THEORETICAL ANALYSIS OF A STOCHASTIC APPROXIMATION APPROACH FOR COMPUTING QUASI-STATIONARY DISTRIBUTIONS

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Abstract. This paper studies a method, which has been proposed in the Physics literature by [8, 7, 10], for estimating the quasi-stationary distribution. In contrast to existing methods in eigenvector estimation, the method eliminates the need for explicit transition matrix manipulation to extract the principal eigenvector. Our paper analyzes the algorithm by casting it as a stochastic approximation algorithm (Robbins-Monro) [23, 16]. In doing so, we prove its convergence and obtain its rate of convergence. Based on this insight, we also give an example where the rate of convergence is very slow. This problem can be alleviated by using an improved version of the algorithm that is given in this paper. Numerical experiments are described that demonstrate the effectiveness of this improved method.

1. Introduction

The motivation for this algorithm came from physicists’ need to estimate the quasi-stationary distribution of interacting particle systems (IPS) [8, 7, 10, 17]. A quasi-stationary distribution can be computed via the left principal eigenvector of the substochastic transition matrix over the non-absorbing states (transition rate matrix in continuous-time). However, the eigenvalue problem suffers from the curse of dimensionality, and is especially prohibitive in IPS where the state space is very large.

A sampling based method has been proposed by these physicists based on a heuristic manipulation of the Kolmogorov forward equation. The validity of this method actually has been a priori proven by [1, 2, 21] who casted it as a generalized urn process. Results on rates of convergence have been obtained. This result involves a Central Limit Theorem (CLT) for a specific set of functionals corresponding to non-principal eigenvectors of the underlying substochastic matrix.

Our main contribution are as follows

1. Our paper recognizes the algorithm as a stochastic approximation algorithm (Section 4.2).
2. This allows us to prove convergence and sufficient conditions for a stronger CLT (Theorem 3) that is not restricted only to specific functionals.
3. More importantly, we recognized common scenarios (Section 5.1) where the CLT fails and significantly hamper the performance of the algorithm (i.e. very slow rate of convergence).
4. At the end, we came up with an improved algorithm (Section 5.2) which exhibits a valid CLT under all scenarios by using projection and iterate averaging [22].

Section 2 reviews some background material to the contact process, quasi-stationary distributions, mentions a less powerful method of proof via urn processes, and reviews the relevant related literature on eigenvector estimations and points out their shortcomings. Section 3 explains the the basis for the original heuristic and outlines the algorithm. Section 4 goes over the stochastic approximation formulation and sketches the proof of convergence (the full proof is given in the Appendix 8.1). Section 5 gives an improved version of the algorithm using projection along with its faster rate of convergence result. Section 6 briefly studies the algorithm adapted for continuous-time Markov chains. Section 7 goes over several important numerical experiments.
2. Background and Related Literature

2.1. Quasi-Stationary Distribution.

2.1.1. Discrete-Time Version. The paper \cite{5} proposed the concepts of quasi-stationary distribution and quasi-limiting distribution for discrete-time Markov chains. Assume that 0 is the absorbing state and 1, \ldots, n are non-absorbing, we can partition the Markov transition matrix as

\[ P = \begin{bmatrix} 1 & 0 \\ \alpha & Q \end{bmatrix} \]

where \( Q \) is a \( n \)-by-\( n \) matrix.

First we define the conditional transition probabilities

\[ d_\pi^j(n) = \mathbb{P}(X_n = j | X_0 \sim \pi, X_1, \ldots, X_{n-1} \neq 0) = \pi' Q^n e_j / \pi' Q^n e \]

where \( \{e_i\} \) is the standard basis for \( \mathbb{R}^n \), \( \pi \) is a probability distribution, and \( e \) is the vector of all 1’s. \( d_\pi^r(n) \) is the vector whose \( j \)-th component is \( d_\pi^j(n) \). This leads to the following definition.

Definition 1. If there is a distribution \( \pi \) over the transient states such that \( d_\pi^r(n) \) is independent of \( n \), then we call \( d_\pi^r \) the quasi-stationary distribution.

Under the assumption that the substochastic matrix \( Q \) is irreducible (though not necessarily aperiodic), it is straightforward to see that the quasi-stationary distribution exists and is the unique solution to principal eigenvector problem

\[ d' Q = \rho d' \]

This existence and uniqueness (assuming that \( d \) is normalized to be a probability vector) can be obtained by the Perron-Frobenius theorem \cite{?}.

The paper \cite{19} explores the existence of quasi-stationary distribution for countable and general state space Markov chains where \( Q \) is replaced with the generator and \( d \) is a measure.

2.1.2. Continuous-Time. If we think about the transition rate matrix of a CTMC under similar setup (irreducibility), then it \cite{6} can be said that

\[ d_\pi^j(t) \to d_j + o(e^{(\rho' - \rho_1)t}) \]

where \( d \) is the principal left-eigenvector of the rate matrix corresponding to the transient states with associated eigenvalue \( \rho_1 \), i.e.

\[ d' R = \rho_1 d' \]

where \( R \) is the rate matrix of the CTMC.

2.2. Linear Algebra Methods. Classical linear algebra methods such as the power method \cite{13} suffers from the curse of dimensionality. Monte Carlo power methods by \cite{11} can be adapted to produce eigenvectors but requires an explicit computation of the substochastic transition matrix on the fly and is expensive to do for interacting particle systems. There exists a set of stochastic approximation methods for determining principal eigenvalue/eigenvector where the matrix is random; however, it too requires explicit matrix multiplication \cite{15, 14, 20} which is infeasible in interacting particle system case.

Interacting particle systems such as the contact process (Section 7.3) suffers heavily from the curse of dimensionality and renders existing classical methods infeasible. This is an important class of problems for physicists \cite{10, 8, 13, 17} in the study of phase-transition property of certain non-equilibrium systems.
Lastly, a large number of adaptive algorithms has been designed for estimating principal eigenvector of only covariance matrices (positive semi-definite) where you observe an i.i.d. sequence of random vectors with that particular covariance matrix [4].

2.3. Fleming-Viot method. The Fleming-Viot method [19, 12, 3] is an interacting particle system that allows us to compute quasi-stationary distributions of countable Markov chains and diffusion processes. It consists of $N$ particles evolving independently according to the dynamics of the Markov process. If one particle gets absorbed, it is immediately restarted from a position uniformly picked from the remaining $N-1$ particles. As both time and $N$ goes to infinity, this would converge to the quasi-stationary distribution. When the state space is large, you need $N$ to be large enough to have a good approximation to the true quasi-stationary distribution. This would be prohibitive in interacting particle systems. Furthermore, it is generally computationally expensive to increase both the number of particles $N$ and the time of the simulation.

2.4. Urn Processes. The algorithm which will be described below has been previously analyzed as a generalized Polya’s urn [2, 1]. The overview paper [21] is a comprehensive survey of urn processes. However, the rate of convergence results of these urn processes are not as strong as our result. They only offer a CLT along the non-principal right eigenvectors of the rate matrix whereas we offer a CLT along every direction in the space. The set of non-principal right eigenvectors can never span the whole space (which in this case can be taken to be the hyperplane orthogonal to $1$) because the principal left eigenvector $\bar{\mu}$ is orthogonal to all the non-principal right eigenvectors. Unless if $\bar{\mu}$ is a multiple of $1$, we may only examine the CLT along the space orthogonal to $\bar{\mu}$ as opposed to the whole hyperplane that is orthogonal to $1$. In summary, our results are a strict extension of the available corresponding results on urn processes. However, more importantly, our approach is fundamentally different and builds on the well-studied machinery of stochastic approximations and therefore allows us to obtain significant algorithmic improvements that we shall explain (Theorems 4 and 5) and experimentally demonstrate (Section 7).

3. Heuristic Motivation

3.1. Motivation from the Physics Literature. This section reviews the heuristic origin of the algorithm from the physics literature [10, 8, 7]. Under the setting of a continuous-time Markov chain with rate matrix $R$ and absorbing state $0$ (without loss of generality, we can combine all absorbing states into one state), if we define $p_{ij}(t) = P(X_t = j | X_0 = i)$ and $P_{i0}(t) = 1 - p_{i0}(t)$, then we have that the quasi-stationary distribution $d_j = \lim_{t \to \infty} \frac{p_{ij}(t)}{P_{i0}(t)}$. If we apply the Kolmogorov forward equation (known to physicists as the master equation), we get that

\[
\frac{dp_{ij}(t)}{dt} = \sum_k p_{ik}(t) R_{kj}
\]

and

\[
\frac{dP_{i0}(t)}{dt} = \frac{d}{dt}(1 - p_{i0}(t)) = -\sum_k p_{ik}(t) R_{k0}.
\]
Intuitively by the definition of \( d_j \), we have that \( p_{ij}(t) \approx d_j P_{is}(t) \) in the quasi-stationary time window \( t \) large enough. So we can apply this to the preceding two equations and get

\[
d_j \left( \frac{dP_{is}(t)}{dt} \right) = \sum_k d_k P_{is}(t) R_{kj} \\
\frac{dP_{is}(t)}{dt} = -\sum_k d_k P_{is}(t) R_{k0}.
\]

Combine the two and we get

\[
d_j \left( \sum_k d_k R_{k0} \right) + \sum_k d_k R_{kj} = 0.
\]

This gives us a non-linear equation for the equilibrium condition for the quasi-stationary distribution \( d \). We can think of this as the stationary point of the forward equation

\[
\frac{d(d_j)}{dt} = \sum_k d_k R_{kj} + d_j \left( \sum_k d_k R_{k0} \right).
\]

The first part of this equation is the standard Kolmogorov forward equation, while the second part redeposits the probability of hitting the absorbing states onto all the non-absorbing states according to the current distribution \( d_j \).

This previous discussion suggests the following algorithm:

**Algorithm 1** Algorithm for estimating quasi-stationary distribution

1. Initialize a vector \( \mu = 0 \) with dimension equal to the number of non-absorbing states in the Markov chain. (Each component represents the total number of visits to the corresponding non-absorbing state.)
2. Select any non-absorbing state of the chain, say state \( i \) and let \( X_0 = i \)
3. Simulate the Markov chain starting from state \( X_0 \) up until absorption and update \( \mu \) by adding the number of visits to each state until absorption (so, for example, the number of visits to \( i \) is at least one).
4. Select a non-absorbing state according to the normalized vector \( \mu \) (so that it becomes a probability vector). Let such non-absorbing state be \( X_0 \) and go to Step 3.
5. Repeat Steps 3 and 4 many times and output the normalized vector \( \mu \) as your approximation of the quasi-stationary distribution. You can also output the averaged time to absorption in each tour as an approximation to \( \frac{1}{1-\lambda} \) where \( \lambda \) is the principal eigenvalue of the transition (rate) matrix.

For large enough time, the dynamics of the Markov chain will be governed by Equation (3), which means we can obtain the quasi-stationary distribution by examining the empirical distribution after some large enough time.

4. **Stochastic Approximation Analysis of the Algorithm**

In this section, we will cast Algorithm [1] into a stochastic approximation algorithm. This will let us rigorously prove convergence and CLT for the algorithm.
4.1. Brief Review of Stochastic Approximation and Intuition. Consider the root-finding task of finding $\theta$ such that $f(\theta) = 0$ with the restriction that only access to “noisy” observations of $f(\theta)$, denoted by $F(\theta)$, are available. If $f$ is suitably smooth and the root is simple enough, we can consider the descent method given by

$$\theta_{n+1} = \theta_n + \epsilon_n F(\theta_n)$$

where $\epsilon_n$ is a positive sequence going to zero.

We need to rigorously define the type of noise on the function $F$. There are several conditions on noise which, when imposed, will lead to convergence guarantees on $\{\theta_n\}$. Here we focus on the simplest martingale difference noise type. Let the n-th observation be denoted by $W_n$, which could theoretically depend on the whole history $F_n = \sigma(\theta_k, W_{k-1} | 1 \leq k \leq n)$. In that case the descent method is written as

$$\theta_{n+1} = \theta_n + \epsilon_n W_n$$

The martingale difference noise requires that there exists a $g$ that satisfies

$$\mathbb{E}[W_n | F_n] = g(\theta_n).$$

If we impose the step-size condition $\sum \epsilon_n^2 < \infty$ then $\theta_n \approx \theta_0 + \sum_{k=1}^{n-1} \epsilon_k W_k$. The variance of the last sum is a finite number. Thus if we rewrite the recursion as $\theta_{n+1} - \theta_n = W_n$ and impose the condition $\epsilon_n \downarrow 0$, heuristically we predict that $\theta_n$ should be related to the stationary points of the ODE

$$\dot{\theta}(t) = g(\theta(t)).$$

Furthermore, if we impose $\sum \epsilon_n = \infty$, we know that in some sense, $\theta_n$ would move by $\sum \epsilon_n = \infty$ steps and should converge to the stable attractors (either orbits or points) of this ODE ([16] Theorem 5.2.1).

4.2. Precise Description of the Algorithm. We will now write down a precise description of the above heuristic Algorithm [1] and convert it into stochastic approximation form.

Notation

- $S$ is the state space of the Markov chain whose quasi-stationary distribution we are trying to estimate.
- $T \subseteq S$ is the set of transient states of the Markov chain.
- $Q$ is the substochastic matrix over the transient states $T$.
- $\mu_n$ will be a sequence of probability vectors over the transient states $T$. This vector will store the cumulative empirical distribution up to, and including, the n-th iteration of the algorithm. $\mu_n(x)$ is its value at a particular transient state $x$.
- $\{X_k^{(n)}\}_k$ will be the Markov chain used in the n-th iteration of the algorithm. They’re independent conditioned on the initial distribution. The n-th Markov chain will have initial distribution $\mu_n$.
- $\tau^{(n)} = \min\{k \geq 0 | X_k^{(n)} \notin T\}$. The hitting time of the absorbing state of the n-th iteration.

We can write Algorithm [1] as a recursion

$$\mu_{n+1}(x) = \frac{\left(\sum_{k=0}^{n} \tau^{(k)}\right) \mu_n(x) + \left(\sum_{k=0}^{\tau^{(n+1)}-1} \mathbb{I}(X_k^{(n+1)} = x | X_0^{(n+1)} \sim \mu_n)\right)}{\sum_{k=0}^{\tau^{(n+1)}} \tau^{(k)}} \quad \forall x \in T$$

where we can take the first probability vector $\mu_0$ arbitrarily.

We will transform $\mu_n$ into stochastic approximation form by re-factoring:

$$\mu_{n+1}(x) = \mu_n(x) + \left(\frac{1}{n+1}\right) \left(\sum_{l=0}^{\tau^{(n+1)}-1} \frac{\mathbb{I}(X_l^{(n+1)} = x) - \mu_n(x)}{\frac{1}{n+1} \sum_{j=0}^{\tau^{(n+1)}} \tau^{(j)}}\right).$$
The denominator is problematic because its conditional expectation (on $\mathcal{F}_n$) is not only a function of $\mu_n$ but depends on the whole history of $\mu_n$. To solve this, we artificially add another state $T_n$ in the following way.

$$
\begin{aligned}
T_{n+1} &= T_n + \frac{1}{n+2}(\tau(n+1) - T_n) \quad \text{equivalent to} \quad T_n = \frac{1}{n+1} \sum_{j=0}^{n} \tau(j) \\
\mu_{n+1}(x) &= \mu_n(x) + \\
&\left( \frac{1}{n+1} \right) \left( \frac{\sum_{i=0}^{(n+1)-1} (I(X_i^{(n+1)} = x|X_0^{(n+1)} \sim \mu_n) - \mu_n(x))}{T_n + \frac{\tau(n+1)}{n+1}} \right).
\end{aligned}
$$

We can therefore define

$$Y_n(\mu, T)(x) \triangleq \frac{\sum_{l=0}^{T-1} (I(X_l = x|X_0 \sim \mu) - \mu(x))}{T + \frac{\tau}{n+1}}$$

and rewrite the stochastic approximation recursion as

$$
\begin{aligned}
\mu_{n+1}(x) &= \mu_n(x) + \left( \frac{1}{n+1} \right) Y_n(\mu_n, T_n)(x) \\
T_{n+1} &= T_n + \left( \frac{1}{n+2} \right) Z(\mu_n, T_n).
\end{aligned}
$$

Remark 2. Note:

- The term $Y_n$ has an explicit dependence on $n$. That is fine as that portion is asymptotically negligible. The details are in the Appendix 8.1.
- Please note that the iterates $\mu_n$ are constrained in $H \triangleq \{ x \in \mathbb{R}^n_+ | \sum x_i = 1 \}$ (check by inner producting with 1). This way we automatically satisfy the boundedness requirement in [10].
- We can also define a similar algorithm for the continuous-time Markov chain by keeping track of the amount of time a Markov chain spends in each transient state. This is given in Section 6.

4.3. Convergence. The main result in this section can now be stated.

**Theorem 3.** Given an irreducible absorbing Markov chain over a finite state space $S$, let

(1) The matrix $Q$ denote the transition probabilities over the non-absorbing states
(2) Let $\mu_0$ be an arbitrary probability vector over the non-absorbing states
(3) Let $T_0 \geq 1$.

Then there exists a unique quasi-stationary distribution $\mu$ satisfying the equations

$$
\begin{aligned}
\mu' Q &= \lambda \mu' \\
\mu' 1 &= 1 \\
\mu &\geq 0
\end{aligned}
$$

and Algorithm 1 converges to the point $(\mu, \frac{1}{\lambda})$ with probability 1.

Furthermore, if $\lambda_{PV}$ is the principal eigenvalue of $Q$ and $\lambda_{NPV}$ are the other eigenvalues and they satisfy

$$
\Re \left( \frac{1}{1 - \lambda_{NPV}} \right) < \frac{1}{2} \left( \frac{1}{1 - \lambda_{PV}} \right) \quad \forall \lambda_{NPV} \text{ non-principal eigenvalues},
$$

Then

$$\sqrt{n}(\mu_n - \mu) \to^d N(0, V)$$

for some covariance matrix $V$. 

Proof. The full proof in the Appendix 8.1 but we outline the main idea here. The technique uses the ODE method ([16] Theorem 5.2.1) where we are required to examine the asymptotic behavior of the coupled dynamical system below. Here we neglect the asymptotically negligible dependence on $n$ in order to illustrate the main idea. The dynamical system of interest is

$$\dot{\mu}(t) = \mathbb{E}_{\mu(t), T(t)} \left[ \sum_{l=0}^{\tau-1} \left( \mathbb{I}(X_l = \cdot|X_0) - \tau \mu(t) \right) T(t) \right]$$

$$\dot{T}(t) = \mathbb{E}_{\mu(t)} [\tau] - T(t)$$

where $\mu(t) \in \mathbb{R}^m$ and $T(t) \in \mathbb{R}^+$. ($m$ is the number of non-absorbing states of the Markov chain)

Again in the Appendix 8.1 we are able to show that for a given initial position in the probability simplex, the solution to the above dynamical system exists and converges to its stationary point which is the unique point that satisfies

$$\mu'Q = \rho \mu'$$

$$\sum_i \mu_i = 1$$

$$\mu_i \geq 0$$

and $\rho = 1 - \frac{1}{\mathbb{E}_{\mu}(\tau)}$.

By Theorem 5.2.1 from [16], we can conclude that $\mu_n$ converges to the quasi-stationary distribution for all initial configurations $(\mu_0, T_0)$.

Equation (4) can be analyzed for its rate of convergence. Here we invoke the Theorem 10.2.1 of [16]. Because our algorithm uses a step size of $O\left(\frac{1}{n}\right)$, we eventually conclude that a CLT exists as long as the Jacobian matrix of the ODE vector field has spectral radius less than $-\frac{1}{2}$. This is equivalent to requiring that

$$\text{Re} \left( \frac{1}{1 - \lambda_{N^P}} \right) < \frac{1}{2} \left( \frac{1}{1 - \lambda_{PV}} \right) \forall \lambda_{N^P} \text{ non-principal eigenvalues}$$

where the $\lambda$’s are the eigenvalues of the $Q$ matrix. □

5. Variations on the Existing Algorithm with Improved Rate of Convergence

One interesting question to ask is what happens when the sufficient conditions for CLT are not met. We will study a simple example consisting of two states.

5.1. Counter Example to CLT. Imagine we have a Markov chain with three states $\{0, 1, 2\}$ and transition matrix

$$\begin{bmatrix}
1 & 0 & 0 \\
\epsilon & \frac{1-\epsilon}{2} & \frac{1-\epsilon}{2} \\
\epsilon & \frac{1-\epsilon}{2} & \frac{1-\epsilon}{2}
\end{bmatrix}.$$ 

Obviously the state $\{0\}$ is the absorbing state. In this setup, because of symmetry, our Algorithm 1 reduces to

(1) With probability $\frac{1-\epsilon}{2}$ sample either the state 1 or 2 (without knowing the previous state. This is OK by symmetry) and add to the empirical distribution.
(2) With probability $\epsilon$, sample from either 1 or 2 according to the empirical distribution up until this point.

We recognize this as a self-interacting Markov chain.

A self-interacting Markov chain (SIMC) \cite{9} is a stochastic process $\{X_n\}$ such that

$$
P(X_{n+1} \in dx | F_n) = \Phi(S_n)(dx)
$$

where $\Phi$ is a function that transforms one measure into another measure and $S_n$ is the empirical measure generated by $\{X_k\}_{k=0}^n$.

Our Algorithm \ref{alg:1} for the above "loopy Markov chain" reduces to the empirical process of a SIMC $X_n$ governed by the functional

$$
P(X_{n+1} = dz | F_n) = \int K(x,dz)dS_n(dx)
$$

where the kernel is given by

$$
K(x,dz) = \epsilon \delta_x(dz) + \left( 1 - \frac{\epsilon}{2} \right) [\delta_1(dz) + \delta_2(dz)]
$$

The sufficient condition for CLT (Equation \ref{eq:6}) in this case translates to requiring $\epsilon < 0.5$.

When the CLT is violated however, \cite{9} states that over a very general class of bounded and measurable functions $f$

$$
E[(S_n(f) - \bar{S}_n(f))^2] = \Theta \left( \frac{1}{n^{2(1-\epsilon)}} \right)
$$

where $S_n(f) = \int f(x)dS_n(x)$, $\bar{S}_n(f) = E[S_n(f)]$. Although this doesn’t technically contradict with the existence of a $\sqrt{n}$-CLT, it does suggest that the scaling sequence is $n^{1-\epsilon}$ instead of $\sqrt{n}$.

In the numerical experiment (Section \ref{sec:7}), we simulate this example and demonstrate the slow rate of convergence when $\epsilon < 0.5$.

5.2. Projection Algorithm and Polyak-Ruppert Averaging.

**Doeblinization and the need for strong CLT.** The expected time to absorption $E[\tau]$ is $\frac{1}{\lambda^2}$ where $\lambda$ is the principle eigenvalue of the substochastic matrix $Q$. If $E[\tau]$ is large, then the iterations of the algorithm will take prohibitively long. One trick that can be used is to "Doeblinize" the chain.

If we multiply $Q$ by a constant $\alpha < 1$, this does not change the eigenvector but shrinks the all the eigenvalues by the same proportion. That means we can force the iterations to jump to absorption very quickly. However, because of the non-linearity of $\frac{1}{\lambda^2}$ and its presence in the sufficient condition of the CLT (Equation \ref{eq:6}), the CLT condition will fail to hold if $\alpha$ is too small. We need a technique where CLT can always be guaranteed regardless of the eigenvalues of the matrix $Q$.

Remark: in continuous-time, we can subtract $\alpha I$ matrix from the transition rate matrix to achieve Doeblinization.

**Projection algorithm.** By putting our algorithm into the stochastic approximations framework, we can modify the algorithm into the projection-variant.

$$
\mu_{n+1} = \Theta_H \left[ \mu_n + \epsilon_n \left( \sum_{k=0}^{\tau(n+1)-1} \|X_k^{(n+1)} = \cdot | X_0^{(n+1)} \sim \mu_n \rangle - \mu_n \right) \right]
$$

where the $\Theta_H$ denotes a $L_2$-projection into the probability simplex. Of course we still require $\sum \epsilon_n = \infty$ and $\sum \epsilon_n^2 < \infty$. Notice that in practice, we only need to perform very few number of projections. The expression
inside the projection operator always sum to one. So projection is only needed if any component inside $\Theta$ becomes negative. Breaking it down allows us to gain insight into when it becomes negative

$$\mu_n(1 - \epsilon_n \tau^{(n+1)}) + \epsilon_n \left( \sum I(\ldots) \right).$$

This can only be negative if $\tau > \frac{1}{\epsilon_n}$. But $\epsilon_n \downarrow 0$ means this won’t happen very often. The advantage of this version is that we are free to use slower step sizes that weakens the condition required for CLT to hold.

Specifically, when $\epsilon_n = \Theta\left(\frac{1}{n^\alpha}\right)$ for $\alpha < 0.5$, a $\frac{1}{\sqrt{n}}$-CLT always hold.

**Theorem 4.** Given an irreducible absorbing Markov chain over a finite state space $S$, let

1. The matrix $Q$ denote the transition probabilities over the non-absorbing states
2. Let $\mu_0$ (the initial $\mu$) be a probability vector over the non-absorbing states
3. Let $T_0 \geq 1$.

Then there exists a unique quasi-stationary distribution $\mu$ satisfying the equations

$$\mu^T Q = \lambda \mu,'$$
$$\mu^T 1 = 1$$
$$\mu \geq 0$$

and the projection algorithm (Equation [7]) converges to the point $\mu$ with probability 1.

If step sizes are such that $\epsilon_n = \Theta\left(\frac{1}{n}\right)$ and if $\lambda_{PV}$ is the principal eigenvalue of $Q$ and $\lambda_{NPV}$ are the other eigenvalues and they satisfy

$$\text{Re} \left( \frac{1}{1 - \lambda_{NPV}} \right) < \frac{1}{2} \left( \frac{1}{1 - \lambda_{PV}} \right) \quad \forall \lambda_{NPV} \text{ non-principal eigenvalues.}$$

Furthermore, we can conclude

$$\sqrt{n}(\mu_n - \mu) \rightarrow^d N(0, V)$$

for some covariance matrix $V$.

In the case that the step sizes are such that $\epsilon_n = \Theta\left(\frac{1}{n^\alpha}\right)$ for $0.5 < \alpha < 1$, we can conclude that (regardless of the eigenvalues of $Q$)

$$\sqrt{n^\alpha}(\mu_n - \mu) \rightarrow^d N(0, V)$$

for some covariance matrix $V$.

**Proof.** The proof for the case of step size $\epsilon_n = \Theta\left(\frac{1}{n}\right)$ is almost identical to what’s given in Section 8.1 after omitting the extra dimension $T_n$. In the case of $\epsilon_n = \Theta\left(\frac{1}{n^\alpha}\right)$ for $\alpha < 0.5$, under the notation of Theorem 21 we need to ensure that $J$ is Hurwitz as opposed to the stronger condition that $J + \frac{1}{2}$ is Hurwitz. This is equivalent to the condition that, (again under the notation of Theorem 21)

$$\text{Re}(\lambda_{R}) < \beta$$

which is trivially always true by the Perron-Frobenius theorem [7]. Hence we can conclude that

$$\sqrt{n^\alpha}(\mu_n - \mu) \rightarrow^d N(0, V)$$

by invoking Theorem 10.2.1 of [10]. \(\Box\)
Polyak-Ruppert Averaging. The Polyak-Ruppert averaging technique [22], (Theorem 11.1.1 in [16] can be applied to the projection algorithm to ensure that $\sqrt{n}$-CLT always holds as long as we pick the step sequence to be $\epsilon_n = \Theta\left( \frac{1}{n^\alpha} \right)$ for $\alpha < 0.5$.

Theorem 5. Given an irreducible absorbing Markov chain over a finite state space $S$, let

1. The matrix $Q$ denote the transition probabilities over the non-absorbing states
2. Let $\mu_0$ (the initial $\mu$) be a probability vector over the non-absorbing states
3. Let $T_0 \geq 1$.

Then there exists a unique quasi-stationary distribution $\mu$ satisfying the equations

$$
\mu'Q = \lambda \mu',
\mu'1 = 1,
\mu \geq 0
$$

and the step sizes satisfy $\epsilon_n = \Theta\left( \frac{1}{n^\alpha} \right)$ for $\alpha < 0.5$. We can conclude that the averaged sequence

$$
\nu_n = \frac{1}{n} \sum_{k=1}^{n} \mu_k
$$

converges to the point $\mu$ with probability 1.

Furthermore, a strong CLT always hold

$$
\sqrt{n}(\nu_n - \mu) \to^d N(0, V)
$$

for some covariance matrix $V$.

6. Algorithm for Continuous-Time Markov Chains

6.1. Formulation and Convergence. So far, the exposition has assumed that the Markov chain of interest is a discrete-time process. It is straightforward to adapt our method for continuous-time processes (such as the contact process). If we denote the transition rate matrix of the CTMC in the following block form

$$
T = \begin{bmatrix} 0 & 0 \\ N & Q \end{bmatrix}
$$

then we can write the algorithm as

$$
\mu_{n+1}(x) = \mu_n(x) + \frac{1}{n+1} \int_0^{\tau_{n+1}} \left( \mathbb{I}(X^{n+1}(s) = x|X_0^{n+1} \sim \mu_n) \right) \frac{ds - \tau^{n+1} \mu_n(x)}{\int_0^{\tau_{n+1}} \tau^{l} \sum_{l=0}^{n+1}}

T_{n+1} = T_n + \frac{1}{n+2} (\tau^{n+1} - T_n).

By a similar approach as the discrete-time case, we deduce the related dynamical system

$$
\left\{ \begin{array}{l}
\dot{\mu}(t) = -\frac{1}{T(t)} \left( \mu(t)' Q^{-1} - (\mu(t)' Q^{-1} 1) \mu(t) \right) \\
\dot{T}(t) = -\mu(t)' Q^{-1} 1 - T(t).
\end{array} \right.
$$
It is straightforward to adapt the Perron-Frobenius theorem to transition rate matrices such as $Q$ by decomposing $Q = A - bI$ where $A$ is an irreducible matrix. We know the existence of a principal eigenvector of positive entries $\bar{\mu}$ (with eigenvalue smaller than 0) such that

$$\bar{\mu}' Q = \bar{\lambda} \bar{\mu}' .$$

The rest of the proof is very similar to the discrete-time case. The only trick is to show that $\exp(-Q^{-1})$ is a matrix of non-negative entries. That is included in the Lemma [25]. We summarize it in theorem form

**Theorem 6.** Given an irreducible absorbing Markov chain over a finite state space $S$, let

1. The matrix $Q$ denote the transition rates over the non-absorbing states
2. Let $\mu_0$ (the initial $\mu$) be a probability vector over the non-absorbing states
3. Let $T_0 \geq 1$.

Then there exists a unique quasi-stationary distribution $\mu$ satisfying the equations

$$\mu' Q = \lambda \mu' ,$$

$$\mu' 1 = 1 ,$$

$$\mu \geq 0 ,$$

and the continuous-time algorithm (Equation 8) converges to the point $(\mu, -1/\lambda)$ with probability 1.

**6.2. Rate of Convergence.** In the notation of the definition of Equation 9, the Jacobian of the dynamical system is given by

$$\nabla_\mu \bar{f} = -\frac{1}{T} \left( Q^{-1} - Q^{-1} \mu' - (\mu' Q^{-1}) I \right) ,$$

$$\nabla_{\bar{T}} \bar{f} = \frac{1}{T^2} \left( \mu' Q^{-1} - (\mu' Q^{-1}) \mu' \right) ,$$

$$\nabla_\mu \bar{h} = -Q^{-1} 1 ,$$

$$\nabla_{\bar{T}} \bar{h} = -1 .$$

When evaluated at the stationary point $(\bar{\mu}, \bar{T})$, we get the matrix

$$\begin{bmatrix}
-\bar{\lambda} \left( Q^{-1} - Q^{-1} \mu' - \frac{1}{\bar{T}} I \right) & -Q^{-1} 1 \\
0 & -1
\end{bmatrix} .$$

Using similar techniques as the discrete-time case (given in Appendix 8.1), we conclude that if $\lambda_{NPV}$ is any non-principal eigenvalue of $Q$, then the sufficient condition for CLT becomes

$$2\lambda_{PV} > Re(\lambda_{NPV}) .$$

**Theorem 7.** For the continuous-time algorithm (Equation 8), if $\lambda_{PV}$ is the principal eigenvalue of $Q$ and $\lambda_{NPV}$ are the other eigenvalues and they satisfy

$$2\lambda_{PV} > Re(\lambda_{NPV}) .$$

Furthermore, we can conclude

$$\sqrt{n}(\mu_n - \mu) \to^d N(0, V)$$

for some covariance matrix $V$.

We can easily convert Equation 8 to the projected version and similar theorems regarding projection and Polyak-averaging (Theorems 4 and 5) hold.
6.3. **Uniformization.** Because these CTMC have finite state space, we can form the associated uniformized Markov chain. Let $Q$ be the transition rate matrix of the non-absorbing states and let $\nu = \max_i (-q_{ii})$, we can form a discrete-time transition matrix

$$\tilde{Q} = I + \frac{1}{\nu} Q.$$ 

It is straightforward to verify that any principal left-eigenvector to $Q$ is also a principal left-eigenvector to $\tilde{Q}$. Hence we apply the discrete-time algorithm to this DTMC.

7. **Numerical Experiments**

7.1. **Loopy Markov Chain.** Let’s consider the loopy Markov chain given by the full transition probability matrix

$$
\begin{pmatrix}
1 & 0 & 0 \\
\epsilon & \frac{1}{1-\epsilon} & \frac{1-\epsilon}{1-\epsilon} \\
\epsilon & \frac{1}{1-\epsilon} & \frac{1-\epsilon}{1-\epsilon}
\end{pmatrix}.
$$

The eigenvalues of the sub-stochastic matrix are $1 - \epsilon$ and 0. Hence the sufficient condition for CLT to hold is to require $\epsilon < 0.5$. We tested the original algorithm and the Polyak averaging algorithm for the case of $\epsilon = 0.98$, well outside of the CLT sufficient condition. The result can be seen in Figure 1 where the improved Polyak averaging algorithm significantly outperforms the vanilla algorithm.

7.2. **M/M/1 queue with finite capacity and absorption.** We also simulated a M/M/1 queue where the system has a queue capacity as well as an absorbing state when the system is empty. A discrete-time Markov chain is created when we considered the arrival times of new customers. The system we have simulated has a capacity of 100 with $\rho = 1.25$. The expected time to absorption $E(\tau)$ is very large so we Doeblinized the Markov chain by multiplying the probability matrix by 0.95. The Doeblinized Markov chain no longer satisfies the CLT. You can see in Figure 2 that the Polyak averaging algorithm significantly outperforms the vanilla algorithm.

7.3. **Contact Process on Complete graph.** We now introduce the contact process. It’s a class of models that fall within the interacting particle systems framework whose quasi-stationary distribution are important to physicists [10, 8, 18, 7].

**Definition 8.** A contact process is a continuous-time Markov chain (CTMC) $(X^1_t,...,X^n_t) \in \{0,1\}^n$, where $t \geq 0$ is the time, with an associated connected graph $(V,E)$ such that

- $|V| = n$.
- Individual nodes transition from 1 to 0 at an exponential rate of 1.
- Individual nodes transition from 0 to 1 at rate $\lambda r$ where $r$ is the fraction of neighbors that are in state 1.

This CTMC has $2^n$ states. The state $(0,0,\ldots,0)$ is an absorbing state and the remaining states are all transient.

This CTMC will eventually reach the absorbing state but physicists are interested in the “pseudo-equilibrium” behavior in the period before absorption happens [10, 8, 18, 7]. In another words, we need an algorithm for estimating the quasi-stationary distribution of this process. The difficulty is that the state space is exponential in size save for a few special cases.

Here we simulate the contact process on a complete graph. If the infection rate is changed to 1.5, then each iteration of the algorithm would take an extreme long time. We applied the version of the algorithm designed for continuous-time Markov chains and Doeblinized the Markov chain by subtracting 0.5$I$ from the transition rate matrix. The eigenvalue condition fails resulting in a slow rate of convergence for the vanilla algorithm. The Polyak’s averaging algorithm significantly outperforms the vanilla algorithm. See Figure 3.
8. Discussion and Conclusion

In summary, we have improved upon the algorithm of [7] by recognizing it as a stochastic approximation algorithm as opposed to an urn process. In doing so, we were able to prove its law of large number and CLT. The result is stronger than the results given in the urn process literature[2]. Furthermore, we provided a counterexample that strongly suggests that the sufficient eigenvalues condition for the CLT is also necessary and fails in many common applications. An improved algorithm that uses projection and iterate averaging significantly improves rate of convergence.

We have tested our algorithm on countable state space processes such as the M/M/1/∞ queue with success. Proving the convergence of this algorithm in this countable state space setting is currently an open problem. We're also working on a version of the algorithm for estimating the quasi-stationary distribution of diffusion processes using stochastic approximation.

Another open issue is how to pick the best Doeblinization constant. When $E[\tau]$ is large you’re more likely to satisfy the condition for the CLT but that’s when run-time of the algorithm increases proportionally. There must be a balance between the run-time of each tour and the rate of convergence of $\mu_n$. It is also not clear what the optimal step size should be for the projected algorithm.

Finally, it would be very interesting to investigate the connection between the phase transition critical point of contact processes and its CLT critical point. Unfortunately, preliminary work seems to suggest that those two are unconnected.

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Proof of Main Results

8.1. Proof of Discrete-Time Theorem [3]. We first restate a series of assumptions & notations that is used by Theorem 5.2.1 from [16] which we will invoke. Again the form of the recursion is $\theta_{n+1} = \theta_n + \epsilon_n W_n$ where $W_n$ is a martingale difference sequence with respect to the filtration $\mathcal{F}_n$ that at least contains $\sigma(\theta_i, W_{i-1}, i \leq n)$. Recall that for us, $W_n$ consists of the two components $W_n$ (the probability vector) and $Z_n$ (and added time dimension) defined in Equation 5 and $\theta_n$ consists of $\mu_n$ and $T_n$.

(1) $\epsilon_n \downarrow 0$, $\sum \epsilon_n = \infty$, $\sum \epsilon_n^2 < \infty$. This is trivially satisfied for our $\epsilon_n = \frac{1}{n}$.

(2) The observed responses have to have uniformly bounded variance: $\sup_n E|W_n|^2 < \infty$. See Lemma 10.

(3) (A local-averaging condition) Let $g_n(\mu, T) = E[W_n | \mathcal{F}_n]$. The functions $g_n(\mu, T)$ need to be continuous uniformly in $n$, and there needs to exist a continuous function $\bar{g}(\mu, T)$ such that for each $(\mu, T)$

$$\lim_{n \to \infty} \left| \sum_{i=n}^{m(t_n+t)} \epsilon_i [g_i(\mu, T) - \bar{g}(\mu, T)] \right| \to 0$$

for each $t > 0$. For the proof see Lemma 9.

Under these assumptions, Theorem 5.2.1 of [16] tells us that if the ODE $\frac{d}{dt}(\mu(t), T(t)) = \bar{g}(\mu(t), T(t))$ has an attractor (asymptotically stable point) with domain $A$ and the sequence $(\mu_n, T_n)$ visits a compact subset within the domain infinitely often with probability 1, then $(\mu_n, T_n)$ converges to the attractor with probability 1.
In our situation, it turns out that the entirely probability simplex is the domain for an attractor situated at the quasi-stationary vector. We will first compute the functions $g_n$ and verify condition 3, then the uniformly bounded variance condition 2, and finally the asymptotic behavior of the associated ODE.

8.1.1. Local-averaging of the gradient field.

Lemma 9. Given the gradient field $\bar{g} = \left( \begin{array}{c} \bar{f} \\ \bar{h} \end{array} \right)$ defined by components

$$\bar{f}(\mu, T) \triangleq \mathbb{E}_{\mu, T} \left[ \frac{\sum_{t=0}^{T-1} (I(X_t = \cdot) - \mu)}{T} \right]$$

$$\bar{h}(\mu, T) = \mathbb{E}_{\mu, T}[\tau - T]$$

corresponding respectively to the dynamics of $Y_n$ and $Z_n$, we have for $g_n(\mu_n, T_n) = \mathbb{E}[W_n|\mathcal{F}_n]$

$$\lim_{n \to \infty} \sum_{i=n}^{m(t_n+1)} \epsilon_i[g_i(\mu, T) - \bar{g}(\mu, T)] \to 0$$

for each $t > 0$ pointwise. Furthermore, $g_n$ are continuous uniformly in $n$.

Proof. We treat the $\mu_n$ components and the $T_n$ component of Equation [4] separately. Let us first define and compute $f_n(\mu_n, T_n) \triangleq \mathbb{E}_{\mu_n, T_n}[Y_n|\mathcal{F}_n]$.

It is clear that $Y_n(x, \mu_n, T_n) \to_{n \to \infty} \sum_{i=n}^{m(t_n+1)}(I(X^{n+1}_t=x) - \mu(x))$ where $x$ is a component of the vector $Y_n$ and $\mu_n$, $T_n$ are fixed arguments. We can apply the dominated convergence theorem to arrive at the conclusion

$$f_n(\mu, T) = \mathbb{E}[Y_n|\mathcal{F}_n, \mu_n = \mu, T_n = T] \to_{n \to \infty} \mathbb{E}_{\mu, T} \left[ \frac{\sum_{t=0}^{T-1} (I(X_t = \cdot) - \mu)}{T} \right].$$

Let’s define the limit to be $\bar{f}(\mu, T)$

$$\bar{f}(\mu, T) \triangleq \mathbb{E}_{\mu, T} \left[ \frac{\sum_{t=0}^{T-1} (I(X_t = \cdot) - \mu)}{T} \right].$$

We now have

$$\lim_{n \to \infty} \sum_{i=n}^{m(t_n+1)} \epsilon_i(f_i(\mu, T) - \bar{f}(\mu, T)) \leq \lim_{n \to \infty} \sum_{i=n}^{m(t_n+1)} |\epsilon_i(f_i(\mu, T) - \bar{f}(\mu, T))|$$

$$\leq \lim_{n \to \infty} \max_{n \leq t \leq m(t_n+1)} |f_i(\mu, T) - \bar{f}(\mu, T)| \to 0.$$
8.1.2. Uniformly bounded variance.

**Lemma 10.** $\sup_n \mathbb{E}|W_n|^2 < \infty$ for the unprojected algorithm

\[
\mathbb{E}[|Y_n|^2|\mu_n, T_n] \leq \mathbb{E}_{\mu_n, T_n} \left[ \sum_{l=0}^{T_n-1} (\mathbb{I}(X_l = \cdot) - \mu_n) \right]^2 \\
\leq \mathbb{E}_{\mu_n}(\tau^2) \\
\leq \sum_{n \geq 0} \mathbb{P}_{\mu_n}(\tau > \sqrt{n}) \\
\leq \mu_n' \left( \sum_{l=0}^{\infty} Q[\sqrt{l}] \right)^1.
\]

**Proof.** Now, $\mathbb{E}[|Y_n|^2] = \mathbb{E} \left[ \mathbb{E}[|Y_n|^2|\mu_n, T_n] \right] = \mathbb{E}(\mu_n)' \left( \sum_{l=0}^{\infty} Q[\sqrt{l}] \right)^1$. The infinite sum can be shown to be convergence by an integral test. Since $\mathbb{E}(\mu_n)$ is a vector in the probability simplex, which is compact, it is bounded from above.

For the second $T_n$ component, we have $E[Z_n^2|\mu_n, T_n] = E_{\mu_n, T_n}(\tau - T_n)^2 \leq E_{\mu_n}(\tau^2)$ because $T_n$ is non-negative. Following the argument above, this is also bounded in $n$. \qed

8.1.3. The dynamical system. Lemma 9 show that the dynamical system of interest has gradient field $\bar{g}$ consisting of

\[
\dot{f}(\mu, T) \triangleq \mathbb{E}_{\mu, T} \left[ \sum_{l=0}^{T_n-1} (\mathbb{I}(X_l = \cdot) - \mu) \right] \\
\dot{h}(\mu, T) = \mathbb{E}_{\mu, T}[\tau - T].
\]

After some expansion, they become (writing $\mu$ as a vector ODE)

\[
\dot{\mu}(t)' = \frac{1}{T} \left[ (\mu(t)'(I - Q)^{-1} - (\mu(t)'(I - Q)^{-1})\mu'(t) \right] \\
\dot{T}(t) = \mu(t)'(I - Q)^{-1}1 - T(t).
\]

In the proof of Theorem 5.2.1 of [16], the subsequence limit $\theta(\cdot, \omega)$ is a solution to the above ODE. We only need to prove that these solutions converge to the quasi-stationary distribution. The strategy is to prove the asymptotic limit of all solutions of a reduced ODE starting in $H$ is the quasi-stationary distribution, and then show that these particular solutions (subsequence limits of $\theta(\cdot, \omega)$) of the full ODE (Equation 9) can be converted into solutions for the reduced ODE. Finally we combine these and show that these subsequence solutions that the iterates $(\mu_n, T_n)$ visits a compact subset of $H \times (0, \infty)$ infinitely often almost surely.

The reduced ODE is

\[
\nu'(t) = \nu(t)'(I - Q)^{-1} - (\nu(t)'(I - Q)^{-1}1)\nu(t)' \\
\nu(0) = \mu_0.
\]

For convenience, first define

**Definition 11.** $\Gamma(t) = \int_0^t \frac{1}{T(s)}ds$

It is not hard to see that $\mu(\Gamma^{-1}(t))$ is a solution to the reduced ODE. The following Lemma ensures that the inverse is well defined.
Lemma 12. \( \Gamma(t) \) is non-negative, increasing, and goes to \( \infty \)

Proof. The increasing part is trivial because \( T(s) \) is strictly positive (in both the discrete-time and continuous-time cases). Let’s assume that \( \int_0^\infty \frac{1}{T(s)} < \infty \). This implies

\[
T(t) = T_0 \exp \left( \int_0^t \left[ \frac{E_{\mu(s)}(\tau)}{T(s)} \right] ds - t \right) \\
\leq T_0 \exp \left( \sup_{\mu \in \mathcal{H}} E_{\mu}(\tau) \int_0^t \frac{1}{T(s)} ds - t \right) \\
< T_0 \exp(K \int_0^t \frac{1}{T(s)} ds) \\
< \tilde{K} \quad \forall t.
\]

This means \( \frac{1}{T(t)} \geq \tilde{K} \Rightarrow \int_0^\infty \frac{1}{T(s)} = \infty \) a contradiction. \( \square \)

\( \Gamma^{-1}(0) = 0 \) so \( \mu(\Gamma^{-1}(0)) = \mu(0) \in \mathcal{H} \). Now let’s analyze the asymptotic behavior of any such solution \( \nu(t) \) to Equation 10.

Lemma 13. Given any solution to the reduced ODE 10 such that \( \nu(0) \in \mathcal{H} \), they converge to the quasi-stationary distribution \( \bar{\mu} \).

Proof. If \( v(0) \in \mathcal{H} \), then the entire trajectory stays in \( \mathcal{H} \). Define \( A \equiv (I - Q)^{-1} \). By the Duhamel’s principal, all solutions to \( \nu \) can be represented by

\[
\nu(t)' = v(0)' \exp \left( At - \int_0^t (\nu(s)' A1) ds \right).
\]

Because \( A = \sum_{n=0}^\infty (Q)^n \) is a matrix with only non-negative entries and \( \nu(0) \geq 0 \), we have \( \nu(t) = v(0)' \exp(At) \exp \left( -\int_0^t (\nu(s)' A1) ds \right) \geq 0 \). Along with \( 1' \nu(0) = 1 \), we know that \( \nu(t) \) belongs to the simplex. The gradient field is continuously differentiable over the simplex which is compact. Hence there exists unique solutions to the ODE.

Rearranging the equation gives

\[
\nu(t)' \exp \left( \int_0^t (\nu(s)' A1) ds \right) = \nu(0)' \exp(At) \\
\nu(t)' \exp \left( \int_0^t (\nu(s)' A1) ds - \beta t \right) = \nu(0)' \exp(At - \beta t).
\]

Here, \( \beta \) denotes the Perron-Frobenius eigenvalue for \( A \equiv (I - Q)^{-1} \). Notice that regardless of the periodicity assumption on \( Q \), \( (I - Q)^{-1} \) is a strictly positive matrix. Consequently \( \frac{e^A}{\beta} \) is a strictly positive matrix with spectral radius 1. By Perron-Frobenius theorem ([?] Appendix Theorem 2.1), we have that for some \( w \)

\[
v(0)' \exp(An - \beta n) \to_{t \to \infty} w
\]

where \( w \) is a multiple of the Perron-Frobenius eigenvector of the matrix \( A \). Because \( (A - \beta)/m \) is also a matrix with the same eigenvector, the above convergence will also hold along sequences \( \frac{n}{m} \) for fixed \( m \) as \( n \to \infty \). The exponential is an uniformly continuous function in this case, so the convergence also holds along the real numbers as \( t \to \infty \).
Now, take inner product of Equation 12 with 1 to obtain
\[
\exp\left(\int_0^t (\nu(s)'A1)ds - \beta t\right) \to_{t \to \infty} \gamma \triangleq <w, 1>.
\]
We now rewrite the original representation in the following way
\[
\nu(t) = \nu(0)' \exp\left(At - \int_0^t (\nu(s)'A1)ds\right)
\]
\[
= \nu(0)' \exp(At - \beta t) \exp(-\left(\int_0^t (\nu(s)'A1)ds - \beta t\right))
\]
\[
\to_{t \to \infty} \frac{w}{\gamma}.
\]

Now the limit is a normalized quasi-stationary vector. The last fact that finishes the Lemma is that the Perron-Frobenius eigenvector of Lemma 15.

**Theorem 14.** Any solution (if exists) solving
\[
\dot{\mu}'(t) = \frac{1}{T} \left[(\mu(t)'(I-Q)^{-1} - (\mu(t)'(I-Q)^{-1}1)(\mu(t)'\right]
\]
\[
\dot{T}(t) = \mu(t)'(I-Q)^{-1}1 - T(t)
\]
with initial conditions \(\mu_0 \in H\) and \(T_0 > 0\) converges to the quasi-stationary distribution in \(\mu\) and \(E_{\bar{\mu}}(\tau) = \frac{1}{1-\lambda}\) in \(T\) where \(\lambda\) is the principal eigenvalue of \(Q\). The random iterates \((\mu_n, T_n)\) visits a compact subset (might depend on \(\omega\)) of this attractor space \((H \times (0, \infty))\) almost always. This implies that \(\mu_n \to \bar{\mu}\) and \(T_n \to \frac{1}{1-\lambda}\) with probability one.

**Proof.** Here we chain together the above few lemmas. We find that \(\mu(\Gamma^{-1}(t))\) is a solution to the reduced ODE with initial condition \(\mu(0)\). Therefore Lemma 13 tells us that \(\mu(\Gamma^{-1}(t)) \to \bar{\mu}\). Furthermore, Lemma 12 implies \(\Gamma^{-1}(t) \to \infty\). Together, it means \(\mu(t) \to \bar{\mu}\).

\(T(t)\) can be solved using the formula
\[
T(t) = \int_0^t E_{\mu(s)}[\tau] e^s ds + T_0.
\]

Because \(E_{\mu(s)}[\tau] \to E_{\bar{\mu}}[\tau]\), we can use L’Hopital’s rule and get
\[
\lim_{t \to \infty} T(t) = \lim_{t \to \infty} \frac{E_{\mu(t)}[\tau] e^t}{e^t} = E_{\bar{\mu}}[\tau] = \frac{1}{1-\lambda}.
\]

Now one might notice that \(T_n\) does not lie in a bounded set. This could potentially lead to problems when the proof of [16] Theorem 5.2.1 assumes that \(\int_0^t f(\mu^n(s), T^n(s))ds\) and \(\int_0^t h(\mu^n(s), T^n(s))ds\) are equicontinuous classes of functions (for almost every \(\omega\)).

However, \(T_n = \frac{1}{\gamma} \sum_{k=1}^n \tau^{(k)}\), and we can show that \(T_n\) is bounded almost surely by a finite random variable by Lemma 15. This means \(T^n(s, \omega)\) lives on a compact set for each fixed \(\omega\) in a set of full measure.

We now satisfy all the requirements of Theorem 4.2.1 of [16] and our iterates \((\mu_n, T_n)\) remains within the domain of attraction \((H \times (0, \infty))\) of \((\bar{\mu}, \frac{1}{1-\lambda})\) infinitely often. Hence the stochastic approximation algorithm iterates converge to that point with probability 1. \(\square\)

**Lemma 15.** \(T_n\) is almost surely bounded by a finite random variable
Proof. Recall that \( T_n = \frac{1}{n+1} \sum_{k=1}^{n} \tau^{(k)} \). We can consider \( \tilde{\tau}(x) \) which is the stopping time of a Markov chain starting from state \( x \) and define

\[
\tilde{\tau} \triangleq \max\{\tilde{\tau}(x) | \forall x \in S\}.
\]

As a consequence,

\[
P(\tau^{(k)} > y) \leq P(\tilde{\tau} > y).
\]

That means we can couple the random variable \( \tau^{(k)} \) with a sequence of i.i.d. random variables \( \tilde{\tau}^{(k)} \). Each one has finite expectations because

\[
E[\tilde{\tau}] = \sum_{n \geq 0} P(\tilde{\tau} > n) \leq \sum_{n \geq 0} \sum_{x \in S} P(\tilde{\tau}(x) > n) = \sum_{x \in S} E(\tilde{\tau}(x)) < \infty.
\]

This means \( \lim_n T_n \leq \lim_n \frac{1}{n+1} \sum_{k=1}^{n} \tilde{\tau}^{(k)} \rightarrow E[\tilde{\tau}] \). Hence \( T_n \) is almost surely bounded by a finite random variable. \( \square\)

8.2. Rate of convergence proof. In trying to obtain a rate of convergence result for main algorithm in the form of Equation 4, we invoke Theorem 10.2.1 of [16]. There’s a whole set of assumptions that need to be checked. Here, recall that \( \theta_n \) contains two components, \( \mu_n \) and \( T_n \) (Equation 4) and that the notation is \( E_n(Y_n) \triangleq E[Y_n | F_n] \). We list the sufficient conditions here.

1. \( \{ W_n I_{\{|\theta_n - \bar{\theta}| \leq\rho \}} \} \) has to be uniformly integrable where \( \bar{\theta} \) is the w.p. 1 limit of \( \theta_n \). This is trivial because \( \sup_n E|W_n|^2 < \infty \) by Lemma 10.

2. \( \bar{\theta} \), the limit point of the ODE, is an isolated stable point. Again, it’s trivial.

3. \( E(W_n | F_n) = g_n(\theta_n) \) can be expanded as

\[
g_n(\theta) = g_n(\bar{\theta}) + (Dg_n)(\bar{\theta})(\theta - \bar{\theta}) + o(|\theta - \bar{\theta}|)
\]

where the error \( o \) is uniform in \( n \). This is not so trivial and the proof is given below in Lemma 16.

4. We need the sequence \( \{ \frac{\theta_n - \bar{\theta}}{\sqrt{n}} \} \) to be tight. See Lemma 17.

5. \( \lim_{n,m} \frac{1}{\sqrt{m}} \sum_{i=n}^{n+m-1} g_i(\bar{\theta}) = 0 \) uniformly for each small t-interval. See Lemma 19.

6. There exists a matrix \( A \) such that \( A + I/2 \) is Hurwitz and

\[
\lim_{n,m} \frac{1}{\sqrt{m}} \sum_{i=n}^{n+m-1} [(Dg_i)(\bar{\theta}) - A] = 0.
\]

Let \( A = (D\bar{g})(\bar{\theta}) \) then the above is true because \( Dg_i(\bar{\theta}) \rightarrow D\bar{g}(\bar{\theta}) \) by Lemma 20. Conditions for \( A + I/2 \) being Hurwitz is given in Theorem 21.

7. Define \( \delta M_n = W_n - E_n(W_n) \). There exists a \( p > 0 \) such that

\[
\sup_n E[|\delta M_n|^{2+p}] < \infty
\]

and a non-negative definite matrix \( \Sigma \) such that

\[
E_n \delta M_n \delta M_n' \rightarrow \Sigma.
\]

This is proven in Lemma 24.
8.2.1. Uniformity of the error terms.

**Lemma 16.** $\mathbb{E}(W_n|F_n) = g_n(\theta_n)$ can be expanded as

$$g_n(\theta) = g_n(\bar{\theta}) + (Dg_n)(\bar{\theta})(\theta - \bar{\theta}) + o(|\theta - \bar{\theta}|)$$

where the error $o$ is uniform in $n$.

*Proof.* Refer to proof of [16] for the components of $g_n$. Again, the $n$ component causes no problem because it is independent of $n$. By defining $v(x,s) = \mathbb{E}[e^{-s\tau}|X_0 = x]$, $f_n(\mu, T)$, the $\mu$ component of $g_n$, can be expanded as

$$f_n(\mu, T)(x) = \mathbb{E}_{\mu, T} \left[ \int_0^\infty e^{-(T+\bar{\tau})u} \left( \sum_{k=0}^{\infty} (I(X_k = x) - \mu(x)) \right) du \right]$$

$$= \int_0^\infty \mathbb{E}_{\mu, T} \left[ e^{-(T+\bar{\tau})u} \sum_{k=0}^{\infty} (I(\tau > k, X_k = x) - I(\tau > k)\mu(x)) \right] du$$

$$= \int_0^\infty e^{-Tu} \sum_{k=0}^{\infty} e^{-k\bar{\tau}} E_{\mu} \left[ e^{-(r-k)\bar{\tau}} (I(\tau > k, X_k = x) - I(\tau > k)\mu(x)) \right] du$$

$$= \int_0^\infty e^{-Tu} \sum_{k=0}^{\infty} e^{-k\bar{\tau}} \{v(x, u/n + 1) - v(\cdot, u/n + 1)\} du$$

$$= \int_0^\infty e^{-Tu} \left[ v(x, u/n + 1) - v(\cdot, u/n + 1) \right] du.$$

It is easy to see that integration and (partial) differentiation can be interchanged in this case because of the integrand’s smoothness and integrability. $v(x,s)$ is bounded by 1 and 0 for $s \geq 0$. The integrand consists of a second-order expression in $\mu$ multiplied by an exponential damping factor $e^{-Tu}$. It is now clear that all the mixed second partial derivatives of $f_n$ will be bounded uniformly in $n$ in a neighborhood around the stationary point $\bar{\theta} = (\bar{\mu}, \bar{T})$ since $T > 0$. \hfill $\Box$

8.2.2. Tightness of the normalized iterates. In order for the CLT to hold, the normalized iterates $\left\{ \theta_n - \bar{\theta} \over \sqrt{\epsilon_n} \right\}$ has to be tight.

**Lemma 17.** The normalized iterates $\left\{ \theta_n - \bar{\theta} \over \sqrt{\epsilon_n} \right\}$ is tight.

*Proof.* Here make a slight modification to the proof of Theorem 10.4.1 in [16]. We let $A = (Dg)(\bar{\theta})$. For any positive definite matrix $C$, there exists a positive definite solution $P$ to the equation

$$A'P + PA = -C.$$

We take this $P$ and for each $A_n = (Dg_n)(\bar{\theta})$, we obtain a sequence of matrices $C_n$ via

$$A'_nP + PA_n = -C_n.$$

Obviously $C_n \to C$ and because $C$ is strictly positive definite, there exists a $\lambda > 0$ such that $C_n \geq \lambda P$ in the positive-definite sense.
Lemma 18. which trivially leads to tightness.

The first part can be bounded by Cauchy-Schwartz inequality

\[ \mathbb{E}[V(\theta_{n+1})|F_n] - V(\theta_n) = 2\epsilon_n(\theta_n - \bar{\theta})' Pg_n(\theta_n) + \epsilon_n^2 \mathbb{E}(W_n' P W_n) \]

\[ = 2\epsilon_n(\theta_n - \bar{\theta})' Pg_n(\theta_n) + 2\epsilon_n(\theta_n - \bar{\theta})' PA_n(\theta_n - \bar{\theta}) \]

\[ + 2\epsilon_n(\theta_n - \bar{\theta})' Po(\theta_n - \bar{\theta}) + O(\epsilon_n^2) \]

\[ = O \left( \frac{1}{n} \right) - \epsilon_n(\theta_n - \bar{\theta})' C_n(\theta_n - \bar{\theta}) + 2\epsilon_n(\theta_n - \bar{\theta})' Po(\theta_n - \bar{\theta}) + O(\epsilon_n^2) \]

\[ \leq O(\epsilon_n^2) - \epsilon_n \lambda V(\theta_n) \]

where the several facts are used

1. \( C_n \geq \lambda P \) for large \( n \) (the inequality is in the positive-definite sense).
2. \( (\theta_n - \bar{\theta})' Po(\theta_n - \bar{\theta}) \leq \delta V(\theta_n) \) for small \( \delta \) and all \( n \) large enough by Cauchy-Schwartz.
3. The error term \( o(|\theta_n - \bar{\theta}|) \) of the Taylor series expansion is uniform for all \( \theta_n \) as proven in Lemma 16.
4. \( g_n(\theta) = O(\frac{1}{n}) \). This point is proven in Lemma 18 below.

At this point, we can use the rest of the proof of Theorem 10.4.1 of [16] to show that \( \mathbb{E}[V(\theta_{n+1})|F_n] = O(\epsilon_n) \) which trivially leads to tightness.

Lemma 18. \( g_n(\theta) = O(\frac{1}{n}) \)

Proof. At \( \bar{\theta} \), the gradient field \( \bar{h} \) corresponding to the \( T_n \) component is always 0 at the stationary point so we focus on the \( f_n \) part.

\[ f_n(\theta) = \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \sum_{k=0}^{\tau-1} \frac{1}{(1 + \frac{\tau}{nT})} \mathbb{I}(X_k = \cdot - \mu(\cdot)) \mathbb{I}(\tau > \sqrt{n}) \right] \]

\[ + \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \sum_{k=0}^{\tau-1} \frac{1}{(1 + \frac{\tau}{nT})} \mathbb{I}(X_k = \cdot - \mu(\cdot)) \mathbb{I}(\tau \leq \sqrt{n}) \right] \]

The first part can be bounded by Cauchy-Schwartz inequality

\[ \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \sum_{k=0}^{\tau-1} \frac{1}{(1 + \frac{\tau}{nT})} \mathbb{I}(X_k = \cdot - \mu(\cdot)) \mathbb{I}(\tau > \sqrt{n}) \right] \leq \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \sum_{k=0}^{\tau-1} \frac{1}{(1 + \frac{\tau}{nT})} \mathbb{I}(X_k = \cdot - \mu(\cdot)) \right]^{\frac{1}{2}} \frac{\mathbb{P}(\tau > \sqrt{n})}{\sqrt{n}} \]

\[ = O(e^{-\epsilon \sqrt{n}}). \]

The second part in the expansion of \( f_n(\bar{\theta}) \) can be further expanded using Taylor polynomial

\[ \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \sum_{k=0}^{\tau-1} \frac{1}{(1 + \frac{\tau}{nT})} \mathbb{I}(\tau \leq \sqrt{n}) \right] = \quad \checkmark \]

\[ \frac{1}{T} \mathbb{E}_{\mu,T} \left[ \left( \sum_{k=0}^{\tau-1} \mathbb{I}(X_k = \cdot - \mu(\cdot)) \right) \left( 1 - \frac{\tau}{nT} + \frac{2}{(1-c)^3 n^2 T^2} \right) \mathbb{I}(\tau \leq \sqrt{n}) \right] = \quad \checkmark \]

\[ (1) + (2) + (3) \]
where (1), (2), and (3) are obtained by multiplying \( \sum_{k=0}^{\tau-1} (\mathbb{I}(X_k = \cdot) - \bar{\mu}(\cdot)) \) through the second bracket. \( c \) is a number between 0 and \( \frac{\tau}{nT} \). To get a bound on (1), we have

\[
E_{\mu, T} \left[ \left( \sum_{k=0}^{\tau-1} (\mathbb{I}(X_k = \cdot) - \bar{\mu}(\cdot)) \right)^2 \right] \leq \frac{\tau}{nT} \sum_{k=0}^{\tau-1} \mathbb{I}(\tau \leq \sqrt{n}) = O \left( \frac{1}{n} \right).
\]

Modulus of (2) becomes bounded by

\[
E_{\mu, T} \left[ \sum_{k=0}^{\tau-1} (\mathbb{I}(X_k = \cdot) - \bar{\mu}(\cdot)) \right] \leq \frac{\tau}{nT} \mathbb{I}(\tau \leq \sqrt{n}) = O \left( \frac{1}{n} \right).
\]

Modulus of (3) becomes bounded by

\[
E_{\mu, T} \left[ \sum_{k=0}^{\tau-1} (\mathbb{I}(X_k = \cdot) - \bar{\mu}(\cdot)) \right] \leq \frac{4\tau^2}{nT^2} \mathbb{I}(\tau \leq \sqrt{n}) = O \left( \frac{1}{n} \right).
\]

8.2.3. \( \sqrt{n} \)-averaging.

**Lemma 19.** \( \lim_{n,m} \frac{1}{\sqrt{m}} \sum_{i=n}^{n+mt-1} g_i(\tilde{\theta}) = 0 \) uniformly in each small t-interval.

**Proof.** By Lemma 18, the expression becomes \( \frac{1}{\sqrt{m}} \sum_{i=n}^{n+mt-1} O \left( \frac{1}{n} \right) = \frac{1}{\sqrt{m}} O(\log(n + mt - 1) - \log n) \). If we maximize \( n \) for every \( m \), we find that the log difference is maximized when \( n = 1 \). Hence the limit becomes bounded by

\[
\frac{1}{\sqrt{m}} O(\log(mt)) \to 0
\]

uniformly on a small t-interval. \( \square \)

8.2.4. Hurwitz condition.

**Lemma 20.** \( (Dg_n)(\tilde{\theta}) \to (D\bar{g})(\tilde{\theta}) \)

**Proof.** By Lemma 18 we know

\[
g_n(\theta) = g_n(\tilde{\theta}) + (Dg_n)(\tilde{\theta} - \theta) + o(|\theta - \tilde{\theta}|).
\]

If we take the limit as \( n \to \infty \) we get

\[
\bar{g}(\theta) = 0 + \lim_n (Dg_n)(\theta - \tilde{\theta}) + o(|\theta - \tilde{\theta}|).
\]

Expand the left hand side by Taylor series and get

\[
(D\bar{g})(\tilde{\theta}) = \lim_n (Dg_n)(\tilde{\theta} - \theta) + o(|\theta - \tilde{\theta}|)
\]

\[
\limsup_n \left| (Dg_n - D\bar{g})(\theta) \right| = \frac{o(|\theta - \tilde{\theta}|)}{|\theta - \tilde{\theta}|}
\]

and the right hand side is arbitrarily small so the limsup is 0. \( \square \)
The overall Jacobian would, in block form, look like

\[
\begin{bmatrix}
J & 0 \\
1' B & -1 \\
\end{bmatrix}
\]

This has the same eigenvalues as \( J \) with the addition of the eigenvalue -1. That would not violate the Hurwitz condition. Hence we need to ensure that \( J + \frac{I}{2} \) is Hurwitz.

Recall from equation 9 that \( g \) contains the \( f \) component as well as the \( h \) component. With the notation \( B \triangleq (I - Q^T)^{-1} \), the Jacobians are given by

\[
\nabla_\mu f(\mu, T) = \frac{1}{\beta} \left[ B - (1' B \mu) I - \mu 1' B \right] \\
\nabla_T f(\mu, T) = -\frac{1}{\beta^2} \left[ B\mu - (1' B \mu) \mu \right] \\
\nabla_\mu h(\mu, T) = 1' B \\
\nabla_T h(\mu, T) = -1 \quad \text{(scalar)}.
\]

At the stationary point \((\bar{\mu}, \bar{T})\), if we define \( \beta = 1' B \bar{\mu} = \bar{T} \), the \( f \) component becomes

\[
\nabla_\mu f(\bar{\mu}, \bar{T}) = \frac{1}{\beta} \left[ B - \beta I - \bar{\mu} 1' B \right] \quad \text{call this matrix } J \\
\nabla_T f(\bar{\mu}, \bar{T}) = 0.
\]

We will now established a 1-1 correspondence between the eigenvectors of \( J \) and the eigenvectors of \( B \). The overall Jacobian would, in block form, look like

\[
\begin{bmatrix}
J & 0 \\
1' B & -1 \\
\end{bmatrix}
\]

This has the same eigenvalues as \( J \) with the addition of the eigenvalue -1. That would not violate the Hurwitz condition. Hence we need to ensure that \( J + \frac{I}{2} \) is Hurwitz.

Given a vector \( y \) such that \( Jy = \lambda_J y \) and \( y \) linearly independent of \( \bar{\mu} \). Define \( x \triangleq y + r \bar{\mu} \). That means \( Bx = \beta(\lambda_J + 1)y + (r \beta + 1' B y) \bar{\mu} \). The correct \( r \) that would make \( x \) an eigenvector of \( B \) is such that \( r \beta \lambda_J = 1' B y \). Here \( \beta \) is the principal eigenvalue of \( B \) so it is strictly positive. That means there exists such \( r \) if \( \lambda_J \neq 0 \). The corresponding eigenvalue for \( B \) would be \( \lambda_B \triangleq \beta(\lambda_J + 1) \). If \( y \) is a multiple of \( \bar{\mu} \), then its \( J \) eigenvalue would be -1 and its \( B \) eigenvalue would be \( \beta \). Below in Lemma 23, we show that \( \lambda_J \) can never be 0. This would imply every eigenvector of \( J \) is an eigenvector of \( B \).

Conversely, given a vector \( z \), \( Bz = \lambda_B z \), we can define \( u \triangleq z + r \bar{\mu} \). If we choose \( r = \frac{\beta + \lambda_B (1' z)}{\beta - \lambda_B} \) then \( Ju = (\frac{\lambda_B}{\beta} - 1) u \). This would work when \( z \) is not the principal right-eigenvector of \( B \). If it is, i.e. \( z = \bar{\mu} \), then trivially \( Jz = -z \).

Hence we can conclude that there is a one-to-one correspondence between the eigenvector/eigenvalues of \( J \) and \( B \) and the relation is given by

\[
\lambda_J = \frac{\lambda_B}{\beta} - 1 \quad \text{for } \lambda_B \neq \beta \text{ or } \lambda_J \neq 0 \\
\lambda_J = -1 \text{ when } \lambda_B = \beta.
\]
Hence, in order to ensure that $J + \frac{1}{2}$ is Hurwitz, we require
\[
Re\left(\frac{\lambda_B}{\beta} - \frac{1}{2}\right) < 0 \quad \forall \lambda_B \neq \beta
\]
\[
\Rightarrow Re(\lambda_B) < \frac{\beta}{2} \quad \forall \lambda_B \neq \beta
\]
\[
\Rightarrow \max_{\lambda \in NPV} Re\left(\frac{1}{1 - \lambda}\right) < \frac{1}{2} \left(\frac{1}{1 - \lambda_{PV}}\right).
\]

\[\Box\]

Remark 22. If you carefully examine the proof in [10], you will notice that the Jacobian $J$ is drift of an Ornstein-Uhlenbeck process $U(t)$ that lives on the subspace orthogonal to $1$. Hence, in order for the OU process to have a stationary distribution, it is enough to require that all the eigenvectors that live on this hyperplane have real part of their eigenvalue less than $\frac{1}{2}$. If we are given an eigenvector $Jy = \lambda y$, we can dot this with $1$ and arrive at
\[
Jy = \lambda y
\]
\[
\Rightarrow -1' y = \lambda 1'y.
\]
This implies that if $\lambda \neq -1$, then $1'y = 0$ which is in $y \in 1^\perp$ so it is a relevant eigenvector. If $\lambda = -1$, it would not affect the Hurwitz condition anyways. So our sufficient condition above is not overly strong.

Lemma 23. $\lambda_J \neq 0$

Proof. Assume there exists a $y$ such that $Jy = 0$. That means
\[
By = \beta y + \mu 1' By
\]
\[
(1 - \mu 1')By = \beta y.
\]
We recognize that $P \triangleq (I - \mu 1')$ is a (non-orthogonal) projection. Also $P\mu = 0$ and $1' P = 0$. This means $\beta$ is an eigenvalue of $PB$, that means there would exists a left eigenvector $x$ such that
\[
x' PB = \beta x'
\]
\[
x' P = \beta x' B^{-1}.
\]
We decouple this into two equations
\[
x' P = z
\]
\[
z' = \beta x' B^{-1}.
\]
If the equation $x' P = z'$ has a solution $x$, we must require $z' \mu = 0$. That would mean $x$ can be decomposed as a fundamental solution added to a null solution. The null space is $c1$ and $z' P = z' - z' \mu 1' = z'$. So $x' = c1' + z'$ would span the entire solution space. However, remember that we’re interested in $z' = \beta x' B^{-1}$. We dot this with $\mu$ and arrive at
\[
0 = \beta x' (I - Q) \mu
\]
\[
0 = \beta (x' \mu - \lambda x' \mu)
\]
\[
x' \mu = \lambda x' \mu
\]
\[
x' \mu = 0 \quad \text{because $0 < \lambda < 1$.}
Now we can conclude that $c = 0$:

$$
x' = cI' + z' \quad x'\mu = cI'\mu + z'\mu \quad 0 = c + 0.
$$

This means $x' = z' = \beta x'B^{-1} \Rightarrow x'B = \beta x'$. This would mean $x'$ is the principle left-eigenvector and all its components are strictly positive. In that case, it would be impossible to have $x'\mu = 0$. So there is no eigenvalue $\beta$ for the matrix $PB$. Hence $J$ cannot have a zero eigenvalue.

8.2.5. Quadratic variation of the martingales.

**Lemma 24.** Define $\delta M_n = W_n - \mathbb{E}_n(W_n)$. There exists a $p > 0$ such that

$$
\sup_n \mathbb{E}|\delta M_n|^{2+p} < \infty
$$

and a non-negative definite matrix $\Sigma$ such that

$$
\mathbb{E}_n\delta M_n\delta M_n' \to \Sigma.
$$

**Proof.** Recall that $W_n = (Y_n, Z_n)$ in Equation 4. Pick $p = 2$, we can use Jensen’s inequality and arrive at

$$
|\delta M_n|^4 \leq 2 \left(|Y_n - \mathbb{E}_n(Y_n)|^4 + |Z_n - \mathbb{E}_n(Z_n)|^4\right) \leq 16 \left(|Y_n|^4 + |\mathbb{E}_n(Y_n)|^4 + |Z_n|^4 + |\mathbb{E}_n(Z_n)|^4\right).
$$

Due to the facts

(1) $|Y_n| \leq \tau(\mu_n)$, here $\tau(\mu_n)$ is the stopping time given the initial distribution $\mu_n$,

(a) $\mathbb{E}_n|Y_n|^2 \leq \mathbb{E}_n(|Y_n|^4)$,

(b) $|Z_n| \leq \tau(\mu_n)$,

(c) $\mathbb{E}_n(Z_n)^4 \leq \mathbb{E}_n(Z_n^4)$,

(d) $\tau(\mu) \leq \tau(\mu) \forall \mu$ where $\widetilde{\tau} = \max\{\tau(\mu) | \mu = \delta_x, \forall x \in S\}$ by stochastic dominance followed by Skorohod representation.

Proof. We can conclude that $\sup_n \mathbb{E}|\delta M_n|^4 < \infty$.

We now use dominated theorem on $\mathbb{E}_n\delta M_n\delta M_n'$. We can think in block form matrix $\delta M_n\delta M_n'$

$$
\delta M_n\delta M_n' = \begin{bmatrix}
(Y_n(\theta_n) - f_n(\theta_n))(Y_n(\theta_n) - f_n(\theta_n))' & (Y_n(\theta_n) - f(\theta_n))(Z_n(\theta_n) - h_n(\theta_n))' \\
(Z_n(\theta_n) - h_n(\theta_n))(Y_n(\theta_n) - f_n(\theta_n))' & (Z_n(\theta_n) - h_n(\theta_n))(Z_n(\theta_n) - h_n(\theta_n))'
\end{bmatrix}.
$$

In absolute value conditioned on $\mathcal{F}_n$, each entry of this matrix is dominated by $2\tau(\theta_n) \leq 2\widetilde{\tau}$. $\delta M_n\delta M_n'$ is dominated entry-wise by $2\widetilde{\tau}$ uniformly for all possible admissible $\theta_n$. With a few more steps, we can show the convergence to a non-negative matrix.

$f_n(\theta_n) \to 0$ and $h_n(\theta_n) \to 0$ by Lemma 18. $Z_n(\theta) = \tau(\theta) - T$ can be represented in a way that is continuous in $\theta$ (by writing $\tau$ as a mixture of the initial starting points). Hence $Z_n(\theta_n) \to Z(\theta) = \tau(\theta) - T$.

$Y_n(\theta) = \sum_{k=0}^{\tau(\theta_n)-1} \mathbb{I}(X_k = |X_0 - \bar{\mu}| \sim \mu) / \tau(\theta_n)$ can also be written in a way that is continuous in $\theta$ and uniformly convergent (over $\theta$) the random variable $Y(\theta)$. Hence

$$
Y_n(\theta_n) \to_{n \to \infty} \sum_{k=0}^{\tau(\theta_n)-1} \frac{\mathbb{I}(X_k = |X_0 - \bar{\mu}| \sim \mu)}{\tau} \triangleq Y(\theta).
$$
can also be shown to be entry-wise dominated, hence its expected value is well defined. It is obviously a non-negative definite matrix because of the form $xx'$.

Together with dominated convergence and the fact that $L_1$-convergence implies convergence in probability, we have the conclusion where $\Sigma = \mathbb{E}\left[\begin{pmatrix} Y(\bar{\theta}) & Z(\bar{\theta}) \end{pmatrix}\begin{pmatrix} Y(\bar{\theta}) & Z(\bar{\theta}) \end{pmatrix}\right].$ □

8.3. Continuous-Time version proof. The ODE associated with the continuous-time algorithm can be arrived by similar technique as the discrete-time case.

$$\dot{\mu}(t) = -\frac{1}{T(t)} \left( \mu(t)' Q^{-1} - (\mu(t)' Q^{-1} 1) \mu(t)' \right)$$

$$\dot{T}(t) = -\mu(t)' Q^{-1} 1 - T(t).$$

Note that instead of $(I - Q)^{-1}$ appearing we now have $-Q^{-1}$ where $Q$ is a transition rate matrix. The Perron-Frobenius theorem still applies to matrix of the form $M - D$ where $M$ consists of off-diagonal non-negative entries and $D$ is a non-positive diagonal matrix. In the discrete-time proof, we often used the fact that $\exp(I - Q)^{-1}$ is a matrix of non-negative entries. We need to now show that $\exp(-Q)^{-1}$ is also a matrix of non-negative entries.

Lemma 25. Given a transition rate matrix $Q$, $\exp(-Q)^{-1}$ is a matrix of non-negative entries.

Proof. Let $\alpha$ be the maximum of the diagonal element of $-Q$. Notice that $-Q^{-1} = \alpha \left[ I - \left( \frac{1}{\alpha} Q + I \right) \right]^{-1} = \alpha \sum_{k \geq 0} \left( \frac{1}{\alpha} Q + I \right)^k$ for $\alpha$ large enough. $\frac{1}{\alpha} Q + I$ is a non-negative irreducible matrix hence the infinite sum is also a positive matrix. □

Lemma 26. The principal eigenvalue of $Q$ is real and smaller than 0, and also the left and right principal eigenspaces are one-dimensional.

Proof. The spectral radius is bounded above by $\|Q\|_{\infty} \leq 0$. $Q + cI$ can be made into a irreducible non-negative matrix for some large $c$. All the properties follow after applying Perron-Frobenius to that. □

Analogous to Lemma 15 we need to show that $T_n$ is bounded above and below almost surely.

Lemma 27. The $T_n$ sequence in the continuous-time case is bounded above and below almost surely by finite random variables.

Proof. The upper bound is identical to the discrete-time case (Lemma 15). For the lower bound, we consider a random variable $\tilde{s}$ that is an exponential rate corresponding to the slowest holding rate of the Markov chain. This way, $\tilde{s}^{(k)}$ can be coupled to the first holding time of the Markov chain during the k-th iteration. This way, $\tau^{(k)} \geq a.s. \tilde{s}^{(k)}$. Hence $\lim_n T_n \geq \mathbb{E}(\tilde{s})$ implying that its bounded below by a finite random variable. □
**Figure 1.** This figure is the time vs. error plot of the main algorithm ran on a loopy Markov chain with eigenvalues well outside the CLT regime ($\epsilon = 0.98 > 0.5$). The plot is a log/log plot where the y-axis is the Mean-Squared-Error. It is clear that the Polyak-Ruppert Averaging (the red line) converges much faster than the original algorithm (green line).
Figure 2. This is the simulation of a M/M/1 queue with 100 queue capacity and \( \rho = 1.25 \). We are considering the embedded discrete-time chain at the jump times of the system. We had to Doeblinize the process (multiply transition matrix by 0.95) in order to deal with the large \( E[\tau] \) due to the system being in heavy-traffic regime. As you can see, the Polyak-Ruppert averaging (red) is significantly better than the original algorithm (green) on the log-log plot. The eigenvalue condition for the CLT is not satisfied after Doeblinization.
Figure 3. This is a simulation of the contact process on a complete graph where $\lambda = 1.5$ with 100 nodes. The plot is the log-log plot of the number of steps vs. MSE. The sufficient condition for CLT cannot be met in this case after subtracting $0.5I$ from the rate matrix. The Polyak's averaging algorithm (red) significantly outperforms the vanilla algorithm (green).
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