

Stochastic Processes

Ergodic Theorem, Markov Chain Monte Carlo Methods

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• If x is transient, then

$$\lim_{n\to\infty} P_{x,x}^n = 0, \qquad \qquad \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^n P_{x,x}^k = 0.$$

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In addition, if x is aperiodic, then

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• For an irreducible Markov chain,

Unique stationary distribution exists \iff Markov chain is positive recurrent. Furthermore, in this case, $\pi(x) = \frac{1}{u_{rec}} > 0$ for all x.



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In addition, if *y* is positive recurrent, then

$$\lim_{n\to\infty} P_{x,y}^n = \frac{1}{\mu_{yy}} = \pi(y).$$



Ergodicity and Convergence to Stationary Distribution

Theorem (Ergodicity and Convergence to Stationary Distribution)

Consider a time-homogeneous DTMC $\{X_n\}_{n=0}^{\infty}$ on a discrete state space $\mathcal X$ with TPM P. Assume that $X_0=x$, and for each $n\in\mathbb N$, let π_n denote the PMF of X_n . If P is ergodic with associated stationary distribution π , then

$$\lim_{n o \infty} d_{\mathrm{TV}}(\pi_n, \pi) = \lim_{n o \infty} rac{1}{2} \|\pi_n - \pi\|_1 = 0,$$

where d_{TV} denotes the total variation distance.



Ergodic Theorem



Ergodic Theorem

Theorem (Ergodic Theorem)

For an ergodic Markov chain $\{X_n\}_{n=0}^{\infty}$ on a finite state space \mathcal{X} with TPM P, stationary distribution π , and any starting state $X_0 = x \in \mathcal{X}$,

$$rac{N_{\gamma}(n)}{n} \stackrel{\mathrm{a.s.}}{\longrightarrow} \pi(\gamma) \qquad orall \gamma \in \mathcal{X},$$

where $N_y(n)$ is the number of times the Markov chain visits state y up to time n. More generally, for any bounded, continuous function $f: \mathcal{X} \to \mathbb{R}$ and for any starting state $X_0 = x \in \mathcal{X}$,

$$\frac{1}{n}\sum_{k=1}^{n}f(X_{k}) \xrightarrow{\text{a.s.}} \sum_{\mathbf{y}\in\mathcal{X}}f(\mathbf{y})\,\pi(\mathbf{y}).$$



Proof of Theorem

• Proof of first part of the theorem is an exercise (see Homework 6)

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- To prove the second part of the theorem, observe that

$$\frac{1}{n} \sum_{k=1}^{n} f(X_k) = \sum_{\gamma \in \mathcal{X}} f(x) \frac{N_{\gamma}(n)}{n}$$

The result then follows from part 1



Markov Chain Monte Carlo Methods

Objective

To evaluate a sum of the form

$$I = \sum_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \, \pi(\mathbf{x}),$$

for given functions $f, \pi : \mathcal{X} \to \mathbb{R}$, where π is a probability distribution on \mathcal{X} . Here, $\mathcal{X} \subseteq \mathbb{R}^d$ for some d.

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- Direct sampling from π (via ITT or rejection sampling methods) may be difficult
- High dimensionality: d may be large (e.g., 10000)
- h and/or π may have complex expressions, making it difficult to compute the sum



Metropolis-Hastings Algorithm



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• The method also applies when ${\mathcal X}$ is countable or uncountable



• Let Q be any row-stochastic matrix on $\mathcal{X} \times \mathcal{X}$, i.e.,

$$Q_{\mathbf{x},\mathbf{y}} > 0, \qquad \sum_{\mathbf{y}} Q_{\mathbf{x},\mathbf{y}} = 1 \qquad \forall \mathbf{x},\mathbf{y} \in \mathcal{X}.$$



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- The entries of S are chosen in such a way that $0 < A_{x,y} \le 1$ for all $x, y \in \mathcal{X}$
- A is called the acceptance matrix



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• Claim: The TPM of $\{X_n\}_{n=0}^{\infty}$ will have π as the unique stationary distribution!

• For any $x, y \in \mathcal{X}$, we have

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• It then follows that for all $x, y \in \mathcal{X}$,

$$\pi(x) P_{x,y} = \left(\pi(x) Q_{x,y} \pi(y) Q_{y,x} \right) \cdot \frac{S_{x,y}}{\pi(x) Q_{x,y} + \pi(y) Q_{y,x}} = \pi(y) P_{y,x}.$$

• Therefore, $\pi(x) = \sum_{y} \pi(y) P_{x,y}$ for all x, thus proving that π is a stationary distribution



References



Monte carlo sampling methods using markov chains and their applications. *Biometrika*, 1970.

N Metropolis, A Rosenbluth, MN Rosenbluth, AH Teller, and E Teller. Perspective on "equation of state calculations by fast computing machines". *J. Chem. Phys.*, 21:1087–1092, 1953.