# Accelerated simulated annealing with fast cooling

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# Introduction

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- As we shall see, it involves studying the convergence of a non-homogeneous Markov chain/process.
- Our focus today is an accelerated version of simulated annealing proposed by Choi.
- Reference: "An accelerated variant of simulated annealing that converges under fast cooling" arXiv:1901.10269

# Introduction

- Let $\pi$ be a discrete or continuous distribution.
  **Goal**: Sample from $\pi$ or estimate $\pi(f)$, where

$$\pi(f) = \sum_x f(x)\pi(x), \quad \text{or} \quad \pi(f) = \int f(x)\pi(dx).$$

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- **Difficulty**: At times it is impossible to apply classical Monte Carlo methods, since $\pi$ is often of the form
  $$\pi(x) = \frac{e^{-\beta H(x)}}{Z},$$
  where $Z$ is a normalization constant that cannot be computed.
- **Idea of Markov chain Monte Carlo (MCMC)**: Construct a Markov chain that converges to $\pi$, which only depends on the ratio
  $$\frac{\pi(y)}{\pi(x)}.$$
  Thus there is no need to know $Z$.

# The Metropolis-Hastings algorithm

- In our talk today, we will focus on **continuous-time** Metropolis-Hastings algorithm.
- Two ingredients:
  **(i). Target distribution**: $\pi$
  **(ii). Proposal chain** with generator $Q = (Q(x, y))_{x,y}$.

# The Metropolis-Hastings algorithm

**Algorithm 1:** The Metropolis-Hastings algorithm

**Input:** Proposal chain $Q$, target distribution $\pi$

1 (Generate the proposal): Given $X_t$, propose the next jump $Y_{t+s} \sim Q(X_t, \cdot)$ according to Q, say at time $t+s$

2 (Acceptance-rejection): Take

$$X_{t+s} = \begin{cases} Y_{t+s}, & \text{with probability } \alpha(X_t, Y_{t+s}), \\ X_t, & \text{with probability } 1 - \alpha(X_t, Y_{t+s}), \end{cases}$$

where

$$\alpha(x, y) := \min \left\{ \frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}, 1 \right\}$$

is known as the acceptance probability.

# The Metropolis-Hastings algorithm

## Definition

The Metropolis-Hastings algorithm, with proposal chain $Q$ and target distribution $\pi$, is a Markov chain $X = (X_t)_{t \geq 0}$ with generator

$$M_1(x,y) = \begin{cases} \alpha(x,y)Q(x,y), & \text{for } x \neq y, \\ -\sum_{y;\ y \neq x} M_1(x,y), & \text{for } x = y. \end{cases}$$

# The Metropolis-Hastings (MH) algorithm

**Theorem**

*Given target distribution $\pi$ and proposal chain $Q$, the Metropolis-Hastings chain is*

- ***reversible*** *with respect to $\pi$, that is, for all $x, y$,*

$$\pi(x)M_1(x,y) = \pi(y)M_1(y,x).$$

- *(Ergodic theorem of MH) If $P$ is irreducible, then*

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t f(X_s)\, ds = \pi(f).$$

# Simulated annealing

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# Simulated annealing

- **Goal**: Find the global minimizers of a target function $U$.
- **Idea of simulated annealing**: Construct a **non-homogeneous** Metropolis-Hastings Markov chain that converges to $\pi_\infty$, which is supported on the set of global minima of $U$.
- Target distribution: Gibbs distribution $\pi_{T(t)}$ with temperature $T(t)$ that depends on time $t$

$$\pi_{T(t)}(x) = \frac{e^{-U(x)/T(t)}}{Z_{T(t)}},$$

$$Z_{T(t)} = \sum_x e^{-U(x)/T(t)}.$$

Proposal chain $Q$: symmetric

# Simulated annealing

- The temperature cools down $T(t) \to 0$ as $t \to \infty$, and we expect the Markov chain get "frozen" at the set of global minima $U_{min}$:

$$\pi_\infty(x) := \lim_{t\to\infty} \pi_{T(t)}(x) = \begin{cases} \dfrac{1}{|U_{min}|}, & \text{for } x \in U_{min}, \\ 0, & \text{for } x \notin U_{min}. \end{cases}$$

$$U_{min} := \{x;\ U(x) \le U(y) \text{ for all } y\}.$$

# Simulated annealing

**Algorithm 2:** Simulated annealing

**Input:** Symmetric proposal chain $Q$, target distribution $\pi_{T(t)}$, temperature schedule $T(t)$

1 (Generate the proposal): Given $X_t$, propose the next jump $Y_{t+s} \sim Q(X_t, \cdot)$ according to Q, say at time $t+s$

2 (Acceptance-rejection): Take

$$X_{t+s} = \begin{cases} Y_{t+s}, & \text{with probability } \alpha_t(X_t, Y_{t+s}), \\ X_t, & \text{with probability } 1 - \alpha_t(X_t, Y_{t+s}), \end{cases}$$

where

$$\alpha_t(x,y) := \min\left\{ \frac{\pi_{T(t)}(y)Q(y,x)}{\pi_{T(t)}(x)Q(x,y)}, 1 \right\} = \min\left\{ e^{\frac{U(x)-U(y)}{T(t)}}, 1 \right\}$$

is the acceptance probability.

# Simulated annealing

## Definition

Simulated annealing, with proposal chain $Q$, target distribution $\pi_{T(t)}$ and temperature schedule $T(t)$, is a non-homogeneous Markov chain with generator at time $t$ to be

$$M_{1,t}(x,y) = \begin{cases} \alpha_t(x,y)Q(x,y), & \text{for } x \neq y, \\ -\sum_{y;\ y \neq x} M_{1,t}(x,y), & \text{for } x = y. \end{cases}$$

# Optimal cooling schedule

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**Theorem (Hajek '88, Holley and Stroock '88)**

*The Markov chain generated by simulated annealing converges to $\pi_\infty$ in total variation distance if and only if for any $\epsilon > 0$,*

$$T(t) = \frac{c_{M_1} + \epsilon}{\ln(t+1)},$$

*where $c_{M_1}$ is known as the optimal hill-climbing constant that depends on the target function $U$ and proposal chain $Q$.*

# What is $c_{M_1}$?

- $c_{M_1}$ is the highest hill one need to climb from a local minimum to a global minimum.
- **A path $\gamma$ from $x$ to $y$**: any sequence of points starting from $x_0 = x, x_1, x_2, \ldots, x_n = y$ such that $Q(x_{i-1}, x_i) > 0$ for $i = 1, 2, \ldots, n$.

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- $\Gamma^{x,y}$ := set of paths from $x$ to $y$.
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- $\text{Elev}(\gamma)$ := highest elevation along a path $\gamma \in \Gamma^{x,y} = \max\{U(\gamma_i); \gamma_i \in \gamma\}$
- $H(x, y) := \min\{\text{Elev}(\gamma);\ \gamma \in \Gamma^{x,y}\}$.

**Definition**

$$c_{M_1} = c_{M_1}(Q, U) := \max_{x,y}\{H(x, y) - U(x) - U(y)\}.$$

# Accelerated Metropolis-Hastings $M_2$

- There are many variants of Metropolis-Hastings with improved convergence, e.g. lifting (Chen et al. '99), non-reversible MH (Hwang et al. 93, Bierkens '16), ...

# Accelerated Metropolis-Hastings $M_2$

- There are many variants of Metropolis-Hastings with improved convergence, e.g. lifting (Chen et al. '99), non-reversible MH (Hwang et al. 93, Bierkens '16), ...
- Today we will focus on a variant that we call $M_2$ (Choi SPA '19+, Choi and Huang JTP '19+)

# Accelerated Metropolis-Hastings $M_2$

## Definition

With proposal chain $Q$ and target distribution $\pi$, the accelerated MH is a Markov chain with generator $M_2$ given by

$$M_2(x,y) = \begin{cases} \max\left\{ \dfrac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)}, 1 \right\} Q(x,y), & \text{for } x \neq y, \\ -\sum_{y;\ y \neq x} M_2(x,y), & \text{for } x = y. \end{cases}$$

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- Recall that $M_1(x,y) = \min\left\{\dfrac{\pi(y)Q(y,x)}{\pi(x)Q(x,y)}, 1\right\}Q(x,y)$ for $x \neq y$.

# Accelerated Metropolis-Hastings $M_2$

We write $\langle f, g\rangle_\pi := \sum f(x)g(x)\pi(x)$ and $\lambda_2(M_i) := \inf_{\langle 1,f\rangle_\pi=0;\ \langle f,f\rangle_\pi\leq 1}\langle -M_i f, f\rangle_\pi$ is the spectral gap of $M_i$ for $i = 1, 2$.

**Theorem (Comparison between $M_1$ and $M_2$)**

*Given target distribution $\pi$ and proposal chain $Q$, $M_2$ is*

- ***reversible*** *with respect to $\pi$, that is, for all $x, y$,*

$$\pi(x)M_2(x, y) = \pi(y)M_2(y, x).$$

- $\langle M_2 f, f\rangle_\pi \leq \langle M_1 f, f\rangle_\pi$
- $\lambda_2(M_2) \geq \lambda_2(M_1)$.

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- $\langle M_2 f, f\rangle_\pi \leq \langle M_1 f, f\rangle_\pi$
- $\lambda_2(M_2) \geq \lambda_2(M_1)$.

For more comparison results between $M_1$ and $M_2$, see Choi and Huang '19+.

# Accelerated simulated annealing

## Definition

Accelerated simulated annealing, with proposal chain $Q$, target distribution $\pi_{T(t)}$ (i.e. the Gibbs distribution) and temperature schedule $T(t)$, is a non-homogeneous Markov chain with generator at time $t$ to be

$$M_{2,t}(x,y) = \begin{cases} \max\left\{ \dfrac{\pi_{T(t)}(y)Q(y,x)}{\pi_{T(t)}(x)Q(x,y)}, 1 \right\} Q(x,y), & \text{for } x \neq y, \\ -\sum_{y;\ y \neq x} M_{2,t}(x,y), & \text{for } x = y. \end{cases}$$

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- Recall the dynamics of classical simulated annealing:

$$M_{1,t}(x,y) = \min\left\{ \frac{\pi_{T(t)}(y)Q(y,x)}{\pi_{T(t)}(x)Q(x,y)}, 1 \right\} Q(x,y) \text{ for } x \neq y.$$

# Main results

- The general message is that we can operate **faster** cooling schedule on $M_{2,t}$ than $M_{1,t}$!

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- The general message is that we can operate **faster** cooling schedule on $M_{2,t}$ than $M_{1,t}$!
- Similar to the classical case, the convergence behaviour of $M_{2,t}$ depends critically on a constant we call $c_{M_2}$.

# Main results

**Theorem (Choi '19)**

- ***Case 1:*** $c_{M_2} > 0$
  *The Markov chain generated by* $M_{2,t}$ *converges to* $\pi_\infty$ *in total variation distance if for any* $\epsilon > 0$,

$$T(t) = \frac{c_{M_2} + \epsilon}{\ln(t+1)}.$$

# Main results

## Theorem (Choi '19)

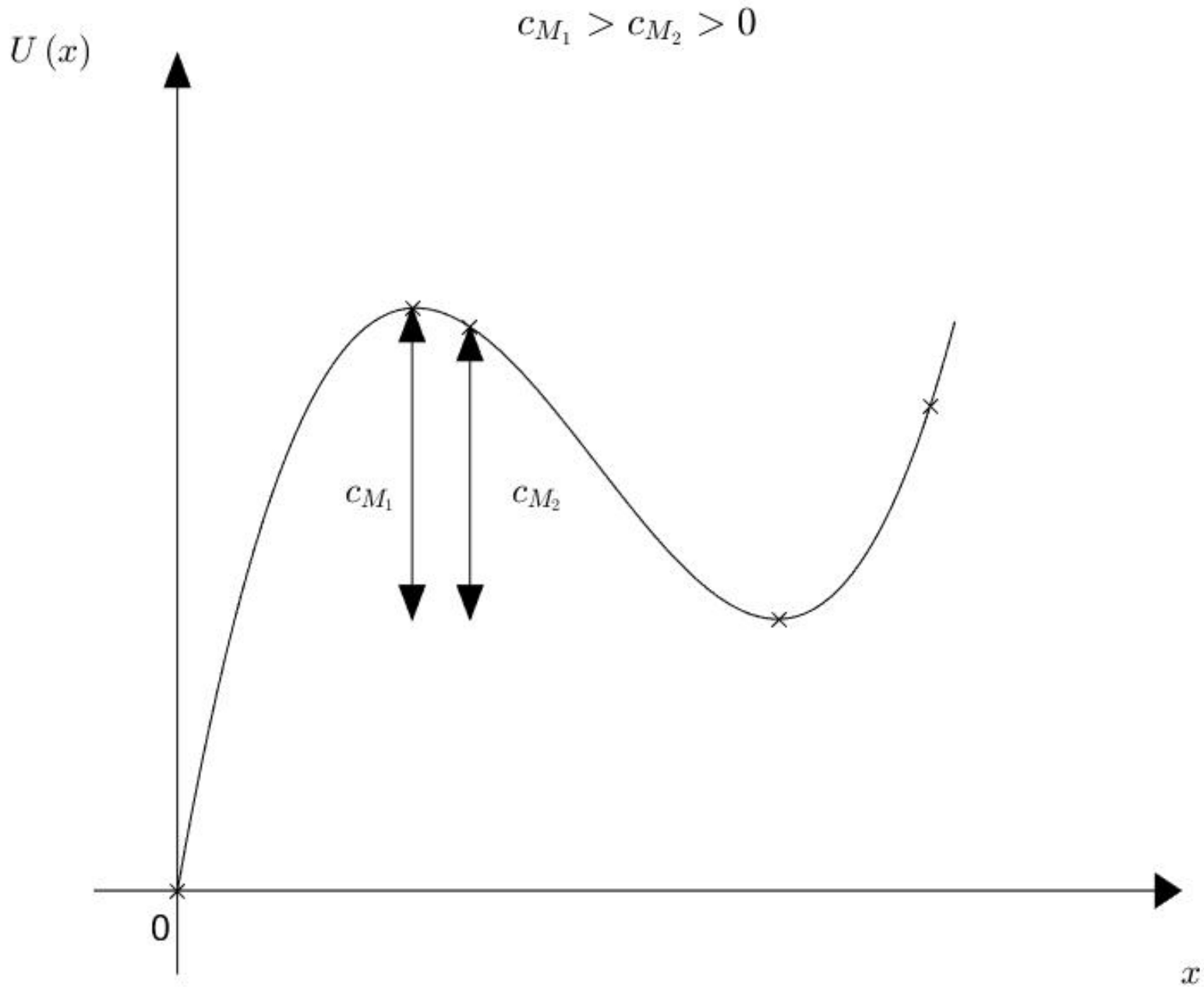
- ***Case 2:*** $c_{M_2} \leq 0$
  *The Markov chain generated by $M_{2,t}$ converges to $\pi_\infty$ in total variation distance if $T(t)$ satisfies*

$$\lim_{t\to\infty} \left(\frac{d}{dt}T(t)\right) \frac{e^{\frac{c_{M_2}}{T(t)}}}{T(t)^2} = 0.$$

  *Examples of fast cooling schedule that satisfy the above requirement are*

  1. *(power law cooling)* $T(t) = (t+1)^{-\alpha}$, *where* $\alpha \in (0,1)$.
  2. *(powers of logarithmic cooling)* $T(t) = (\log(t+1))^{-k}$, *where* $k > 1$.
  3. $T(t) = (t+1)^{-\alpha}\,(\log(t+1))^{-1}$, *where* $\alpha \in (0,1)$.

# What is $c_{M_2}$?



# What is $c_{M_2}$?

- $c_{M_1} := \max_{x,y \in \mathcal{X}} \{H(x,y) - U(x) - U(y)\}$ = largest hill to climb from a local minimum to a global minimum.

# What is $c_{M_2}$?

- $c_{M_1} := \max_{x,y \in \mathcal{X}} \{H(x,y) - U(x) - U(y)\}$ = largest hill to climb from a local minimum to a global minimum.
- $c_{M_2} := \max_{x,y \in \mathcal{X}} \left\{ \max_{\substack{z,w \in \gamma^{x,y},\ z=\gamma_i^{x,y}, w=\gamma_{i+1}^{x,y} \text{ for some } i \\ \text{Elev}(\gamma^{x,y}) = H(x,y)}} U(z) \wedge U(w) - U(x) - U(y) \right\} \approx$ second largest hill to climb from a local minimum to a global minimum
- $c_{M_1} \geq c_{M_2}$. When $U$ has distinct values, $c_{M_1} > c_{M_2}$.

# Main results

**Theorem ($X^{M_2}$ effectively escapes local minimum while $X^{M_1}$ may get trapped under fast cooling)**

*Suppose that $x$ is a local minimum of $U$ and under any cooling schedule,*

$$\mathbb{P}_x(X_t^{M_2} = x \ \forall t \geq 0) = 0.$$

*Under cooling schedule of the form*

$$T(t) = \frac{d}{\log(t+1)},$$

*where $d < c_{M_1}$, then*

$$\mathbb{P}_x(X_t^{M_1} = x \ \forall t \geq 0) > 0.$$

# Summary

- Propose an accelerated simulated annealing $M_{2,t}$
  - ✓ Convergence guarantee under **fast** cooling that depends on $c_{M_2}$. The optimal cooling schedule can be faster than logarithmic cooling depending on $Q$ and $U$.
  - ✓ With probability 1 it will escape local minimum even under fast cooling
  - × Relatively hard to simulate

# Summary

- Propose an accelerated simulated annealing $M_{2,t}$
  - ✓ Convergence guarantee under **fast** cooling that depends on $c_{M_2}$. The optimal cooling schedule can be faster than logarithmic cooling depending on $Q$ and $U$.
  - ✓ With probability 1 it will escape local minimum even under fast cooling
  - × Relatively hard to simulate
- Classical simulated annealing $M_{1,t}$
  - × Convergence guarantee under **slow** cooling that depends on $c_{M_1}$
  - × With positive probability it can get stuck in local minimum under fast cooling
  - ✓ Relatively easy to simulate

Thank you! Question(s)?