Fast Bidirectional Probability Estimation in Markov Models

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Abstract

We develop a new bidirectional algorithm for estimating Markov chain multi-step transition probabilities: given a Markov chain, we want to estimate the probability of hitting a given target state in \( \ell \) steps after starting from a given source distribution. Given the target state \( t \), we use a (reverse) local power iteration to construct a random variable with the desired mean but having small variance – this can then be sampled efficiently by a Monte Carlo algorithm. This method extends to any Markov chain on a discrete (finite or countable) state-space, and can be extended to compute functions of multi-step transition probabilities such as PageRank, graph diffusions, hitting/return times, etc. Surprisingly, we also show that in ‘sparse’ Markov Chains – wherein the number of transitions between states is comparable to the number of states – the running time of our algorithm for a uniform-random target node is orderwise smaller than Monte Carlo and power iteration based algorithms; in particular, our method can estimate a probability \( p \) using only \( O(1/\sqrt{p}) \) running time.

1 Introduction

Markov chains are one of the workhorses of stochastic modeling, finding use across a variety of applications – MCMC algorithms for simulation and statistical inference; to compute network centrality metrics for data mining applications; statistical physics; operations management models for reliability, inventory and supply chains, etc. In this paper, we consider a fundamental problem associated with Markov chains, which we refer to as the multi-step transition probability estimation (or MSTP-estimation) problem: given a Markov Chain on state space \( S \) with transition matrix \( P \), an initial source distribution \( \sigma \) over \( S \), a target state \( t \in S \) and a fixed length \( \ell \), we are interested in computing the \( \ell \)-step transition probability from \( \sigma \) to \( t \). Formally, we want to estimate:

\[
 p_\sigma^\ell[t] := \langle \sigma P^\ell, e_t \rangle = \sigma P^\ell e_T^T,
\]

where \( e_t \) is the indicator vector of state \( t \). A natural parametrization for the complexity of MSTP-estimation is in terms of the minimum transition-probabilities we want to detect; formally, given a desired minimum detection threshold \( \delta \), we want algorithms that give estimates with multiplicative guarantees for any \((\sigma, t, \ell)\) such that \( p_\sigma^\ell[t] > \delta \).

Parametrizing in terms of the detection threshold \( \delta \) can be thought of as benchmarking against a standard Monte-Carlo algorithm, wherein we estimate \( p_\sigma^\ell[t] \) by sampling independent \( \ell \)-step paths, each starting from a random state sampled from \( \sigma \). An alternate technique for MSTP-estimation is based on linear algebraic iterations, in particular, the (local) power iteration. We discuss these in more detail in Section 1.2. Crucially, however, both Monte Carlo and linear algebraic techniques have a running time of \( \Omega(1/\delta) \) for testing if \( p_\sigma^\ell[t] > \delta \); moreover this is true not only for worst case

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choices of target state $t$, but rather, for many Markov chains (in particular, Markov chains with high conductance), this is true for most choices of target states (cf. Section 1.2).

### 1.1 Our Results

To the best of our knowledge, our work gives the first bidirectional algorithm for MSTP-estimation which works for general discrete state-space Markov chains\(^1\). Surprisingly, the algorithm we develop is very simple, both in terms of implementation and analysis. Moreover, we prove that in many settings, it is orderwise faster than existing techniques.

The bidirectional-MSTP estimation algorithm is formally presented in Section 2.1. Briefly: it consists of two distinct components, which we refer to as reverse-work and forward-work:

- **Reverse-work**: Starting from the target node $t$, we perform a sequence of reverse local power iterations. In particular, we use the REVERSE-PUSH operation defined in Algorithm 1.
- **Forward-work**: We next sample $n_f$ random trajectories of length $\ell$, starting from $\sigma$ and transitioning according to $P$, and return the sum of residues on the trajectory as an estimate of $p^\ell_\sigma[t]$.

The above procedure, which is encoded on Algorithm 2, works for all countable-state Markov chains, and gives us the following accuracy result:

**Theorem 1** (For details, refer Section 2.3). Given any Markov chain $P$, source distribution $\sigma$, terminal state $t$, length $\ell$, threshold $\delta$ and relative error $\epsilon$, the Bidirectional-MSTP estimator (Algorithm 2) returns an unbiased estimate $\tilde{p}^\ell_\sigma[t]$ for $p^\ell_\sigma[t]$, which, with high probability, satisfies:

$$|\tilde{p}^\ell_\sigma[t] - p^\ell_\sigma[t]| < \max\{\epsilon p^\ell_\sigma[t], \delta\}.$$  

Since we dynamically adjust the number of REVERSE-PUSH operations to ensure that all residues are small, the proof of the above theorem follows from straightforward concentration bounds – see Section 2.3 for details. A natural concern now is the running time of the algorithm; it is easy to see that this could be large in the worst case – for example, if $t$ has more than $1/\delta$ in-neighbors. Surprisingly we show that in sparse Markov chains and for typical target states, this is not the case:

**Theorem 2** (For details, refer Section 2.3). Given any Markov chain $P$, source distribution $\sigma$, length $\ell$, threshold $\delta$ and desired accuracy $\epsilon$; then for a uniform random choice of $t \in S$, the Bidirectional-MSTP estimation algorithm has a running time of $\tilde{O}(\ell^{3/2} \sqrt{d}/\delta)$, where $d$ is the average number of neighbors of nodes in $S$.

Thus, for typical targets, we can estimate transition probabilities of order $\delta$ in time only $O(1/\sqrt{\delta})$. Note that we do not need for every state that the number of neighboring states is small, but rather, that they are small on average – for example, this is true in "power-law" networks, where some nodes have very high degree, but the average degree is small. The proof of this result is based on a modification of an argument in [2] – refer Section 2.3 for details.

Estimating transition probabilities to a target state is one of the fundamental primitives in Markov chain models – hence, we believe that our algorithm can prove useful in a variety of application domains. In Section 3, we briefly describe how to adapt our method for some of these applications – estimating hitting/return times and stationary probabilities, extensions to non-homogenous Markov chains (in particular, for estimating graph diffusions and heat kernels), connections to local algorithms and expansion testing. However, in addition, our MSTP-estimator could be useful in several other applications – estimating ruin probabilities in reliability models, buffer overflows in queueing systems, in statistical physics simulations, in numerical linear algebra (via variants of the von Neumann-Ulam method [3]), etc.

### 1.2 Existing Approaches for MSTP-Estimation

There are two main techniques used for MSTP-estimation. First, a natural method is via a direct Monte-Carlo algorithm: we can estimate $p^\ell_\sigma[t]$ by sampling independent $\ell$-step paths, each starting from a random state sampled from $\sigma$. A simple concentration argument shows that for a given value\(^1\)

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\(^1\)Bidirectional estimators have been developed before for reversible Markov chains [1]; our method however is not only more general, but conceptually and operationally simpler than these techniques (cf. Section 1.2).
of $\delta$, we need $\Theta(1/\delta)$ samples to get an accurate estimate of $p_s^t$, irrespective of the choice of $t$, and the structure of $P$. Note however that this algorithm is agnostic of the terminal state $t$; moreover, if $|S| = n$, then using $\Theta(\log n/\delta)$ samples results in an accurate estimate for any $t$ such that $p_s^t > \delta$. On the other hand, the problem also admits a natural linear algebraic solution, via the forward or reverse power iterations (by writing Equation (1) as $p_s^t := \sigma(e_s(P^T)^T)^T$. When the state space is large, performing a direct power iteration is infeasible – however, there are localized versions of the power iteration that are still efficient. Such algorithms have been developed, among other applications, for PageRank estimation \cite{4,5} and for heat kernel estimation \cite{6}. Although slow in the worst case (for example, if a state has a very large in/out neighborhood in case of reverse/forward local update respectively), such local update algorithms are often fast in practice, as unlike Monte-Carlo methods they exploit the local structure of the chain. However even in sparse Markov chains and for a large fraction of target states, their running time can be $\Omega(1/\delta)$. For example, consider a random walk on a random $d$-regular graph and let $\delta = o(1/n)$ – then for $\ell \sim \log_d(1/\delta)$, verifying $p_s^\ell > \delta$ is equivalent to uncovering the entire $\log_d(1/\delta)$ neighborhood of $s$. However since a large random $d$-regular graph is (whp) an expander, this neighborhood has $\Omega(1/\delta)$ distinct nodes.

For reversible Markov chains, one can get a bidirectional algorithms for estimating $p_s^\ell$ based on colliding random walks. For example, consider the problem of estimating length-2$\ell$ random walk transition probabilities in a regular undirected graph $G(V,E)$ on $n$ vertices \cite{1,7}. The main idea is that to test if a random walk goes from $s$ to $t$ in $2\ell$ steps with probability $\geq \delta$, we can generate two independent random walks of length $\ell$, starting from $s$ and $t$ respectively, and detect if they terminate at the same intermediate node. Suppose $p_w, q_w$ are the probabilities that a length-$\ell$ walk from $s$ and $t$ respectively terminate at node $w$ – then from the reversibility of the chain, we have that $p_s^\ell[t] = \sum_{w \in V} p_w q_w$; this is also the collision probability. The critical observation is that if we generate $\sqrt{1/\delta}$ walks from $s$ and $t$, then we get $1/\delta$ potential collisions, which is sufficient to detect if $p_s^\ell > \delta$. This argument forms the basis of the birthday-paradox, and similar techniques used in a variety of estimation problems (eg., see \cite{8}). Showing concentration for this estimator is tricky as the samples are not independent; moreover, to control the variance of the samples, the algorithms often need to separately deal with ‘heavy’ intermediate nodes, where $p_w$ or $q_w$ are much larger than $O(1/n)$. Our proposed approach is much simpler both in terms of algorithm and analysis, and more significantly, it extends beyond reversible chains to any general discrete state-space Markov chain.

The most similar approach to ours is the recent FAST-PPR algorithm of Lofgren et al. \cite{2} for PageRank estimation; our algorithm borrows several ideas and techniques from that work. However, the FAST-PPR algorithm relies heavily on the structure of PageRank – in particular, the fact that the PageRank walk has Geometric($\alpha$) length (and hence can be stopped and restarted due to the memoryless property). Our work provides an elegant and powerful generalization of the FAST-PPR algorithm, extending the approach to general Markov chains. Moreover, although \cite{2} presents a theoretical unbiased estimator, it is too complicated to implement in practice (the FAST-PPR algorithm itself is a simpler approximate estimator). In contrast, we give a simple unbiased estimator which is easy to implement, as demonstrated by our experiments.

# 2 The Bidirectional MSTP-estimation Algorithm

Notation: For a Markov chain with finite state-space $S$ and transition probability matrix $P$, we denote $|S| = n$ and denote $m$ to be the number of non-zero elements of $P$; the average number of neighbors of states in $S$ is thus $d = \frac{m}{n}$.

## 2.1 Algorithm

As described in Section 1.1, given a target state $t$, our bidirectional MSTP algorithm keeps track of a pair of vectors – the estimate vector $q_k^t$ and the residual vector $r_k^t$ – for each length $k \in \{0, 1, 2, \ldots, \ell\}$. The vectors are initially all set to $\emptyset$ (i.e., the all-0 vector), except $r_0^t$ which is initialized as $q_2$. Moreover, they are updated using a reverse push operation defined as:
Before formally analyzing the performance of our MSTP-estimation algorithm, we first build some intuition as to why it works. In particular, it is useful to interpret the estimates and residues in probabilistic/combinatorial terms. In Figure 2.2, we have considered a simple Markov chain on three states – Red, Green and Blue (henceforth \((R, G, B)\)). On the right side, we have illustrated an intermediate stage of reverse work using \(R\) as the target, after performing the REVERSE-PUSH operations: Given the Markov chain on the left with \(R\) as the target, we perform REVERSE-PUSH operations \((R, 0), (G, 1), (B, 1), (R, 2)\).
operations \((R, 0), (G, 1), (B, 1)\) and \((R, 2)\) in that order. Each push at level \(i\) uncovers a collection of length-\((i + 1)\) paths terminating at \(R\) – for example, in the figure, we have uncovered all length 2 and 3 paths, and several length 4 paths. The crucial observation is that each uncovered path of length \(i\) starting from a node \(v\) is accounted for in either \(q_t^i\) or \(r_t^i\). In particular, in Figure 2.2, all paths starting at solid nodes are stored in the estimates of the corresponding states, while those starting at blurred nodes are stored in the residue. Now we can use this set of pre-discovered paths to boost the estimate returned by Monte-Carlo trajectories generated starting from the source distribution. The dotted line in the figure represents the current reverse-work frontier – it separates the fully uncovered neighborhood of \((R, 0)\) from the remaining states \((v, i)\).

In a sense, what the REVERSE-PUSH operation does is construct a sequence of importance-sampling weights, which can then be used for Monte-Carlo. An important novelty here is that the importance-sampling weights are: (i) adapted to the target state, and (ii) dynamically adjusted to ensure the Monte Carlo estimates have low variance. Viewed in this light, it is easy to see how the algorithm can be modified to applications beyond basic MSTP-estimation: for example, to non-homogenous Markov chains, or for estimating the probability of hitting a target state \(t\) for the first time in \(\ell\) steps (cf. Section 3). Essentially, we only need an appropriate reverse-push/dynamic programming update for the quantity of interest (with associated invariant, as in Equation (2)).

2.3 Performance Analysis

We first formalize the critical invariant introduced in Equation (2); the proof follows the outline of a similar result in Andersen et al. [5] for PageRank estimation:

**Lemma 1.** Given a terminal state \(t\), suppose we initialize \(q_t^0 = 0, r_t^0 = e_v, \) and \(q_t^k, r_t^k = 0\) \(\forall k \geq 0\). Then for any source distribution \(\sigma\) and length \(\ell\), after any arbitrary sequence of REVERSE-PUSH\((v,k)\) operations, the vectors \(\{ q_t^\ell, r_t^\ell \} \) satisfy the invariant:

\[ p_t^\ell [t] = \langle \sigma, q_t^\ell \rangle + \sum_{k=0}^{\ell} \langle \sigma P^k, r_t^{\ell-k} \rangle \]  

(3)

**Proof.** First, note that Equation (3) can be re-written as \( p_t^\ell [t] = \langle \sigma, q_t^\ell \rangle + \sum_{k=0}^{\ell} r_t^{\ell-k} (P^k)^T \rangle \).

Note that under the initial conditions specified in Algorithm 2, for any \(\sigma, \ell\), the invariant reduces to: \( p_t^\ell [t] = \langle \sigma, q_t^\ell \rangle + \sum_{k=0}^{\ell} r_t^{\ell-k} (P^k)^T \rangle = \langle \sigma, e_v (P^T)^\ell \rangle = \langle \sigma P^\ell, e_v \rangle \), which is true by definition.

We now prove the invariant by induction. Suppose at some stage, vectors \(\{ q_t^\ell, r_t^\ell \}\) satisfy Equation (3); to complete the proof, we need to show that for any pair \((v,i)\), the REVERSE-PUSH\((v,i)\) operation preserves the invariant. Let \((\tilde{q}_t^\ell, \tilde{r}_t^\ell)\) denote the estimate and residual vectors after the REVERSE-PUSH\((v,i)\) operation is applied, and define:

\[ \Delta_v^i = \left( \tilde{q}_t^i - q_t^i \right) + \left( \tilde{r}_t^i - r_t^i \right) = \langle \tilde{r}_t^i, e_v \rangle - \langle r_t^i, e_v \rangle = 0 \]

Now, to prove the invariant, it is sufficient to show \(\Delta_v^i = 0\) for any choice of \((v,i)\). Clearly this is true if \(\ell < i\); this leaves us with two cases:

- If \(\ell = i\) we have: \(\Delta_v^i = \left( \tilde{q}_t^i - q_t^i \right) + \left( \tilde{r}_t^i - r_t^i \right) = \langle \tilde{r}_t^i, e_v \rangle - \langle r_t^i, e_v \rangle = 0\)
- If \(\ell > i\), we have:

\[ \Delta_v^i = \left( \tilde{r}_t^{i+1} - r_t^{i+1} \right) + \left( \tilde{r}_t^i - r_t^i \right) (P^T)^{\ell-i-1} = \left( \tilde{r}_t^i, e_v \right) \langle e_v P^T \rangle - \left( r_t^i, e_v \right) \langle e_v P^T \rangle \left( P^T \right)^{\ell-i-1} = 0 \]

This completes the proof of the lemma.

**Theorem 1.** We are given any Markov chain \(P\), source distribution \(\sigma\), terminal state \(t\), maximum length \(\ell_{\text{max}}\) and also parameters \(\delta, p_f\) and \(\epsilon\) (i.e., the desired threshold, failure probability and relative error). Suppose we choose any reverse threshold \(\delta > \delta\) and number of sample-paths
Forward-work (i.e., for generating trajectories): we generate 

$$n_f = c\delta_r/\delta,$$

where $c = \max \{6e/e^2, 1/\ln 2\} \ln (2\ell_{\max}/p_f)$; then for any length $\ell \leq \ell_{\max}$ with probability at least $1 - p_f$, the estimate returned by Bidirectional-MSTP satisfies:

$$|\hat{p}_\sigma^f[t] - p_\sigma^f[t]| < \max \{\epsilon p_\sigma^f[t], \delta\}.$$

**Proof.** Given any Markov chain $P$ and terminal state $t$, note first that for a given length $\ell \leq \ell_{\max}$, Equation (2) shows that the estimate $\hat{p}_\sigma^f[t]$ is an unbiased estimator. Now, for any random-trajectory $T_k$, we have that the score $S_{t,k}^f$ obeys: (i) $\mathbb{E}[S_{t,k}^f] \leq p_\sigma^f[t]$ and (ii) $S_{t,k}^f \in [0, \ell\delta_r]$; the first inequality again follows from Equation (2), while the second follows from the fact that we executed REVERSE-PUSH operations until all residual values were less than $\delta_r$.

Now consider the random variable $X_k = S_{t,k}^f/(\ell\delta_r)$ and $X = \sum_{k \in [n_f]} X_k$; then we have that $X_k \in [0, 1]$, $\mathbb{E}[X] \leq (n_f/\ell\delta_r)p_\sigma^f[t]$ and also $(X - \mathbb{E}[X]) = (n_f/\ell\delta_r)(\hat{p}_\sigma^f[t] - p_\sigma^f[t])$. Moreover, using standard Chernoff bounds (cf. Theorem 1.1 in [9]), we have that:

$$\mathbb{P}[|X - \mathbb{E}[X]| > \epsilon\mathbb{E}[X]] < 2 \exp \left(-\frac{\epsilon^2\mathbb{E}[X]}{3}\right)$$

and

$$\mathbb{P}[X > b] \leq 2^{-b} \text{ for any } b > 2\epsilon\mathbb{E}[X].$$

Now we consider two cases:

1. $\mathbb{E}[S_{t,k}^f] > \delta/2e$ (i.e., $\mathbb{E}[X] > n_f\delta/2e\ell\delta_r = c/2e$): Here, we can use the first concentration bound to get:

$$\mathbb{P}\left[\left|\hat{p}_\sigma^f[t] - p_\sigma^f[t]\right| \geq \epsilon p_\sigma^f[t]\right] = \mathbb{P}\left[|X - \mathbb{E}[X]| \geq \frac{c n_f}{\ell\delta_r} p_\sigma^f[t]\right] \leq \mathbb{P}\left[|X - \mathbb{E}[X]| \geq \epsilon\mathbb{E}[X]\right]$$

$$\leq 2 \exp \left(-\frac{\epsilon^2\mathbb{E}[X]}{3}\right) \leq 2 \exp \left(-\frac{\epsilon^2c}{6e}\right),$$

where we use that $n_f = c\ell_{\max}\delta_r/\delta$ (cf. Algorithm 2). Moreover, by the union bound, we have:

$$\mathbb{P}\left[\bigcup_{t \leq \ell_{\max}} \left\{\left|\hat{p}_\sigma^f[t] - p_\sigma^f[t]\right| \geq \epsilon p_\sigma^f[t]\right\}\right] \leq 2\ell_{\max} \exp \left(-\frac{\epsilon^2c}{32e}\right),$$

Now as long as $c \geq \left(6e/e^2\right) \ln (2\ell_{\max}/p_f)$, we get the desired failure probability.

2. $\mathbb{E}[S_{t,k}^f] < \delta/2e$ (i.e., $\mathbb{E}[X] < c/2e$): In this case, note first that since $X > 0$, we have that $p_\sigma^f[t] - \hat{p}_\sigma^f[t] = (n_f/\ell\delta_r)\mathbb{E}[X] \leq \delta/2e < \delta$. On the other hand, we also have:

$$\mathbb{P}\left[\hat{p}_\sigma^f[t] - p_\sigma^f[t] \geq \delta\right] = \mathbb{P}\left[X - \mathbb{E}[X] \geq \frac{n_f\delta}{\ell\delta_r}\right] \leq \mathbb{P}[X \geq c] \leq 2^{-c},$$

where the last inequality follows from our second concentration bound, which holds since we have $c > 2e\mathbb{E}[X]$. Now as before, we can use the union bound to show that the failure probability is bounded by $p_f$ as long as $c \geq \log_2 (\ell_{\max}/p_f)$.

Combining the two cases, we see that as long as $c \geq \max \{6e/e^2, 1/\ln 2\} \ln (2\ell_{\max}/p_f)$, then we have

$$\mathbb{P}\left[\bigcup_{t \leq \ell_{\max}} \left\{\left|\hat{p}_\sigma^f[t] - p_\sigma^f[t]\right| \geq \max\{\epsilon, \delta p_\sigma^f[t]\}\right\}\right] \leq p_f.$$

One aspect that is not obvious from the intuition in Section 2.2 or the accuracy analysis is if using a bidirectional method actually improves the running time of MSTP-estimation. This is addressed by the following result, which shows that for typical targets, our algorithm achieves significant speedup:

**Theorem 2.** Given any Markov chain $P$, source distribution $\sigma$, maximum length $\ell_{\max}$ and parameters $\delta, p_f$ and $c$. Suppose we set $\delta_r = \sqrt{\ell_{\max}\log(\ell_{\max}/p_f)}$: then for a uniform random choice of $t \in S$, the Bidirectional-MSTP estimation algorithm has a running time of $\tilde{O}\left(\ell_{\max}^{3/2}\sqrt{\delta/\delta_r}\right)$.

**Proof.** The runtime of Algorithm 2 consists of two parts:

- **Forward-work** (i.e., for generating trajectories): we generate $n_f = c\ell_{\max}\delta_r/\delta$ sample trajectories,
each of length $\ell_{\max}$ – hence the running time is $O\left(c^2\ell_{\max}^2/\delta\right)$ for any Markov chain $P$, source distribution $\sigma$ and target node $t$. Substituting for $c$ from Theorem 1, we get that the forward-work running time $T_f = O\left(\ell_{\max}^2 \log(\ell_{\max}/p_f)\right)$ for any Markov chain $P$, source distribution $\sigma$ and target node $t$. Substituting for $c$ from Theorem 1, we get that the forward-work running time $T_f = O\left(\ell_{\max}^2 \log(\ell_{\max}/p_f)\right)$ for any Markov chain $P$, source distribution $\sigma$ and target node $t$.

Reverse-work (i.e., for REVERSE-PUSH operations): Let $T_r$ denote the reverse-work runtime for a uniform random choice of $t \in S$. Then we have:

$$E[T_r] = \frac{1}{|S|} \sum_{t \in S} \left(\sum_{k=0}^{\ell_{\max}} \sum_{v \in S} (d^l(v) + 1) I\left\{\text{REVERSE-PUSH}(v,k) \text{ is executed}\right\}\right)$$

Now for a given $t \in S$ and $k \in \{0, 1, \ldots, \ell_{\max}\}$, note that the only states $v \in S$ on which we execute REVERSE-PUSH$(v,k)$ are those with residual $r^l_k(v) > \delta_r$ – consequently, for these states, we have that $q^l_k(v) > \delta_r$, and hence, by Equation (3), we have that $p^k_{e_{\sigma}}[t] \geq \delta_r$ (by setting $\sigma = \mathbb{E}_{v}$, i.e., starting from state $v$). Moreover, a REVERSE-PUSH$(v,k)$ operation involves updating the residuals for $d^l(v) + 1$ states. Note that $\sum_{t \in S} p^k_{e_{\sigma}}[t] = 1$ and hence, via a straightforward counting argument, we have that for any $v \in S$, $\sum_{t \in S} I\{p^k_{e_{\sigma}}[t] \geq \delta_r\} \leq 1/\delta_r$. Thus, we have:

$$E[T_r] \leq \frac{1}{|S|} \sum_{t \in S} \left(\sum_{k=0}^{\ell_{\max}} \sum_{v \in S} (d^l(v) + 1) I\left\{p^k_{e_{\sigma}}[t] \geq \delta_r\right\}\right) = \frac{1}{|S|} \sum_{v \in S} \left(\ell_{\max} + 1 \cdot (d^l(v) + 1) \cdot I\left\{p^k_{e_{\sigma}}[t] \geq \delta_r\right\}\right) = O\left(\frac{\ell_{\max}}{\delta_r}\right).$$

Finally, we choose $\delta_r = \frac{c^2\delta}{\ell_{\max} \log(\ell_{\max}/p_f)}$ to balance $T_f$ and $T_r$ and get the result. \hfill \qed

### 3 Applications of MSTP estimation

- **Estimating the Stationary Distribution and Hitting Probabilities:** MSTP-estimation can be used in two ways to estimate stationary probabilities $\pi[t]$. First, if we know the mixing time $\tau_{\text{mix}}$ of the chain $P$, we can directly use Algorithm 2 to approximate $\pi[t]$ by setting $\ell_{\max} = P$ and using any source distribution $\sigma$. Theorem 2 then guarantees that we can estimate a stationary probability of order $\delta$ in time $O(\tau_{\text{mix}}/\delta)$. In comparison, Monte Carlo has $O(\tau_{\text{mix}}/\delta)$ runtime. We note that in practice, we usually do not know the mixing time – in such a setting, our algorithm can be used to compute an estimate of $\pi[t]$ for all values of $\ell \leq \ell_{\max}$.

An alternate method is to modify Algorithm 2 to estimate the probability of hitting $t$ for the first time in $\ell$ steps (i.e., estimate $P[T_t \leq \ell]$). To do this, we modify Algorithm 2 as follows: at each stage $i \in \{1, 2, \ldots, \ell_{\max}\}$ (note: not $i = 0$), instead of REVERSE-PUSH$(t,i)$, we update $q^l_i(t) = q^l_i(t) + r^l_i(t)$, set $r^l_i(t) = 0$ and do not push back $r^l_i(t)$ to the in-neighbors of $t$ in the $(i+1)^{th}$ stage. The remaining algorithm remains the same. Denote the resulting quantity as $p^l_{T_t \leq \ell}$. It is easy to see from the discussion in Section 2.2 that this is an unbiased estimate of $P[T_t \leq \ell | X_0 \sim \sigma]$ – we omit a formal proof due to lack of space.

Now, by setting $\sigma \equiv \mathbb{E}_{v}$, we can get an estimate for the truncated expected return time $E[T_t | T_t \leq \ell_{\max}]$ by computing $\sum_{\ell \leq \ell_{\max}} \ell p^l_{T_t \leq \ell}$ Finally, using that fact that $\pi[t] = 1/E[T_t]$, we get an estimate which for all $\ell_{\max}$ is $\leq \pi[t]$, and moreover converges to $\pi[t]$ as $\ell_{\max} \to \infty$.

- **Exact Stationary Probabilities in Strong Doeblin chains:** A strong Doeblin chain [10] is obtained by mixing a Markov chain $P$ and a distribution $\sigma$ – at each transition, it proceeds according to $P$ with probability $\alpha$, else samples state from $\sigma$. They are widely used in ML applications – special cases include the celebrated PageRank metric [11], variants such as HITS and SALSA [12], and other algorithms for other applications such as ranking [13] and structured prediction [14]. An important property of these chains is that if we sample a starting node $V_0$ from $\sigma$ and sample a trajectory of length $Geometric(\alpha)$ starting from $V_0$, then the terminal node is an unbiased sample from the stationary distribution [15]. There are two ways in which our algorithm can be used for this purpose: one is to replace the REVERSE-PUSH algorithm with a corresponding local update algorithm for the strong Doeblin chain (similar to the one in Andersen et al. [5] for PageRank), and then sample random trajectories of length $Geometric(\alpha)$ A more direct technique is to choose some $\ell_{\max} >> 1/\alpha$, estimate $\{p^l_{\sigma} \forall \ell \in \ell_{\max}\}$ and then directly compute the stationary distribution as $\pi[t] = \sum_{\ell=1}^{\ell_{\max}} \alpha^{\ell-1}(1-\alpha)p^l_{\sigma}[t]$. 

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• **Graph Diffusions:** The second approach proposed above shows that we can use MST-estimation as a subroutine to estimate the $t$th element of any given polynomial of the transition matrix: $f(P,σ)[t] := \sum_{i=0}^{∞} α_i (σ^t P^i)[t]$. For random walks on a (weighted) graph, the such functions called graph diffusions [16], and are used in a variety of applications. The case where $α_i = α^{t-1}(1 - α)$ corresponds to PageRank. If instead the length is drawn according to a Poisson distribution (i.e., $α_k = e^{-α}α^k/k!$), then the resulting function is called the heat kernel $h(G, α)$; this too has several applications, including finding communities (clusters) in large networks [6].

Note that for any function $f$ as defined above, the truncated sum $f_{t_{max}} = \sum_{i=0}^{t_{max}} α_i (p_r^T P^i)$ obeys: $|f - f_{t_{max}}|_{∞} ≤ \sum_{i=t_{max}+1}^{∞} α_i$. Thus a guarantee on an estimate for the truncated sum (as given by our algorithm) directly translates to a guarantee on the estimate for the diffusion.

We perform numerical experiments on heat kernel estimation in the next section.

• **Conductance Testing in Graphs:** MST-estimation is an essential primitive for conductance testing in large Markov chains [1]. In particular, in regular undirected graphs, Kale et al [7] develop a sublinear bidirectional estimator based on counting collisions between walks in order to identify ‘weak’ nodes – those which belong to sets with small conductance. Our algorithm can be used to extend this process to any graph, including weighted and directed graphs.

• **Local Algorithms:** There is significant interest of late on local algorithms – those which perform computations given only a small neighborhood of a source node [17]. In this regard, we note that Algorithm 2 is naturally local (and hence so are the applications mentioned above); given a $k$-hop neighborhood around the source and target, we set $t_{max}$ to $k$. This essentially follows from the fact that Equation (2) holds after any sequence of REVERSE-PUSH operations.

4 Experiments

To demonstrate the efficiency of our algorithm on large Markov chains, we use heat kernel estimation (cf. Section 3) as an example application. The heat kernel is a non-homogenous Markov chain, defined as the probability of stopping at the target on a random walk from the source, where the walk length is sampled from a Poisson($t$) Distribution. It is important in practice as it has empirically been shown to detect communities well.

We use our estimator to compute heat kernels on diverse, real-world graphs that range from millions to billions of edges. For each graph, for random (source, target) pairs, we compute the heat kernel. We set average walk-length $t = 5$, but our qualitative running-time results are not sensitive to the choice of $t$. We set a maximum length of 10 standard deviations above the expectation $t + 10\sqrt{t} ≈ 27$; the probability of a walk being longer than this is $10^{-12}$, so we can ignore that event.

We compare Algorithm 2 to two state of the art algorithms: The natural Monte Carlo algorithm, and the push forward algorithm introduced in [6]. All three have parameters which allow them to trade off speed and accuracy. For a fair comparison, we choose parameters such that the mean relative error of all three algorithms is around 10%, and for those parameters we measure the mean running time of all three algorithms. We implemented all three algorithms in Scala (for the push forward algorithm, our implementation follows the code linked from [6]).

Our results are presented in Figure 4. We find that on these four graphs, our algorithm is 100x faster (per $(s, t)$ pair) than these state-of-the-art algorithms. For example, on the Twitter graph, our algorithm can estimate a heat kernel score is 0.1 seconds, while the state-of-the-art algorithms both take more than 4 minutes. We note though that the state-of-the-art algorithms were designed for community detection, and return scores from the source to all targets, rather than just one target. Our algorithm’s advantage applies in applications where we want the score from a source to a single target or small set of targets.

The Pokec [18], Live Journal [19], and Orkut [19] datasets were downloaded from the Stanford SNAP project [20]. The Twitter-2010 [21] was downloaded from the Laboratory for Web Algorithmics [22]. For reproducibility, the source code of our experiments will be available on our website.

Note that for larger values of $t$, the walk mixes into the stationary distribution, “forgetting” where it started.
Figure 2: Estimating heat kernels: Bidirectional MSTP-estimation vs. Monte-Carlo, Forward Push. Notice that our algorithm is 100 times faster per (source, target) pair than state-of-the-art algorithms.

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