

# Monte Carlo Markov Chain methods

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# Markov Chains

- Defined by transition probability  $T_m(Z^m, Z^{m+1})$
- For time homogeneous chains  $T_m$  is same for all  $m$ .

# Markov Chains (cont)

## Stationary Distribution

A distribution  $p$  is stationary with respect to Markov chain defined by transition probability  $T$  if

$$p(z) = \sum_{z'} T(z', z) p(z')$$

# Detailed Balance

## Theorem

*Given  $p$ , if we choose  $T$  such that detailed balance equation is satisfied then  $p$  will be stationary distribution for this  $T$ .*

$$p(z)T(z, z') = p(z')T(z', z)$$

## Proof.

$$\begin{aligned}\sum_{z'} p(z')T(z', z) &= \sum_{z'} p(z)T(z, z') && \text{by hypothesis} \\ &= p(z) \sum_{z'} T(z, z') \\ &= p(z)\end{aligned}$$



# Metropolis-Hastings Algorithm

- Generalizes Metropolis algorithm
- No need for proposal distribution to be symmetric
- Acceptance probability for proposal of  $z^*$  from  $z^\tau$

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

Where  $\tilde{p}(z)$  is the unnormalized density at  $z$  and  $q(z|z')$  is a proposal distribution at  $z'$ .

- Note that for symmetric  $q$ , this boils down to Metropolis algorithm
- Transition probability is given by

$$T(z^\tau, z^*) = q(z^*|z^\tau)A(z^*, z^\tau)$$

We will prove that our target distribution  $p$  (i.e. normalized version of  $\tilde{p}$ ) is stationary distribution with respect to transition probability defined in last slide by proving that it satisfies detailed balance condition. (detailed balance  $\implies$  stationary distribution)

## Proof.

$$\begin{aligned} p(z)T(z, z') &= p(z)q(z'|z)A(z', z) \\ &= p(z)q(z'|z)\min\left(1, \frac{\tilde{p}(z')q(z|z')}{\tilde{p}(z)q(z'|z)}\right) \\ &= \min\left(p(z)q(z'|z), p(z)q(z'|z)\frac{\tilde{p}(z')q(z|z')}{\tilde{p}(z)q(z'|z)}\right) \\ &= \min(p(z)q(z'|z), p(z')q(z|z')) \\ &= \min(p(z')q(z|z'), p(z)q(z'|z)) \\ &= p(z')q(z|z')\min\left(1, \frac{p(z)q(z'|z)}{p(z')q(z|z')}\right) \\ &= p(z')q(z|z')\min\left(1, \frac{\tilde{p}(z)q(z'|z)}{\tilde{p}(z')q(z|z')}\right) \\ &= p(z')T(z', z) \end{aligned}$$

# Gibbs Sampling

Metropolis-Hastings algorithm can be inefficient if proposal distribution is not chosen properly, as seen in demo. However if our target distribution is over  $m$  variables and we can compute conditional distribution  $p(z_m | z_{-m})$  where  $z_{-m}$  denotes all variables other than  $z_m$ , Gibbs sampling is efficient algorithm.



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## Algorithm

- initialize  $z_i \quad \forall i \in [1, 2, \dots, m]$
- for next step  $\tau + 1$ 
  - $z_1^{\tau+1} \sim p(z_1|z_2^\tau, z_3^\tau, \dots, z_m^\tau)$
  - $z_2^{\tau+1} \sim p(z_2|z_1^{\tau+1}, z_3^\tau, \dots, z_m^\tau)$
  - $\vdots$
  - $z_m^{\tau+1} \sim p(z_m|z_1^{\tau+1}, z_2^{\tau+1}, \dots, z_{m-1}^{\tau+1})$

First we will prove that this transitions leads to stationary distribution.

Proof.

$$\begin{aligned}& \sum_{z'} p(z') T(z', z) \\&= \sum_{z'_i} \sum_{z'_{-i}} T(z', z) p(z'_i | z'_{-i}) p(z'_{-i}) \\&= \sum_{z'_i} T(z', z) p(z'_i | z'_{-i}) p(z'_{-i}) \\&= p(z'_{-i}) \sum_{z'_i} p(z_i | z'_{-i}) p(z'_i | z'_{-i}) \\&= p(z'_{-i}) p(z_i | z'_{-i}) \sum_{z'_i} p(z'_i | z'_{-i}) \\&= p(z_{-i}) p(z_i | z_{-i}) \quad \text{because } z'_{-i} = z_{-i} \\&= p(z)\end{aligned}$$



# Gibbs sampling as a special case of Metropolis-Hastings

Gibbs sampling is a special case of Metropolis-Hastings in which proposal distribution is univariate conditional and no proposals are rejected. Thus is more efficient than simple MH algorithm.

Proof.

Suppose we are at about to do  $k$ th update in this iteration. Our proposal distribution is  $q(z^*|z) = p(z_k^*|z_{-k})$ . Let's calculate ratio of MH algorithm.

$$\begin{aligned} & \frac{p(z^*)q(z|z^*)}{p(z)q(z^*|z)} \\ &= \frac{p(z_k^*|z_{-k}^*)p(z_{-k}^*)p(z_k|z_{-k}^*)}{p(z_k|z_{-k})p(z_{-k})p(z_k^*|z_{-k})} \\ &= 1 \end{aligned} \quad \text{as } z_{-k}^* = z_{-k}$$