

Confidence intervals for the mixing time of a reversible Markov chain from a single sample path

Daniel Hsu[†] Aryeh Kontorovich[#] Csaba Szepesvári^{*}

[†]Columbia University, [#]Ben-Gurion University, ^{*}University of Alberta

ITA 2016

Problem

- ▶ Irreducible, aperiodic, time-homogeneous Markov chain

$$X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \dots$$

Problem

- ▶ Irreducible, aperiodic, time-homogeneous Markov chain

$$X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \dots$$

- ▶ There is a unique **stationary distribution** π with

$$\lim_{t \rightarrow \infty} \mathcal{L}(X_t \mid X_1 = x) = \pi, \quad \text{for all } x \in \mathcal{X}.$$

Problem

- ▶ Irreducible, aperiodic, time-homogeneous Markov chain

$$X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \dots$$

- ▶ There is a unique **stationary distribution** π with

$$\lim_{t \rightarrow \infty} \mathcal{L}(X_t \mid X_1 = x) = \pi, \quad \text{for all } x \in \mathcal{X}.$$

- ▶ The **mixing time** t_{mix} is the earliest time t with

$$\sup_{x \in \mathcal{X}} \|\mathcal{L}(X_t \mid X_1 = x) - \pi\|_{\text{tv}} \leq 1/4.$$

Problem

- ▶ Irreducible, aperiodic, time-homogeneous Markov chain

$$X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \dots$$

- ▶ There is a unique **stationary distribution** π with

$$\lim_{t \rightarrow \infty} \mathcal{L}(X_t \mid X_1 = x) = \pi, \quad \text{for all } x \in \mathcal{X}.$$

- ▶ The **mixing time** t_{mix} is the earliest time t with

$$\sup_{x \in \mathcal{X}} \|\mathcal{L}(X_t \mid X_1 = x) - \pi\|_{\text{tv}} \leq 1/4.$$

Problem:

Determine (confidently) if $t \geq t_{\text{mix}}$ after seeing X_1, X_2, \dots, X_t .

Problem

- ▶ Irreducible, aperiodic, time-homogeneous Markov chain

$$X_1 \rightarrow X_2 \rightarrow X_3 \rightarrow \dots$$

- ▶ There is a unique **stationary distribution** π with

$$\lim_{t \rightarrow \infty} \mathcal{L}(X_t \mid X_1 = x) = \pi, \quad \text{for all } x \in \mathcal{X}.$$

- ▶ The **mixing time** t_{mix} is the earliest time t with

$$\sup_{x \in \mathcal{X}} \|\mathcal{L}(X_t \mid X_1 = x) - \pi\|_{\text{tv}} \leq 1/4.$$

Problem:

Given $\delta \in (0, 1)$ and $X_{1:t}$, determine non-trivial $I_t \subseteq [0, \infty]$ with

$$\mathbb{P}(t_{\text{mix}} \in I_t) \geq 1 - \delta.$$

Some motivation from machine learning and statistics

Chernoff bounds for Markov chains $X_1 \rightarrow X_2 \rightarrow \dots$:

for suitably well-behaved $f: \mathcal{X} \rightarrow \mathbb{R}$, with probability at least $1 - \delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \underbrace{\tilde{O} \left(\sqrt{\frac{t_{\text{mix}} \log(1/\delta)}{t}} \right)}_{\text{deviation bound}}.$$

Bound depends on t_{mix} , which may be unknown *a priori*.

Some motivation from machine learning and statistics

Chernoff bounds for Markov chains $X_1 \rightarrow X_2 \rightarrow \dots$:

for suitably well-behaved $f: \mathcal{X} \rightarrow \mathbb{R}$, with probability at least $1 - \delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \underbrace{\tilde{O} \left(\sqrt{\frac{t_{\text{mix}} \log(1/\delta)}{t}} \right)}_{\text{deviation bound}}.$$

Bound depends on t_{mix} , which may be unknown *a priori*.

Examples:

Bayesian inference Posterior means & variances via MCMC

Reinforcement learning Mean action rewards in an MDP

Supervised learning Error rates of hypotheses from non-iid data

Some motivation from machine learning and statistics

Chernoff bounds for Markov chains $X_1 \rightarrow X_2 \rightarrow \dots$:

for suitably well-behaved $f: \mathcal{X} \rightarrow \mathbb{R}$, with probability at least $1 - \delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \underbrace{\tilde{O} \left(\sqrt{\frac{t_{\text{mix}} \log(1/\delta)}{t}} \right)}_{\text{deviation bound}}.$$

Bound depends on t_{mix} , which may be unknown *a priori*.

Examples:

Bayesian inference Posterior means & variances via MCMC

Reinforcement learning Mean action rewards in an MDP

Supervised learning Error rates of hypotheses from non-iid data

Need *observable* deviation bounds.

Observable deviation bounds from mixing time bounds?

Suppose an estimator $\hat{t}_{\text{mix}} = \hat{t}_{\text{mix}}(X_{1:t})$ of t_{mix} satisfies:

$$\mathbb{P}(t_{\text{mix}} \leq \hat{t}_{\text{mix}} + \varepsilon_t) \geq 1 - \delta.$$

Observable deviation bounds from mixing time bounds?

Suppose an estimator $\hat{t}_{\text{mix}} = \hat{t}_{\text{mix}}(X_{1:t})$ of t_{mix} satisfies:

$$\mathbb{P}(t_{\text{mix}} \leq \hat{t}_{\text{mix}} + \varepsilon_t) \geq 1 - \delta.$$

Then with probability at least $1 - 2\delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \tilde{O} \left(\sqrt{\frac{(\hat{t}_{\text{mix}} + \varepsilon_t) \log(1/\delta)}{t}} \right).$$

Observable deviation bounds from mixing time bounds?

Suppose an estimator $\hat{t}_{\text{mix}} = \hat{t}_{\text{mix}}(X_{1:t})$ of t_{mix} satisfies:

$$\mathbb{P}(t_{\text{mix}} \leq \hat{t}_{\text{mix}} + \varepsilon_t) \geq 1 - \delta.$$

Then with probability at least $1 - 2\delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \tilde{O} \left(\sqrt{\frac{(\hat{t}_{\text{mix}} + \varepsilon_t) \log(1/\delta)}{t}} \right).$$

But \hat{t}_{mix} is computed from $X_{1:t}$, so ε_t may also depend on t_{mix} .

Observable deviation bounds from mixing time bounds?

Suppose an estimator $\hat{t}_{\text{mix}} = \hat{t}_{\text{mix}}(X_{1:t})$ of t_{mix} satisfies:

$$\mathbb{P}(t_{\text{mix}} \leq \hat{t}_{\text{mix}} + \varepsilon_t) \geq 1 - \delta.$$

Then with probability at least $1 - 2\delta$,

$$\left| \frac{1}{t} \sum_{i=1}^t f(X_i) - \mathbb{E}_{\pi} f \right| \leq \tilde{O} \left(\sqrt{\frac{(\hat{t}_{\text{mix}} + \varepsilon_t) \log(1/\delta)}{t}} \right).$$

But \hat{t}_{mix} is computed from $X_{1:t}$, so ε_t may also depend on t_{mix} .

Deviation bounds for point estimators are insufficient.
Need (observable) confidence intervals for t_{mix} .

What we do

What we do

1. Shift focus to **relaxation time** t_{relax} to enable spectral methods.

What we do

1. Shift focus to **relaxation time** t_{relax} to enable spectral methods.
2. **Lower/upper bounds** on sample path length for point estimation of t_{relax} .

What we do

1. Shift focus to **relaxation time** t_{relax} to enable spectral methods.
2. **Lower/upper bounds** on sample path length for point estimation of t_{relax} .
3. **New algorithm** for constructing confidence intervals for t_{relax} .

Relaxation time

- ▶ Let P be the **transition operator** of the Markov chain, and let λ_* be its **second-largest eigenvalue modulus** (i.e., largest eigenvalue modulus other than 1).

Relaxation time

- ▶ Let P be the **transition operator** of the Markov chain, and let λ_* be its **second-largest eigenvalue modulus** (i.e., largest eigenvalue modulus other than 1).
- ▶ **Spectral gap**: $\gamma_* := 1 - \lambda_*$.
Relaxation time: $t_{\text{relax}} := 1/\gamma_*$.

$$(t_{\text{relax}} - 1) \ln 2 \leq t_{\text{mix}} \leq t_{\text{relax}} \ln \frac{4}{\pi_*}$$

for $\pi_* := \min_{x \in \mathcal{X}} \pi(x)$.

Relaxation time

- ▶ Let P be the **transition operator** of the Markov chain, and let λ_* be its **second-largest eigenvalue modulus** (i.e., largest eigenvalue modulus other than 1).
- ▶ **Spectral gap**: $\gamma_* := 1 - \lambda_*$.
Relaxation time: $t_{\text{relax}} := 1/\gamma_*$.

$$(t_{\text{relax}} - 1) \ln 2 \leq t_{\text{mix}} \leq t_{\text{relax}} \ln \frac{4}{\pi_*}$$

for $\pi_* := \min_{x \in \mathcal{X}} \pi(x)$.

Assumptions on P ensure $\gamma_*, \pi_* \in (0, 1)$.

Relaxation time

- ▶ Let P be the **transition operator** of the Markov chain, and let λ_\star be its **second-largest eigenvalue modulus** (i.e., largest eigenvalue modulus other than 1).
- ▶ **Spectral gap**: $\gamma_\star := 1 - \lambda_\star$.
Relaxation time: $t_{\text{relax}} := 1/\gamma_\star$.

$$(t_{\text{relax}} - 1) \ln 2 \leq t_{\text{mix}} \leq t_{\text{relax}} \ln \frac{4}{\pi_\star}$$

for $\pi_\star := \min_{x \in \mathcal{X}} \pi(x)$.

Assumptions on P ensure $\gamma_\star, \pi_\star \in (0, 1)$.

Spectral approach: construct CI's for γ_\star and π_\star .

Our results (point estimation)

We restrict to **reversible Markov chains** on **finite state spaces**.

Let d be the (known *a priori*) cardinality of the state space \mathcal{X} .

Our results (point estimation)

We restrict to **reversible Markov chains** on **finite state spaces**.
Let d be the (known *a priori*) cardinality of the state space \mathcal{X} .

1. Lower bound:

To estimate γ_* within a constant multiplicative factor,
every algorithm needs (w.p. $1/4$) sample path of length

$$\geq \Omega\left(\frac{d \log d}{\gamma_*} + \frac{1}{\pi_*}\right).$$

Our results (point estimation)

We restrict to **reversible Markov chains** on **finite state spaces**.
Let d be the (known *a priori*) cardinality of the state space \mathcal{X} .

1. Lower bound:

To estimate γ_* within a constant multiplicative factor, every algorithm needs (w.p. $1/4$) sample path of length

$$\geq \Omega\left(\frac{d \log d}{\gamma_*} + \frac{1}{\pi_*}\right).$$

2. Upper bound:

Simple algorithm estimates γ_* and π_* within a constant multiplicative factor (w.h.p.) with sample path of length

$$\tilde{O}\left(\frac{\log d}{\pi_* \gamma_*^3}\right) \quad (\text{for } \gamma_*), \quad \tilde{O}\left(\frac{\log d}{\pi_* \gamma_*}\right) \quad (\text{for } \pi_*).$$

Our results (point estimation)

We restrict to **reversible Markov chains** on **finite state spaces**.
Let d be the (known *a priori*) cardinality of the state space \mathcal{X} .

1. Lower bound:

To estimate γ_* within a constant multiplicative factor, every algorithm needs (w.p. 1/4) sample path of length

$$\geq \Omega\left(\frac{d \log d}{\gamma_*} + \frac{1}{\pi_*}\right).$$

2. Upper bound:

Simple algorithm estimates γ_* and π_* within a constant multiplicative factor (w.h.p.) with sample path of length

$$\tilde{O}\left(\frac{\log d}{\pi_* \gamma_*^3}\right) \quad (\text{for } \gamma_*), \quad \tilde{O}\left(\frac{\log d}{\pi_* \gamma_*}\right) \quad (\text{for } \pi_*).$$

But point estimator $\not\Rightarrow$ confidence interval.

Our results (confidence intervals)

3. **New algorithm:** Given $\delta \in (0, 1)$ and $X_{1:t}$ as input, constructs intervals $I_t^{\gamma_\star}$ and $I_t^{\pi_\star}$ such that

$$\mathbb{P}(\gamma_\star \in I_t^{\gamma_\star}) \geq 1 - \delta \quad \text{and} \quad \mathbb{P}(\pi_\star \in I_t^{\pi_\star}) \geq 1 - \delta.$$

Widths of intervals converge a.s. to zero at $\sqrt{\frac{\log \log t}{t}}$ rate.

Our results (confidence intervals)

3. **New algorithm:** Given $\delta \in (0, 1)$ and $X_{1:t}$ as input, constructs intervals $I_t^{\gamma_\star}$ and $I_t^{\pi_\star}$ such that

$$\mathbb{P}(\gamma_\star \in I_t^{\gamma_\star}) \geq 1 - \delta \quad \text{and} \quad \mathbb{P}(\pi_\star \in I_t^{\pi_\star}) \geq 1 - \delta.$$

Widths of intervals converge a.s. to zero at $\sqrt{\frac{\log \log t}{t}}$ rate.

4. **Hybrid approach:** Use new algorithm to turn error bounds for point estimators into observable CI's.
(This improves asymptotic rate for π_\star interval.)

Plug-in estimator

Plug-in estimator

- ▶ Reversibility grants the symmetry of

$$M := \text{diag}(\pi)P = \left\{ \mathbb{P}_{X_1 \sim \pi}(X_1 = x, X_2 = x') \right\}_{x, x' \in \mathcal{X}}$$

(doublet state probabilities in stationary chain).

Plug-in estimator

- ▶ Reversibility grants the symmetry of

$$M := \text{diag}(\pi)P = \left\{ \mathbb{P}_{X_1 \sim \pi}(X_1 = x, X_2 = x') \right\}_{x, x' \in \mathcal{X}}$$

(doublet state probabilities in stationary chain).

- ▶ Moreover, eigenvalues of

$$L := \text{diag}(\pi)^{-1/2} M \text{diag}(\pi)^{-1/2}$$

are real, and satisfy

$$\begin{aligned} 1 = \lambda_1 &> \lambda_2 \geq \dots \geq \lambda_d > -1, \\ \gamma_\star &= 1 - \max\{\lambda_2, |\lambda_d|\}. \end{aligned}$$

Plug-in estimator

- ▶ Reversibility grants the symmetry of

$$M := \text{diag}(\pi)P = \left\{ \mathbb{P}_{X_1 \sim \pi}(X_1 = x, X_2 = x') \right\}_{x, x' \in \mathcal{X}}$$

(doublet state probabilities in stationary chain).

- ▶ Moreover, eigenvalues of

$$L := \text{diag}(\pi)^{-1/2} M \text{diag}(\pi)^{-1/2}$$

are real, and satisfy

$$\begin{aligned} 1 &= \lambda_1 > \lambda_2 \geq \dots \geq \lambda_d > -1, \\ \gamma_\star &= 1 - \max\{\lambda_2, |\lambda_d|\}. \end{aligned}$$

- ▶ **Plug-in estimator:** estimate π and M from $X_{1:t}$ (using empirical frequencies), then plug-in to formula for γ_\star .

Chicken-and-egg problem

(Matrix) Chernoff bound (for Markov chains) gives error bounds for estimates of π and M (and ultimately of L and γ_*): e.g., w.h.p.,

$$|\hat{\gamma}_* - \gamma_*| \leq \|\hat{L} - L\| \leq O\left(\sqrt{\frac{\log(d) \log(t/\pi_*)}{\gamma_* \pi_* t}}\right).$$

Chicken-and-egg problem

(Matrix) Chernoff bound (for Markov chains) gives error bounds for estimates of π and M (and ultimately of L and γ_*): e.g., w.h.p.,

$$|\hat{\gamma}_* - \gamma_*| \leq \|\hat{L} - L\| \leq O\left(\sqrt{\frac{\log(d) \log(t/\pi_*)}{\gamma_* \pi_* t}}\right).$$

This has *inverse dependence* on γ_* .

Chicken-and-egg problem

(Matrix) Chernoff bound (for Markov chains) gives error bounds for estimates of π and M (and ultimately of L and γ_*): e.g., w.h.p.,

$$|\hat{\gamma}_* - \gamma_*| \leq \|\hat{L} - L\| \leq O\left(\sqrt{\frac{\log(d) \log(t/\pi_*)}{\gamma_* \pi_* t}}\right).$$

This has *inverse dependence* on γ_* .

Can't "solve the bound" for γ_*
(unlike "empirical Bernstein" inequalities).



Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

- ▶ **Key advantage:** observable confidence intervals for P via “empirical Bernstein” inequality for martingales.

Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

- ▶ **Key advantage:** observable confidence intervals for P via “empirical Bernstein” inequality for martingales.

Two problems:

Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

- ▶ **Key advantage:** observable confidence intervals for P via “empirical Bernstein” inequality for martingales.

Two problems:

1. Without appealing to symmetry structure, can argue

$$\|\hat{P} - P\| \leq \varepsilon \implies |\hat{\gamma}_* - \gamma_*| \leq O(\varepsilon^{1/(2d)}),$$

but this implies **exponential slow-down in rate**.

Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

- ▶ **Key advantage:** observable confidence intervals for P via “empirical Bernstein” inequality for martingales.

Two problems:

1. Without appealing to symmetry structure, can argue

$$\|\hat{P} - P\| \leq \varepsilon \implies |\hat{\gamma}_* - \gamma_*| \leq O(\varepsilon^{1/(2d)}),$$

but this implies **exponential slow-down in rate**.

2. Direct appeal to symmetry structure of

$$L = \text{diag}(\pi)^{1/2} P \text{diag}(\pi)^{-1/2}$$

gives bounds that depend on π , which is unknown.

Direct estimation of P

Alternative: directly estimate P from $X_{1:t}$.

- ▶ **Key advantage:** observable confidence intervals for P via “empirical Bernstein” inequality for martingales.

Two problems:

1. Without appealing to symmetry structure, can argue

$$\|\hat{P} - P\| \leq \varepsilon \implies |\hat{\gamma}_* - \gamma_*| \leq O(\varepsilon^{1/(2d)}),$$

but this implies **exponential slow-down in rate**.

2. Direct appeal to symmetry structure of

$$L = \text{diag}(\pi)^{1/2} P \text{diag}(\pi)^{-1/2}$$

gives bounds that depend on π , which is unknown.

Our approach:

Directly estimate P , and *indirectly* estimate π via \hat{P} .

Indirect estimation of π

1. We ensure that \hat{P} is transition operator for an ergodic chain (easy via Laplace smoothing).

Indirect estimation of π

1. We ensure that \hat{P} is transition operator for an ergodic chain (easy via Laplace smoothing).
2. **Key step:** estimate π via \hat{P} via **group inverse** $\hat{A}^\#$ of $I - \hat{P}$.

Indirect estimation of π

1. We ensure that \hat{P} is transition operator for an ergodic chain (easy via Laplace smoothing).
2. **Key step:** estimate π via \hat{P} via **group inverse** $\hat{A}^\#$ of $I - \hat{P}$.
 - ▶ $\hat{A}^\#$ contains “virtually everything that one would want to know about the chain” [with transition operator \hat{P}] (Meyer, 1975).

Indirect estimation of π

1. We ensure that \hat{P} is transition operator for an ergodic chain (easy via Laplace smoothing).
2. **Key step:** estimate π via \hat{P} via **group inverse** $\hat{A}^\#$ of $I - \hat{P}$.
 - ▶ $\hat{A}^\#$ contains “virtually everything that one would want to know about the chain” [with transition operator \hat{P}] (Meyer, 1975).
 - ▶ Reveals unique stationary distribution $\hat{\pi}$ w.r.t. \hat{P} .
This is our indirect estimate of π .

Indirect estimation of π

1. We ensure that \hat{P} is transition operator for an ergodic chain (easy via Laplace smoothing).
2. **Key step:** estimate π via \hat{P} via **group inverse** $\hat{A}^\#$ of $I - \hat{P}$.
 - ▶ $\hat{A}^\#$ contains “virtually everything that one would want to know about the chain” [with transition operator \hat{P}] (Meyer, 1975).
 - ▶ Reveals unique stationary distribution $\hat{\pi}$ w.r.t. \hat{P} .
This is our indirect estimate of π .
 - ▶ Tells us how to bound $\|\hat{\pi} - \pi\|_\infty$ in terms of $\|\hat{P} - P\|$.
Hence, from this, we construct a confidence interval for π .

Overall algorithm (outline)

1. Form empirical estimate and confidence intervals for P
(exploit Markov property & “empirical Bernstein”-type bounds).
2. Form estimate and confidence intervals for π
(via group inverse of $I - \hat{P}$).
3. Form estimate and confidence interval for γ_*
(via confidence intervals for π and P , & eigenvalue perturbation theory).

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.
- ▶ Strongly exploit Markov property and ergodicity in confidence intervals for P and π .

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.
- ▶ Strongly exploit Markov property and ergodicity in confidence intervals for P and π .
- ▶ **Problem #1:** close gap between lower and upper bounds on sample path length (for point estimation).

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.
- ▶ Strongly exploit Markov property and ergodicity in confidence intervals for P and π .
- ▶ **Problem #1:** close gap between lower and upper bounds on sample path length (for point estimation).
- ▶ **Problem #2:** overcome computational bottlenecks from matrix operations.

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.
- ▶ Strongly exploit Markov property and ergodicity in confidence intervals for P and π .
- ▶ **Problem #1:** close gap between lower and upper bounds on sample path length (for point estimation).
- ▶ **Problem #2:** overcome computational bottlenecks from matrix operations.
- ▶ **Problem #3:** handle large/continuous state spaces under suitable assumptions.

Recap and future work

- ▶ We resolve “chicken-and-egg” problem of observable confidence intervals for mixing time from a single sample path.
- ▶ Strongly exploit Markov property and ergodicity in confidence intervals for P and π .
- ▶ **Problem #1:** close gap between lower and upper bounds on sample path length (for point estimation).
- ▶ **Problem #2:** overcome computational bottlenecks from matrix operations.
- ▶ **Problem #3:** handle large/continuous state spaces under suitable assumptions.

Thanks!