STA 4273H:
Statistical Machine Learning

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Lecture 7

Approximate Inference

• When using probabilistic graphical models, we will be interested in evaluating the posterior distribution $p(\mathbf{Z}|\mathbf{X})$ of the latent variables $\mathbf{Z}$ given the observed data $\mathbf{X}$.

• For example, in the EM algorithm, we need to evaluate the expectation of the complete-data log-likelihood with respect to the posterior distribution over the latent variables.

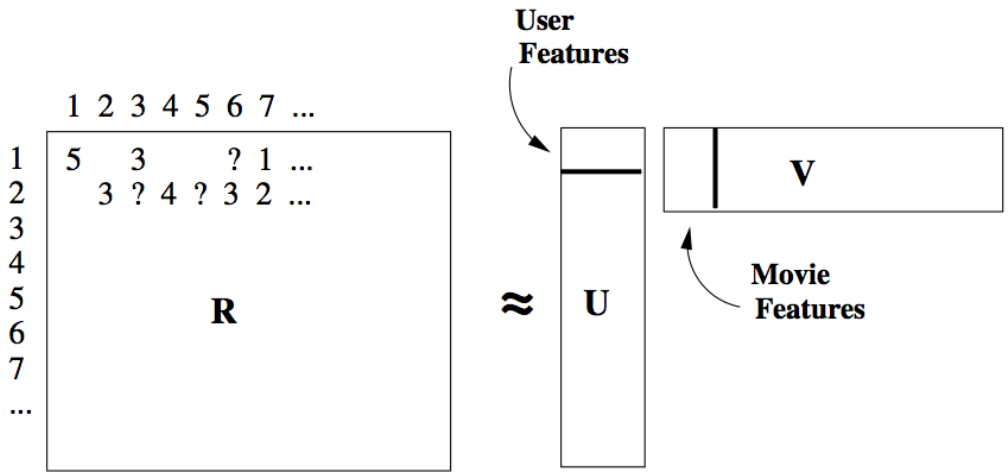
• For more complex models, it may be infeasible to evaluate the posterior distribution, or compute expectations with respect to this distribution.

• Last class we looked at variational approximations, including mean-field, variational Bayes.

• We now consider sampling-based methods, known as Monte Carlo techniques.

Bayesian Matrix Factorization

- Let us first look at a few examples.



- We have N users, M movies, and integer rating values from 1 to K.

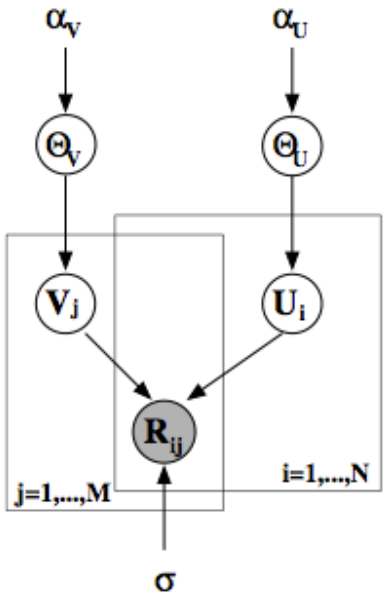
- Let r_{ij} be the rating of user i for movie j, and $U \in R^{D \times \mathcal{N}}$, and $V \in R^{D \times \mathcal{M}}$ be latent user and movie feature matrices:

$$R \approx U^T V.$$

- Our goal is to predict missing values (missing ratings).

Bayesian Matrix Factorization

- We can define a probabilistic bilinear model with Gaussian observation noise:



$$p(r_{ij}|U, V, \sigma^2) = \mathcal{N}(r_{ij}|u_i^T v_j, \sigma^2).$$

- We can place Gaussian priors over latent variables:

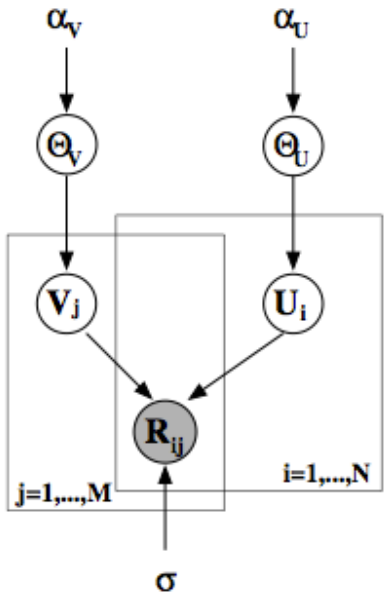
$$p(U|\mu_U, \Lambda_U) = \prod_{i=1}^{N} \mathcal{N}(u_i|\mu_U, \Lambda_U^{-1}),$$

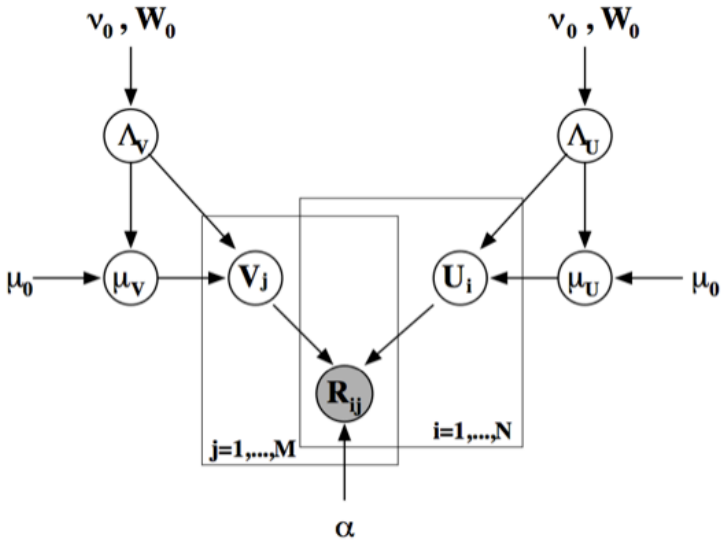
$$p(V|\mu_V, \Lambda_V) = \prod_{j=1}^{M} \mathcal{N}(v_j|\mu_V, \Lambda_V^{-1}).$$

- We next introduce Gaussian-Wishart priors over the user and movie hyper-parameters:

$$\Theta_U = \{\mu_U, \Lambda_U\},\ \Theta_V = \{\mu_V, \Lambda_V\}.$$

Bayesian Matrix Factorization





$$p(r_{ij}|U,V,\sigma^2) = \mathcal{N}(r_{ij}|u_i^T v_j, \sigma^2).$$

$$\Theta_U = \{\mu_U, \Lambda_U\},$$

$$\Theta_V = \{\mu_V, \Lambda_V\}.$$

$$p(U|\mu_U,\Lambda_U) = \prod_{i=1}^{N} \mathcal{N}(u_i|\mu_U,\Lambda_U^{-1}),$$

$$p(V|\mu_V,\Lambda_V) = \prod_{j=1}^{M} \mathcal{N}(v_j|\mu_V,\Lambda_V^{-1}).$$

Predictive Distribution

- Consider predicting a rating r^*_{ij} for user and query movie j.

$$p(r^*_{ij}|R) = \iint p(r^*_{ij}|u_i, v_j)\underbrace{p(U, V, \Theta_U, \Theta_V|R)}_{\text{Posterior over parameters and hyperparameters}}d\{U, V\}d\{\Theta_U, \Theta_V\}$$

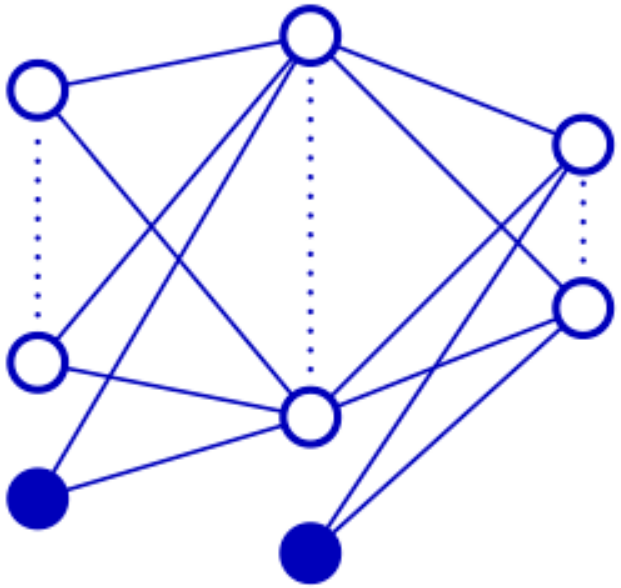
- Exact evaluation of this predictive distribution is analytically intractable.
- Posterior distribution over parameters and hyper-parameters is complicated and does not have a closed-form expression.
- Need to approximate.

- One option would be to approximate the posterior using factorized distribution Q and use variational framework.
- Alternative would be to resort to Monte Carlo methods.

Bayesian Neural Networks

• Another example is to consider Bayesian neural nets, that often give state-of-the art results for a range of regression problems.

• Regression problem: We are given a set of i.i.d. observations $\mathbf{X} = \{x^1,\ldots,x^N\}$ with corresponding targets $T = \{t^1,\ldots,t^N\}$.



• Likelihood:

$$p(\mathbf{T}|\mathbf{X},\mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}(t^n|y(\mathbf{x}^n,\mathbf{w}),\beta^2)$$

• The mean is given by the output of the neural network:

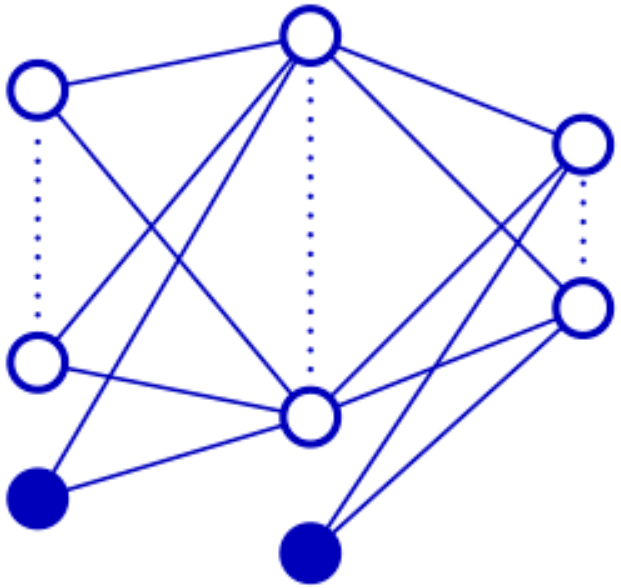
$$y_k(\mathbf{x},\mathbf{w}) = \sum_{j=1}^{M} w_{kj}^{(2)} \sigma\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i\right)$$

where $\sigma(x)$ is the sigmoid function.

• We place Gaussian prior over model parameters: $p(\mathbf{w}) = \mathcal{N}(0,\alpha I)$.

Bayesian Neural Networks

- We therefore have:



- Likelihood:

Nonlinear function of inputs.

$$p(\mathbf{T}|\mathbf{X},\mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}(t^n|y(\mathbf{x}^n,\mathbf{w}),\beta^2)$$

- Gaussian prior over parameters:

$$p(\mathbf{w}) = \mathcal{N}(0,\alpha I).$$

- The posterior is analytically intractable:

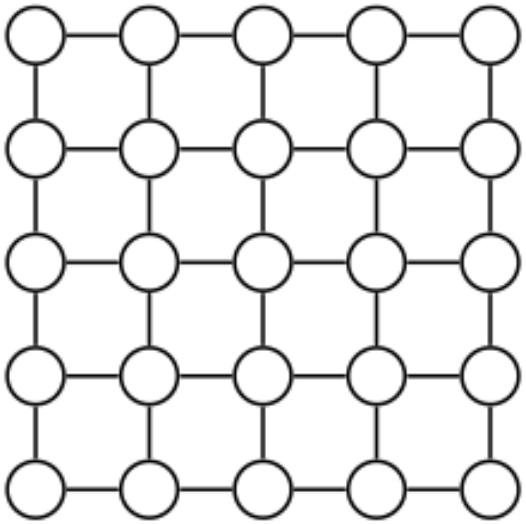
$$p(\mathbf{w}|\mathbf{T},\mathbf{X}) = \frac{p(\mathbf{T}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{\int p(\mathbf{T}|\mathbf{X},\mathbf{w})p(\mathbf{w})\mathrm{d}\mathbf{w}}$$

Cannot analytically compute normalizing constant.

- We need the posterior to compute predictive distribution for t given a new input x.

Undirected Graphical Models

• Let **x** be a binary random vector with $x_i \in \{-1.1\}$:



$$P_\theta(\mathbf{x}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij \in E} x_i x_j \theta_{ij} + \sum_{i \in V} x_i \theta_i \Big)$$

where $Z(\theta)$ is a normalizing constant (also known as partition function):

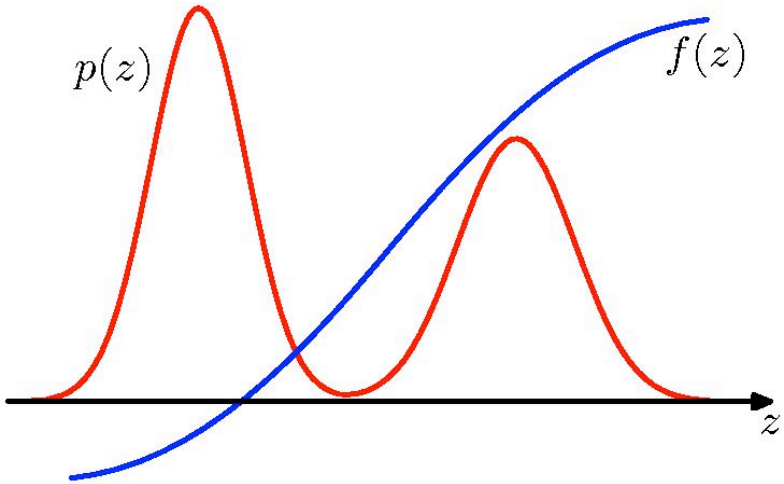
$$\mathcal{Z}(\theta) = \sum_{\mathbf{x}} \exp\Big(\sum_{ij \in E} x_i x_j \theta_{ij} + \sum_{i \in V} x_i \theta_i \Big).$$

• If **x** is 100-dimensional, we need to sum over 2^{100} terms.

• The sum might decompose, which would be the case for the tree structured graphical models (or models with low tree-width). Otherwise, we need to approximate.

Notation

• For most situations, we will be interested in evaluating expectations (for example in order to make predictions):



$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})\mathrm{d}\mathbf{z}.$$

where the integral will be replaced with summation in case of discrete variables.

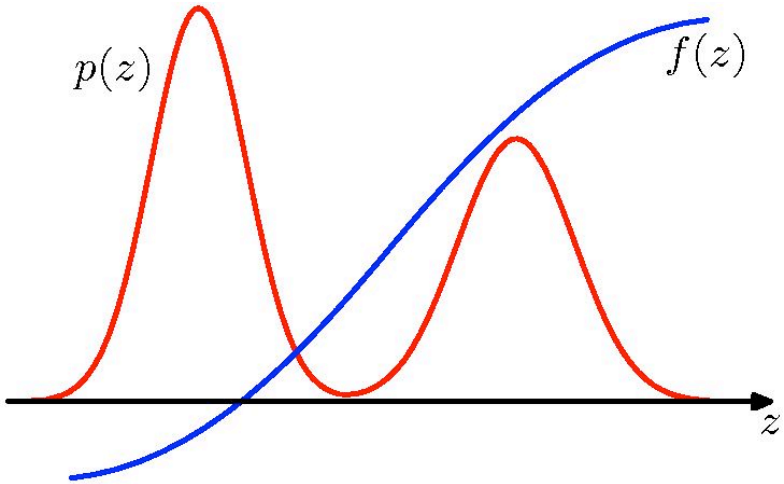
• We will make use of the following notation: $p(\mathbf{z}) = \dfrac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}$.

• We can evaluate $\tilde{p}(\mathbf{z})$ pointwise but cannot evaluate $\mathcal{Z}$.

- Posterior distribution: $p(\theta|\mathcal{D}) = \dfrac{1}{p(\mathcal{D})}p(\mathcal{D}|\theta)p(\theta)$.
- Markov Random Fields: $p(\mathbf{x}) = \dfrac{1}{\mathcal{Z}}\exp(-E(\mathbf{x}))$.

Simple Monte Carlo

• General Idea: Draw independent samples $\{z^1,..,z^n\}$ from distribution p(z) to approximate expectation:



$$\mathbb{E}[f] = \int f(z)p(z)dz \approx \frac{1}{N}\sum_{n=1}^{N} f(z^n) = \hat{f}.$$

Note that:

$$\mathbb{E}[f] = \mathbb{E}[\hat{f}].$$

so the estimator has correct mean (unbiased).

• The variance:

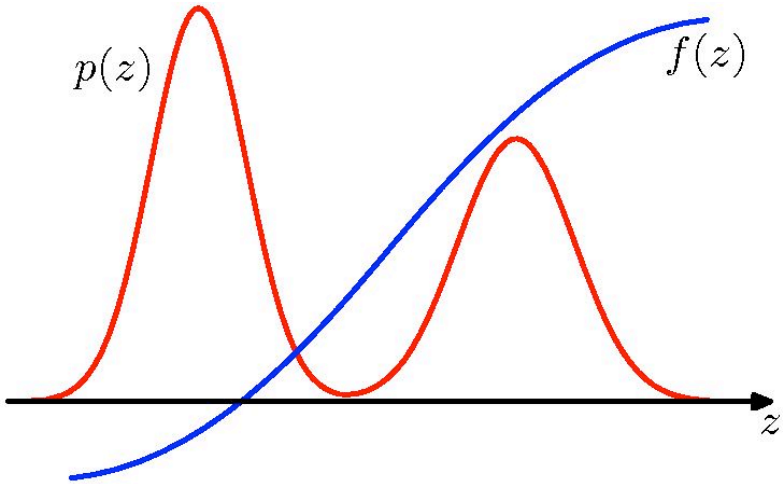
$$\mathrm{var}[\hat{f}] = \frac{1}{N}\mathbb{E}\left[(f - \mathbb{E}[f])^2\right].$$

• Variance decreases as 1/N.

• **Remark**: The accuracy of the estimator does not depend on dimensionality of z.

Simple Monte Carlo

- High accuracy may be achieved with a small number N of independent samples from distribution p(z).



$$\mathrm{var}[\hat{f}] = \frac{1}{N}\mathbb{E}\left[(f - \mathbb{E}[f])^2\right].$$

- **Problem 1**: we may not be able to draw independent samples.

- **Problem 2**: if f(z) is large in regions where p(z) is small (and vice versa), then the expectations may be dominated by regions of small probability. Need larger sample size.

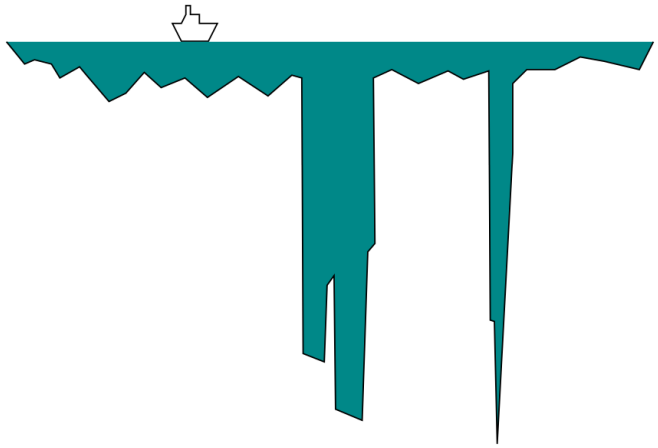
Simple Monte Carlo

- In general:

$$\mathbb{E}[f] = \int f(z)p(z)dz \approx \frac{1}{N}\sum_{n=1}^{N} f(z^n), \quad z^n \sim p(z).$$

- Predictive distribution:

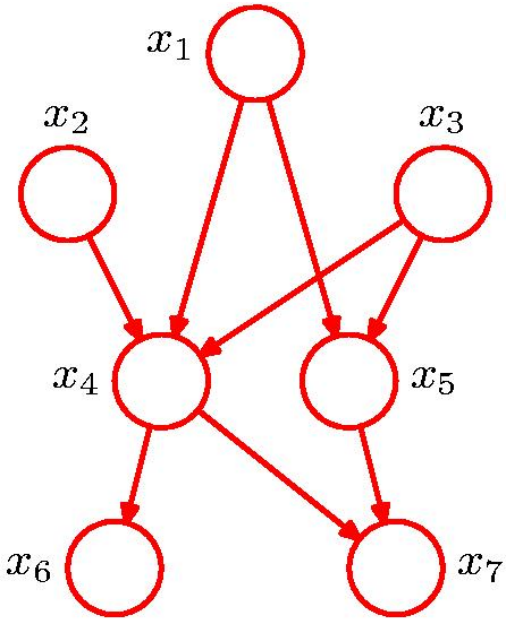
$$p(x^*|\mathcal{D}) = \int p(x^*|\theta,\mathcal{D})p(\theta|\mathcal{D})d\theta$$
$$\approx \frac{1}{N}\sum_{n=1}^{N} p(x^*|\theta^n), \quad \theta^n \sim p(\theta|\mathcal{D}).$$



- **Problem**: It is hard to draw exact samples from p(z).

Directed Graphical Models

• For many distributions, the joint distribution can be conveniently specified in terms of a graphical model.



• For directed graphs with no observed variables, sampling from the joint is simple:

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$

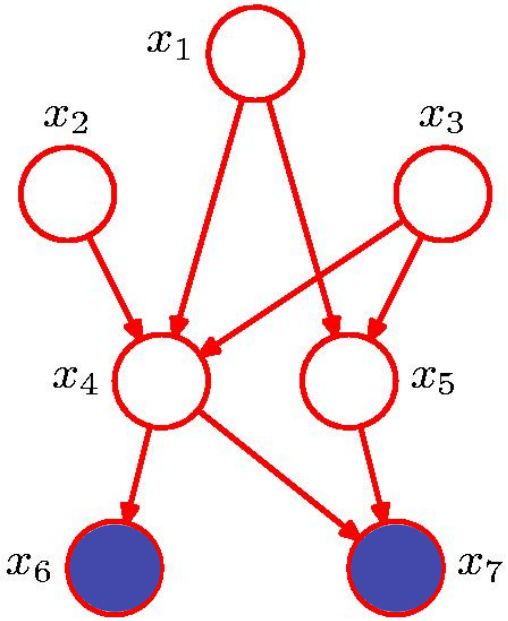
$$\hat{x}_1 \sim p(x_1)$$
$$\hat{x}_2 \sim p(x_2)$$
$$\hat{x}_3 \sim p(x_3)$$
$$\hat{x}_4 \sim p(x_4|\hat{x}_1, \hat{x}_2, \hat{x}_3)$$
$$\hat{x}_5 \sim p(x_5|\hat{x}_1, \hat{x}_3)$$

The parent variables are set to their sampled values

• After one pass through the graph, we obtain a sample from the joint.

Directed Graphical Models

- Consider the case when some of the nodes are observed.



- Naive idea: Sample from the joint.

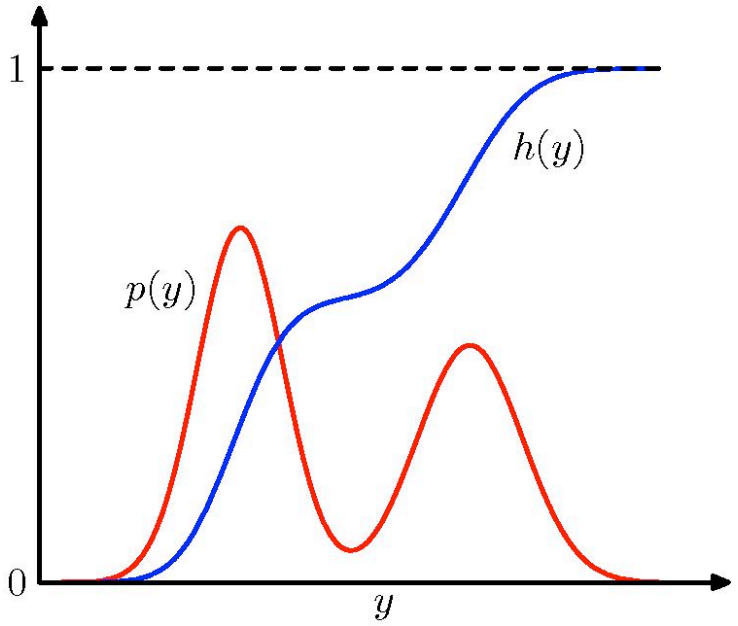
$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$

- If the sampled values agree with the observed values, we retain the sample.
- Otherwise, we disregard the whole sample.

- The algorithm samples correctly from the posterior.
- The overall probability of accepting the sample from the posterior decreases rapidly as the number of observed variables increases.
- Rarely used in practice.

Basic Sampling Algorithm

• How can we generate samples from simple non-uniform distributions assuming we can generate samples from uniform distribution.



• Define:

$$h(y) = \int_{-\infty}^{y} p(\hat{y}) d\hat{y}.$$

• Sample:

$$z \sim \mathrm{U}[0, 1]$$

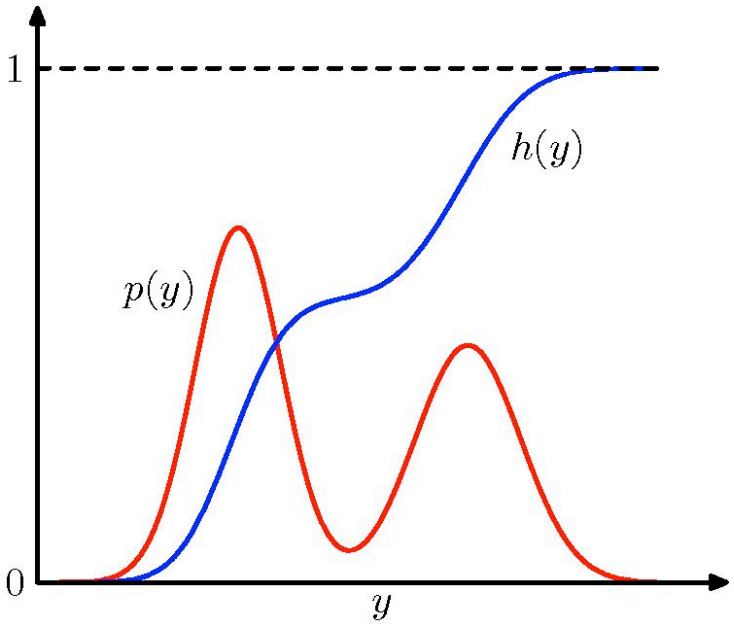
• Then $y = h^{-1}(z)$

is a sample from p(y).

Basic Sampling Algorithm

- For example, consider the exponential distribution:

$$p(y) = \lambda \exp(-\lambda y).$$



- In this case:

$$h(y) = \int_0^y p(\hat{y}) d\hat{y} = 1 - \exp(-\lambda y).$$

- Sample:

$$z \sim \mathrm{U}[0, 1]$$

- Then

$$y = h^{-1}(z) = -\lambda^{-1} \ln(1 - z)$$

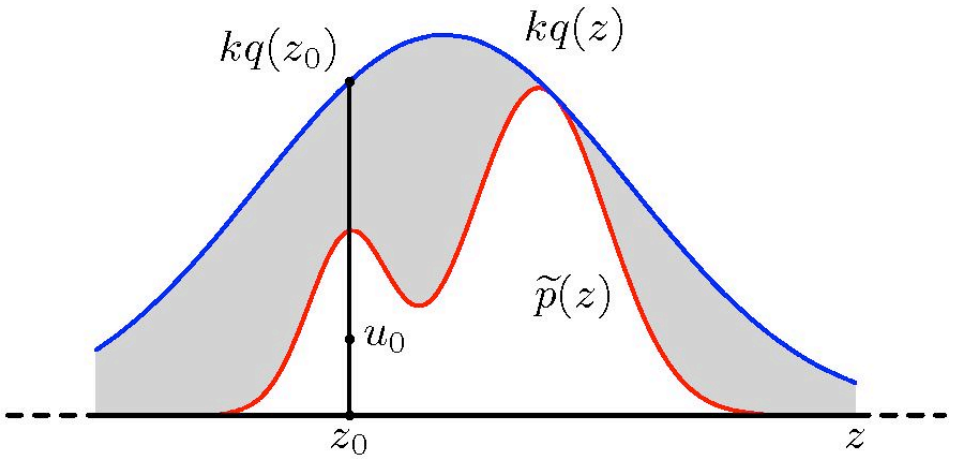
is a sample from p(y).

- **Problem**: Computing h(y) is just as hard!

Rejection Sampling

• Sampling from the target distribution $p(z) = \tilde{p}(z)/\mathcal{Z}_p$ is difficult. Suppose we have an easy-to-sample proposal distribution q(z), such that:

$$kq(z) \geq \tilde{p}(z), \ \forall z.$$



• Sample:

$$z_0 \sim q(z),$$

• Sample:

$$u_0 \sim \text{Uniform}[0, kq(z_0)].$$

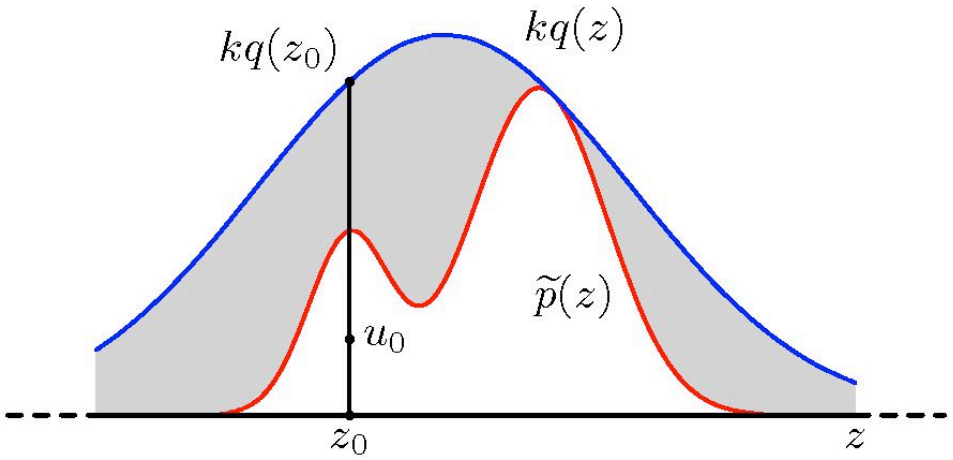
• Sample (z_0, u_0) has uniform distribution under the curve of $kq(z)$.

• If $u_0 > \tilde{p}(z_0)$, the sample is rejected.

Rejection Sampling

- Probability that a sample is accepted is calculated as:

$$p(\text{accept}) = \int \frac{\tilde{p}(z)}{kq(z)} q(z)dz$$
$$= \frac{1}{k} \int \tilde{p}(z)dz.$$

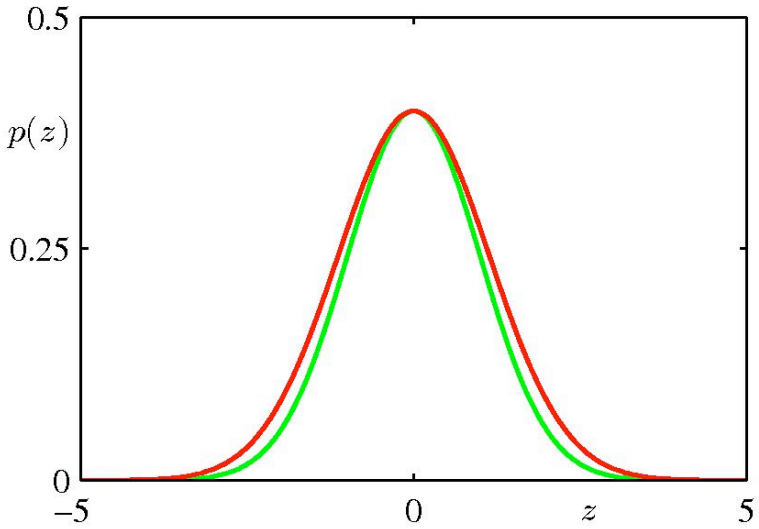


- The fraction of accepted samples depends on the ratio of the area under $\tilde{p}(z)$ and $kq(z)$.

- It is often hard to find q(z) with optimal k.

Rejection Sampling

- Consider the following simple problem:



- Target distribution:

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \sigma_p^2 I),$$

- Proposal distribution:

$$q(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \sigma_q^2 I).$$

- We must have:

$$\sigma_q^2 \geq \sigma_p^2.$$

- The optimal k is given by: $k = \left(\frac{\sigma_q}{\sigma_p}\right)^D$.

- Hence the acceptance rate diminishes exponentially!

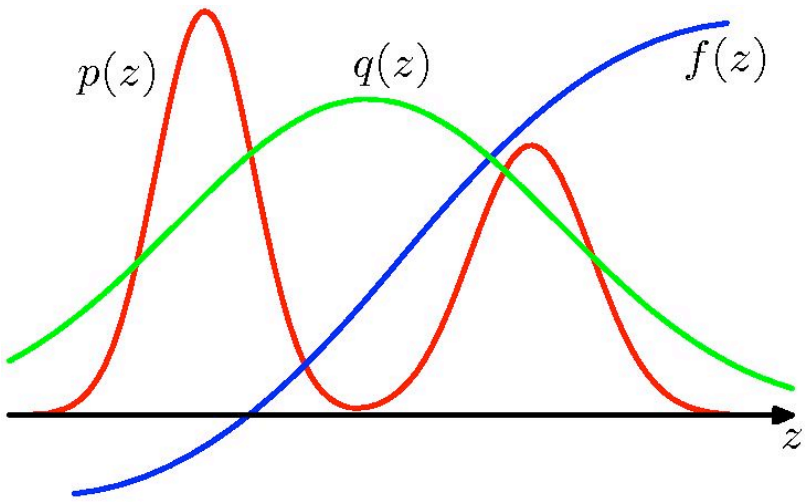
- Useful technique in one or two dimensions. Typically applies as a subroutine in more advanced techniques.

Importance Sampling

- Suppose we have an easy-to-sample proposal distribution q(z), such that

$$q(z) > 0 \quad \text{if} \quad p(z) > 0.$$

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



$$= \int f(z)\frac{p(z)}{q(z)}q(z)dz$$

$$\approx \frac{1}{N}\sum_n \frac{p(z^n)}{q(z^n)}f(z^n), \quad z^n \sim q(z).$$

- The quantities

$$w^n = p(z^n)/q(z^n)$$

are known as **importance weights**.

- Unlike rejection sampling all samples are retained.
- But wait: we cannot compute $p(z) = \frac{\tilde{p}(z)}{Z}$.

Importance Sampling

- Let our proposal be of the form: $q(z) = \tilde{q}(z)/\mathcal{Z}_q$.

$$\mathbb{E}[f] = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz = \frac{Z_q}{Z_p}\int f(z)\frac{\tilde{p}(z)}{\tilde{q}(z)}q(z)dz$$
$$\approx \frac{\mathcal{Z}_q}{\mathcal{Z}_p}\frac{1}{N}\sum_n \frac{\tilde{p}(z^n)}{\tilde{q}(z^n)}f(z^n) = \frac{\mathcal{Z}_q}{\mathcal{Z}_p}\frac{1}{N}\sum_n w^n f(z^n),$$

- But we can use the same weights to approximate $\mathcal{Z}_q/\mathcal{Z}_p$:

$$\frac{\mathcal{Z}_p}{\mathcal{Z}_q} = \frac{1}{\mathcal{Z}_q}\int \tilde{p}(z)dz = \int \frac{\tilde{p}(z)}{\tilde{q}(z)}q(z)dz \approx \frac{1}{N}\sum_n \frac{\tilde{p}(z^n)}{\tilde{q}^n(z)} = \frac{1}{N}\sum_n w^n.$$

- Hence:

$$\mathbb{E}[f] \approx \sum_{n=1}^{N} \frac{w^n}{\sum_{m=1}^{N} w^m} f(z^n), \qquad z^n \sim q(z).$$

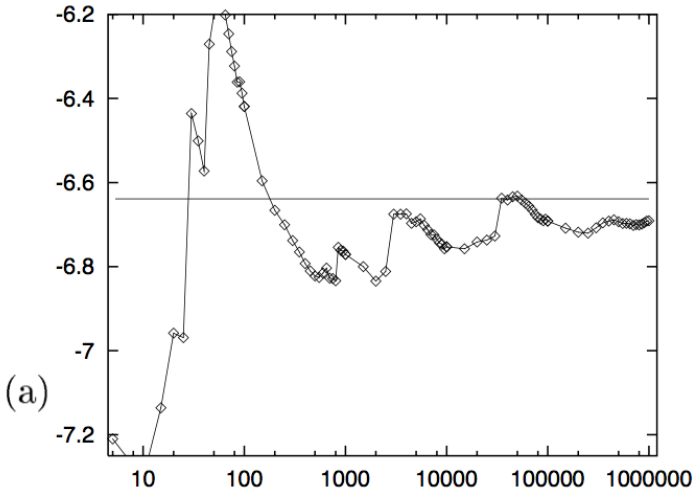
Consistent but biased.

Importance Sampling: Example

- With importance sampling, it is hard to estimate how reliable the estimator is:

$$\hat{f} = \sum_{n=1}^{N} \frac{w^n}{\sum_{m=1}^{N} w^m} f(z^n), \qquad \mathbb{E}[f] = \int f(z) \frac{p(z)}{q(z)} q(z) dz$$

- Huge variance if the proposal density q(z) is small in a region where |f(z)p(z)| is large



(a)

- Example of using Gaussian distribution as a proposal distribution (1-d case).

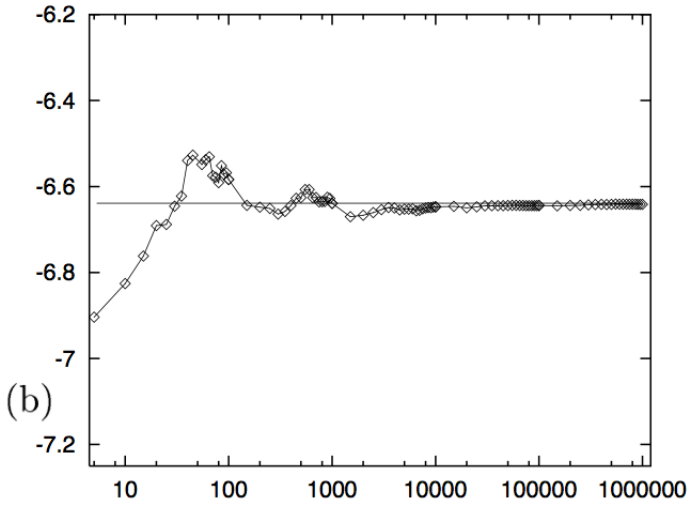
- Even after 1 million samples, the estimator has not converged to the true value.

Importance Sampling: Example

• With importance sampling, it is hard to estimate how reliable the estimator:

$$\hat{f} = \sum_{n=1}^{N} \frac{w^n}{\sum_{m=1}^{N} w^m} f(z^n), \qquad \mathbb{E}[f] = \int f(z) \frac{p(z)}{q(z)} q(z) dz$$

• Huge variance if the proposal density q(z) is small in a region where |f(z)p(z)| is large



• Example of using Cauchy distribution as a proposal distribution (1-d case).

• After 500 samples, the estimator appears to converge

• Proposal distribution should have heavy tails.

Monte Carlo EM

- Sampling algorithms can also be used to approximate the E-step of the EM algorithm when E-step cannot be performed analytically.
- We are given visible (observed) variables **X**, hidden (latent) variables **Z** and model parameters θ.
- In the M-step, we maximize the expected complete data log-likelihood:

$$\mathcal{Q}(\theta, \theta^{old}) = \int p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) \mathrm{d}\mathbf{Z}.$$

- We can approximate the integral with:

$$\mathcal{Q}(\theta, \theta^{old}) \simeq \frac{1}{L} \sum_{l=1}^{L} \ln p(\mathbf{X}, \mathbf{Z}^l|\theta), \quad \mathbf{Z}^l \sim p(\mathbf{Z}|\mathbf{X}, \theta^{old}).$$

- The samples are drawn from the current estimate of the posterior distribution.
- The Q function is optimized in the usual way in the M-step.

IP Algorithm

- Suppose we move from the maximum likelihood approach to the fully Bayesian approach.
- In this case, we would like to get samples from the joint p($\mathbf{Z}$,θ | $\mathbf{X}$), but let us assume that this is difficult.
- We also assume that it is easy to sample from the complete-data parameter posterior p(θ | $\mathbf{Z}$,$\mathbf{X}$).
- This inspires the data-augmentation algorithm, which alternates between two steps:
  - I-step (imputation step), analogous to E-step.
  - P-step (posterior step), analogous to M-step.

IP Algorithm

- Let us look at the two steps:
- I-step: We want to sample from p(**Z** | **X**), but we can not do it directly. However:

$$p(\mathbf{Z}|\mathbf{X}) = \int p(\mathbf{Z}|\mathbf{X},\theta)p(\theta|\mathbf{X})\mathrm{d}\theta.$$

- Approximate by:
  - For l=1,…,L, draw: $\theta^l \sim p(\theta|\mathbf{X})$
  - For l=1,…,L, draw: $\mathbf{Z}^l \sim p(\mathbf{Z}|\theta^l,\mathbf{X}).$
- P-step: Use the relation:

$$p(\theta|\mathbf{X}) = \int p(\theta|\mathbf{Z},\mathbf{X})p(\mathbf{Z}|\mathbf{X})\mathrm{d}\mathbf{Z}.$$

- Using samples Z^l we obtained in the I-step, we approximate:

$$p(\theta|\mathbf{X}) \simeq \frac{1}{L}\sum_l p(\theta|\mathbf{Z}^l,\mathbf{X}),$$

which is, by assumption, easy to sample from.

Summary so Far

- If our proposal distribution q(z) poorly matches our target distribution p(z) then:
  - Rejection sampling: almost always rejects
  - Importance Sampling: has large, possibly infinite, variance (unreliable estimator).

- For high-dimensional problems, finding good proposal distributions is very hard.

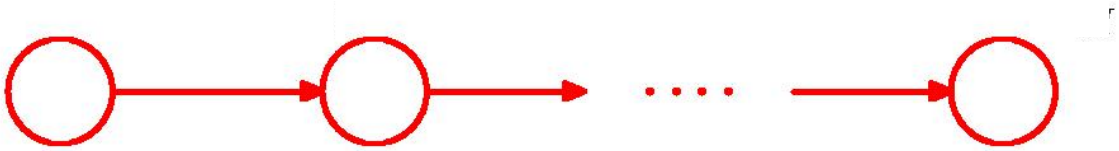
What can we do?

- Markov Chain Monte Carlo.

Markov Chains

• A first-order Markov chain: a series of random variables $\{z^1, ..., z^N\}$, such that the following conditional independence property holds for $n \in \{z^1, ..., z^{N-1}\}$:

$$p(z^{n+1}|z^1, .., z^n) = p(z^{n+1}|z^n).$$



• We can specify Markov chain:

- Probability distribution for initial state $p(z^1)$.
- Conditional probability for subsequent states in the form of transition probabilities:

$$T(z^{n+1} \leftarrow z^n) = p(z^{n+1}|z^n).$$

• $T(z^{n+1} \leftarrow z^n)$ is often called a **transition kernel**.

Markov Chains

• A marginal probability of a particular state can be computed as:

$$p(z^{n+1}) = \sum_{z^n} T(z^{n+1} \leftarrow z^n) p(z^n).$$

• A distribution π(z) is said to be **invariant** or **stationary** with respect to a Markov chain if each step in the chain leaves π(z) invariant:

$$\pi(z) = \sum_{z'} T(z \leftarrow z') \pi(z').$$

• A given Markov chain may have many stationary distributions.

• For example:

$$T(z \leftarrow z') = I(z = z')$$

is the identity transformation. Then any distribution is invariant.

Detailed Balance

• A sufficient (but not necessary) condition for ensuring that π(z) is invariant is to choose a transition kernel that satisfies a **detailed balance property**:

$$\pi(z')T(z \leftarrow z') = \pi(z)T(z' \leftarrow z).$$

$$T(z' \leftarrow z) = p(z'|z).$$

• A transition kernel that satisfies detailed balance will leave that distribution invariant:

$$\sum_{z'} \pi(z')T(z \leftarrow z') = \sum_{z'} \pi(z)T(z' \leftarrow z)$$

$$= \pi(z) \sum_{z'} T(z' \leftarrow z) = \pi(z).$$

• A Markov chain that satisfies detailed balance is said to be **reversible**.

Example

- Discrete example:

$$P^\star = \begin{pmatrix} 3/5 \\ 1/5 \\ 1/5 \end{pmatrix} \qquad T = \begin{pmatrix} 2/3 & 1/2 & 1/2 \\ 1/6 & 0 & 1/2 \\ 1/6 & 1/2 & 0 \end{pmatrix} \qquad T_{ij} = T(x_i \leftarrow x_j)$$

- In this case P^* is **invariant distribution** of T since $TP^* = P^*$, or:

$$\sum_{z'} P^*(z')T(z \leftarrow z') = P^*(z).$$

- P^* is also the **equilibrium distribution** of T since:

$$T^{100} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3/5 \\ 1/5 \\ 1/5 \end{pmatrix} = P^\star$$

Example credit: Iain Murray.

Markov Chains

• We want to sample from the target distribution (e.g. posterior distribution, or a Markov Random Field): $\pi(z) = \tilde{\pi}(z)/\mathcal{Z}.$

• Obtaining independent samples is difficult.

- Set up a Markov chain with transition kernel T(z' ← z) that leaves our target distribution π(z) invariant.
- If the chain is ergodic, then the chain will converge to this unique equilibrium distribution.
- We obtain dependent samples drawn approximately from π(z) by simulating a Markov chain for some time.

• **Ergodicity** requires: There exists K, such that for any starting z, we have

$$T^K(z' \leftarrow z) > 0 \text{ for all } \pi(z') > 0.$$

A state i is said to be ergodic if it is aperiodic and positive recurrent. If all states in an irreducible Markov chain are ergodic, then the chain is said to be ergodic.

Combining Transition Operators

• In practice, we often construct the transition probabilities from a set of "**base**" transition operators $B_1,\ldots,B_K$.

• One option is to consider a mixture distribution of the form:

$$T(z' \leftarrow z) = \sum_{k=1}^{K} \alpha_k B_k(z' \leftarrow z),$$

where mixing coefficients satisfy: $\alpha_k \geq 0, \quad \sum_k \alpha_k = 1.$

• Another option is to combine through successive application:

$$T(z' \leftarrow z) = \sum_{z^1} \ldots \sum_{z^{n-1}} B_1(z' \leftarrow z^1) \ldots B_K(z^{K-1} \leftarrow z).$$

• If a distribution is invariant with respect to each of the base transitions, then it will also be invariant with respect to T(z' $\leftarrow$ z).

Combining Transition Operators

- For the case of the mixture:

$$T(z' \leftarrow z) = \sum_{k=1}^{K} \alpha_k B_k(z' \leftarrow z),$$

If each of the base distributions satisfies the detailed balance, then the mixture transition T will also satisfy detailed balance.

- For the case of using composite transition probabilities:

$$T(z' \leftarrow z) = \sum_{z^1} ... \sum_{z^{n-1}} B_1(z' \leftarrow z^1) ... B_K(z^{K-1} \leftarrow z).$$

this does not hold.

- A simple idea is to **symmetrize** the order of application of the base transitions:

$$B_1, B_2, ..., B_K, B_K, ..., B_2, B_1.$$

- A common example of using composite transition probabilities is where each base transition changes only a subset of variables.

Metropolis-Hasting Algorithm

• A Markov chain transition operator from the current state z to a new state z' is defined as follows:

- A new "candidate" state z^* is proposed according to some proposal distribution $q(z^*|z)$.
- A candidate z^* is accepted with probability:

$$\min\left(1, \frac{\tilde{\pi}(z^*)}{\tilde{\pi}(z)}\frac{q(z|z^*)}{q(z^*|z)}\right).$$

- If accepted, set $z' = z^*$. Otherwise $z = z'$, or the next state is the copy of the current state.

• Note: there is no need to compute normalizing constant.

• For symmetric proposals, e.g. $N(z,\sigma^2)$, the acceptance probability reduces to:

$$\min\left(1, \frac{\tilde{\pi}(z^*)}{\tilde{\pi}(z)}\right).$$

Metropolis-Hasting Algorithm

• We can show that M-H transition kernel leaves π(z) invariant by showing that it satisfies detailed balance:

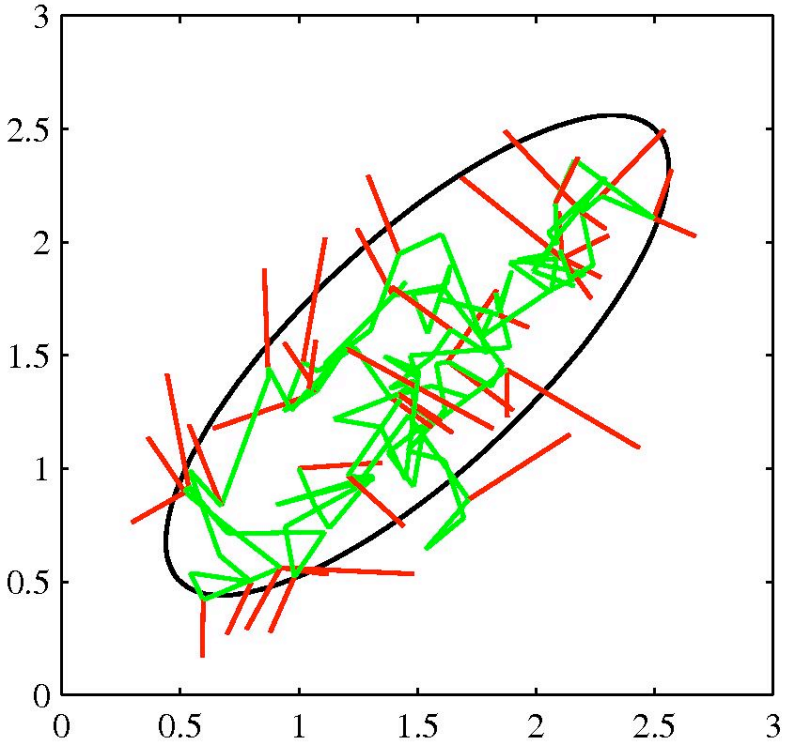
$$\begin{aligned}
\pi(z)T(z' \leftarrow z) &= \pi(z)q(z'|z)\min\left(1, \frac{\pi(z')}{\pi(z)}\frac{q(z|z')}{q(z'|z)}\right) \\
&= \min\left(\pi(z)q(z'|z), \pi(z')q(z|z')\right) \\
&= \pi(z')q(z|z')\min\left(\frac{\pi(z)}{\pi(z')}\frac{q(z'|z)}{q(z|z')}, 1\right) \\
&= \pi(z')T(z \leftarrow z').
\end{aligned}$$

• Note that whether the chain is ergodic will depend on the particulars of the stationary distribution π and proposal distribution q.

Metropolis-Hasting Algorithm

- Using Metropolis algorithm to sample from Gaussian distribution with proposal

$$q(z'|z) = \mathcal{N}(z, 0.04).$$



- accepted (green), rejected (red).
- 150 samples were generated and 43 were rejected.
- Note that generated samples are not independent.

Random Walk Behaviour

- Consider a state-space consisting of integers with

$$p(z^{t+1} = z^t) = 0.5$$
$$p(z^{t+1} = z^t + 1) = 0.25$$
$$p(z^{t+1} = z^t - 1) = 0.25$$

- If the initial state is $z^1 = 0$, then by symmetry:

$$\mathbb{E}[z^t] = 0,$$

- and

$$\mathbb{E}[(z^t)^2] = t/2.$$

- Hence after t steps, the random walk traveled a distance that is on average proportional to the square root of t.

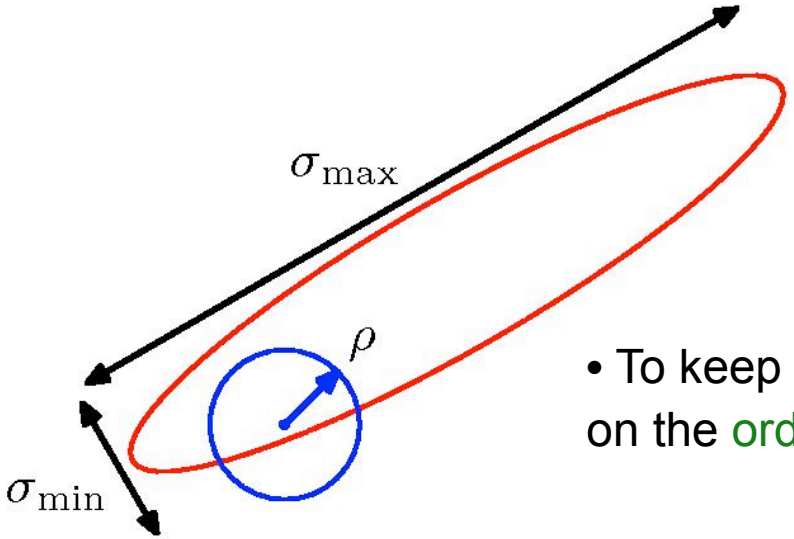
- This square root dependence is typical of random walk behavior.

- Ideally, we would want to design MCMC methods that avoid random walk behavior.

Choice of Proposal

• Suppose that our goal is to sample from the correlated multivariate Gaussian distribution.

• Consider a Gaussian proposal: centered on the current state:



$$q(z'|z) = \mathcal{N}(z, \rho^2 I)$$

• ρ large -- many rejections

• ρ small -- chain moves too slowly.

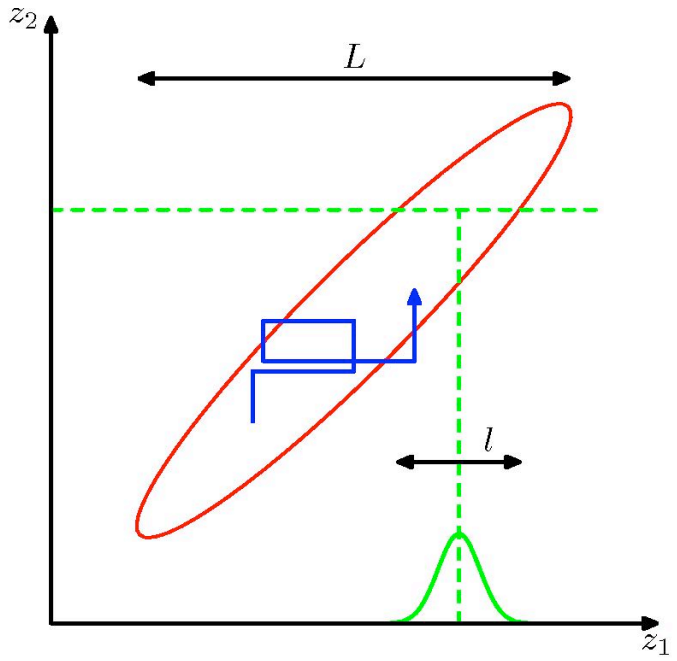
• To keep the rejection rate low, the scale ρ should be on the order of the smallest standard deviation σ_{min}.

• Random walk behaviour: The number of steps separating states that are approximately independent is of order: $(\sigma_{max}/\sigma_{min})^2$.

• The specific choice of proposal can greatly affect the performance of the algorithm.

Gibbs Sampler

• Consider sampling from $p(z_1,\ldots,z_N)$:



• Initialize z_i, i=1,..,N.

• For t=1:T

- Sample: $z_1^{t+1} \sim p(z_1 | z_2^t, ..., z_N^t)$
- Sample: $z_2^{t+1} \sim p(z_2 | z_1^{t+1}, z_3^t, ..., z_N^t)$
- …
- Sample: $z_N^{t+1} \sim p(z_N | z_1^{t+1}, z_2^{t+1}, ..., z_{N-1}^{t+1})$

• This procedure samples from the required distribution p(z).

• When sampling $p(z_n|\mathbf{z}_{-n})$ the marginal distribution $p(\mathbf{z}_{-n})$ is clearly invariant, as it does not change.

• Each step samples from the correct conditional, hence the joint distribution is itself invariant.

Gibbs Sampler

• Applicability of the Gibbs sampler depends on how easy it is to sample from conditional probabilities $p(z_n|\mathbf{z}_{-n})$.

• For discrete random variables with a few discrete settings:

$$p(z_n|\mathbf{z}_{-n}) = \frac{p(z_n, \mathbf{z}_{-n})}{\sum_{z_n} p(z_n, \mathbf{z}_{-n})},$$

where the sum can be performed analytically.

• For continuous random variables:

$$p(z_n|\mathbf{z}_{-n}) = \frac{p(z_n, \mathbf{z}_{-n})}{\int p(z_n, \mathbf{z}_{-n}) dz_n},$$

• The integral is univariate and is often analytically tractable or amenable to standard sampling methods.

Gibbs Sampler

- Gibbs sampler is a particular instance of M-H algorithm with proposals: $q_n(\mathbf{z}^*|\mathbf{z}) = p(z_n^*|\mathbf{z}_{-n})$.

- Note that $\mathbf{z}_{-n}^* = \mathbf{z}_{-n}$ because these components are unchanged by the sampling step.

- Let us look at the factor that determines acceptance probability in M-H.

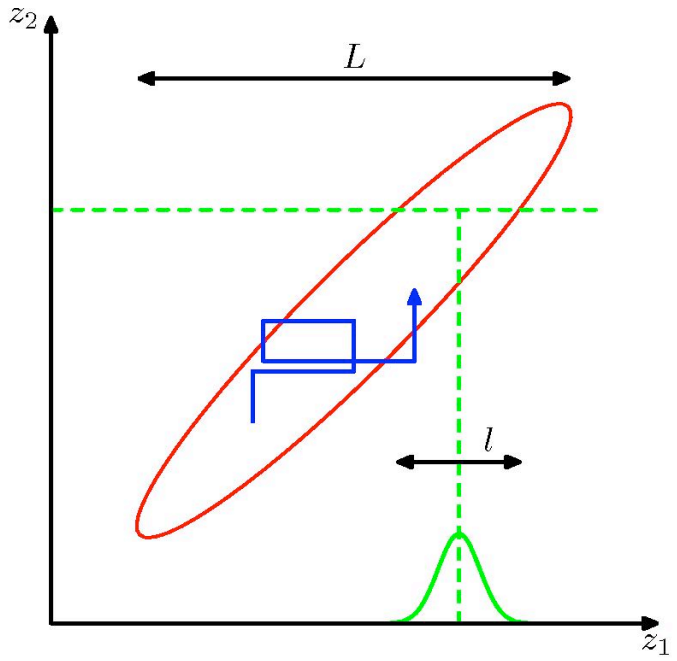
$$A(\mathbf{z}^*, \mathbf{z}) = \frac{p(\mathbf{z}^*)}{p(\mathbf{z})} \times \frac{q_n(\mathbf{z}|\mathbf{z}^*)}{q_n(\mathbf{z}^*|\mathbf{z})}$$
$$= \frac{p(z_n^*|\mathbf{z}_{-n}^*)p(\mathbf{z}_{-n}^*)}{p(z_n|\mathbf{z}_{-n})p(\mathbf{z}_{-n})} \times \frac{p(z_n|\mathbf{z}_{-n}^*)}{p(z_n^*|\mathbf{z}_{-n})} = 1.$$

- Thus MH steps are always accepted.

- Let us look at the behavior of Gibbs.

Gibbs Sampler

• As with MH, we can get some insight into the behavior of Gibbs sampling.



• Consider a correlated Gaussian having conditional distributions of width l and marginal distributions of width L.

• Random walk behavior: The typical step size is governed by the conditional and will be of order l.

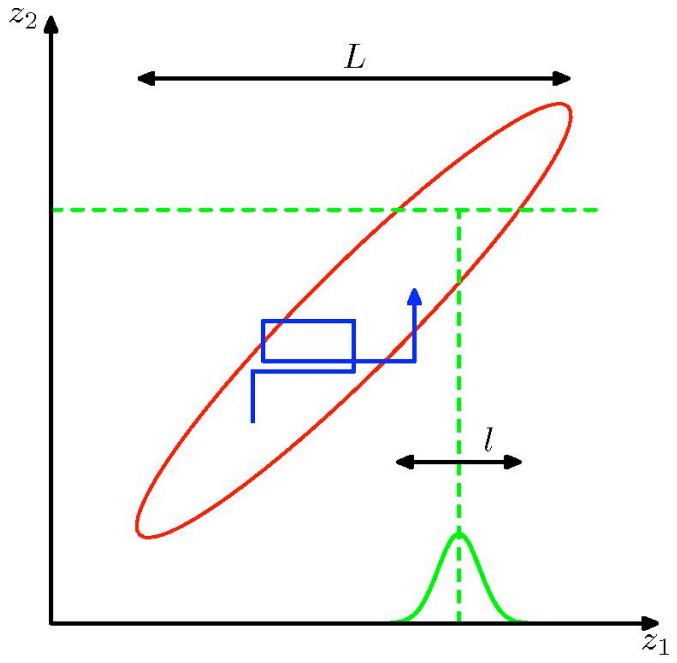
• The number of steps separating states that are approximately independent is of order:

$$O((L/l)^2).$$

• If the Gaussian distribution were uncorrelated, then the Gibbs sampling would be optimally efficient.

Over-Relaxation

• One approach to reducing random walk behavior is called over-relaxation:



• Consider conditional distributions that are Gaussian.

• At each step of the Gibbs sampler, the conditional distribution for z_i is:

$$p(z_n|\mathbf{z}_{-n}) = \mathcal{N}(z_n|\mu_n, \sigma_n^2).$$

• In the over-relaxed framework, the value of z_n is replaced with:

$$z'_n = \mu_n + \alpha(z_n - \mu_n) + \sigma_n(1-\alpha_n^2)^{1/2}\nu,$$
$$\nu \sim \mathcal{N}(0,1).$$

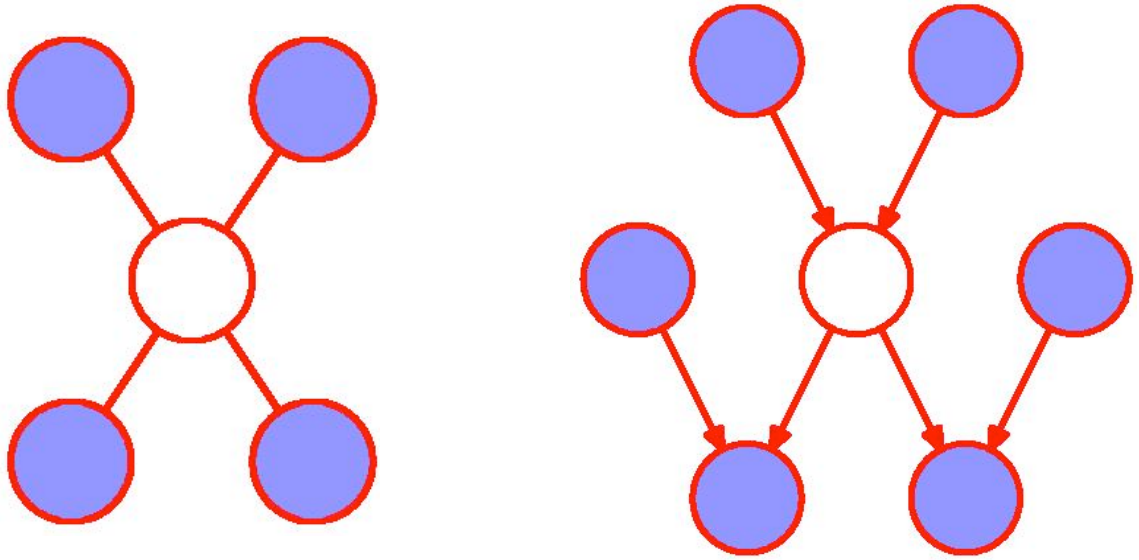
• Setting α = 0, we recover standard Gibbs.

• The step leaves the desired distribution invariant because if z_n has mean μ_n and standard deviation σ_n, then so does z'_n.

• This encourages directed motion through the state space when the variables are high correlated.

Graphical Models

• For graphical models, the conditional distribution is a function only of the states of the nodes in the Markov blanket.



• **Block Gibbs**: Choose blocks of variables (not necessarily disjoint) and then sample jointly from the variables in each block in turn, conditioned on the remaining variables.

Bayesian PMF

- Consider predicting a rating r^*_{ij} for user i and query movie j.

$$p(r^*_{ij}|R) = \iint p(r^*_{ij}|u_i, v_j)\underbrace{p(U, V, \Theta_U, \Theta_V|R)}_{\text{Posterior over parameters and hyperparameters}} d\{U, V\} d\{\Theta_U, \Theta_V\}$$

- Use Monte Carlo approximation:

$$p(r^*_{ij}|R) \approx \frac{1}{N} \sum_n p(r^*_{ij}|u_i^{(n)}, v_j^{(n)}).$$

- The samples (u_i^n, v_j^n) are generated by running a Gibbs sampler, whose stationary distribution is the posterior distribution of interest.

Bayesian PMF

- Monte Carlo approximation:

$$p(r_{ij}^*|R) \approx \frac{1}{N} \sum_n p(r_{ij}^*|u_i^{(n)}, v_j^{(n)}).$$

- The conditional distributions over the user and movie feature vectors are Gaussians → easy to sample from:

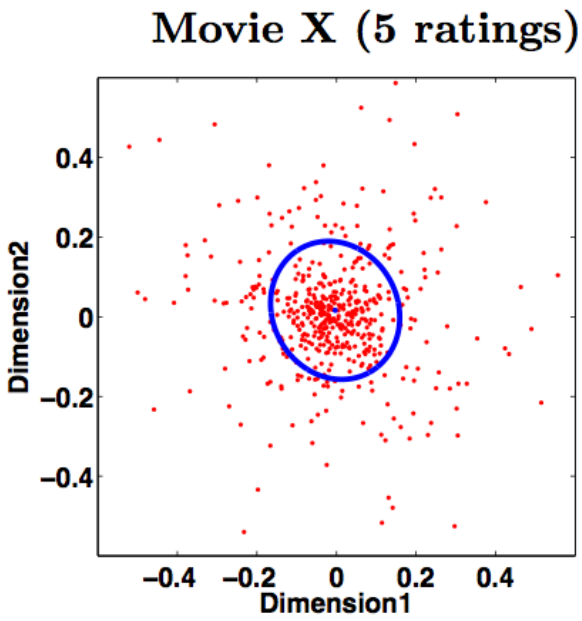
$$p(u_i|R, V, \Theta_U) = \mathcal{N}(u_i|\mu_i, \Sigma_i)$$
$$p(v_i|R, U, \Theta_V) = \mathcal{N}(v_j|\mu_j, \Sigma_j)$$

- The conditional distributions over hyperparameters also have closed form distributions → easy to sample from.

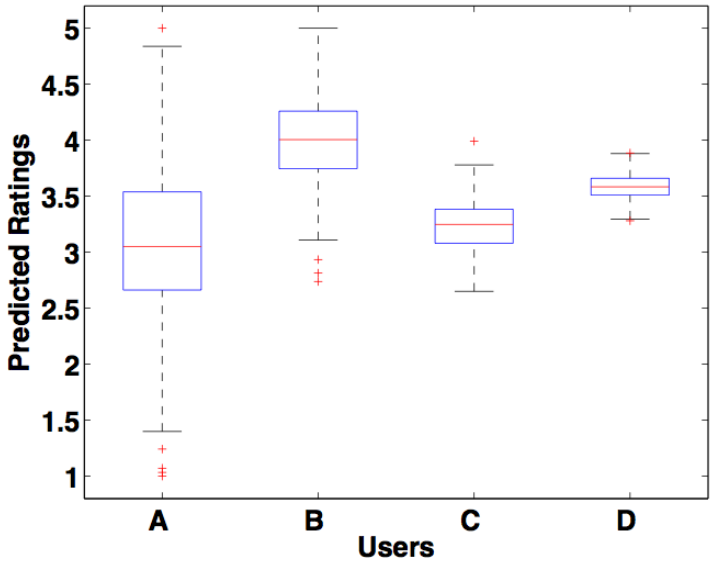
- The Netflix dataset – Bayesian PMF can handle over 100 million ratings.

Bayesian PMF

• Sample from the posterior of a movie with 5 ratings: Non-Gaussian.



• Assessing uncertainty in predicted values can be crucial.



• Variational approximation in this case works much worse compared to Gibbs.

• Predicted ratings for a test movie by users A,B,C, and D that have 4, 23, 319, and 660 observed ratings.

Auxiliary Variables

- The goal of MCMC is to marginalize out variables.
- But sometimes it is useful to introduce additional, or auxiliary variables.

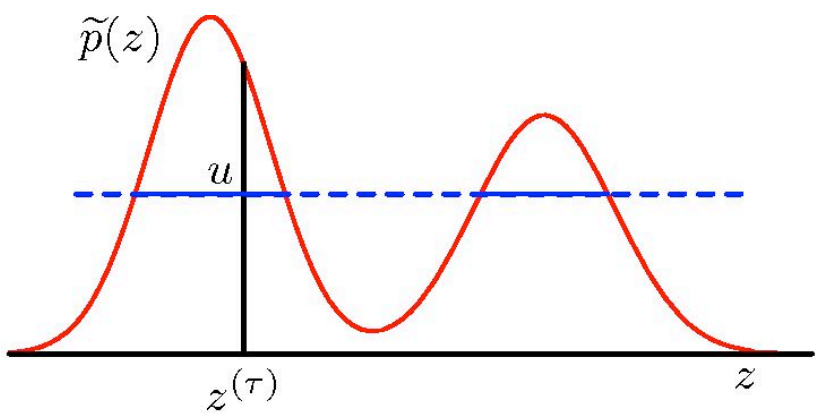
$$\int f(z)p(z)dz = \int f(z)p(z,u)dzdu$$

$$\approx \frac{1}{L}\sum_{l=1}^{L} f(z^l), \qquad (z,u) \sim p(z,u).$$

- We would want to do this if:
  - Sampling from conditionals p(z | u) and p(u | z) is easy.
  - It is easier to deal with p(z,u).
- Many MCMC algorithms use this idea.

Slice Sampling

- M-H algorithm is sensitive to the step size.
- Slice sampling provides an adaptive step size that is automatically adjusted.
- We augment z with an additional (auxiliary) variable u and then draw samples from the joint (z,u) space.



(a)

- The goal is to sample uniformly from the area under the distribution:

$$\hat{p}(z,u) = \begin{cases} 1/\mathcal{Z}_p & 0 \leq u \leq \tilde{p}(z) \\ 0 & \text{otherwise} \end{cases}$$

- The marginal distribution over z is:

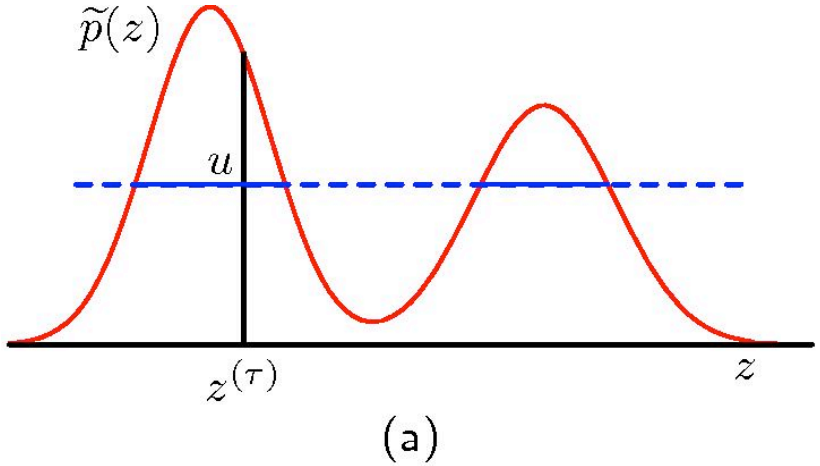
$$\int \tilde{p}(z,u)\mathrm{d}u = \int_0^{\tilde{p}(z)} \frac{1}{\mathcal{Z}_p}\mathrm{d}u = \frac{\tilde{p}(z)}{\mathcal{Z}_p} = p(z),$$

which is the target distribution of interest.

Slice Sampling

- The goal if sample uniformly from the area under the distribution:

$$\hat{p}(z,u) = \begin{cases} 1/\mathcal{Z}_p & 0 \leq u \leq \tilde{p}(z) \\ 0 & \text{otherwise} \end{cases}$$



- Given z, we sample u uniformly from:

$$0 \leq u \leq \tilde{p}(z),$$

which is easy.

- Given u, we sample z uniformly from the **slice** through the distribution defined:

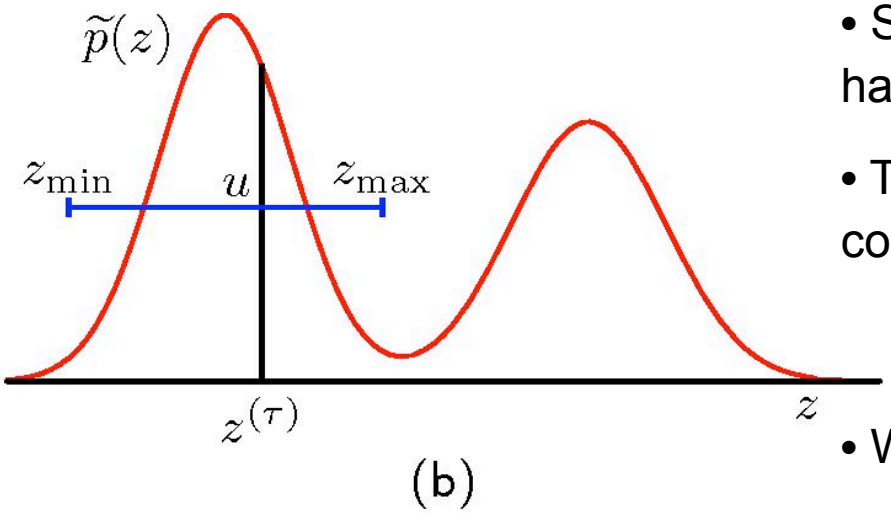
$$\{z : \tilde{p}(z) > u\}.$$

- In practice, sampling directly from a slice might be difficult.
- Instead we can define a sampling scheme that leaves the distribution $\hat{p}(z,u)$ invariant.

Slice Sampling

- The goal if sample uniformly from the area under the distribution:

$$\hat{p}(z,u) = \begin{cases} 1/\mathcal{Z}_p & 0 \leq u \leq \tilde{p}(z) \\ 0 & \text{otherwise} \end{cases}$$



(b)

- Suppose the current state is z^{τ}, and we have obtained a corresponding sample u.
- The next value of z is obtained by considering the region:

$$z_{min} \leq z \leq z_{max}.$$

- We can adapt the region.

- Start with a region containing z^{τ} having some width w.
- Linearly step out until the end point lies outside the region.
- Sample uniformly from the region, shrinking if the sample if off slice.
- Satisfies detailed balance.

Using MCMC in Practice

- The samples we obtain from MCMC are not independent. Should we thin, i.e. only keep every Kth sample?
- We often start MCMC from arbitrary starting points. Should be discard a burn-in period?
- Should we perform multiple runs as opposed to one long run?
- How do we know whether we have run our chain for long enough?