

MARKOV CHAIN MONTE CARLO

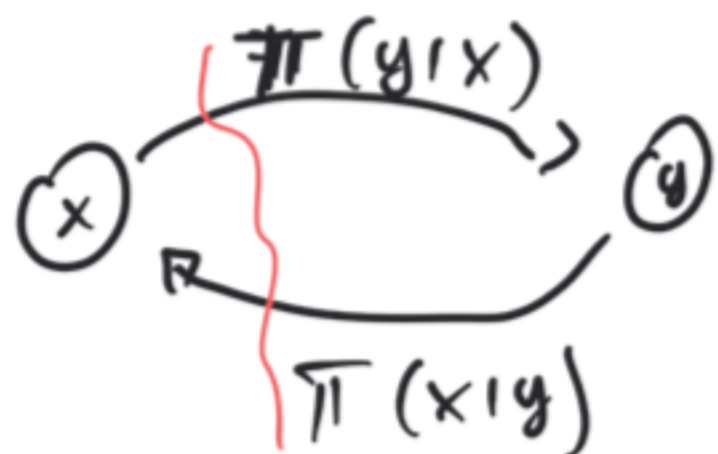
$p(x)$ difficult to sample.

1) SAMPLE $p(x)$

2) COMPUTE $E[f(x)] = \int f(x)p(x)dx$

Idea: construct ~~new~~ DTMC s.t. $p(x)$ is steady state for it.

DETAILED BALANCE



$$p(x) \pi(y|x) = p(y) \pi(x|y)$$

If p satisfies detailed balance, then

$$\underline{p} = \underline{p} \underline{\pi}, \text{ i.e. } p \text{ is invariant.}$$

For continuous state space, we have a KERNEL $K(x|y)$, $x, y \in S$ (here $\mathbb{R}, \mathbb{R}^n, S \subseteq \mathbb{R}^n$), t.c. measurable in y and is a distribution w.r.t. x .

$$\text{Typically } K(x|y) = \mathcal{N}(y, \sigma^2)$$

UPDATE RULE ↓ METROPOLIS-HASTINGS

GOAL: SAMPLE $p(x)$

FIX A PROPOSAL DISTRIBUTION (KERNEL):

$$q(x^* | x).$$

ERGODIC (IRREDUCIBLE)
(POSITIVE RECURRENT)

1) SAMPLE x^* FROM $q(x^* | x)$ (we are in x)

2) ACCEPT x^* with probability

$$A(x^* | x) = \min \left\{ 1, \frac{p(x^*) q(x | x^*)}{p(x) q(x^* | x)} \right\}$$

$$\left. \frac{p(x^*) q(x | x^*)}{p(x) q(x^* | x)} \right\}$$

otherwise stay in x .

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$$K(y | x) = \underbrace{q(y | x) A(y | x)}_{y \neq x} + \underbrace{\int_{x^*} \delta(y - x^*) p(x^*)}_{y = x}$$

$$r(x) = 1 - \int q(z | x) A(z | x) dz$$

prob. of staying in x

Let's prove the DBC! Fix $x \neq y$

$$P(x) q(y|x) A(y|x) = \min \left\{ P(x) q(y|x), \frac{P(y) q(x|y)}{P(x) q(y|x)} \right\}$$

this is
the DBC

$$= \min \{ P(x) q(y|x), P(y) q(x|y) \}$$

$$= P(y) q(x|y) A(x|y)$$

$P(x)$ is invariant, hence it is steady state!

$$\lim_{n \rightarrow \infty} P(X_n = x) = P(x)!$$

$$A = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_N \end{pmatrix}$$

$$A^n = \begin{pmatrix} \lambda_1^n & & 0 \\ & \ddots & \\ 0 & & \lambda_N^n \end{pmatrix}$$

$$\sum \lambda_i = 1, \lambda_1^n = 1$$

$$\text{So } \lambda_2, \dots, \lambda_N < 1 \quad \lambda_j^n \rightarrow 0$$

$$\lambda_2 > \lambda_3 > \dots > \lambda_N$$

$$\lambda_2^n > \lambda_3^n > \dots > \lambda_N^n$$

MIXING COEFFICIENT.

$$A(y|x) = \min \left\{ 1, \frac{P(y) q(x|y)}{P(x) q(y|x)} \right\}$$

[We just need to know $P(x)$ up to a normalization coefficient!

If $q(x|y) = q(y|x)$ is symmetric, then

$A(y|x) = \min\left\{1, \frac{p(y)}{p(x)}\right\}$ \rightarrow METROPOLIS update rule!

On: The VARIANCE of the proposal distribution q is crucial to have a chain that MIXES WELL

MIXTURES AND CYCLES OF UPDATE KERNELS

Let q_1 and q_2 be two proposal distributions.

1) APPLY q_1 and q_2 in sequence $q_1(y|x) A_1(y|x) q_2(z|y) A_2(z|y) A_1(z|y) A_2(y|x)$

2) MIXTURES, $\alpha > 0, \alpha < 1$ $q(y|x) = \alpha q_1(y|x) + (1-\alpha) q_2(y|x)$

GIBBS SAMPLER

We have $p(x_1, \dots, x_n)$ and we know how to sample from $p(x_j | \vec{x}_{-j})$

update step: SAMPLE $p(x_1 | x_{-1}) \leftarrow$

SAMPLE $p(x_j | x_{-j}) \leftarrow$

SAMPLE $p(x_n | x_{-n})$

$$q_j(y|x) = \begin{cases} p(y_j | x_{-j}) & \text{if } y_j = x_j \\ 0 & \text{otherwise} \end{cases}$$

$$\vec{x}_{-j} = x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n$$

$$q_j(y|x) = \int_0^1 P(y_j | x_{-j}) \quad \text{if } y_j = x_j$$

$$q_j(y|x) = \min \left\{ 1, \frac{P(y) q_j(x|y)}{P(x) q_j(y|x)} \right\}$$

In the Gibbs sampler,
we accept every step
with prob. 1.
(FIXED SCAN G.S.)

$$\frac{P(y) P(y_j | y_{-j}) P(x_j | y_{-j})}{P(x) P(x_j | x_{-j}) P(y_j | x_{-j})} = 1$$

$P(x)$

$$x_{-j} = y_{-j}$$

RANDOM SEQUENCE SCAN G.S.

SAMPLE $\{j \in \{1, \dots, n\} \text{ unif.}\}$
SAMPLE FROM q_j

We need to check $P(x_j | x_{-j})$ is ergodic
(This is true if $P(x_j | x_{-j})$ is non-zero everywhere in S)