Approximate Inference via Sampling (1)

CS698X: Topics in Probabilistic Modeling and Inference

Piyush Rai

Plan

- Sampling to approximate distributions
- Basic sampling methods
- Markov Chain Monte Carlo (MCMC)

Sampling for Approximate Inference

- Some typical tasks that we have to solve in probabilistic/fully-Bayesian inference

Posterior distribution

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} = \frac{p(\mathcal{D}|\theta)p(\theta)}{\int p(\mathcal{D}|\theta)p(\theta)d\theta}$$

Posterior predictive distribution

$$p(\mathcal{D}^{new}|\mathcal{D}) = \int p(\mathcal{D}^{new}|\theta)p(\theta|\mathcal{D})d\theta = \mathbb{E}_{p(\theta|\mathcal{D})}[p(\mathcal{D}^{new}|\theta)]$$

Needed for model selection (and in computing posterior too)

Marginal likelihood

$$p(\mathcal{D}|m) = \int p(\mathcal{D}|\theta)p(\theta|m)d\theta = \mathbb{E}_{p(\theta|m)}[p(\mathcal{D}|\theta)]$$

Needed in EM

Expected complete data log-likelihood

$$\text{Exp-CLL} = \int p(z|\theta, x)p(x, z|\theta)dz = \mathbb{E}_{p(z|\theta,x)}[p(x, z|\theta)]$$

Needed in VI

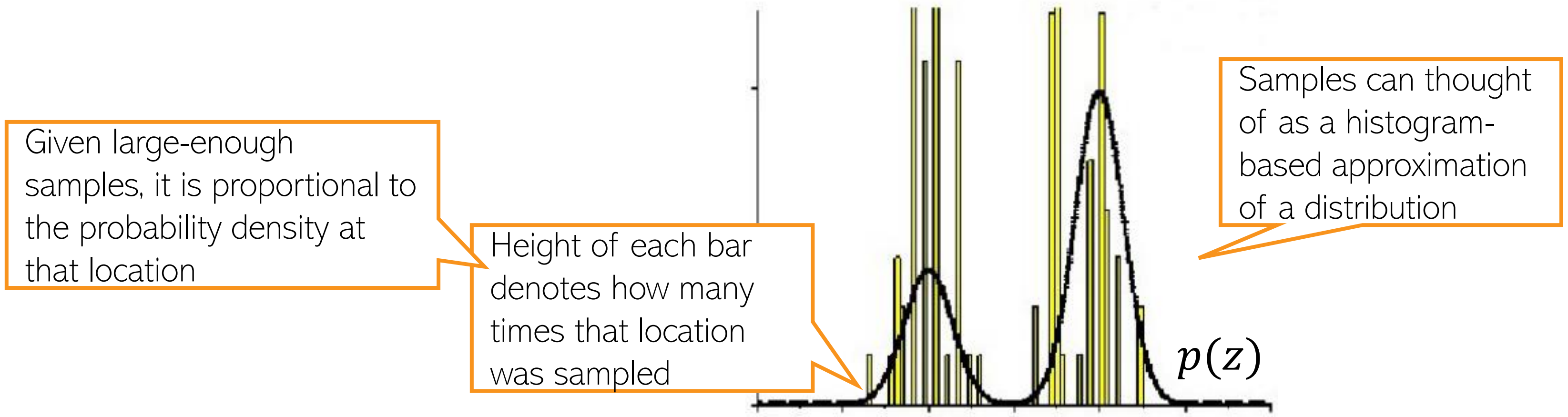
Evidence lower bound (ELBO)

$$\mathcal{L}(q) = \mathbb{E}_q[\log p(x, z)] - \mathbb{E}_q[\log p(z)]$$

- Sampling methods provide a general way to (approximately) solve these problems

Approximating a Prob. Distribution using Samples

- Can approximate any distribution using a set of randomly drawn samples from it



- The samples can also be used for computing expectations (Monte-Carlo averaging)
- Usually straightforward to generate samples if it is a simple/standard distribution
- The interesting bit: Even if the distribution is "difficult" (e.g., an intractable posterior), it is often possible to generate random samples from such a distribution, as we will see.

The Empirical Distribution

- Sampling based approx. can be formally represented using an empirical distribution
- Given L points/samples $\boldsymbol{z}^{(1)}, \boldsymbol{z}^{(2)}, \dots, \boldsymbol{z}^{(L)}$, empirical distr. defined by these is

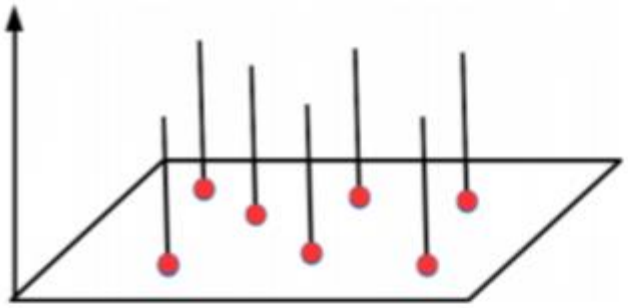
Dirac Distribution with finite support at $\boldsymbol{z}^{(1)}, \boldsymbol{z}^{(2)}, \dots, \boldsymbol{z}^{(L)}$

Weights sum to 1

Weight of point $\boldsymbol{z}^{(\ell)}$

$$p_L(A) = \sum_{\ell=1}^{L} w_\ell \delta_{\boldsymbol{z}^{(\ell)}}(A)$$

Can think of A as being the area over which we want to evaluate the distribution



Dirac Distribution

$$\delta_{\boldsymbol{z}}(A) = \begin{cases} 0 & \text{if} \quad \boldsymbol{z} \notin A \\ 1 & \text{if} \quad \boldsymbol{z} \in A \end{cases}$$

Sampling: Some Basic Methods

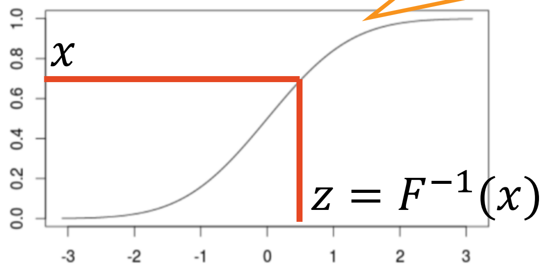
$$p(z) = q(x)\left|\frac{\partial x}{\partial z}\right|$$

Determinant of Jacobian

- Most of these basic methods are based on the idea of transformation
  - Generate a random sample x from a distribution $q(x)$ which is easy to sample from
  - Apply a transformation on x to make it random sample z from a complex distr $p(z)$

- Some popular examples of transformation methods
  - Inverse CDF method

$F(z)$: CDF of $p(z)$



$$x \sim \text{Unif}(0,1) \Rightarrow z = \text{Inv-CDF}_{p(z)}(x) \sim p(z)$$

  - Reparametrization method

$$x \sim \mathcal{N}(0,1) \Rightarrow z = \mu + \sigma x \sim \mathcal{N}(\mu, \sigma^2)$$

  - Box-Mueller method: Given (x_1, x_2) from $\mathbf{Unif}(-1,+1)$, generate (z_1, z_2) from $\mathcal{N}(\mathbf{0}, \mathbf{I}_2)$

$$z_1 = \sqrt{-2\ln x_1}\cos(2\pi x_2), \quad z_1 = \sqrt{-2\ln x_1}\sin(2\pi x_2)$$

- Transformation Methods are simple but have limitations
  - Mostly limited to standard distributions and/or distributions with very few variables

Rejection Sampling

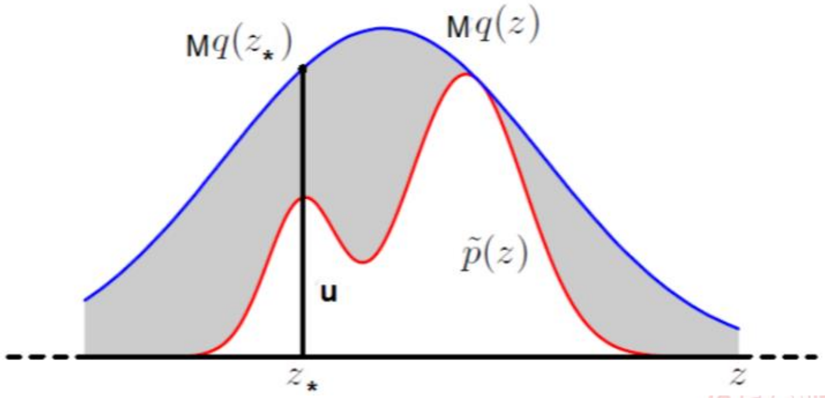
- Goal: Generate a random sample from a distribution of the form $p(z) = \frac{\tilde{p}(z)}{Z_p}$, assuming
  - We can only evaluate the value of numerator $\tilde{p}(z)$ for any z
  - The denominator (normalization constant) Z_p is intractable and we don't know its value

Should have the same support as $p(z)$

- Assume a proposal distribution $q(z)$ we can generate samples from, and

$$Mq(\mathbf{z}) \geq \tilde{p}(\mathbf{z}) \qquad \forall \mathbf{z} \quad (\text{where } M > 0 \text{ is some const.})$$

- Rejection Sampling then works as follows
  - Sample an random variable z_* from $q(z)$
  - Sampling a uniform r.v. $u \sim \text{Unif}[0, Mq(z_*)]$
  - If $u \leq \tilde{p}(z_*)$ then accept z_*, otherwise reject it



- All accepted z_*'s will be random samples from $p(z)$. Proof on next slide

Rejection Sampling

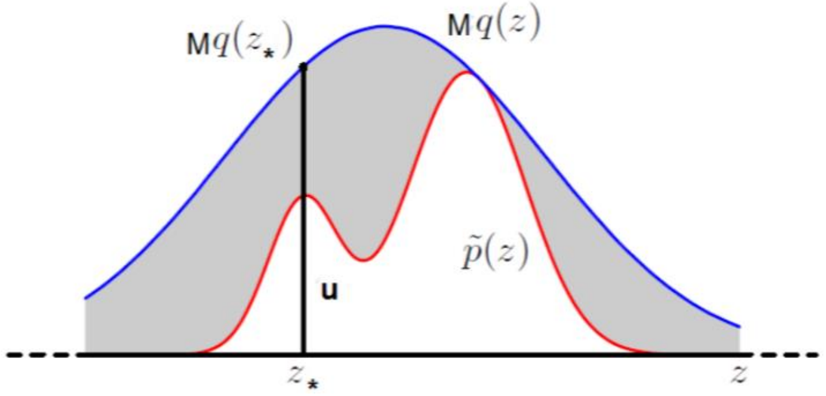
- Why $z \sim q(z)$ + accept/reject rule is equivalent to $z \sim p(z)$?
- Let's look at the pdf of the z's that were accepted, i.e., $p(z|\text{accept})$

$$p(\text{accept}|z) = \int_0^{\tilde{p}(z)} \frac{1}{Mq(z)} du = \frac{\tilde{p}(z)}{Mq(z)}$$

$$p(z, \text{accept}) = q(z) p(\text{accept}|z) = \frac{\tilde{p}(z)}{M}$$

$$p(\text{accept}) = \int \frac{\tilde{p}(z)}{M} dz = \frac{Z_p}{M}$$

$$p(z|\text{accept}) = \frac{p(z, \text{accept})}{p(\text{accept})} = \frac{\tilde{p}(z)}{Z_p} = p(z)$$



Computing Expectations via Monte Carlo Sampling

- Often we are interested in computing expectations of the form

$$\mathbb{E}[f] = \int f(z)p(z)dz$$

where $f(z)$ is some function of the random variable $z \sim p(z)$

- A simple approx. scheme to compute the above expectation: Monte Carlo integration
  - Generate L independent samples from $p(z)$: $\{z^{(\ell)}\}_{\ell=1}^{L} \sim p(z)$

    Assuming we know how to sample from $p(z)$

  - Approximate the expectation by the following empirical average

$$\mathbb{E}[f] \approx \hat{f} = \frac{1}{L}\sum_{\ell=1}^{L} f(z^{(\ell)})$$

- Since the samples are independent of each other, we can show the following

Unbiased expectation

$$\mathbb{E}[\hat{f}] = \mathbb{E}[f] \quad \text{and} \quad \text{var}[\hat{f}] = \frac{1}{L}\text{var}[f] = \frac{1}{L}\mathbb{E}[(f - \mathbb{E}[f])^2]$$

Variance in our estimate decreases as L increases

Computing Expectations via Importance Sampling

- How to compute Monte Carlo expec. if we don't know how to sample from $p(z)$?
- One way is to use transformation methods or rejection sampling
- Another way is to use Importance Sampling (assuming $p(z)$ can be evaluated at least)
  - Generate L indep samples from a proposal $q(z)$ we know how sample from: $\{z^{(\ell)}\}_{\ell=1}^{L} \sim q(z)$
  - Now approximate the expectation as follows

$$\mathbb{E}[f] = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz \approx \frac{1}{L}\sum_{\ell=1}^{L} f(z^{(\ell)})\frac{p(z^{(\ell)})}{q(z^{(\ell)})}$$

- This is basically "weighted" Monte Carlo integration
  - $w^{(\ell)} = \frac{p(z^{(\ell)})}{q(z^{(\ell)})}$ denotes the importance weight of each sample $z^{(\ell)}$

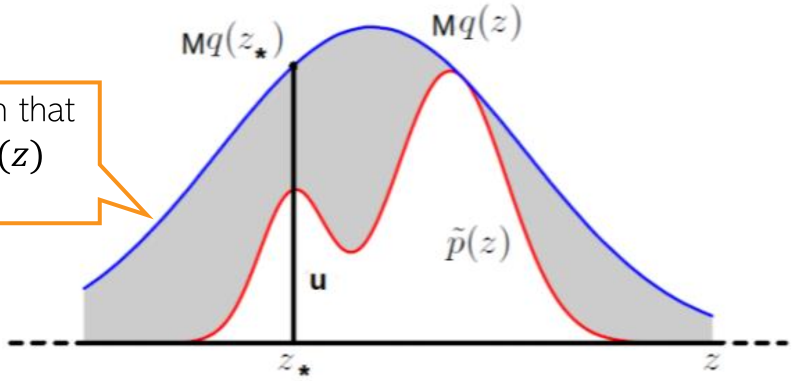
See PRML 11.1.4

- IS works even when we can only evaluate $p(z) = \frac{\tilde{p}(z)}{Z_p}$ up to a prop. constant
- Note: Monte Carlo and Importance Sampling are NOT sampling methods!
  - These are only uses for computing expectations (approximately)

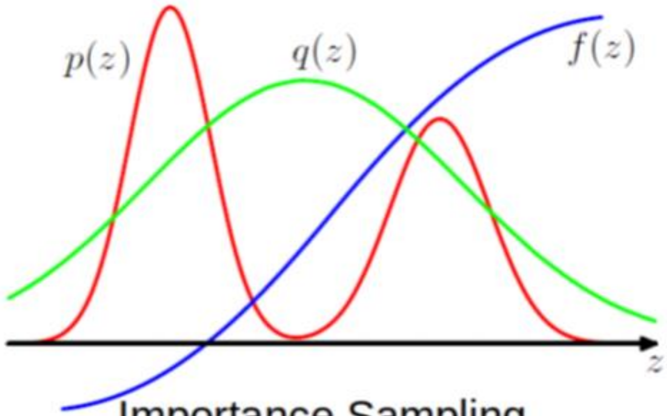
Limitations of the Basic Methods

- Transformation based methods: Usually limited to drawing from standard distributions
- Rejection Sampling and Importance Sampling: Require good proposal distributions

$q(z)$ should be such that $Mq(z)$ envelopes $\tilde{p}(z)$ everywhere



Rejection Sampling



Importance Sampling

$$\mathbb{E}[f] \approx \frac{1}{L}\sum_{\ell=1}^{L} f(z^{(\ell)})\frac{p(z^{(\ell)})}{q(z^{(\ell)})}$$

Ideally, would like $q(z)$ to give samples from where $p(z)$ is large or $f(z)p(z)$ is large

Difficult to guarantee so if z is high-dimensional

- In general, difficult to find good prop. distr. especially when z is high-dim
- More sophisticated sampling methods like MCMC work well in such high-dim spaces

Markov Chain Monte Carlo (MCMC)

If the target is a posterior, it will be conditioned on data, i.e., $p(\boldsymbol{z}|\boldsymbol{x})$

- Goal: Generate samples from some target distribution $p(\boldsymbol{z}) = \frac{\tilde{p}(\boldsymbol{z})}{Z_p}$

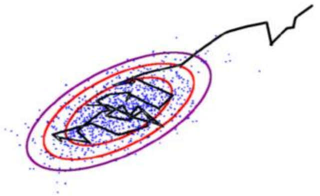
$\boldsymbol{z}$ usually is high-dim

- Assume we can evaluate $p(\boldsymbol{z})$ at least up to a proportionality constant

Means we can at least evaluate $\tilde{p}(\boldsymbol{z})$

- MCMC uses a Markov Chain which, when converged, starts giving samples from $p(z)$

$$\underbrace{\boldsymbol{z}^{(1)} \rightarrow \boldsymbol{z}^{(2)} \rightarrow \boldsymbol{z}^{(3)} \rightarrow}_{\text{initial samples typically garbage}} \ldots \rightarrow \underbrace{\boldsymbol{z}^{(L-2)} \rightarrow \boldsymbol{z}^{(L-1)} \rightarrow \boldsymbol{z}^{(L)}}_{\text{after convergence, actual samples from } p(\boldsymbol{z})}$$

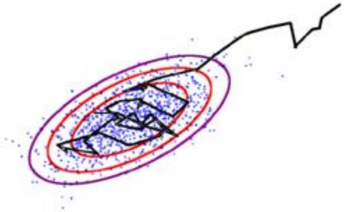


- Given current sample $\boldsymbol{z}^{(\ell)}$ from the chain, MCMC generates the next sample $\boldsymbol{z}^{(\ell+1)}$ as
  - Use a proposal distribution $q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$ to generate a candidate sample $\boldsymbol{z}_*$
  - Accept/reject $\boldsymbol{z}_*$ as the next sample based on an acceptance criterion (will see later)
  - If accepted, set $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}_*$. If rejected, set $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^{(\ell)}$

Should also have the same support as $p(\boldsymbol{z})$

- Important: The proposal distribution $q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$ depends on the previous sample $\boldsymbol{z}^{(\ell)}$

MCMC: The Basic Scheme



- The chain run infinitely long (i.e., upon convergence) will give ONE sample from $p(\boldsymbol{z})$
- But we usually require several samples to approximate $p(\boldsymbol{z})$

MCMC is exact in theory but approximate in practice since we can't run the chain for infinitely long in practice

Thus we say that the samples are approximately from the target distribution

- This is done as follows
  - Start the chain at an initial $\boldsymbol{z}^{(0)}$
  - Using the proposal $q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$, run the chain long enough, say T_1 steps
  - Discard the first $T_1 - 1$ samples (called "burn-in" samples) and take last sample $\boldsymbol{z}^{(T_1)}$
  - Continue from $\boldsymbol{z}^{(T_1)}$ up to T_2 steps, discard intermediate samples, take last sample $\boldsymbol{z}^{(T_2)}$
    - This discarding (called "thinning") helps ensure that $\boldsymbol{z}^{(T_1)}$ and $\boldsymbol{z}^{(T_2)}$ are uncorrelated
  - Repeat the same for a total of S times
  - In the end, we now have S *approximately independent* samples from $p(\boldsymbol{z})$

Will treat it as our first sample from $p(\boldsymbol{z})$

Requirement for Monte Carlo approximation

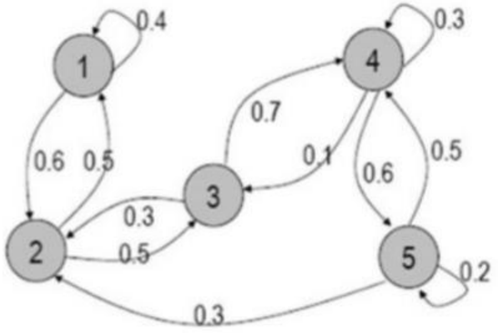
- Note: Good choices for T_1 and $T_i - T_{i-1}$ (thinning gap) are usually based on heuristics

MCMC: Some Basic Theory

- A first order Markov Chain assumes $p\left(\boldsymbol{z}^{(\ell+1)} | \boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\ell)}\right) = p(\boldsymbol{z}^{(\ell+1)} | \boldsymbol{z}^{(\ell)})$
- A 1st order Markov Chain $\boldsymbol{z}^{(0)}, \boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(L)}$ is a sequence of r.v.'s and is defined by
  - An initial state distribution $p(\boldsymbol{z}^{(0)})$
  - A Transition Function (TF): $T_\ell\left(\boldsymbol{z}^{(\ell)} \rightarrow \boldsymbol{z}^{(\ell+1)}\right) = p(\boldsymbol{z}^{(\ell+1)} | \boldsymbol{z}^{(\ell)})$
- TF is a distribution over the values of next state given the value of the current state
- Assuming a K-dim discrete state-space, TF will be $K \times K$ probability table

Transition probabilities can be defined using a *K*x*K* table if **z** is a discrete r.v. with *K* possible values

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0.4 & 0.6 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 0.3 & 0.0 & 0.7 & 0.0 \\ 0.0 & 0.0 & 0.1 & 0.3 & 0.6 \\ 0.0 & 0.3 & 0.0 & 0.5 & 0.2 \end{bmatrix} \end{array}$$



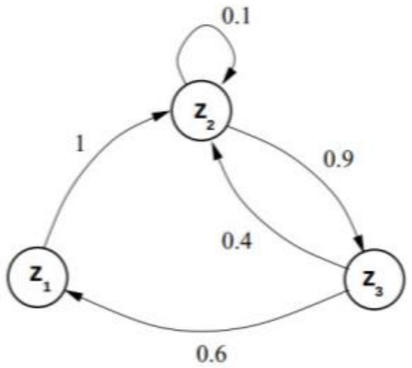
- Homogeneous Markov Chain: The TF is the same for all ℓ , i.e., $T_\ell = T$

MCMC: Some Basic Theory

- Consider the following Markov Chain with a $K = 3$ discrete state-space

$$p(\boldsymbol{z}^{(0)}) = p\left(z_1^{(0)}, z_2^{(0)}, z_3^{(0)}\right) = [0.5, 0.2, 0.3]$$

$$T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix}$$



$$p(\boldsymbol{z}^{(1)}) = p(\boldsymbol{z}^{(0)}) \times T = [0.2, 0.6, 0.2]$$ (rounded to single digit after decimal)

After doing it a few more (say some m) times

Stationary/Invariant Distribution $p(\boldsymbol{z})$ of this Markov Chain

$p(\boldsymbol{z})$ is multinoulli with $\pi = [0.2, 0.4, 0.4]$

$$p(\boldsymbol{z}^{(0)}) \times T^m = [0.2, 0.4, 0.4]$$ (rounded to single digit after decimal)

- $p(\boldsymbol{z})$ being Stationary means no matter what $p(\boldsymbol{z}^{(0)})$ is, we will reach $p(\boldsymbol{z})$
- A Markov Chain has a stationary distribution if T has the following properties
  - Irreducibility: T's graph is connected (ensures reachability from anywhere to anywhere)
  - Aperiodicity: T's graph has no cycles (ensures that the chain isn't trapped in cycles)

MCMC: Some Basic Theory

- A Markov Chain with transition function $\boldsymbol{T}$ has stationary distribution $\boldsymbol{p(z)}$ if $\boldsymbol{T}$ satisfies

Known as the Detailed Balance condition

$$p(\boldsymbol{z})T(\boldsymbol{z}'|\boldsymbol{z}) = p(\boldsymbol{z}')T(\boldsymbol{z}|\boldsymbol{z}')$$

Here $T(b|a)$ denotes the transition probability of going from state $\boldsymbol{b}$ to state $\boldsymbol{a}$

- Integrating out (or summing over) detailed balanced condition on both sides w.r.t. $\boldsymbol{z}'$

Thus $p(z)$ is the stationary distribution of this Markov Chain

$$p(\boldsymbol{z}) = \int p(\boldsymbol{z}')T(\boldsymbol{z}|\boldsymbol{z}')d\boldsymbol{z}'$$

- Thus a Markov Chain with detailed balance always converges to a stationary distribution
- Detailed Balance ensures reversibility
- Detailed balance is sufficient but not necessary condition for having a stationary distr.

Coming Up Next

- MCMC algorithms
  - Metropolis Hastings (MH)
  - Gibbs sampling (special case of MH)