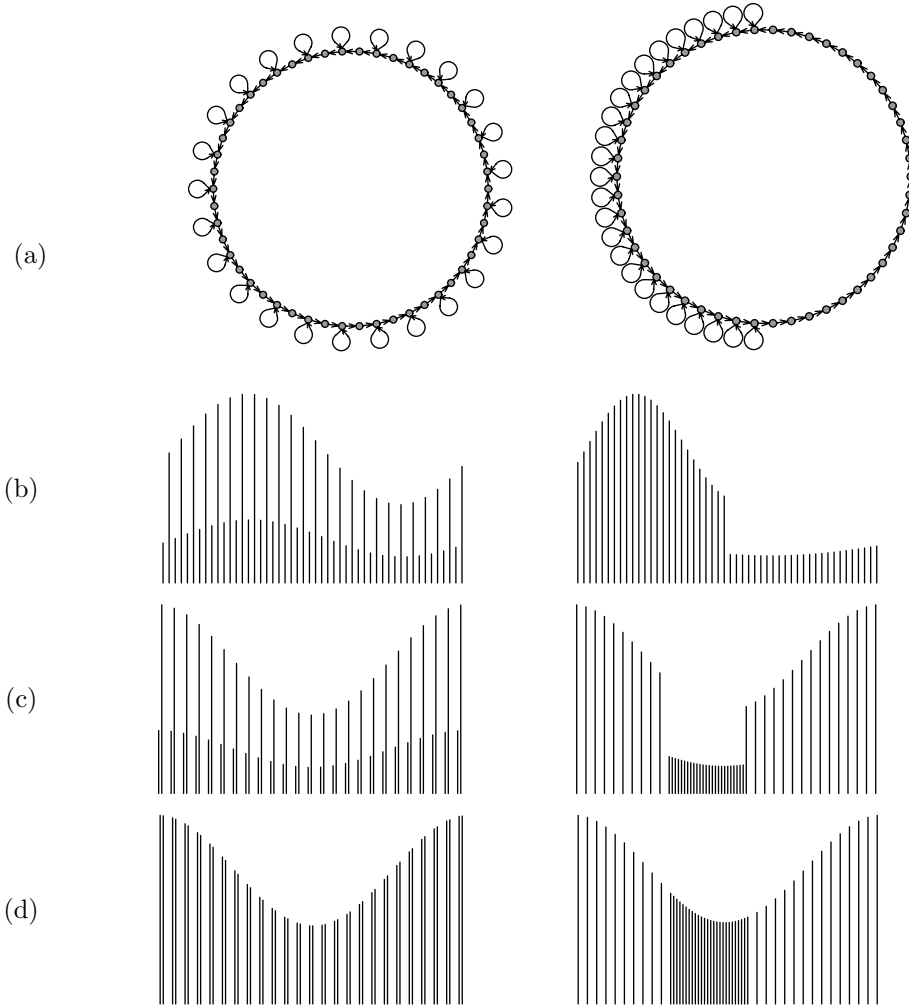


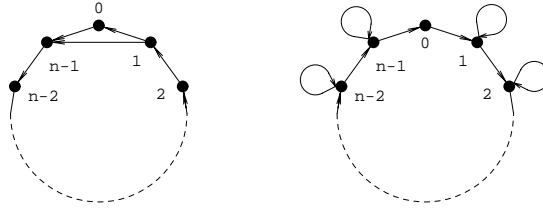
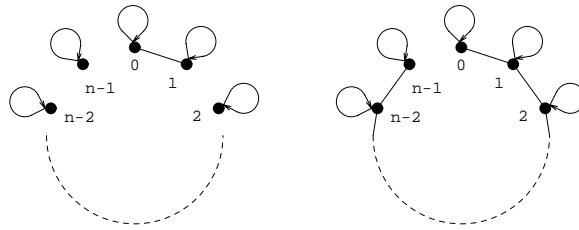
FIGURE 2. (a) Underlying graphs of two homogeneous stop/go chains;  $n = 50$ ,  $m = 25$ ,  $R(i) = \lfloor (i + 1)/2 \rfloor$  and  $R(i) = \min(i, n/2)$ . (b)  $P_n^t(0, \cdot)$  for the two chains above;  $p = 2/3$  and  $t = 530$ . (c)  $P_n^t(0, \cdot)$  rearranged. (d)  $P_n^t(0, \cdot)$  rearranged and normalized.

flip is maximized. However, this family converges at time scale

$$\frac{(qn + p \lfloor kn \rfloor)^3}{pq \lfloor kn \rfloor} = \frac{(q + pk)^3}{p q k} n^2 + O(n).$$

The coefficient of  $n^2$  is minimized when

$$p = \frac{-k + \sqrt{k^2 - k + 1}}{1 - k}.$$

FIGURE 3. The underlying graphs of  $P_n$  and  $P_n^{n-1}$ .FIGURE 4. The underlying graphs of  $M(P_n)$  and  $K_n = M(P_n^{n-1})$ .

This optimizing probability is a decreasing function of  $k$  which approaches 1 as  $k \rightarrow 0$  and  $1/2$  as  $k \rightarrow 1$ .

**Comparison with other methods.** While it is generally difficult to apply the usual techniques for bounding rates of convergence to our nearly-periodic examples, there is a linked pair of examples which are susceptible. For these, we find that a Nash inequality of Diaconis and Saloff-Coste [7] is correct, up to a constant factor, while the symmetrized second-largest-eigenvalue bound of Fill [9] is off by a log factor.

Let  $0 < p < 1$ ,  $q = 1 - p$ , and let

$$P_n = \begin{bmatrix} 0 & 0 & 0 & \dots & 1 \\ q & 0 & 0 & \dots & p \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 0 \end{bmatrix}, \quad \text{so that} \quad P_n^{n-1} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & p & q & \dots & 0 \\ 0 & 0 & p & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & q \\ q & 0 & \dots & 0 & p \end{bmatrix}.$$

See Figure 3. The chain  $P_n$  has one bead and  $n-1$  link states; its bead has  $\mu = 1+q$  and  $\sigma^2 = pq$ . Theorem 2 gives a convergence time scale of  $(n-p)^3/pq$  for  $\{P_n\}$ .

However,  $P_n^{n-1}$  is also a necklace chain, with  $n$  link states and  $n-1$  simple beads; the outer cycle has changed direction. By equation (10), the family  $\{P_n^{n-1}\}$

has convergence time scale  $(n - p)^3/pq(n - 1)$  (consistent with the time scale for  $\{P_n\}$ ).

*Symmetrize and compare.* When  $P$  is a Markov chain, let  $\overleftarrow{P}$  be the time reversal of  $P$  and  $M(P) = P\overleftarrow{P}$  be the multiplicative symmetrization of  $P$ . Fill [9] showed that

$$(11) \quad \|P^t(x_0, \cdot) - \pi(\cdot)\|_{TV} \leq \frac{1}{2\sqrt{\pi(x_0)}}\beta_1(M(P))^{t/2},$$

where  $\beta_1(M(P))$  is the second largest eigenvalue of  $M(P)$ .

Unfortunately, the underlying graph of  $M(P_n)$  is almost completely disconnected and thus  $\beta_1(M(P_n)) = 1$  (see [7] for several similar examples). However,

$$K_n = M(P_n^{n-1}) = \begin{bmatrix} q & p & 0 & \dots & 0 \\ pq & p^2 + q^2 & pq & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & pq & p^2 + q^2 & pq \\ 0 & \dots & 0 & pq & 1 - pq \end{bmatrix}$$

has underlying graph an  $n$ -path (see Figure 4). Because  $K_n$  has non-trivial edge weights, we cannot compute  $\beta_1(K_n)$  explicitly—as can be done for simpler random walks on the path. However, the identical underlying graphs allow us to use the comparison method of Diaconis and Saloff-Coste [6]. Specializing their result to  $K_n$  yields

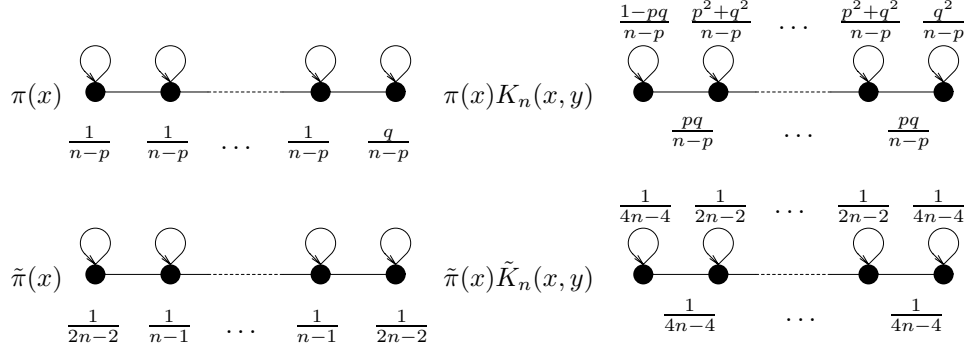
$$(12) \quad \beta_1(K_n) \leq 1 - \left( \min_x \frac{\tilde{\pi}_n(x)}{\pi_n(x)} \right) \left( \min_{\substack{K_n(x,y) > 0 \\ x \neq y}} \frac{\pi_n(x)K_n(x,y)}{\tilde{\pi}_n(x)\tilde{K}_n(x,y)} \right) (1 - \beta_1(\tilde{K}_n)),$$

whenever  $\tilde{K}_n$  is a chain on the same state space as  $K_n$  with the property that  $K_n(x, y) > 0$  implies  $\tilde{K}_n(x, y) > 0$ ; here  $\tilde{\pi}_n$  is the stationary distribution of  $\tilde{K}_n$ .

It is convenient to take

$$\tilde{K}_n = \begin{bmatrix} 1/2 & 1/2 & 0 & \dots & 0 \\ 1/4 & 1/2 & 1/4 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 1/4 & 1/2 & 1/4 \\ 0 & \dots & 0 & 1/2 & 1/2 \end{bmatrix},$$

the “lazy” simple random walk on the  $n$ -path. Substituting the stationary distributions and edge weights of  $K_n$  and  $\tilde{K}_n$  (as shown in Figure 5) and  $\beta_1(\tilde{K}_n) =$

FIGURE 5. Stationary distributions and edge weights of  $K$  and  $\tilde{K}$ .

$\frac{1}{2} + \frac{1}{2} \cos\left(\frac{\pi}{n-1}\right)$  into (12) and (11) now gives

$$\beta_1(K_n) = 1 - \frac{pq\pi^2}{2(n-1)^2} + O\left(\frac{1}{(n-1)^4}\right)$$

and

$$\left\| P_n^{(n-1)t}(x_0, \cdot) - \pi \right\|_{TV} \leq \frac{1}{2\sqrt{\pi(x_0)}} \left( 1 - \frac{pq\pi^2}{2(n-1)^2} + O\left(\frac{1}{(n-1)^4}\right) \right)^{t/2}.$$

Since  $\frac{q}{n-p} \leq \pi(x_0) \leq \frac{1}{n-p}$ , we have shown that  $O(n^2 \log n)$  steps suffice for  $P_n^{n-1}$  to be within a fixed distance of stationarity, while  $O(n^3 \log n)$  suffice for  $P_n$ . As can happen for bounds using only the second-largest eigenvalue, these results are a factor of  $\log n$  larger than necessary.

*Nash inequalities.* Diaconis and Saloff-Coste [7] bound convergence to stationarity using Nash inequalities. Their results are often sharper than second-largest-eigenvalue bounds for slowly-converging chains. Here, we extract only a few pieces of their analysis.

Given an edge set  $E$  on a state space  $S$ , let  $d(x, y)$  be the length of a shortest path from  $x$  to  $y$  via  $E$ . Let  $B(x, r) = \{y : d(x, y) \leq r\}$ . Given a measure  $\pi$  on  $S$ , let  $V(x, r) = \sum_{y \in B(x, r)} \pi(y)$ . Let  $\gamma = \max_{x, y} d(x, y)$  be the diameter of  $E$ .

Say  $(S, E, \pi)$  has  $(A, d)$ -moderate growth if

$$V(x, r) \geq \frac{1}{A} \left( \frac{r+1}{\gamma} \right)^d \quad \text{for } 0 \leq r \leq \gamma.$$

It is easily checked that the underlying graph and stationary distribution of  $M(P_n^{n-1})$  have  $\left(\frac{1}{q} + \frac{1}{n-1}, 1\right)$ -moderate growth.

**Proposition 5** (Diaconis and Saloff-Coste [7]). *Let  $K$  be a Markov chain on a finite set  $S$  with stationary distribution  $\pi$ . Let  $M(K)$  be the multiplicative symmetrization of  $K$ , and  $E$  the edge set of the underlying graph of  $M(K)$ . Assume*

$(S, E, \pi)$  has  $(A, d)$ -moderate growth. Let  $\{\gamma_{xy}\}$  be a collection of paths in  $E$  joining each pair of states in  $S$ , and let

$$a = \max_{\substack{(x,y) \in E \\ 0 \leq r \leq \gamma}} \frac{2}{r^2 \pi(x) M(K)(x, y)} \left\{ \sum_{\substack{\gamma_{zw} \ni (x,y) \\ d(z,w) \leq r}} |\gamma_{zw}| \frac{\pi(z)\pi(w)}{V(z, r)} \right\}.$$

Then

$$\|P^t(x_0, \cdot) - \pi\|_{TV} \leq \frac{1}{2} a_1 e^{-m/(a\gamma^2)}, \quad \text{for } t = a\gamma^2 + m + 1,$$

when  $m \geq 0$  and  $a_1 = (e(1+d)A)^{1/2}(4(2+d))^{d/4}$ .

Following example 5(a) of [7], we take the paths  $\{\gamma_{xy}\}$  in  $K_n = M(P_n^{n-1})$  to be geodesics and bound  $a$ . From the values in Figure 5 we see that

$$\frac{2}{\pi(x)M(K_n)(x, y)} \leq \frac{2(n-p)}{\min(q^2, pq)} \quad \text{and} \quad \pi(z)\pi(w) \leq \frac{(1-pq)^2}{(n-p)^2}.$$

The number of terms in the sum is at most  $r(r+1)/2$  and  $|\gamma_{zw}| \leq r$ . Finally,  $\left(\frac{1}{q} + \frac{1}{n-1}, 1\right)$ -moderate growth implies that

$$V(z, r) \geq \frac{q(r+1)}{n-p}.$$

Combining these estimates yields

$$a \leq \frac{(1-pq)^2}{q \min(q^2, pq)}.$$

We can conclude that  $O(n^2)$  steps suffice for the chain  $P_n^{n-1}$  to be close to stationarity, and thus  $O(n^3)$  suffice for the chain  $P_n$ .

*Remark.* Although it is difficult to compare the asymptotic statement of Theorem 2 and the direct inequalities of Proposition 5, the Nash inequality estimate of the lead term constant appears to worsen as  $q$  decreases to 0.

In order to force  $\|P_n^{t(n-1)}(x_0, \cdot) - \pi\|_{TV} \leq \epsilon$  using Theorem 2, we need a  $\tau$  such that

$$\left( \int_{\mathbb{R}/\mathbb{Z}} |\theta_\tau(x) - 1| dx \right)^{1/2} < \epsilon.$$

Then  $t > \frac{\tau(n-p)^3}{pq(n-1)} = \frac{cn^2}{pq} + O(n)$  steps suffice. In Proposition 5, we must have

$$m > \log\left(\frac{a_1}{\epsilon}\right) a\gamma^2,$$

which implies

$$t > \frac{(1-pq)^2}{q \min(q^2, pq)} \left( 1 + \frac{1}{4} \log(48e^2) + \frac{1}{2} \log\left(\frac{1}{q}\right) - \log \epsilon \right) (n-1)^2 + 1.$$

As  $q \rightarrow 0$ , the lead term is  $O\left(\frac{1}{q^3} \log \frac{1}{q}\right) n^2$ , as opposed to  $O\left(\frac{1}{q}\right) n^2$  for the asymptotic bound.

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