Abstract—Estimation of missing mass with the popular Good-
Turing (GT) estimator is well-understood in the case where samples are independent and identically distributed (iid). In this
article, we consider the same problem when the samples come
from a stationary Markov chain with a rank-2 transition matrix,
which is one of the simplest extensions of the iid case. We develop
an upper bound on the absolute bias of the GT estimator in
terms of the spectral gap of the chain and a tail bound on the
occupancy of states. Borrowing tail bounds from known
concentration results for Markov chains, we evaluate the bound
using other parameters of the chain. The analysis, supported by
simulations, suggests that, for rank-2 irreducible chains, the GT
estimator has bias and mean-squared error falling with number
of samples at a rate that depends loosely on the connectivity of
the states in the chain.

I. INTRODUCTION

A. Preliminaries

Consider a Markov chain \( X^n = (X_1, X_2, \ldots, X_n) \) with the
states \( X_i \in \mathcal{X} = [K] \triangleq \{1, 2, \ldots, K\} \) and
\[ \Pr(X_i=x_i|X_{i-1}=x_{i-1}, \ldots, X_1=x_1) = \Pr(X_2=x_2|X_1=x_1) \]
for \( i = 2, \ldots, n \) and all \( x_i \in \mathcal{X} \). The transition probability
matrix (t.p.m) of the Markov chain, denoted \( P \), is the \( K \times K \)
matrix with \((i, j)\)-th element \( P_{ij} \triangleq \Pr(X_2=j|X_1=i) \). A
distribution \( \pi = [\pi_1, \ldots, \pi_K] \) on \( \mathcal{X} = [K] \) is said to be
a stationary distribution if \( \pi P = \pi \) \( \|1\| \). We will consider stationary Markov chains
for which the distribution of \( X_1 \) (and all \( X_i \)) is a stationary
distribution.

For \( x \in \mathcal{X} \), let
\[
F_x(X^n) \triangleq \sum_{i=1}^{n} I(X_i = x),
\]
where \( I(\cdot) \) is an indicator random variable, denote the number
of occurrences of \( x \) in \( X^n \). For a stationary Markov chain with
state distribution \( \pi \), the missing mass or the total probability
of letters that did not appear in \( X^n \), denoted \( M_0(X^n, \pi) \), is
defined as
\[
M_0(X^n, \pi) \triangleq \sum_{x \in \mathcal{X}} \pi_x I(F_x(X^n) = 0).
\]
For \( l \geq 0 \), let
\[
\phi_l(X^n) \triangleq \sum_{x \in \mathcal{X}} I(F_x(X^n) = l)
\]
denote the number of letters that have occurred \( l \) times in
\( X^n \). The popular and standard Good-Turing estimator \( \phi_1 \)
for \( M_0(X^n, \pi) \) is defined as
\[
G_0(X^n) \triangleq \frac{\phi_1(X^n)}{n}. \tag{1}
\]
We will drop the arguments \( X^n, \pi \) whenever it is non-
ambiguous.

II. PRIOR WORK AND PROBLEM SETTING

When the t.p.m has a rank of 1, the chain is iid and the
bias of Good-Turing estimators falls as \( 1/n \) \( \|3\| \). So, in the iid
case, the number of letters occurring once (i.e. \( \phi_1 \)) acts as a
good proxy for the missing letters in a sequence. However,
the Markov case can be very different, in general. Consider a
t.p.m with \( P_{ii} = 1 - \eta \) and \( P_{ij} = \eta/(K-1), i \neq j \). For small
\( \eta \), every state is "sticky" and \( \phi_1 \) appears to be inadequate to
capture the mass of missing letters. As expected, a simulation
of Good-Turing estimators for such sticky chains shows a non-
vanishing bias.

Markov models occur naturally in language modeling \( \|4\| \)
and several other applications in practice, where Good-Turing
estimators and their modifications are routinely used. There-
fore, it is interesting to analytically understand and study
Good-Turing estimators for missing mass in Markov chains.
Missing mass has been studied extensively in the iid case \( \|3\|, \|5\| - \|10\| \),
estimation in Markov chains has been studied as well \( \|11\| - \|14\| \).
Recently, there has been interest in studying concentration
and estimation of missing mass in Markov chains \( \|15\|, \|16\| \).

The sticky chain example above has a full-rank t.p.m, while
the iid case has a rank-1 t.p.m. This naturally motivates the
study of Good-Turing estimators for chains with t.p.m.s of
other ranks. In particular, in this article, we consider chains
with rank-2 t.p.m.s, which are, in some sense, the simplest in
the non-iid Markovian case.

Consider a Markov chain with a rank-2 t.p.m \( P \), which we
will call, loosely, as a rank-2 Markov chain. Since \( P \) has all
entries in \( [0, 1] \) with each row adding to 1 and it has rank 2,
the eigenvalues of \( P \) will be \( 1, \lambda_2, 0, \ldots, 0 \), and \( -1 \leq \lambda_2 \leq 1 \) (by
Perron-Frobenius theorem) \( \|17\| \). The value of \( \lambda_2 \) determines
several important properties of the chain. If \( \lambda_2 = 1 \), the chain
is reducible. If \( \lambda_2 = -1 \), the chain is periodic with period 2.
For \( -1 < \lambda_2 < 1 \), the chain is irreducible and aperiodic.
III. Results

The main results of this article provide bounds on the absolute bias of Good-Turing estimators of missing mass $|E[G_0(X^n) - M_0(X^n, \pi)]|$ on rank-2 stationary Markov chains. To the best of our knowledge, these are perhaps the first such bounds to have appeared in the literature.

For the purpose of bounding, the bias is split into two significant components. The first component has contributions from states $x$ for which $\pi_x$ is low. This component is bounded in terms of the spectral gap

$$\beta(P) \triangleq 1 - \lambda_2 \in [0, 2].$$  

For bounding the remaining part of the bias, we use tail bounds on the occupancy $F_x(X^n)$ for states $x$ with a high enough value of $\pi_x$.

The following theorem states the main starting point of our bounds on bias. We let $\mathbf{c} \triangleq 1 - x$.

**Theorem 1.** Let $X^n$ be a stationary Markov chain with state distribution $\pi$ and a rank-2 t.p.m with spectral gap $\beta$. Let $1/n < \delta \leq \beta/5$. Then, there exist universal constants $c_1 > 0$ and $c_2 > 0$ such that

$$|E[G_0(X^n) - M_0(X^n, \pi)]| \leq \frac{\delta}{\beta} \left( c_1 + \frac{c_2}{n\beta} \right) + 2 \max_{x : \pi_x > \mathbf{c}, P_{x,\mathbf{x}} \neq 0} \Pr(F_x(X^n) \leq 1) + O(1/n).$$  

As $\beta \to 0$, the chain becomes reducible, and the bias bound grows unbounded as expected because consistent estimation is not possible for missing mass in reducible chains [15]. For example, consider the chain with t.p.m

$$\begin{bmatrix} (2/K) \mathbf{1}_{K/2 \times K/2} & 0 \mathbf{1}_{K/2 \times K/2} \\ 0 \mathbf{1}_{K/2 \times K/2} & (2/K) \mathbf{1}_{K/2 \times K/2} \end{bmatrix},$$

where $b_{r \times c}$ denotes the $r \times c$ all-$b$ matrix, with the uniform distribution on all states as $\pi$. This chain does not visit half the states making the estimation of missing mass inconsistent.

For a non-vanishing $\beta$, using Theorem 1 with a specific tail bound for $\Pr(F_x \leq 1)$ and a choice for $\delta$, we obtain bounds that depend only on the chain’s parameters. Tail bounds, obtained from concentration inequalities for Markov chains, typically use other parameters derived from the t.p.m.s. The inequality of Kontorovich and Raman in [18] uses a parameter $\theta(P)$ defined as

$$\theta(P) \triangleq \sup_{x, x' \in \mathcal{X}} d_{TV}(P(\cdot|x), P(\cdot|x')),$$

where $d_{TV}(p, q) = \frac{1}{2} \sum_{x \in \mathcal{X}} |p_x - q_x|$ is the total variation (TV) distance between two distributions $p$ and $q$ on the same alphabet $\mathcal{X}$. We will call $\theta(P)$ or simply $\theta$ as the maximum TV gap of the chain.

**Corollary 2.** For a rank-2 Markov chain with spectral gap $\beta$ and maximum TV gap $\theta$ satisfying $\beta \geq \beta_0 \triangleq 5 \left( 1/n^c + 1/n \right)$ for some $c \in (0, 0.5)$, we have

$$|E[G_0(X^n) - M_0(X^n, \pi)]| \leq \frac{1}{\beta} \left( \frac{1}{n} + \frac{1}{\theta n^c} \right) c_1 + \frac{c_2}{n\beta} + 4e^{-0.5n(1-2c)} + O(1/n).$$  

In the above corollary, a tail bound from the concentration inequality of [18] is used for $\Pr(F_x \leq 1)$ in Theorem 1 with $\delta = \beta_0/5$. The bias bound is now expressed in terms of $n$, the spectral gap $\beta$ and the maximum TV gap $\theta$, and the rate of fall of absolute bias with $n$ is bounded by how the two gap parameters $\beta$ and $\theta$ vary with $n$.

If two rows of the t.p.m are disjoint in their non-zero positions, we get $\theta = 1$ and Corollary 2 does not apply. We will need to use other concentration inequalities in such cases.

The concentration inequality for Markov chains due to Naor, Rao and Regev in [19] uses a parameter $\lambda_\pi(p, \pi)$ defined as

$$\lambda_\pi(p, \pi) \triangleq \sup_{z : \sum_i \pi_i z_i^2 = 1} \left( \sum_{i=1}^K \pi_i \left( \sum_{j=1}^K (P_{ij} - \pi_j) z_j \right)^2 \right)^{1/2},$$

which is the norm of $P - 1_{K \times 1} \pi$ in the Hilbert space $L_2(\pi)$ with $\|z\|_2^2 = \sum_i \pi_i z_i^2$. If $P$ is orthonormally diagonalizable in $L_2(\pi)$, $\lambda_\pi$ is equal to the absolute second eigenvalue $|\lambda_2|$ in the rank-2 case. However, in most other cases, the optimization in (6) needs to be evaluated to find $\lambda_\pi$, and the evaluation is usually feasible in the rank-2 case. We will call the parameter $\lambda_\pi(P)$ or simply $\lambda_\pi$ as the non-iid weighted norm of the chain.

**Corollary 3.** For a rank-2 Markov chain with spectral gap $\beta$ and non-iid weighted norm $\lambda_\pi$ satisfying $\beta \geq \beta_1 \triangleq 15 \sqrt{\frac{\ln n}{n\lambda_\pi}} + 5/n$, we have

$$|E[G_0(X^n) - M_0(X^n, \pi)]| \leq \frac{1}{\beta} \left( c_1 + \frac{c_2}{n\beta} \right) \left( 3 \sqrt{\frac{\ln n}{\lambda_\pi n}} + \frac{1}{n} \right) + O(1/n),$$

where $c_1, c_2 > 0$ are universal constants.

In the above corollary, a tail bound from the concentration inequality of [19] is used for $\Pr(F_x \leq 1)$ in Theorem 1 with $\delta = \beta_1/5$.

We will now consider a few specific types of rank-2 irreducible chains and use Corollaries 2 and 3 to bound the absolute bias of the Good-Turing estimator for missing mass in terms of $\beta$, $\theta$ and non-iid weighted norm $\lambda_\pi$.

**Chains with $\theta = 0$ (IID):** The iid case $P = 1_{K \times 1} \pi$ (i.e. each row equal to $\pi$) has $\beta = 1$ and $\theta = 0$ resulting in a $1/\sqrt{n}$ upper bound from Corollary 2 which, while capturing the fall of bias to zero, is poorer in rate than the well-known $1/n$ bound.
Non-iid chains: Consider the following $K \times K$ rank-2 t.p.ms.

$$P_1 = \begin{bmatrix}
\frac{a}{K} & \frac{1}{K} & \frac{1}{K} & 0 \\
0 & \frac{a}{K} & \frac{1}{K} & \frac{1}{K} \\
\frac{a}{K} & \frac{1}{K} & \frac{1}{K} & \frac{1}{K} \\
0 & 0 & 0 & 0
\end{bmatrix},$$

$$P_2 = \begin{bmatrix}
\frac{1}{K} & 0 & 0 & 0 \\
0 & \frac{1}{K} & 0 & 0 \\
0 & 0 & \frac{1}{K} & 0 \\
0 & 0 & 0 & \frac{1}{K}
\end{bmatrix},$$

$$P_3 = \begin{bmatrix}
\frac{1}{K} & 0 & 0 & 0 \\
0 & \frac{1}{K} & 0 & 0 \\
0 & 0 & \frac{1}{K} & 0 \\
0 & 0 & 0 & \frac{1}{K}
\end{bmatrix},$$

where $a = 2/(K + K_1)$ and 0 is an all-zero matrix of appropriate size. In all of the three cases above, States 1 to $K/2$ and States $K/2 + 1$ to $K$ are connected only through the $K_1$ states from $(K - K_1)/2 + 1$ to $(K + K_1)/2$. Motivated by the iid worst case, we let $K = n$ and consider $K_1 = \Theta(n^\kappa)$ for $\kappa \leq 1$ to control the connectivity in the chains. Table I lists the dominant terms in the parameters $\beta$, $\bar{\beta}$, $\bar{\lambda}_n$, and the bounds from Corollaries 2 and 3 for the t.p.ms $P_1$, $P_2$ and $P_3$ (up to a multiplicative constant). The three chains considered above illustrate different regimes of values for the parameters $\theta$ and $\lambda$. The corollaries apply when $\bar{\theta} \neq 0$ or $\bar{\lambda} \neq 0$ and when $\kappa$ is large enough to satisfy the lower bound on the spectral gap $\beta$ in the corollaries. The case of $\kappa = 1$ results in a bound tending to $1/\sqrt{n}$, and lower $\kappa$ results in weaker bounds.

Fig. 1 shows simulation plots of the rate of fall of absolute bias and mean-squared error versus $n$ for the three t.p.ms above with $\kappa = 1$ and $\kappa = 1/4$. We observe that both the absolute bias and the mean-squared error fall with $n$ in all cases. For the highly connected case of $\kappa = 1$, the rate of fall in simulations is close to $1/n$. As $\kappa$ decreases and connectivity reduces, the rate of fall of both absolute bias and MSE reduce.

Periodic case: Consider the following $n \times n$ t.p.m

$$\begin{bmatrix}
0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1 \\
1 & 0 & 0 & \cdots & 0
\end{bmatrix}_{r \times r} \otimes \begin{bmatrix}
\frac{r}{n} & \cdots & \frac{r}{n} \\
\vdots & \ddots & \vdots \\
\frac{r}{n} & \cdots & \frac{r}{n}
\end{bmatrix}_{n/r \times n/r},$$

which is a Kronecker product of an $r \times r$ right-shift-by-1 permutation matrix and an $n/r \times n/r$ matrix with each entry equal to $r/n$. The rank of the above t.p.m is $r$, the chain is irreducible and periodic with all states having a period $r$, and the uniform distribution is the unique stationary distribution. For $r = 2$, we get the rank-2 irreducible, period-2 chain. Using a direct computation in a manner similar to the iid case, we obtain the following exact characterization of bias:

$$|\mathbb{E}[G_0(X^n) - M_0(X^n, \pi)]| = \frac{r}{n} \left(1 - \frac{r}{n}\right)^{\frac{n}{r} - 1}. \quad (8)$$

For sub-linear $r$, we see that bias tends to zero. However, for $r \approx n$, we get a bias that is constant.

In summary, we see that the bias of the Good-Turing estimator for missing mass in rank-2 Markov chains can be analytically bounded using the spectral gap $(\beta)$ and other parameters such as the maximum TV gap $(\theta)$ or the non-iid weighted norm $(\bar{\lambda}_n)$ that control the concentration of state occupancies. If better tail bounds can be developed, the rate of fall of bias predicted from the bounds can be tightened further.

From examples such as the sticky chain and the periodic case above, we expect a constant bias for the Good-Turing estimator in certain higher rank Markov chains. Improvement in estimation methods for missing mass is needed for such higher rank chains.

### Table I: Dominant terms of $\beta$, $\bar{\beta}$, $\bar{\lambda}_n$ and bounds (up to a multiplicative constant).

| $K = n$ | $K_1 = n^{\kappa}$ | $\beta$ | $\bar{\beta}$ | $\bar{\lambda}_n$ | Cor 2 $\kappa > 3/4$ | Cor 3 $\kappa > 2/3$ |
|---------|------------------|--------|-------------|--------------|----------------|----------------|
| $P_1$   | $n^{\kappa}/n$  | $n^{\kappa}/n$ | $n^{\kappa}/n$ | $\frac{1}{n^{2\kappa - 3/2}}$ | $\sqrt{\ln n / n^{2\kappa}}$ | $\sqrt{\ln n / n^{2\kappa}}$ |
| $P_2$   | $n^{\kappa}/n$  | 0      | 0           | $\frac{1}{n^{2\kappa}}$     | $\sqrt{\ln n / n^{2\kappa}}$ | $\sqrt{\ln n / n^{2\kappa}}$ |
| $P_3$   | $n^{\kappa}/n$  | 0      | $n^{\kappa}/n$ | $\frac{1}{n^{2\kappa}}$     | $\sqrt{\ln n / n^{2\kappa}}$ | $\sqrt{\ln n / n^{2\kappa}}$ |
Lemma 4.

Proof. See Section V

Using Part 1 of Lemma 4 it suffices to upper bound $\sum_{x \in X: P_{xx} \neq \pi_x} \pi_x \Gamma_x$. In order to carry out this analysis, we fix a threshold $\delta$ (to be decided later) and partition the set of states with $P_{xx} \neq \pi_x$ into two sets

$$A(\delta) = \{ x \in X : \pi_x \leq \delta, P_{xx} \neq \pi_x \},$$

$$\bar{A}(\delta) = \{ x \in X : \pi_x > \delta, P_{xx} \neq \pi_x \}.$$

Observe that

$$\pi_x \Gamma_x = \frac{1}{n} \left( \sum_{i=1}^{n} \pi_x \Pr(F_x(X^n) = 0, X_i = x) - \pi_x \Pr(F_x(X^n) = 0, X_i = x) \right)$$

$$= \frac{\pi_x}{n} \left( \sum_{i=1}^{n} \Pr(F_x(X^n) = 0, X_i = x) - \pi_x \Pr(F_x(X^n) = 0) \right)$$

$$= \frac{\pi_x}{n} \Pr(F_x(X^n) = 1) - \pi_x \Pr(F_x(X^n) = 0).$$

Summing over $x \in \bar{A}(\delta)$, we get

$$\left| \sum_{x \in \bar{A}(\delta)} \pi_x \Gamma_x \right|$$

$$= \left| \sum_{x \in \bar{A}(\delta)} \frac{\pi_x}{n} \Pr(F_x(X^n) = 1) - \pi_x \Pr(F_x(X^n) = 0) \right|$$

$$\leq \sum_{x \in \bar{A}(\delta)} \left( \frac{\pi_x}{n} + \pi_x \right) \Pr(F_x(X^n) \leq 1)$$

$$\leq 2 \max_{x \in \bar{A}(\delta)} \Pr(F_x(X^n) \leq 1),$$

where, in the last inequality, we use $\sum x < 1$ and $|\bar{A}(\delta)| \leq 1/\delta < n$. Using Part 2 of Lemma 4 and (10), the proof is complete.

B. Corollaries 2 and 3

For any $x$, we have $E[F_x(X^n)/n] = \pi_x$. For large $\pi_x$, if $F_x(X^n)$ concentrates, we can bound the tail probability $Pr(F_x(X^n) \leq 1)$ using concentration of $F_x(X^n)$ as follows:

$$Pr(F_x(X^n) \leq 1) = Pr(\pi_x - F_x(X^n)/n \geq \pi_x - 1/n) \leq Pr(|\pi_x - F_x(X^n)/n| \geq \pi_x - 1/n).$$

Using the concentration results in [18] and [19], we obtain the following:

Lemma 5. 1) If the chain has maximum TV gap $\theta < 1$,

$$Pr(|\pi_x - F_x(X^n)/n| \geq \epsilon) \leq 2e^{-0.5\theta^2\epsilon^2}.$$

2) If the chain has non-iid weighted norm $\lambda_x < 1$,

$$Pr(|\pi_x - F_x(X^n)/n| \geq \epsilon) \leq C \left( \frac{q}{\lambda_x n} \right)^{\epsilon^2}$$

where $C$ is a constant and $q \geq 2$.

Proof. See Section V

1) Proof of Corollary 2. We consider the set $\bar{A}(\delta)$ with

$$\delta = \frac{1}{\theta n^c} + \frac{1}{n}, \ c \in (0, 0.5).$$

For $x \in \bar{A}(\delta)$, we have $\pi_x - \frac{1}{n} > \frac{1}{\theta n^c}$. So, setting $\epsilon = \frac{1}{\theta n^c}$ in Part 1 of Lemma 5 we get

$$Pr(F_x(X^n) \leq 1) \leq 2e^{-0.5\theta^2\epsilon^2}.$$

Using $\delta$ from (12) and the above bound for $Pr(F_x(X^n) \leq 1)$ in Theorem 1 we get (5) and the proof for Corollary 2 is complete.

2) Proof of Corollary 3. We consider the set $\bar{A}(\delta)$ with

$$\delta = 3 \sqrt{\frac{\ln n}{n \lambda_x}} + \frac{1}{n}.$$

For $x \in \bar{A}(\delta)$, we have $\pi_x - 1/n \geq 3 \sqrt{\frac{\ln n}{n \lambda_x}}$. So, setting $\epsilon = 3 \sqrt{\frac{\ln n}{n \lambda_x}}$ and $q = 3 \ln n$ in Part 2 of Lemma 5 we get

$$\max_{x \in \bar{A}(\delta)} Pr(F_x(X^n) \leq 1) \leq C/n^{1.5}.$$

Using $\delta$ from (13) and the above bound for $Pr(F_x(X^n) \leq 1)$ in Theorem 1 we get (7) and the proof for Corollary 3 is complete.
V. PROOFS OF LEMMAS

Consider a rank-2 $K \times K$ irreducible t.p.m $P$ with stationary distribution $\pi = [\pi_1 \cdots \pi_K]^T$. There exist vectors $u = [u_1 \cdots u_K]^T$ and $v = [v_1 \cdots v_K]^T$ satisfying the following decompositions:

1) If $P$ is diagonalizable with spectral gap $\beta \neq 1$, then

$$P = RDS$$

where $R = [1_{K \times 1} \ v]$, $D = \begin{bmatrix} 1 & 0 \\ 0 & \beta \end{bmatrix}$ and $S = \begin{bmatrix} \pi^T \\ u^T \end{bmatrix}$.

Since $P$ is a t.p.m., we have, for $1 \leq i, j \leq K$,

$$0 \leq \pi_j + (1-\beta)v_j u_j \leq 1.$$  \hspace{1cm} (14)

2) If $P$ is non-diagonalizable with spectral gap $\beta = 1$, then

$$P = RS$$

Since $P$ is a t.p.m., we have, for $1 \leq i, j \leq K$,

$$0 \leq \pi_j + v_i u_j \leq 1.$$

A. Lemma 3 Part 2 (see [20] for Part 1)

The quantity $\Gamma_x$, when $P_{xx} \neq \pi_x$, can be expressed in terms of some more spectral parameters for both the diagonalizable and the non-diagonalizable cases.

**Lemma 6.** If $P$ is diagonalizable and $x \in \mathcal{X}$ with $P_{xx} \neq \pi_x$,

$$\Gamma_x = \beta v_x u_x \left[ \left( (\lambda_{1}^{x})^{n-1} - (\lambda_{2}^{x})^{n-1} \right) \frac{1}{\pi_x} \right.$$

$$- \left( (\lambda_{1}^{x})^{n-1} + (\lambda_{2}^{x})^{n-1} \right) \left( 1 - \frac{2}{\beta} \right) \frac{1}{\Delta_x^2}$$

$$+ \frac{2}{n} \lambda_{1}^{x} - \lambda_{2}^{x} \left( (\lambda_{1}^{x})^{n-2} - (\lambda_{2}^{x})^{n-2} \right) \right], \hspace{1cm} (15)$$

where $\lambda_{i}^{x} = 0.5(\pi_x + \beta(1-v_x u_x) + (1-\beta)^{1+\Delta_x})$, $i = 1, 2$, are the eigenvalues of the matrix $D = \begin{bmatrix} 1_{2 \times 2} - \begin{bmatrix} \pi_x \\ u_x \end{bmatrix} & [1 \ v_x] \end{bmatrix}$, and $\Delta_x^2 = \left[ \beta - \pi_x + \beta v_x u_x \right]^2 + 4\beta \pi_x v_x u_x$.

**Proof.** See [20] for a proof. \hfill \Box

Now, $|\Gamma_x|$ is upper-bounded by the sum of absolute value of all the terms in the RHS of (15). To simplify the bound, we use $|\lambda_{i}^{x}| < 1$ and $1 - 2/n < 1$ to get

$$|\Gamma_x| \leq 2 \left( \frac{1}{\pi_x} + \frac{\beta}{\Delta_x^2} \left( 1 + 2\frac{\Delta_x^{-1}}{n} \right) \right) \beta v_x u_x.$$  \hspace{1cm} (16)

For $x \in A(\delta)$, we have $\pi_x \leq \delta$ and $\delta \leq \beta/5 \leq 2/5$. Using this and (14), it is possible to show that

**Claim 1:** $\Delta_x \geq \beta/3$ for $x \in A(\delta)$.

Using these bounds in (16), we get

$$|\Gamma_x| \leq \frac{2}{\beta} \left( 7 + \frac{27}{n\beta} \right) \beta v_x u_x,$$  \hspace{1cm} (17)

Next we claim that

**Claim 2:** $\sum_{x \in A(\delta)} |\beta v_x u_x| \leq 3$.

Using this and (17), we get

$$\sum_{x \in A(\delta)} \pi_x \beta v_x u_x \leq \frac{6\delta}{\beta} \left( 7 + \frac{27}{n\beta} \right),$$

where we have bounded $\pi_x \leq 1$ and $\pi_x < \delta$. This completes the proof for the diagonalizable case.

1) **Proofs of Claims:** **Claim 1:** Using $\pi_x \leq \delta \leq \beta/5$ for $x \in A(\delta)$ and $\beta v_x u_x \geq -\pi_x$ from (14), we get

- (i) $\pi_x - \beta v_x u_x \geq \beta - 2\pi_x \geq 5\pi_x - 2\pi_x \geq 0$, and (ii) $4\pi_x \beta v_x u_x \geq -4\pi_x^2$.

This implies that,

$$\Delta_x^2 \geq (\pi_x - \beta v_x u_x)^2 + 4\pi_x \beta v_x u_x \geq (\beta - 2\pi_x)^2 - 4\pi_x^2 \geq \beta^2/5 \geq \beta^2/9 \hspace{1cm} (18)$$

and hence $\Delta_x \geq \beta/3$ for $x \in A(\delta)$.

**Claim 2:** To prove this, we partition $A(\delta)$ into two sets, $A_1(\delta) = \{ x \in A(\delta) : \beta v_x u_x \leq 0 \}$ and its complement, $\overline{A}_1(\delta) = A(\delta) \setminus A_1(\delta)$.

1) For $x \in A_1(\delta)$, using $\beta v_x u_x \leq 0$ and $\beta v_x u_x \geq -\pi_x$ from (14), we get

$$0 \geq \sum_{x \in A_1(\delta)} \beta v_x u_x \geq - \sum_{x \in A_1(\delta)} \pi_x \pi_x \geq -1$$

which implies $\sum_{x \in A_1(\delta)} \beta v_x u_x \leq 1$.

2) On the other hand, to deal with the sum over $\overline{A}_1(\delta)$, note that $\sum_{x \in \hat{\mathcal{X}}} v_x u_x = 1$ since the matrix product $SR = I$. Therefore,

$$\sum_{x \in \hat{\mathcal{X}} : \beta v_x u_x > 0} \beta v_x u_x = \beta - \sum_{x \in \hat{\mathcal{X}} : \beta v_x u_x \leq 0} \beta v_x u_x$$

Since the summation on the right in the above equation is bounded above by 1 in absolute value (because of (14) again), we get $\sum_{x \in \overline{A}_1(\delta)} \beta v_x u_x \leq 1 + \beta \leq 2$.

**Lemma 7.** If $P$ is non-diagonalizable and $x \in \mathcal{X}$ with $P_{xx} \neq \pi_x$,

$$\Gamma_x = \frac{v_x u_x \left[ \left( (\lambda_{1}^{x})^{n-1} - (\lambda_{2}^{x})^{n-1} \right) \frac{1}{\pi_x} \right.$$

$$- \left( (\lambda_{1}^{x})^{n-1} + (\lambda_{2}^{x})^{n-1} \right) \left( 1 - \frac{2}{\beta} \right) \frac{1}{\Delta_x^2}$$

$$+ \frac{2}{n} \lambda_{1}^{x} - \lambda_{2}^{x} \left( (\lambda_{1}^{x})^{n-2} - (\lambda_{2}^{x})^{n-2} \right) \right], \hspace{1cm} (19)$$

where $\lambda_{i}^{x} = 0.5(\pi_x - \beta v_x u_x) + (1-\beta)^{1+\Delta_x})$, $i = 1, 2$, are the eigenvalues of the matrix $D = \begin{bmatrix} \pi_x & -\pi_x v_x \\ -v_x u_x & -u_x v_x \end{bmatrix}$ with $\Delta_x^2 = (\pi_x - v_x u_x)^2$ and $\pi_x = (\pi_x - v_x u_x)^2 + 4v_x u_x$.

**Proof.** Similar to that of Lemma 6. \hfill \Box

Bounding $\sum_{x \in A} \pi_x \beta v_x u_x$ using a method similar to the diagonalizable case, completes the proofs.
B. Lemma 5

**Theorem 8 (13).** Suppose that $X^n$ is a Markov chain with state space $X$ and t.p.m $P$ with $\theta(P) < 1$, and $\psi(X^n) : X^n \to \mathbb{R}$ is a d-Lipschitz function with respect to the normalized Hamming metric, then

$$Pr(|\psi(X^n) - E[\psi(X^n)]| \geq \epsilon) \leq e^{-n(1-\theta)^2\epsilon^2/2d^2}. \quad (20)$$

Since $E_x(X^n)/n$ is 1-Lipschitz, Theorem 20 directly results in Part 1. For Part 2, we use the following theorem from [19].

**Theorem 9 (19).** Suppose that $X^n$ is a stationary Markov chain with state space $X = [K]$, stationary distribution $\pi$ and t.p.m $P$ such that $\lambda_\pi(P) < 1$. Then every $f : [K] \to \mathbb{R}$ satisfies the following inequality for every $n \in \mathbb{N}$ and $q \geq 2$, $q \leq n$:

$$\left( E\left[\frac{\sum_{i=1}^{n} f(X_i)}{n}\right] - E[f(X_1)] \right)^{1/2} \leq \sqrt{\frac{q}{(1-\lambda_\pi)n}} \left( E[f(X_1)]^{q/2} \right)^{1/q}, \quad (21)$$

where $D_1 \leq D_2$ implies there exists a universal constant $C > 0$ such that $D_1 \leq CD_2$.

Using Markov's inequality,

$$Pr\left(\left|\pi_x - F_x(X^n)/n\right|^q \geq \epsilon^q\right) \leq E\left[\frac{\pi_x - F_x(X^n)/n}{\epsilon^q}\right] \leq C\left(\frac{q}{\lambda_\pi n}\right)^{q/2} \pi_x \epsilon^{-q}, \quad (22)$$

where (a) follows by setting $f(X_i) = I(X_i = x)$ in (21).

**C. Proofs of Lemma.**

We prove Lemma 6 and part 1, Lemma 6 (for diagonalizable t.p.m.) using the Lemma below. (The proof of part 1 of Lemma 4 for non-diagonalizable t.p.m. follows a similar method and is hence omitted.)

**Lemma 10.** Let $P$ be a rank-2 diagonalizable t.p.m. Let $E_{x\sim m}$ denote the event $F_x(X_{n-m}) = 0$.

1. For $x \in X$ with $P_{xx} = \pi_x$,
   $$Pr(E_{x\sim m} | X_m = x) = Pr(E_{x\sim m} | X_m \neq x) = (\pi_x)^{n-1} \text{ for } m = 1 \text{ to } n.$$
2. For $x \in X$ with $P_{xx} \neq \pi_x$,
   a) for $m = 1$ to $n$,
   $$Pr(E_{x\sim m} | X_m \neq x) = \frac{1}{2^{m-1}} \left( \frac{\lambda_{\pi_x}^m}{\Delta_x} + \frac{\lambda_{\pi_x}^{n-m}}{\Delta_x} \right) \quad (23)$$
   b) for $m = 2$ to $n - 1$,
   $$Pr(E_{x\sim m} | X_m = x) = Pr(E_{x\sim m} | X_m = x) = \left(\frac{\lambda_{\pi_x}^m}{\Delta_x} \frac{\lambda_{\pi_x}^{n-m}}{\Delta_x} \right) = \left[1 - \frac{(1-\beta)v_x u_x}{\pi_x} \right] (S^{\pi_x} R \xi)^{n-2} \left[1 - \pi_x \xi \right]. \quad (26)$$

**Proof.** Appendix

**Lemma 11.** For $m = 1, 2, \ldots, n$

$$Pr(E_{x\sim m} | X_m \neq x) = \left[1 - \frac{(1-\beta)v_x u_x}{\pi_x} \right] (S^{\pi_x} R \xi)^{n-2} \left[1 - \pi_x \xi \right]. \quad (26)$$

**Proof.** Appendix

**Lemma 12.** 1) For $m \geq 2$,

$$Pr(E_{x\sim m} | X_1 = x) = \left[1 - (1-\beta)v_x \xi \right] (S^{\pi_x} R \xi)^{m-2} \left[1 - \pi_x \xi \right]. \quad (27)$$

**Proof.** Appendix
2) \[
Pr(E^x_{1:n-1}|X_n = x) = Pr(E^x_{2:n}|X_1 = x) \tag{28}
\]
For \(m = 2, \ldots, n-1,\)
\[
Pr(E^x_{m}|X_m = x) = Pr(E^x_{2:m}|X_1 = x)
Pr(E^x_{2:m-1}|X_1 = x) \tag{29}
\]

Proof. Appendix

The next lemma gives an expression for \((S^{x} \cdot RD)^l\) \((l \geq 1)\) for various values of \(\pi_x, v_x, \text{ and } u_x.\)

**Lemma 13.** \((S^{x} \cdot RD)^l:\)
1) For \(x \in X,\) with \(v_x = u_x = 0,\)
\[
(S^{x} \cdot RD)^l = \begin{bmatrix}
\pi_x & 0 \\
0 & \beta
\end{bmatrix}
\]
2) For \(x \in X,\) with \(v_x \neq 0, u_x \neq 0,\)
a) \(\pi_x = \beta:\)
\[
(S^{x} \cdot RD)^l = \begin{bmatrix}
-\pi_x l & 0 \\
0 & \pi_x \pi_x - \beta
\end{bmatrix}
\]
b) \(\pi_x \neq \beta:\)
\[
(S^{x} \cdot RD)^l = \begin{bmatrix}
1 & 0 \\
-\pi_x v_x / \pi_x & 1
\end{bmatrix}
\]
3) For \(x \in X,\) with \(v_x \neq 0, u_x = 0,\)
a) \(\pi_x = \beta:\)
\[
(S^{x} \cdot RD)^l = \begin{bmatrix}
\pi_x & 0 \\
0 & \pi_x \pi_x - \beta
\end{bmatrix}
\]
b) \(\pi_x \neq \beta:\)
\[
(S^{x} \cdot RD)^l = \begin{bmatrix}
1 & 0 \\
-\pi_x v_x / \pi_x & 1
\end{bmatrix}
\]
4) For \(x \in X,\) with \(v_x \neq 0, u_x \neq 0,\)
\[
(S^{x} \cdot RD)^l = V^{x} \left(\begin{bmatrix}
(\lambda_1^{x})^l & 0 \\
0 & (\lambda_2^{x})^l
\end{bmatrix}
(V^{x})^{-1}
\right)
\]
where \(V^{x} = \begin{bmatrix}
\frac{1}{2(1-\beta)\pi_x x_v + \Delta_2 x} & \frac{1}{2(1-\beta)\pi_x x_v + \Delta_2 x}
\end{bmatrix}
\]
\[
(V^{x})^{-1} = \begin{bmatrix}
\Delta_2 x + s_x & -(1-\beta)\pi_x x_v \\
\Delta_2 x & \Delta_2 x
\end{bmatrix}
\]
with \(s_x = 1 - \pi_x - (1-\beta)(1-\pi_x x_v), \lambda_1^{x}, \lambda_2^{x}\) and \(\Delta_2 x\) as defined in Lemma 9.

For \(x \in X\) that fall in any of the first three categories in Lemma 13 (which makes \(P^{x} = \pi_x\)), substituting the corresponding form of \((S^{x} \cdot RD)^l\) in (26), (27) and simplifying we get \(Pr(E_{m}|X_m \neq x) = (1 - \pi_x)^{m-1}\) for \(m = 1 \text{ to } n\) and \(Pr(E^x_{2:m}|X_1 = x) = (1 - \pi_x)^{m-1}\), for all \(2 \leq m \leq n\). Using this in (28) and (29), we get \(Pr(E^x_{m}|X_m = x) = (1 - \pi_x)^{m-1}\), for \(m = 1 \text{ to } n\). This completes the proof of the first part of Lemma 10.

For \(x \in X\) with \(v_x \neq 0\) and \(u_x \neq 0\), substituting the expression for \((S^{x} \cdot RD)^l\) from (32) in (27) and simplifying we get
\[
Pr(E^x_{2:m}|X_1 = x) = \frac{\pi_x}{\pi_x - \beta}
\]
\[
Pr(E^x_{m}|X_m \neq x) = \frac{1}{\pi_x - \beta}
\]
\[
Pr(E^x_{m}|X_m = x) = \frac{1}{\pi_x - \beta}
\]
Multiplying we get
\[
Pr(E^x_{m}|X_1 = x) = \frac{1}{\pi_x - \beta}
\]
\[
Pr(E^x_{m}|X_m \neq x) = \frac{1}{\pi_x - \beta}
\]
\[
Pr(E^x_{m}|X_m = x) = \frac{1}{\pi_x - \beta}
\]
for \(m \geq 2\).

Using (33) with \(m = n\) along with (28) completes the proof of (24). Using (33) in (29) and simplifying, we get (25). Lastly, substituting \((S^{x} \cdot RD)^l\) from (32) in (26) and simplifying, we get (29) and the proof is complete.

**APPENDIX**

A. Proof of Lemma 11

To prove Lemma 11 we first note that
\[
Pr(E^x_{n}|X_n \neq x) = \frac{Pr(F_x(X^n) = 0, X_n \neq x)}{Pr(X_n \neq x)}
\]
\[
Pr(F_x(X^n) = 0) = \sum_{y \in X : y \neq x} \pi_y Pr(E^x_{n-1}|X_1 = y).
\]
We can write \(Pr(F_x(X^n) = 0)\) as
\[
Pr(F_x(X^n) = 0) = \sum_{y \in X : y \neq x} \pi_y Pr(E^x_{n-1}|X_1 = y).
\]
Since \(Pr(E^x_{n-1}|X_1 = y)\) is the probability that the Markov chain does not visit the state \(x\) in the steps \(X_2\) through \(X_n\), given that it starts in state \(y\), \(Pr(E^x_{n-1}|X_1 = y)\) equals the row sum of \((P^{x})^{n-1}\) taken along the row corresponding to the state \(y\). Therefore
\[
Pr(F_x(X^n) = 0) = \sum_{y \in X : y \neq x} \pi_y \sum_{z \in X} [(P^{x})^{n-1}]_{y,z}
\]
\[
= \sum_{y \in X : y \neq x} \pi_y \sum_{z \in X} [(RDS^{x})^{n-1}]_{y,z}
\]
\[
= \sum_{y \in X : y \neq x} \pi_y \sum_{z \in X} [RD(S^{x} \cdot RD)^{n-2} S^{x}]_{y,z}
\]
respectively and \( [1 \quad (1 - \beta) v_y] \) is the row of the matrix \( RD \) corresponding to the state \( y \), we have

\[
\text{Pr}(F_y(X^n) = 0) \\
\quad \overset{(b)}{=} \sum_{y \in X, y \neq x} \pi_y \left[ 1 - (1 - \beta) v_y \right] (S^{-x} RD)^{n-2} \left[ 1 - \pi_x \right] \\
\quad \overset{(c)}{=} \left[ 1 - \pi_x \right] (1 - (1 - \beta)\pi_x v_x) (S^{-x} RD)^{n-2} \left[ 1 - \pi_x \right] \]

where we use \( \pi^T 1_{K \times 1} = 1, u^T 1_{K \times 1} = 0 \) (from \( SR = I \)) to sum up the rows of \( S^{-x} \) to get (b) and use \( \pi^T 1_{K \times 1} = 1, u^T v = 0 \) (from \( SR = I \)) to get (c).

Using \( \text{Pr}(E_{z,m}^x | X_m \neq x) = \frac{1}{1 - \pi_x} \text{Pr}(F_x(X^n) = 0) \) for \( m = 1, 2, \ldots n \) completes the proof.

B. Proof of Lemma 12

1) Using a method similar to the proof of Lemma 11 we get

\[
\text{Pr}(E_{2,m}^x | X_1 = x) \\
= \sum_{z \in X} \left[ (P^{x}_{-z} m^{-1})_{x,z} - \sum_{z \in X} [(RDS^{-x})^{m-1}]_{x,z} \right] \\
= \left[ 1 - (1 - \beta) v_x \right] (S^{-x} RD)^{m-2} \left[ 1 - \pi_x \right]
\]

2) We begin with the result of Lemma 8 which states that for a stationary Markov chain \( X^n \),

\[
\text{Pr}(X_j = x, E_{1,j-i}^x) = \text{Pr}(X_1 = x, E_{2,j}^x), \text{ for } 2 \leq j \leq n \]  
(34)

Since

\[
\text{Pr}(E_{1:n-1}^x | X_n = x) = \frac{\text{Pr}(E_{1:n-1}^x, X_n = x)}{\text{Pr}(X_n = x)}
\]

using (34) and the stationarity of \( X^n \), we get

\[
\text{Pr}(E_{n-1}^x | X_n = x) = \text{Pr}(E_{2:n}^x | X_1 = x)
\]

We now factorise \( \text{Pr}(E_{z,m}^x | X_m = x) \) (for \( m = 2, \ldots, n-1 \)) as shown below:

\[
\begin{align*}
\text{Pr}(E_{z,m}^x | X_m = x) \\
\quad \overset{(a)}{=} \text{Pr}(E_{1:m-1}^x | X_m = x) \text{Pr}(E_{m+1:n}^x | X_m = x) \\
\quad \overset{(b)}{=} \text{Pr}(E_{2:m}^x | X_1 = x) \text{Pr}(E_{m+1:n}^x | X_m = x) \\
\quad \overset{(c)}{=} \text{Pr}(E_{2:m}^x | X_1 = x) \text{Pr}(E_{2:n-1}^x | X_1 = x)
\end{align*}
\]

where we use Markov property to get (a), use (28) with \( n = m \) to get (b) and finally use the stationarity of \( X^n \) to get (c). This completes proof of (29).

C. Proof of Lemma 13

Since \( SR = I \), we have \( S^{-x} R = [\pi_x \quad -\pi_x v_x] \) and

\[
S^{-x} RD = \begin{bmatrix} \pi_x & -\pi_x v_x \\ -u_x & 1 - v_x u_x \end{bmatrix}
\]

(35)

1) We substitute \( v_x = u_x = 0 \) in (35) and raise the power on both sides to \( l \).
2a) Substituting \( v_x = 0, \beta = \pi_x \) in (35), we get \( S^{-x} RD \Rightarrow \begin{bmatrix} \pi_x & 0 \\ -u_x & \pi_x \end{bmatrix} \). Using induction on power \( l \), we get \( (S^{-x} RD)^l = \begin{bmatrix} \pi_x & 0 \\ -l u_x \pi_x & \pi_x \end{bmatrix} \).
2b) Substituting \( v_x = 0 \) in (35), we get \( S^{-x} RD = \begin{bmatrix} \pi_x & 0 \\ -u_x & \beta \end{bmatrix} \). We observe that \( \pi_x, \beta \) are the eigenvalues of \( S^{-x} RD \) with \( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) and \( \begin{bmatrix} \pi_x & 1 \\ -u_x \pi_x & \beta \end{bmatrix} \) their respective right eigenvectors resulting in the diagonalised form in (30).
3a) Substituting \( u_x = 0, \beta = \pi_x \) in (35), we get \( S^{-x} RD = \begin{bmatrix} \pi_x & 0 \\ -\pi_x v_x & \pi_x \end{bmatrix} \). Using induction on power \( l \), we get \( (S^{-x} RD)^l = \begin{bmatrix} \pi_x & 0 \\ -l \pi_x v_x & \beta \end{bmatrix} \).
3b) Substituting \( u_x = 0 \) in (35), we get \( S^{-x} RD = \begin{bmatrix} \pi_x & 0 \\ -u_x & \beta \end{bmatrix} \). We observe that \( \pi_x, \beta \) are the eigenvalues of \( S^{-x} RD \) with \( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) and \( \begin{bmatrix} \pi_x & 1 \\ -u_x & \beta \end{bmatrix} \) their respective right eigenvectors resulting in the diagonalised form in (31).

4) Solving \( det(S^{-x} RD - \lambda I) = 0 \), we get \( \lambda_x^{-x} \Rightarrow 0.5(\pi_x + \beta \pi_x (1 - v_x u_x)) + (-1)^{i+1} \Delta_x \), \( i = 1, 2 \), as the eigenvalues of \( S^{-x} RD \) with \( \begin{bmatrix} \frac{1}{2(1-\beta) \pi_x v_x} \\ \frac{1}{2(1-\beta) \pi_x} \end{bmatrix} \) as their respective right eigenvectors, where \( \Delta_x^2 = (\beta - \pi_x + \beta v_x u_x)^2 + 4\beta \pi_x v_x u_x, s_1 = 1 - \pi_x - (1 - \beta)(1 - v_x u_x) \), resulting in the diagonalised form in (32).

This completes the proof of Lemma 13.

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