

Markov Chain Monte Carlo in Statistics - Recent Advances

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Outline

- **Design Principle of a MCMC Scheme**
- **Generalized Gibbs**
- **Multipoint Metropolis Methods**
- **Evolutionary Monte Carlo**
- **Perfect Sampling**
- **Dynamic Weighting**

One Basic Problem of Monte Carlo

- Draw random variable

$$\mathbf{x} \sim \pi(\mathbf{x})$$

often used for simulating complex systems

- It may not be easy to draw \mathbf{x} directly!
→ MCMC (Markov Chain Monte Carlo).

A MCMC Scheme

- A MCMC sampler with transition functions $A_i(\mathbf{x}, \mathbf{y})$

$$\mathbf{x}^{(0)} \xrightarrow{x^{(1)} \sim A_1(\mathbf{x}^{(0)}, \mathbf{x}^{(1)})} \mathbf{x}^{(1)} \xrightarrow{x^{(2)} \sim A_2(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})} \mathbf{x}^{(2)} \dots$$

- Key Theory:

If a Markov chain

- irreducible
- aperiodic
- possesses an invariant distribution π

then the chain will become stationary at π .

- Principle: Design a transition function $A(\mathbf{x}, \mathbf{y})$ that leaves the target distribution $\pi(\mathbf{x})$ invariant.

Invariance and Detailed Balance

- $A(\mathbf{x}, \mathbf{y})$ leaves $\pi(\mathbf{x})$ invariant if

$$\int \pi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) d\mathbf{x} = \pi(\mathbf{y})$$

$$\mathbf{x}^{(t)} = \mathbf{x} \sim \pi \xrightarrow{y \sim A(\mathbf{x}, \mathbf{y})} \mathbf{x}^{(t+1)} = \mathbf{y} \sim \pi$$

- Detailed balance:

$$\pi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{y}) A(\mathbf{y}, \mathbf{x})$$

It ensures invariance since

$$\int \pi(\mathbf{x}) A(\mathbf{x}, \mathbf{y}) d\mathbf{x} = \int \pi(\mathbf{y}) A(\mathbf{y}, \mathbf{x}) d\mathbf{x} = \pi(\mathbf{y}) \int A(\mathbf{y}, \mathbf{x}) d\mathbf{x} = \pi(\mathbf{y})$$

Gibbs Sampler

- Purpose: Draw from a Joint Distribution

$$\mathbf{x} = (x_1, \dots, x_d) \sim \pi(\mathbf{x})$$

- Method: Iterative Conditional Sampling

$$\forall i \quad \mathbf{x} = (x_i, \mathbf{x}_{[-i]})$$

$$\text{draw } x_i' \sim \pi(x_i' | \mathbf{x}_{[-i]})$$

$$\text{let } \mathbf{y} = (x_i', \mathbf{x}_{[-i]})$$

Metropolis-Hastings Algorithm

- Draw \mathbf{y} from a proposal distribution $T(\mathbf{x}, \mathbf{y})$.

- Accept \mathbf{y} with probability

$$r(\mathbf{x}, \mathbf{y}) = \min \left\{ 1, \frac{\pi(\mathbf{y})T(\mathbf{y}, \mathbf{x})}{\pi(\mathbf{x})T(\mathbf{x}, \mathbf{y})} \right\}$$

and stay at \mathbf{x} with probability $1-r(\mathbf{x}, \mathbf{y})$.

Note: One can check that detailed balance is satisfied.

Beyond Invariance

Make the Markov chain explore the relevant space quickly and reach stationarity quickly!

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Gibbs Sampler

$\forall i \quad \mathbf{x} = (x_i, \mathbf{x}_{[-i]})$

draw $x_i' \sim \pi(x_i' | \mathbf{x}_{[-i]})$

let $\mathbf{y} = (x_i', \mathbf{x}_{[-i]})$



draw $\gamma \sim \pi(x_i + \gamma | \mathbf{x}_{[-i]})$
let $\mathbf{y} = \gamma(\mathbf{x}) = (x_i + \gamma, \mathbf{x}_{[-i]})$

a transformation

Group Moves

Try moving along an arbitrary direction...

Given any fixed direction $\mathbf{e} = (e_1, \dots, e_d)$

$$\gamma(\mathbf{x}) = \mathbf{x} + \gamma\mathbf{e} = (x_1 + \gamma e_1, \dots, x_d + \gamma e_d)$$

Try scaling...

$$\gamma(\mathbf{x}) = \gamma\mathbf{x} = (\gamma x_1, \dots, \gamma x_d)$$

* Generalized Gibbs

Form of the transition function $A(\mathbf{x}, \mathbf{y})$:

- selecting a transformation $\gamma \in \Gamma$
- letting $\mathbf{y} = \gamma(\mathbf{x})$.

Question: What distribution should one draw $\gamma \in \Gamma$ from so that $\pi(\mathbf{x})$ is left invariant?

A Theorem

- $\Gamma = \{\text{all } \gamma\}$ is a locally compact group
- L is its left-Haar measure
- $\gamma \sim p_{\mathbf{x}}(\gamma) \propto \pi(\gamma(\mathbf{x})) |J_{\gamma}(\mathbf{x})| L(d\gamma)$

where

$$J_{\gamma}(\mathbf{x}) = \det \left\{ \frac{\partial \gamma(\mathbf{x})}{\partial \mathbf{x}} \right\}$$

is the Jacobian of the transformation

If $\mathbf{x} \sim \pi(\mathbf{x})$, then $\mathbf{y} = \gamma(\mathbf{x}) \sim \pi$.

Note: A left-Haar measure satisfies

$$\forall \gamma_0 \in \Gamma, \forall B \subset \Gamma, L(B) = L(\gamma_0 B)$$

Translation group along an arbitrary direction...

Given any fixed direction $\mathbf{e} = (e_1, \dots, e_d)$

$$\Gamma = \left\{ \gamma \in \mathbb{R}^1 : \gamma(\mathbf{x}) = \mathbf{x} + \gamma \mathbf{e} = (x_1 + \gamma e_1, \dots, x_d + \gamma e_d) \right\}$$

Draw $\gamma \sim p_{\mathbf{x}}(\gamma) \propto \pi(\mathbf{x} + \gamma \mathbf{e})$

Let $\mathbf{y} = \gamma(\mathbf{x}) = \mathbf{x} + \gamma \mathbf{e}$

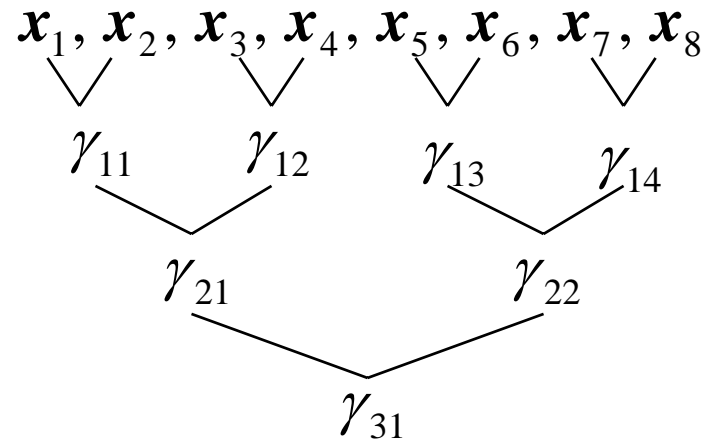
Scale-transformation Group...

$$\Gamma = \{\gamma \in \mathbb{R}^1 \setminus \{0\} : \gamma(\mathbf{x}) = (\gamma x_1, \dots, \gamma x_d)\}$$

Draw $\gamma \sim p_{\mathbf{x}}(\gamma) \propto |\gamma|^{d-1} \pi(\gamma \mathbf{x})$

Let $\mathbf{y} = \gamma(\mathbf{x}) = \gamma \mathbf{x}$

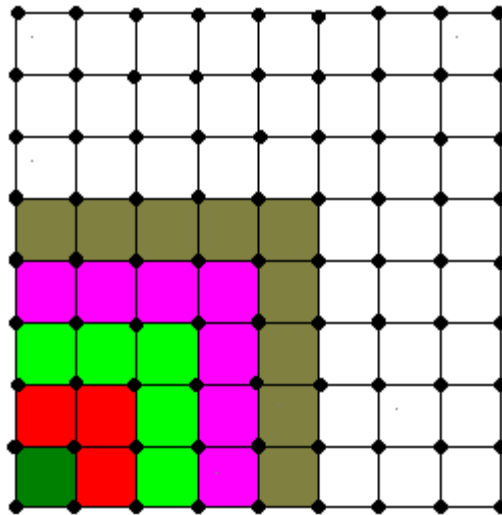
More Examples of Group Moves



In general, for any subset S of $\{1, \dots, 8\}$,
 $\{x_i, i \in S\}$ can be moved together.

$z = \{z_\sigma, \text{ all lattice points}\}$

$$\pi(z) \propto e^{-\beta H(z)}$$



In general, for any subset S of the lattice points, $\{z_\sigma, \sigma \in S\}$ can be moved together.

If we can't directly draw from $p_x(\gamma)$

- MCMC transition function $A_x(\gamma, \gamma')$
 - need to leave $p_x(\gamma)$ invariant
 - need to be “transformation invariant”

$$A_x(\gamma, \gamma') = A_{\gamma_0(x)}(\gamma\gamma_0^{-1}, \gamma'\gamma_0^{-1})$$

group
operation

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Difficulty of Choosing The Proposal Distribution

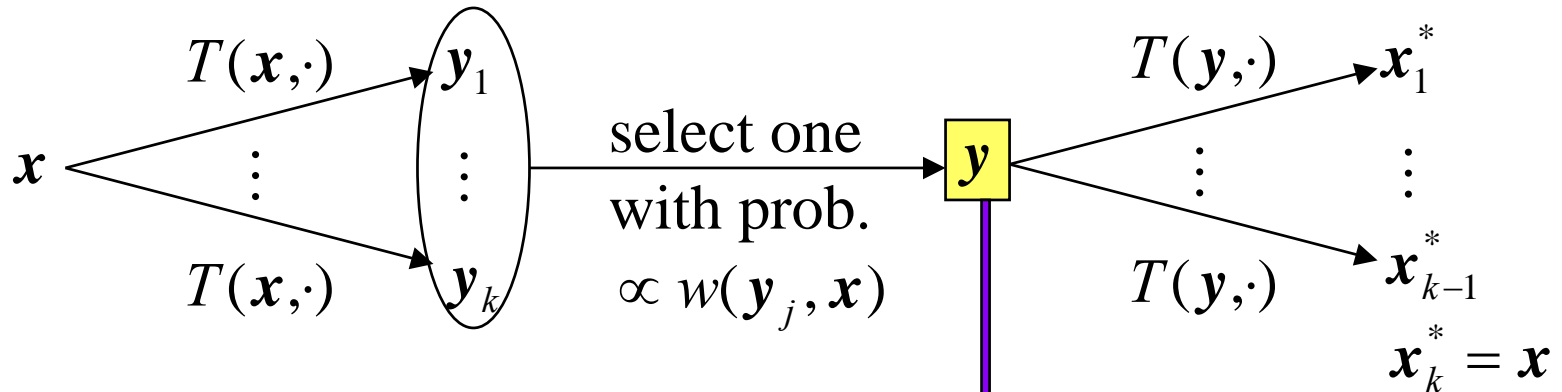
- small step size in the proposal distribution
→ slow movement of the Markov chain
- large step size in the proposal distribution
→ low acceptance rate

In both cases, the chain moves slowly!

* Multipoint Metropolis Methods

- Idea: make multiple proposals and select a good one from them.
- Guiding principle: leaving the target distribution $\pi(\mathbf{x})$ invariant!

Independent Multipoint Proposals



accept with prob. $r_g = \min \left\{ 1, \frac{w(\mathbf{y}_1, \mathbf{x}) + \dots + w(\mathbf{y}_k, \mathbf{x})}{w(\mathbf{x}_1^*, \mathbf{y}) + \dots + w(\mathbf{x}_k^*, \mathbf{y})} \right\}$

reject with prob. $1 - r_g$

- Remark 1:

$$w(\mathbf{x}, \mathbf{y}) = \pi(\mathbf{x})T(\mathbf{x}, \mathbf{y})\lambda(\mathbf{x}, \mathbf{y})$$

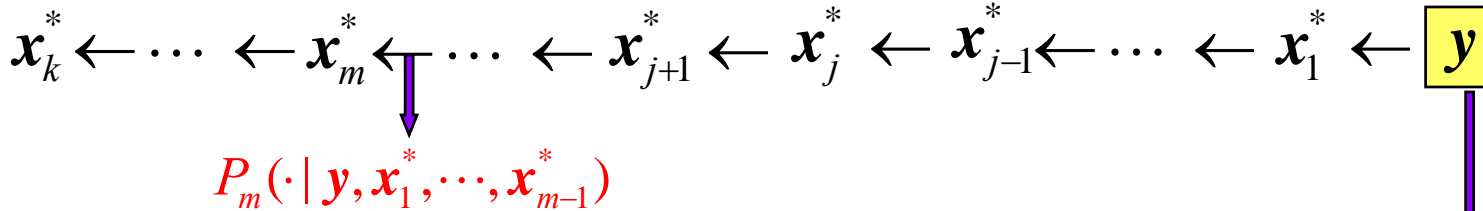
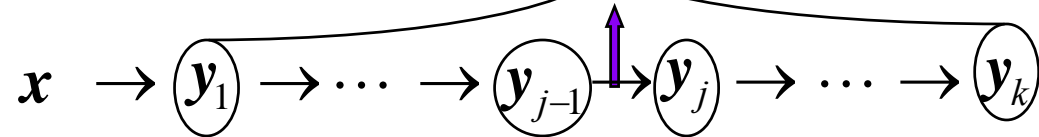
where $\lambda(\mathbf{x}, \mathbf{y})$ is a non-negative symmetric function that can be chosen by the user.

- Remark 2: Detailed balance is satisfied.

Correlated Multipoint Proposals

select one with prob.
 $\propto w(\mathbf{y}_{[l:1]}, \mathbf{x})$

suppose $\mathbf{y} = \mathbf{y}_j$
 $P_j(\cdot | \mathbf{x}, \mathbf{y}_1, \dots, \mathbf{y}_{j-1})$



accept with prob. $r = \min \left\{ 1, \frac{w(\mathbf{y}_1, \mathbf{x}) + \dots + w(\mathbf{y}_{[k:1]}, \mathbf{x})}{w(\mathbf{x}_1^*, \mathbf{y}) + \dots + w(\mathbf{x}_{[k:1]}^*, \mathbf{y})} \right\}$

reject with prob. $1 - r$

■ Remark 1:

$$P_j(\mathbf{y}_{[j:1]} | \mathbf{x}) = P_1(\mathbf{y}_1 | \mathbf{x}) \cdots P_j(\mathbf{y}_j | \mathbf{x}, \mathbf{y}_{[1:j-1]})$$

$$w_j(\mathbf{y}_{[j:1]}, \mathbf{x}) = \pi(\mathbf{x}) P_j(\mathbf{y}_{[j:1]} | \mathbf{x}) \lambda_j(\mathbf{x}, \mathbf{y}_{[1:j]})$$

where $\lambda_j(\mathbf{x}, \mathbf{y}_{[1:j]})$ is a sequentially symmetric function that can be chosen by the user:

$$\lambda_j(a, b, \dots, z) = \lambda_j(z, \dots, b, a)$$

■ Remark 2: Detailed balance is satisfied.

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Population-based “Learning” Strategy

- conduct parallel Monte Carlo Markov chains
- interactions among the multiple chains in the “population”
 - mutation
 - crossover
 - exchange

purpose: improve “fitness” of the members

* Evolutionary Monte Carlo In A Tempering Framework

- Target distribution:

$$\pi(\mathbf{x}) \propto \exp\{-H(\mathbf{x})\}$$

- Population: $\mathbf{X}=\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\}$

$$\pi(\mathbf{x}_i) \propto \exp\{-H(\mathbf{x}_i)/t_i\}$$

$$1=t_1 < t_2 < \dots < t_m$$

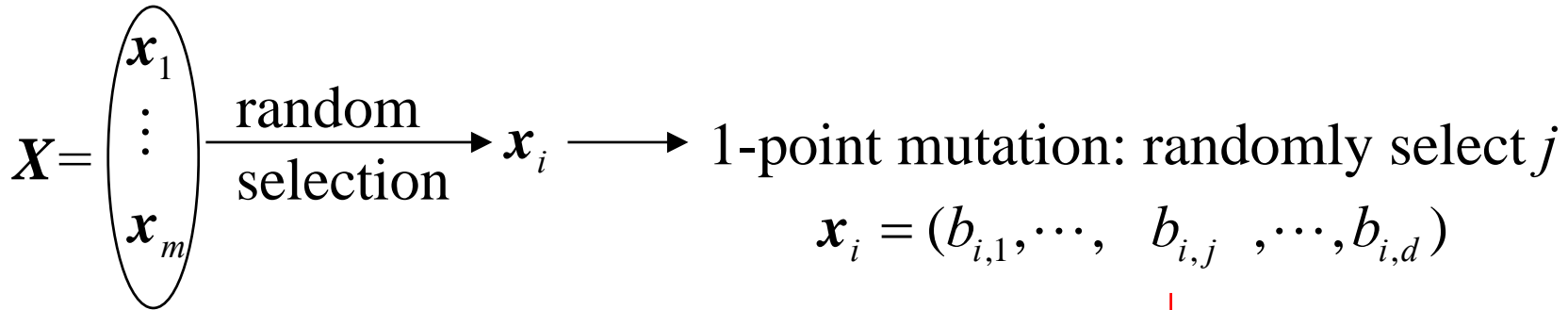
- Target distribution of the population: the augmented Boltzmann distribution

$$\pi(\mathbf{X}) \propto \exp\left\{-\sum_{i=1}^m H(\mathbf{x}_i)/t_i\right\}$$

- Example: binary-coded state space

$$\mathbf{x}_i = (b_{i,1}, \dots, b_{i,d}), \quad i = 1, \dots, m$$

Mutation



$$\mathbf{x}_i = (b_{i,1}, \dots, b_{i,j}, \dots, b_{i,d})$$



$$\mathbf{y}_i = (b_{i,1}, \dots, 1 - b_{i,j}, \dots, b_{i,d})$$

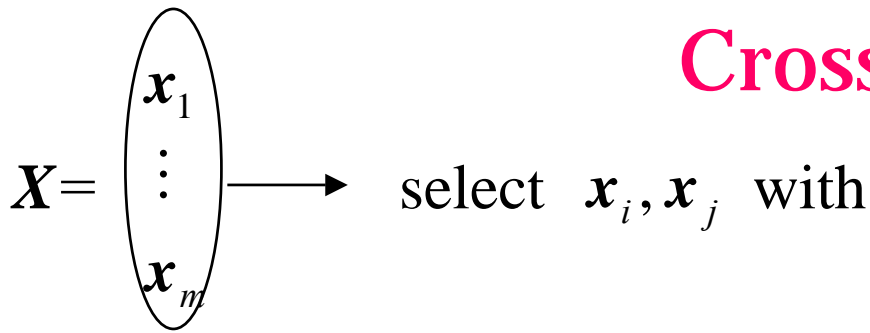
$$\mathbf{Y} = \{\mathbf{x}_1, \dots, \mathbf{y}_i, \dots, \mathbf{x}_m\}$$



accept with prob.

$$\min \left\{ 1, \frac{\pi(\mathbf{Y})}{\pi(\mathbf{X})} = \exp\{-(H(\mathbf{y}_k) - H(\mathbf{x}_k)) / t_k\} \right\}$$

Crossover



$$P((\mathbf{x}_i, \mathbf{x}_j) | \mathbf{X}) \propto [\exp\{-H(\mathbf{x}_i)/t_s\} + \exp\{-H(\mathbf{x}_j)/t_s\}] \quad \mathbf{x}_i \neq \mathbf{x}_j$$

→ 1-point crossover: randomly select position k

$$\mathbf{x}_i = (b_{i,1}, \dots, b_{i,k}, \dots, b_{i,d}) \quad \mathbf{x}_j = (b_{j,1}, \dots, b_{j,k}, \dots, b_{j,d})$$

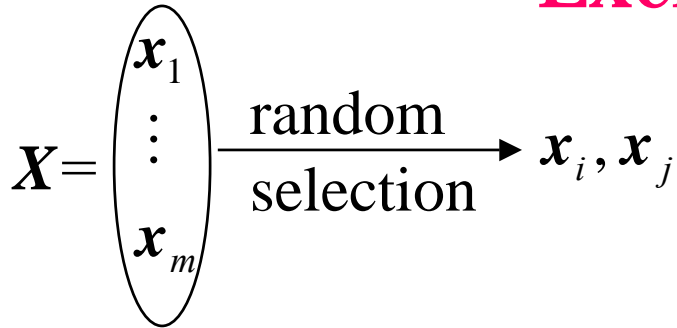
$$\mathbf{y}_i = (b_{i,1}, \dots, b_{j,k}, \dots, b_{i,d}) \quad \mathbf{y}_j = (b_{j,1}, \dots, b_{i,k}, \dots, b_{j,d})$$

$$\mathbf{Y} = \{\mathbf{x}_1, \dots, \mathbf{y}_i, \dots, \mathbf{y}_j, \dots, \mathbf{x}_m\}$$

accept with prob.

$$\min \left\{ 1, \frac{\pi(\mathbf{Y})T(\mathbf{Y}, \mathbf{X})}{\pi(\mathbf{X})T(\mathbf{X}, \mathbf{Y})} = \exp \left\{ -\frac{H(\mathbf{y}_i) - H(\mathbf{x}_i)}{t_i} - \frac{H(\mathbf{y}_j) - H(\mathbf{x}_j)}{t_j} \right\} \frac{T(\mathbf{Y}, \mathbf{X})}{T(\mathbf{X}, \mathbf{Y})} \right\}$$

Exchange



\longrightarrow exchange

$$\mathbf{X} = \{ \mathbf{x}_1, \dots, \mathbf{x}_i, \dots, \mathbf{x}_j, \dots, \mathbf{x}_m \}$$

$$\mathbf{Y} = \{ \mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_i, \dots, \mathbf{x}_m \}$$



accept with prob.

$$\min \left\{ 1, \frac{\pi(\mathbf{Y})}{\pi(\mathbf{X})} = \exp \left\{ - (H(\mathbf{x}_i) - H(\mathbf{x}_j)) (1/t_j - 1/t_i) \right\} \right\}$$

Continuous Sample Space: Mutation

Any kind of Metropolis-Hasting move independently for each chain!

Continuous Sample Space: Snooker Crossover

$$X = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{pmatrix}$$

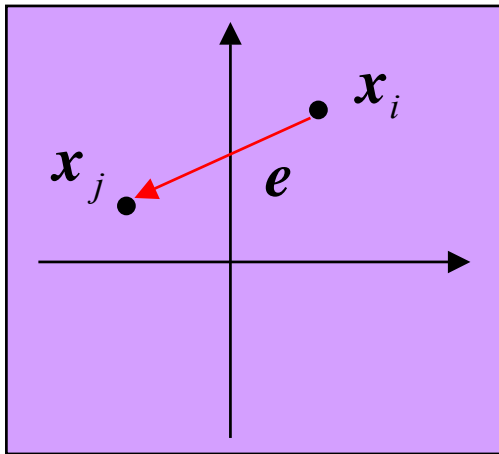
random
selection

$$\mathbf{x}_i$$

select “anchor”

$\mathbf{x}_j \in X \setminus \{\mathbf{x}_i\}$ with prob.

$$\propto \exp\{-H(\mathbf{x}_j)/t_s\}$$



→ let

$$\mathbf{e} = \frac{\mathbf{x}_j - \mathbf{x}_i}{\|\mathbf{x}_j - \mathbf{x}_i\|}$$

draw $\gamma \sim p(\gamma) \propto |\gamma|^{d-1} \pi(\mathbf{x}_i + \gamma \mathbf{e})$

let $\mathbf{y}_i = \pi(\mathbf{x}_i + \gamma \mathbf{e})$

new population

$$Y = \{\mathbf{x}_1, \dots, \mathbf{y}_i, \dots, \mathbf{x}_m\}$$

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An Observation

- If a Markov chain had been started from the infinite past

starting point

$$t = -\infty$$

$$\mathbf{x}_{-\infty}$$

.....

$$t = 0$$

$$\mathbf{x}_0 \sim \pi$$

stationary

The Idea of Coupling

- Assume finite Markov chain: $\mathcal{X} = \{1, \dots, |\mathcal{X}|\}$

$t = -1$

\mathbf{x}_{-1}

$t = 0$

$\mathbf{x}_0 \sim A(\mathbf{x}_{-1}, \cdot)$

$\mathbf{x}_0 = \phi(u_0, \mathbf{x}_{-1})$

(1) Compute

$$G(\mathbf{x}_{-1}, j) = \sum_{k=1}^j A(\mathbf{x}_{-1}, k) = \Pr(\mathbf{x}_0 \leq j \mid \mathbf{x}_{-1})$$

(2) generate $u_0 \sim \text{Uniform}(0, 1)$

(3) Let $\mathbf{x}_0 = j$ if

$$G(\mathbf{x}_{-1}, j-1) < u_0 \leq G(\mathbf{x}_{-1}, j)$$

- The chains starting from all possible states at $t=-1$ are *coupled by the same random number* u_0 .

* Perfect Sampling

- If u_0 makes all the chain “coupled”, that is,

$$\forall i \quad \phi(u_0, i) \equiv j_0$$

then $\mathbf{x}_0 = j_0 \sim \pi$

starting point

$$t = -\infty$$

$$\mathbf{x}_{-\infty}$$

.....

$$t = -1$$

$$\exists i \quad \mathbf{x}_{-1} = i$$

$$t = 0$$

$$\mathbf{x}_0 \equiv j_0$$

stationary

$$\sim \pi$$

If the chains are not coupled in one step...

$$\begin{aligned}\mathbf{x}_{-(n-1)} &= \phi(u_{-(n-1)}, \mathbf{x}_{-n}) \\ \Rightarrow \mathbf{x}_0 &= \phi(u_0, \phi(u_{-1}, \dots, \phi(u_{-(n-1)}, \mathbf{x}_{-n}) \dots))\end{aligned}$$

■ Equivalently,

- The sequence of uniform random variables

$$\dots, u_{-n}, \dots, u_{-1}, u_0$$

are given in advance

- From the infinite past, we compose

$$\dots, \mathbf{x}_{-n}, \dots, \mathbf{x}_{-1}, \mathbf{x}_0$$

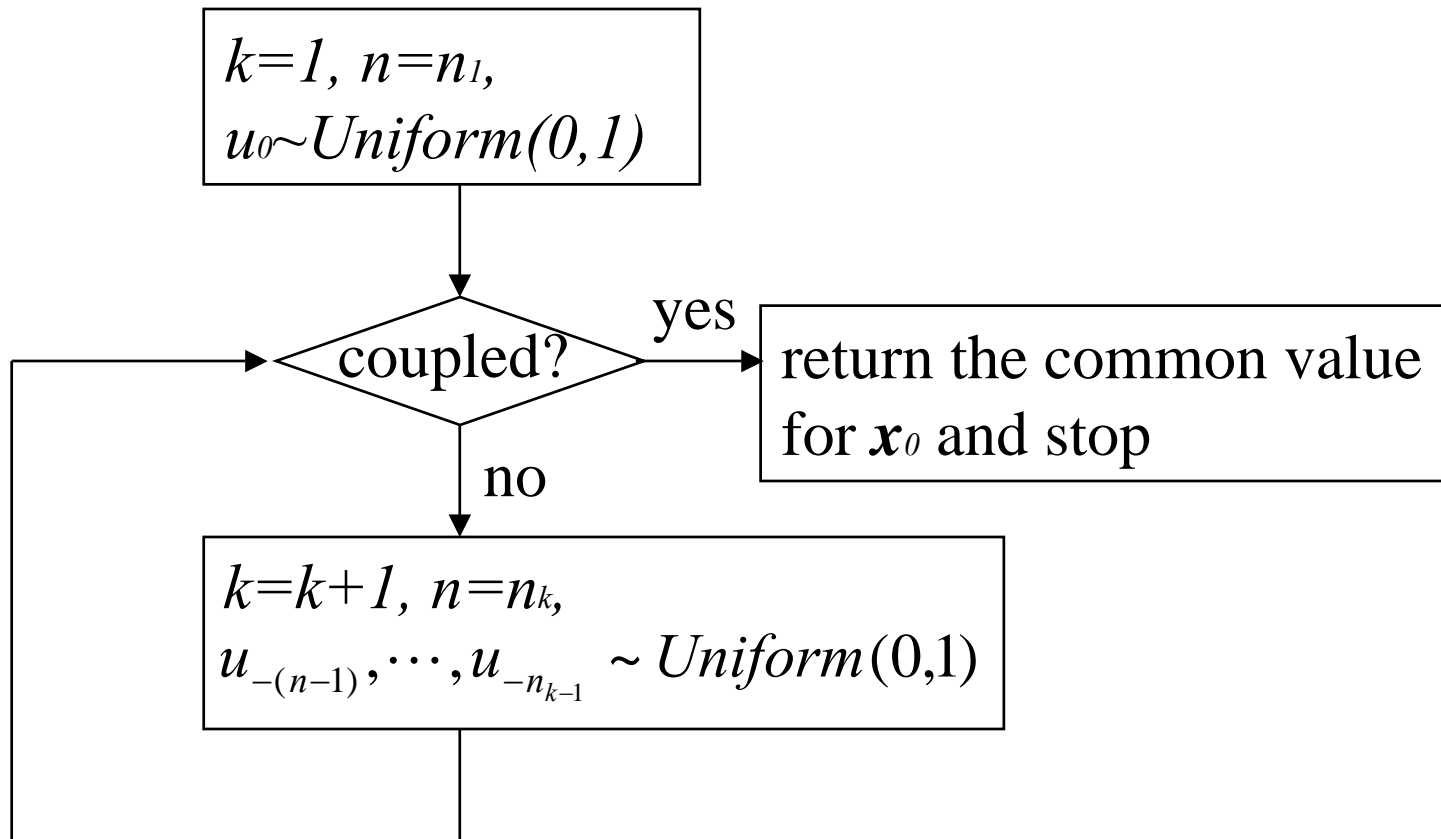
- If $\forall i \phi(u_0, \phi(u_{-1}, \dots, \phi(u_{-(n-1)}, i) \dots)) = j_0$
then $\mathbf{x}_0 = j_0 \sim \pi$

starting point

$$\begin{array}{ccccccc}
 t = -\infty & \dots\dots & t = -n & \dots\dots & t = 0 & \text{stationary} \\
 \mathbf{x}_{-\infty} & & \exists i \quad \mathbf{x}_{-n} = i & & \mathbf{x}_0 \equiv j_0 & \sim \pi
 \end{array}$$

The Conceptual Algorithm

schedule : $1 = n_1 < n_2 < n_3 < \dots$



$\dots \dots u_{-(n_k-1)}, \dots, u_{-n_{k-1}} \dots \dots u_{-(n_2-1)}, \dots, u_{-1} \quad u_0$

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Weighted Sample

- Augment the sample space from \mathcal{X} to $\mathcal{X} \times \mathbb{R}^+$ to include a weight variable for each state.

$$\mathbf{x} \rightarrow (\mathbf{x}, w)$$

- Suppose $f(\mathbf{x}, w)$ is the joint distribution of (\mathbf{x}, w) . \mathbf{x} is correctly weighted by w with respect to π if

$$\sum_w wf(\mathbf{x}, w) \propto \pi(\mathbf{x})$$

Note: we can estimate $E_\pi[h(\mathbf{x})]$ by

$$\frac{\sum_{i=1}^n w_i h(\mathbf{x}_i)}{\sum_{i=1}^n w_i} \quad \text{where } (\mathbf{x}_i, w_i) \sim f, i = 1, \dots, n$$

New Design Principle

- IWIW (Invariance With respect to Importance Weighting).
 - A transition rule $A(\mathbf{x}, w; \mathbf{y}, w')$ satisfies IWIW if

$$f(\mathbf{x}, w) \xrightarrow{A(\mathbf{x}, w; \mathbf{y}, w')} f'(\mathbf{y}, w')$$

correctly
weighted wrt π

correctly
weighted wrt π

* Dynamic Weighting

M-type move: Given $(\mathbf{x}_t, w_t) = (\mathbf{x}, w)$ at iteration t .

- Draw \mathbf{x}_{t+1} from a transition function that leaves π invariant.
- Set $w_{t+1} = w$.

R-type move: Given $(\mathbf{x}_t, w_t) = (\mathbf{x}, w)$ at iteration t .

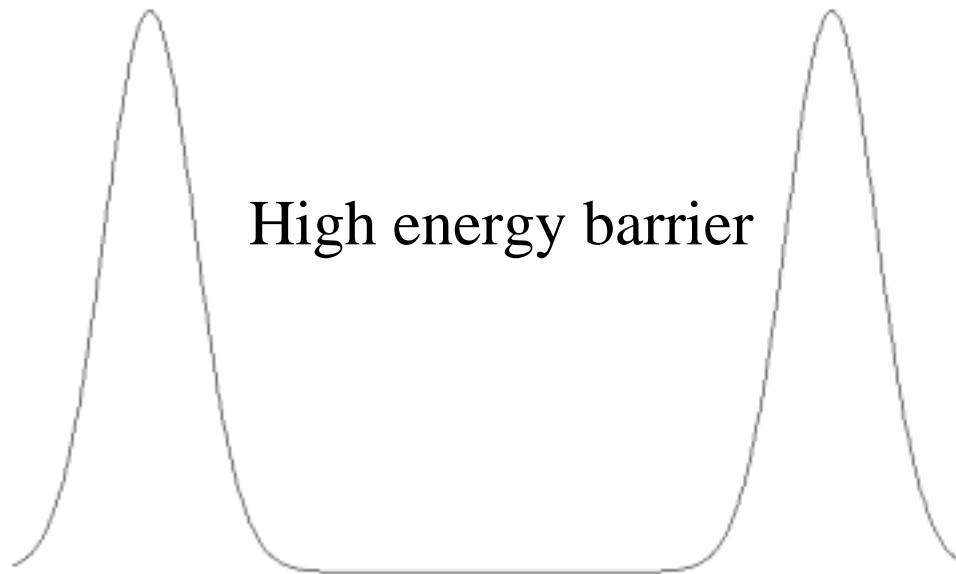
- Propose \mathbf{y} from $T(\mathbf{x}, \mathbf{y})$ and compute

$$r(\mathbf{x}, \mathbf{y}) = \frac{\pi(\mathbf{y})T(\mathbf{y}, \mathbf{x})}{\pi(\mathbf{x})T(\mathbf{x}, \mathbf{y})}$$

- Choose $\theta = \theta(\mathbf{x}, w) > 0$, and draw $U \sim \text{Uniform}(0, 1)$. Let

$$(\mathbf{x}_{t+1}, w_{t+1}) = \begin{cases} (\mathbf{y}, wr(\mathbf{x}, \mathbf{y}) + \theta) & \text{if } U \leq \frac{wr(\mathbf{x}, \mathbf{y})}{wr(\mathbf{x}, \mathbf{y}) + \theta} \\ \left(\mathbf{x}, \frac{w(wr(\mathbf{x}, \mathbf{y}) + \theta)}{\theta} \right) & \text{otherwise} \end{cases}$$

Waiting Time Infinity \rightarrow Importance Weight Infinity



- In the standard Metropolis process, the waiting time to cross over the barriers is infinite.
- The dynamic weighting process can cross the energy barrier, but has “importance weight infinity”.

Combinatory Strategy

- Use the weighted moves when proposing large changes in the system.
- Use the standard Metropolis or Gibbs moves for local exploration.

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Thanks!