Monte Carlo Methods

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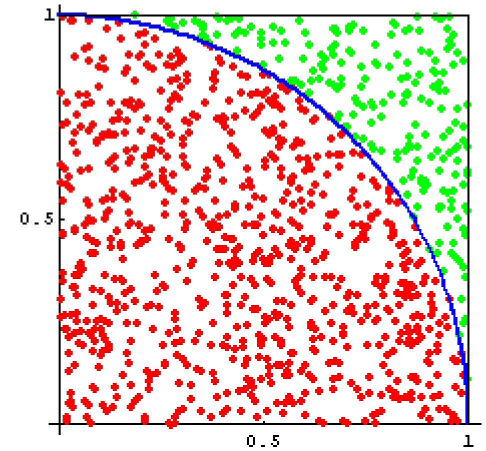
Monte Carlo Methods

- a class of computational algorithms that rely on repeated random sampling to compute their results.
- tend to be used when it is infeasible to compute an exact result with a deterministic algorithm
- was coined in the 1940s by John von Neumann, Stanislaw Ulam and Nicholas Metropolis

Games of Chance

Monte Carlo Methods to Calculate Pi

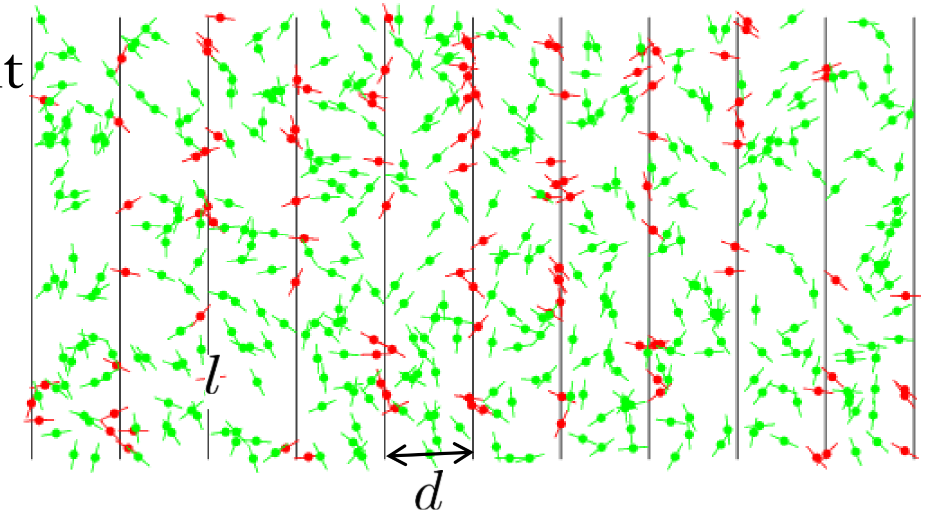
- Computer Simulation



$$\hat{\pi} = 4 \times \frac{m}{N}$$

  - N: # points inside the square
  - m: # points inside the circle

- Bufffon's Needle Experiment

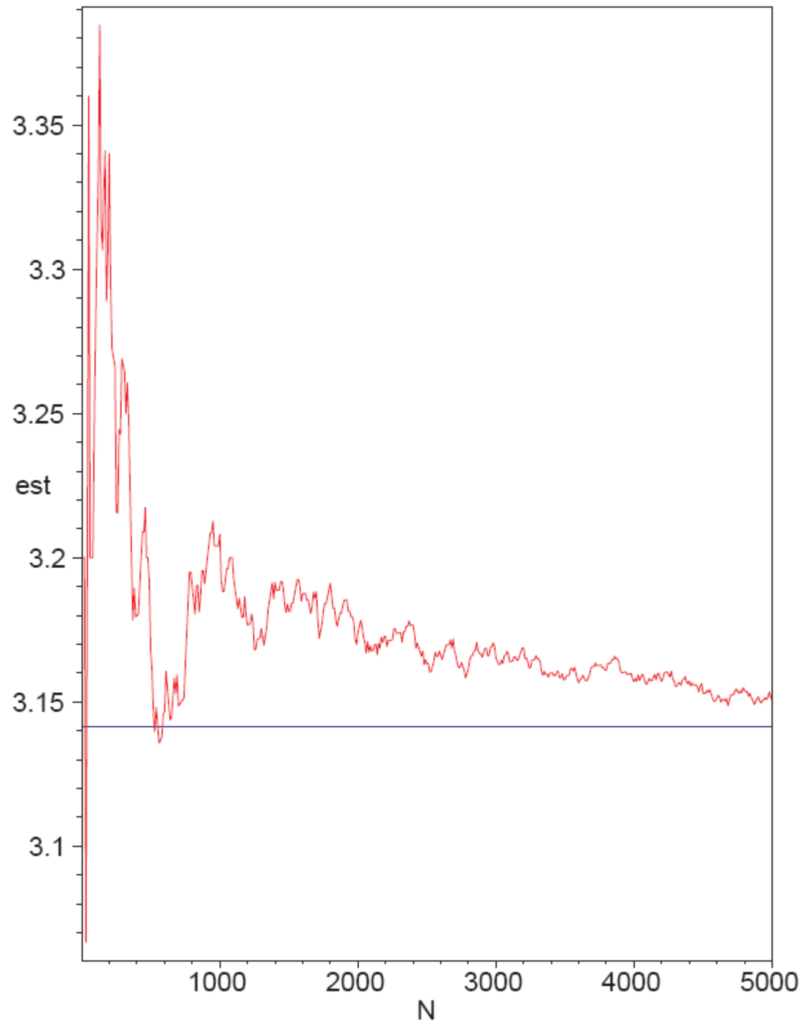


$$\hat{\pi} = \frac{2Nx}{m}$$

  - m: # line crossings

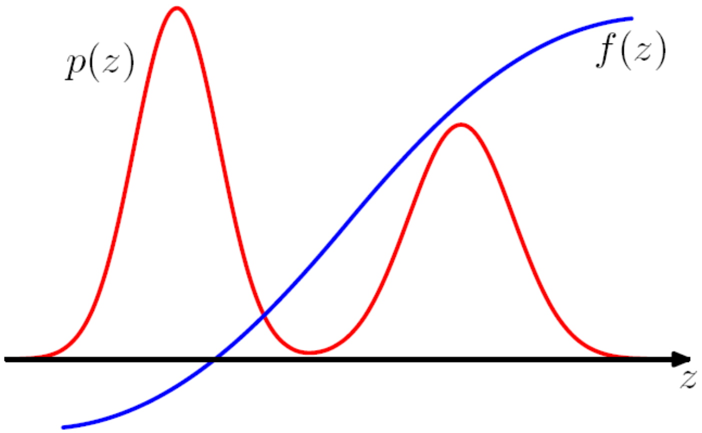
$$x = \frac{l}{d}$$

Typical Outputs with Simulation



Problems to be Solved

- **Sampling**
  - to generate a set of samples $\{\mathbf{z}_l\}_{l=1}^{L}$ from a given probability distribution $p(\mathbf{z})$
  - the distribution is called target distribution
  - can be from statistical physics or data modeling
- **Integral**
  - To estimate expectations of functions under this distribution



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

Use Sample to Estimate the Target Dist.

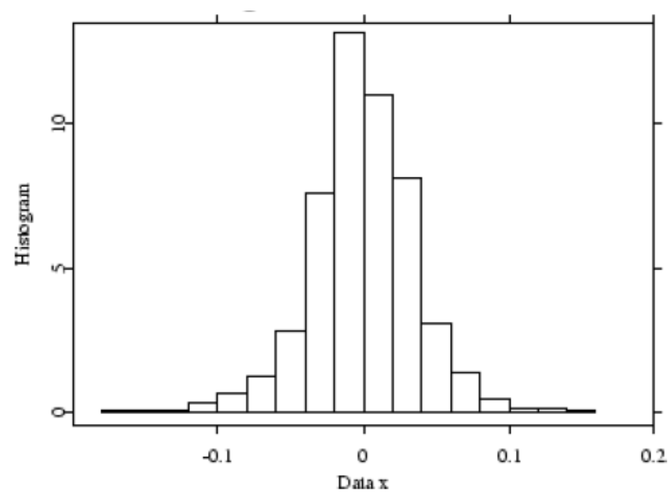
- Draw a set of independent samples (a hard problem)

$$\forall 1 \leq l \leq L, \quad \mathbf{z}^{(l)} \sim p(\mathbf{z})$$

- Estimate the target distribution as count frequency

$$p(\mathbf{z}) \approx \frac{1}{L} \sum_{l=1}^{L} \delta_{\mathbf{z},\mathbf{z}^{(l)}}$$

Histogram with Unique Points as the Bins



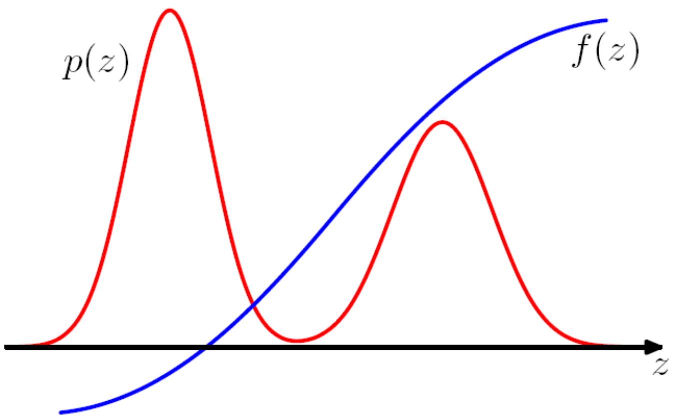
Basic Procedure of Monte Carlo Methods

- Draw a set of independent samples

$$\forall 1 \le l \le L, \quad \mathbf{z}^{(l)} \sim p(\mathbf{z})$$

- Approximate the expectation with

$$\hat{f} = \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^{(l)})$$



  - where is the distribution p?

$$p(\mathbf{z}) \approx \frac{1}{L}\sum_{l=1}^{L} \delta_{\mathbf{z},\mathbf{z}^{(l)}}$$

Histogram with Unique Points as the Bins

  - why this is good?

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

  - Accuracy of estimator does not depend on dimensionality of z
  - High accuracy with few (10-20 independent) samples
  - However, obtaining independent samples is often not easy!

Why Sampling is Hard?

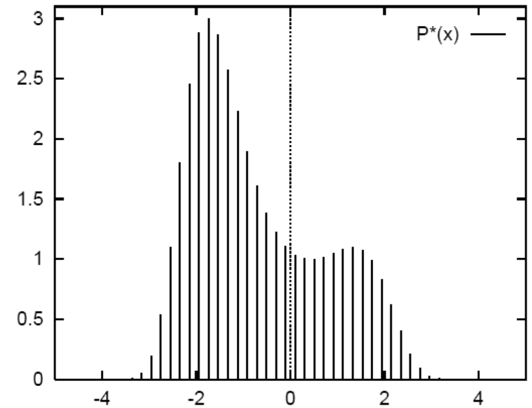
- **Assumption**
  - The target distribution can be evaluated, at least to within a multiplicative constant, i.e.,

$$p(\mathbf{z}) = p^*(\mathbf{z})/Z$$

  - where $p^*(\mathbf{z})$ can be evaluated
- **Two difficulties**
  - Normalizing constant is typically unknown
  - Drawing samples in high-dimensional space is challenging

A Simple Example

- Draw samples from a discrete distribution with a finite set of uniformly distributed points

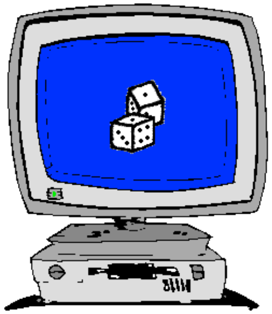


- We can compute the distribution via

$$Z = \sum_i p_i^* \qquad p_i = p_i^* / Z$$

- … then draw samples from the multinomial distribution
- But, the cost grows exponentially with dimension!

Basic Sampling Algorithms



- Strategies for generating samples from a given standard distribution, e.g., Gaussian

- Assume that we have a pseudo-random generator for *uniform distribution over (0,1)*

- For standard distributions we can *transform* uniformly distributed samples into desired distributions

Basic Sampling Algorithms

- If z is uniformly distributed over (0, 1), then $y = f(z)$ has the distribution

$$p(y) = p(z)\left|\frac{dz}{dy}\right|$$

  - where $p(z) = 1$
- Normally, we know *p(y)* and infer *f*. This can be done via

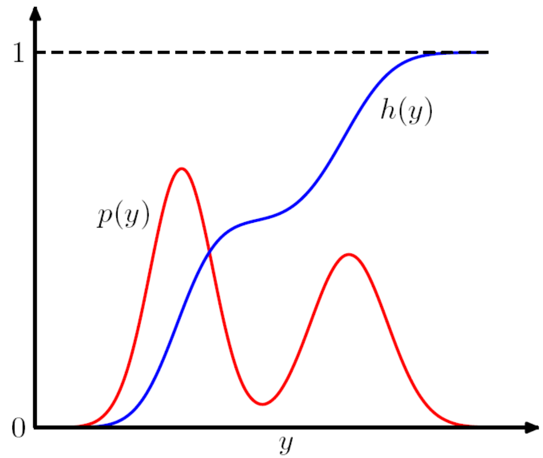
$$z = h(y) = \int_{-\infty}^{y} p(\hat{y})d\hat{y}$$

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

- So we have to transform uniformly distributed random numbers
  - using a function which is the inverse of the indefinite integral of the distribution

Geometry of Transformation

- Generating non-uniform random variables



- $h(y)$ is indefinite integral of desired $p(y)$
- $z \sim \mathrm{Uniform}(0,1)$ is transformed using $y = h^{-1}(z)$
- Results in y being distributed as $p(y)$

Example #1

- How to get the exponential distribution from uniform variable?

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

- Do the integral, we get

$$\begin{aligned} z = h(y) = \int_{-\infty}^{y} p(\hat{y}) d\hat{y} &= \int_{-\infty}^{y} \lambda \exp(-\lambda \hat{y}) d\hat{y} \\ &= 1 - \exp(-\lambda y) \end{aligned}$$

- Thus

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

Example #2

- How to get the standard normal distribution from uniform variable?

$$p(y) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}y^2\right)$$

- Do the integral, we get

$$\begin{aligned} z = h(y) = \int_{-\infty}^{y} p(\hat{y}) d\hat{y} &= \Phi(y) \\ &= \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{y}{\sqrt{2}}\right)\right] \end{aligned}$$

- Thus

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

No closed form!!

Example #2: Box-Muller for Gaussian

- E xample of a bivariate Gaussian

$$p(y_1, y_2) = \Big[\frac{1}{\sqrt{2\pi}} \exp\Big(-\frac{1}{2}y_1^2\Big)\Big]\Big[\frac{1}{\sqrt{2\pi}} \exp\Big(-\frac{1}{2}y_2^2\Big)\Big]$$

- Generate pairs of uniformly distributed random numbers

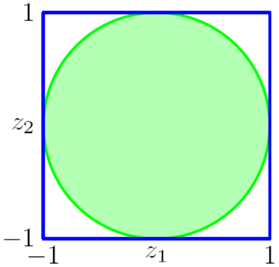
$$z_1,\ z_2 \sim \mathrm{Uniform}(-1, 1)$$

- Discard each pair unless

$$z_1^2 + z_2^2 \leq 1$$

- Leads to uniform distribution of points inside unit circle with

$$p(z_1, z_2) = \frac{1}{\pi}$$



Example #2: Box-Muller for Gaussian

- E valuate the two quantities

$$y_1 = z_1 \left(\frac{-2 \ln z_1}{r^2} \right)^{1/2} \qquad y_2 = z_2 \left(\frac{-2 \ln z_2}{r^2} \right)^{1/2}$$

  - where $r^2 = z_1^2 + z_2^2$
- Then, we have independent standard normal distribution

$$p(y_1, y_2) = \left[\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} y_1^2 \right) \right] \left[\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} y_2^2 \right) \right]$$

- How about non-zero means and non-standard variance?
- How about multivariate Gaussian?

Rejection Sampling

- **Problems with transformation methods**
  - depend on ability to calculate and then invert indefinite integral
  - feasible only for some standard distributions

- **More general strategy is needed**
  - Rejection sampling and importance sampling are limited to univariate distributions
    - Although not applicable to complex problems, they are important components in more general strategies
  - Allows sampling from complex distributions

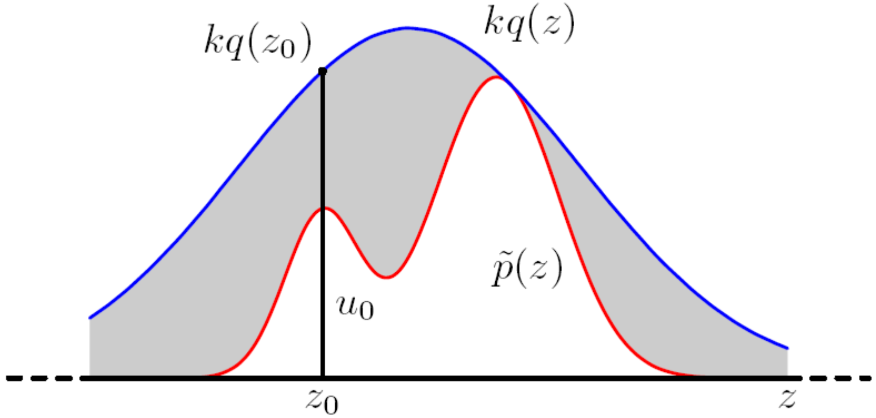
Rejection Sampling

- Wish to sample from distribution $p(z)$
- Suppose we are able to easily evaluate $p(z)$ *for any* given value of z
- Samples are drawn from simple distribution, called proposal distribution $q(z)$
- Introduce constant k whose value is such that $kq(z) \geq p(z)$ for all z
  - Called comparison function

Rejection Sampling

- Samples are drawn from simple distribution $q(z)$
- Rejected if they fall in grey area between $\tilde{p}(z)$ and $kq(z)$

$$p(z) = \frac{\tilde{p}(z)}{Z_p}$$



- Resulting samples are distributed according to *p(z)* which is the normalized version of $\tilde{p}(z)$

How to determine if sample is in shaded region?

- E ach step involves generating two random numbers

$$z_0 \sim q(z) \qquad u_0 \sim \text{Uniform}(0, kq(z_0))$$

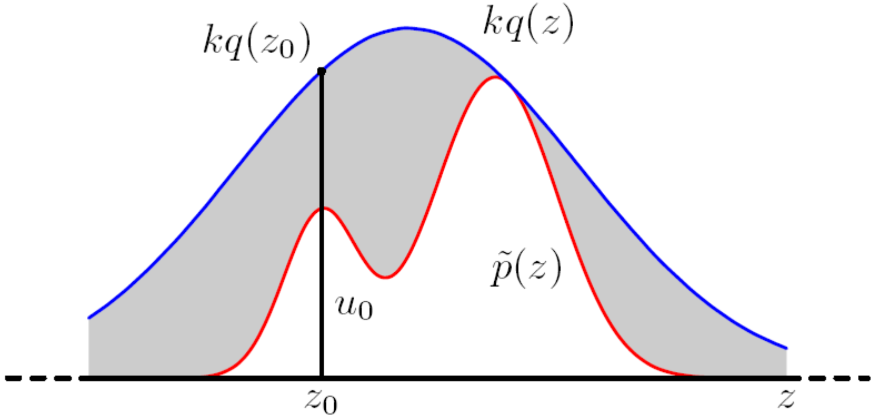
- This pair has uniform distribution under the curve of function $kq(z)$
- If $u_0 > p(z_0)$ the pair is rejected otherwise it is retained
- Remaining pairs have a uniform distribution under the curve of $p(z)$ and hence the corresponding z values are distributed according to $p(z)$ as desired
- Proof?

$$\hat{p}(z) = q(z) \times \frac{\tilde{p}(z)}{kq(z)} \propto \tilde{p}(z)$$

More on Rejection Sampling

- The probability that a sample will be accepted (accept ratio)

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

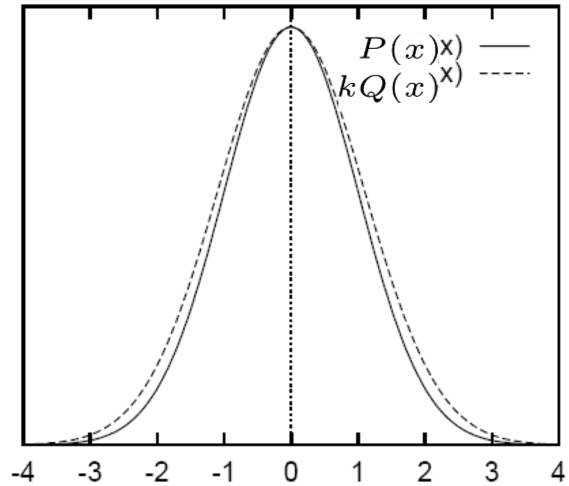


- To have high accept ratio, *k* should be as small as possible
  - … but it needs to satisfy

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

Curse of Dimensionality

- Consider two univariate Gaussian distributions



$$P(x) \sim \mathcal{N}(0, \sigma_p^2)$$

$$Q(x) \sim \mathcal{N}(0, \sigma_q^2)$$

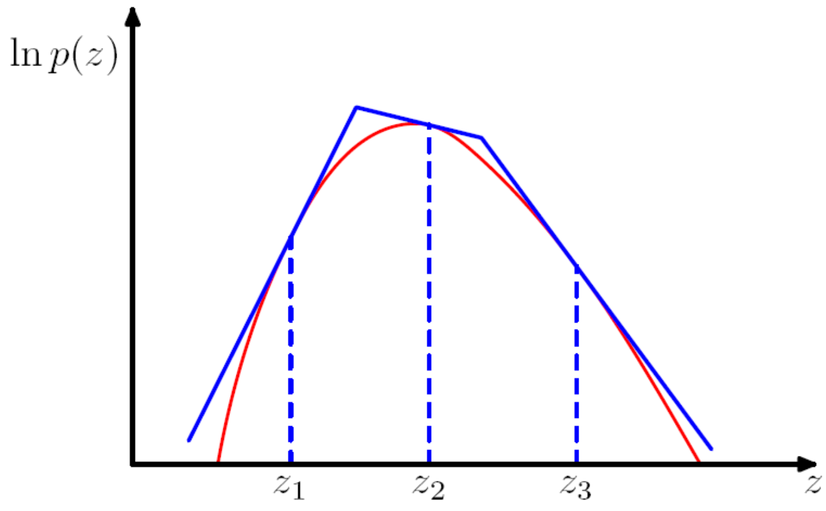
$$\sigma_q > \sigma_p$$

- What is k?
  - At the origin, we have $k \frac{1}{\sqrt{2\pi}\sigma_q} = \frac{1}{\sqrt{2\pi}\sigma_p}$, so $k = \frac{\sigma_q}{\sigma_p}$
  - How about in 1000 dimensions?

$$k = \left(\frac{\sigma_q}{\sigma_p}\right)^{1000} \approx 20,000 \text{ if } \sigma_q = 1.01\sigma_p$$

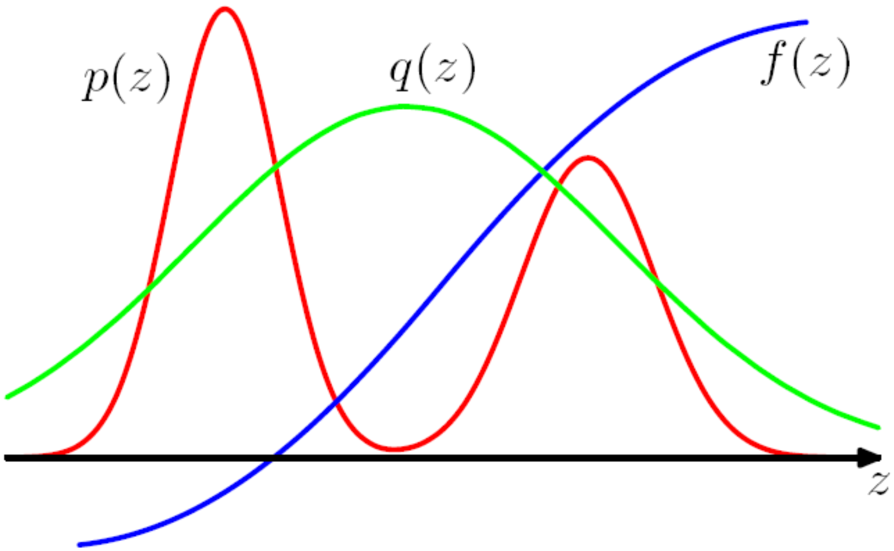
Adaptive Rejection Sampling

- When difficult to find suitable analytic distribution
- Straight-forward when $p(z)$ is log concave
  - When $\ln p(z)$ has derivatives that are non-increasing functions of z
  - Function $\ln p(z)$ and gradients are evaluated at set of grid points
  - Intersections are used to construct envelope ➔ a sequence of linear functions



Importance Sampling

- Evaluating expectation of $f(z)$ with respect to distribution $p(z)$ from which it is difficult to draw samples directly
- Samples $\{z^{(l)}\}$ are drawn from simpler distribution $q(z)$
- Terms in summation are weighted by ratios $\dfrac{p(z^{(l)})}{q(z^{(l)})}$



Importance Sampling

- The expectation can be computed as

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

- Use Monte Carlo methods

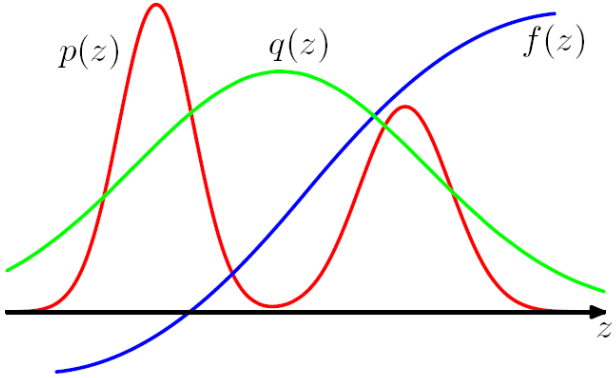
$$\mathbb{E}[f] \approx \frac{1}{L}\sum_{l=1}^{L} r_l f(\mathbf{z}^{(l)})$$

  - where the importance weights are

$$r_l = \frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}$$

  - and the samples are

$$\mathbf{z}^{(l)} \sim q(\mathbf{z})$$



Importance Sampling

- For **unnormalized distributions**

$$p(\mathbf{z}) = \frac{\tilde{p}(\mathbf{z})}{Z_p}, \quad q(\mathbf{z}) = \frac{\tilde{q}(\mathbf{z})}{Z_q}$$

- We have $\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z} = \frac{Z_q}{Z_p}\int f(\mathbf{z})\frac{\tilde{p}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})d\mathbf{z}$

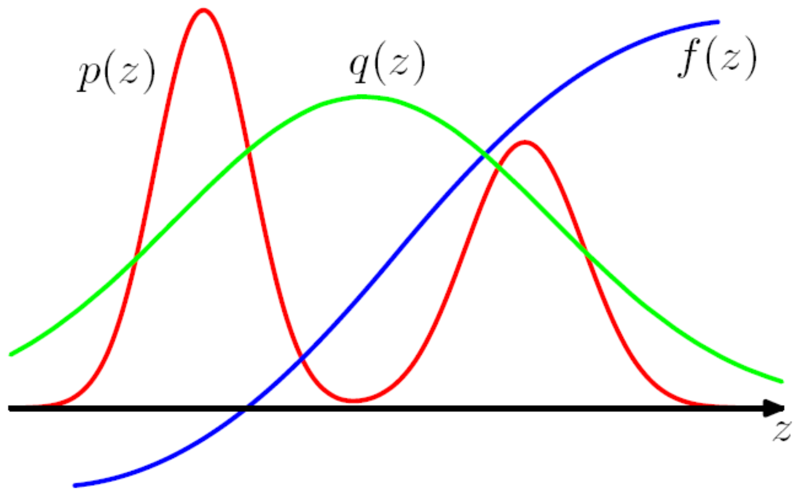
$$\mathbb{E}[f] \approx \frac{Z_q}{Z_p}\frac{1}{L}\sum_{l=1}^{L}\tilde{r}_l f(\mathbf{z}^{(l)}) \quad \text{where } \tilde{r}_l = \frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}$$

- The ratio $\frac{Z_p}{Z_q} = \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})d\mathbf{z} = \int \frac{\tilde{p}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})d\mathbf{z} \approx \frac{1}{L}\sum_{l=1}^{L}\tilde{r}_l$
- Then, the expectation is

$$\mathbb{E}[f] \approx \sum_{l=1}^{L} w_l f(\mathbf{z}^{(l)}), \quad \text{where } w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m}$$

Problems with Importance Sampling

- As with Rejection sampling, the performance depends crucially on how well the proposal matches the target



  - a lot of wastes in the areas where $p(z)f(z)$ is small
  - more serious in high dimensional spaces

Summary so far …

- Monte Carlo methods use samples to estimate expectations
- Rejection sampling and importance sampling are useful when no closed-form transformation is available or is hard
- But they can be inefficient in high-dimensional spaces
    - only works well when the proposal approximate the target well

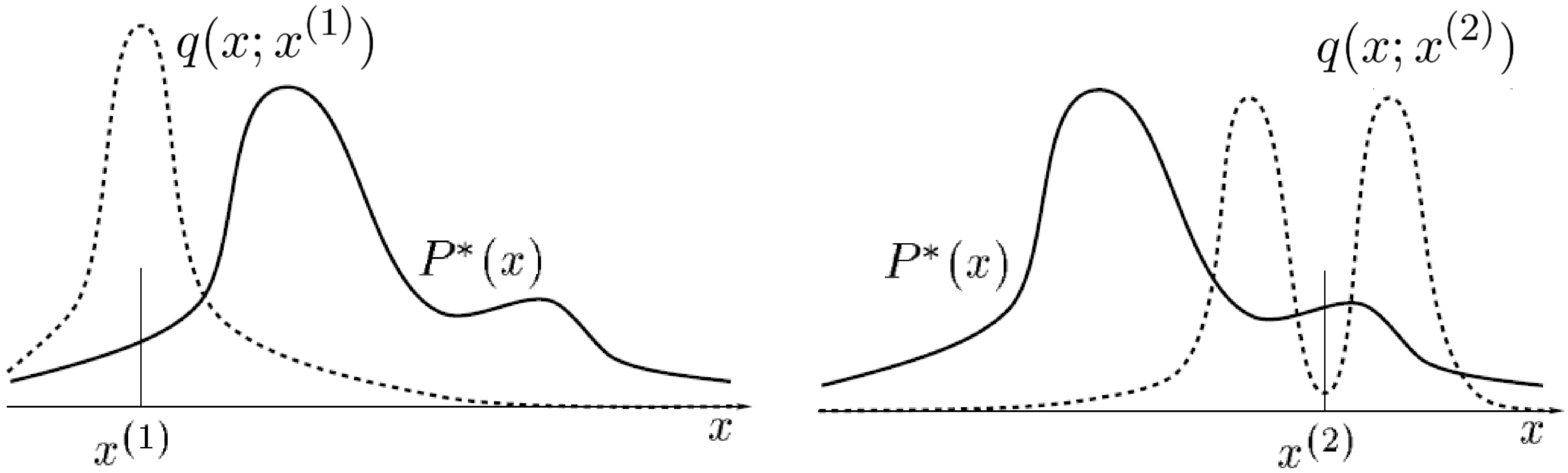
Markov Chain Monte Carlo (MCMC)

- As with rejection and importance sampling, it samples from a proposal distribution
- But, it maintains a record of $\mathbf{z}^{\tau}$, and the proposal distribution depends on current state $q(\mathbf{z}|\mathbf{z}^{\tau})$
- It's not necessary for the proposal to look at all similar to the target
- The sequence $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$ forms a Markov chain

- Configurable components:
  - Proposal distribution
  - Accept strategy

Geometry of MCMC

- Proposal depends on current state
- Not necessarily similar to the target
- Can evaluate the un-normalized target



Metropolis Algorithm

- Proposal distribution is symmetric

$$q(\mathbf{z}|\mathbf{z}') = q(\mathbf{z}'|\mathbf{z})$$

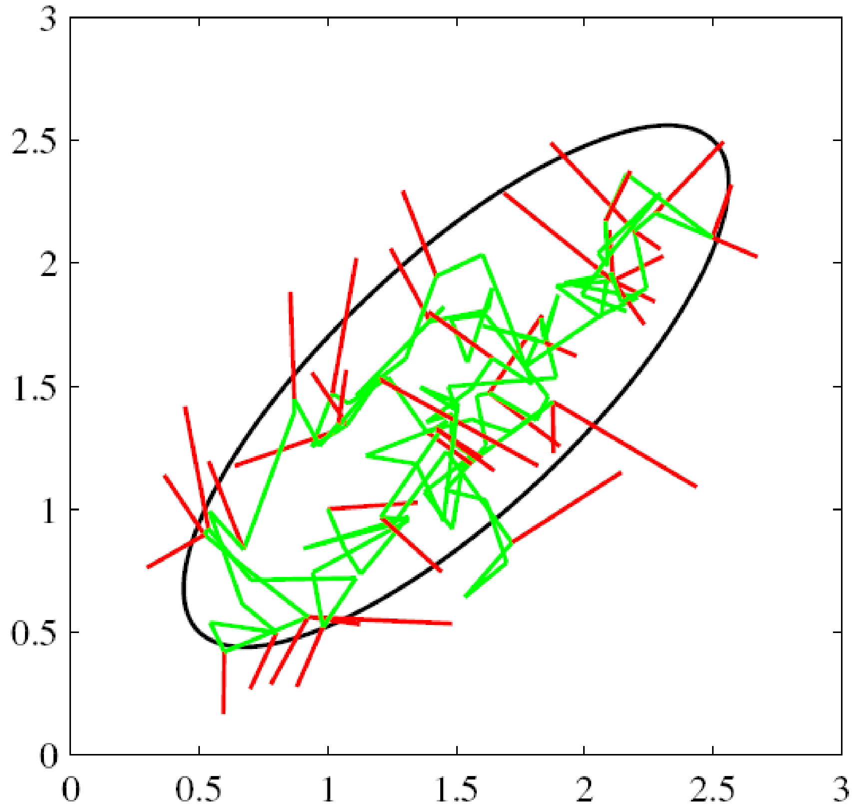
- The candidate sample $\mathbf{z}^*$ is accepted with probability

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

  - The acceptance can be done by
    - draw a random $u \sim \mathrm{Uniform}(0, 1)$
    - accepting the sample if $A(\mathbf{z}^*, \mathbf{z}^{(\tau)}) > u$
- If sample is accepted, set $\mathbf{z}^{(\tau+1)} = \mathbf{z}^*$; otherwise $\mathbf{z}^{(\tau+1)} = \mathbf{z}^{(\tau)}$
- **Note:** $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$ is not a set of independent samples

Geometry of Metropolis Algorithm

- Sample from Gaussian distribution with the proposal being an isotropic Gaussian with std 0.2.
- **Green**: accepted steps; **Red**: rejected steps



Properties of Markov Chains

- $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots, \mathbf{z}^{(M)}$ is a *first-order Markov chain* if conditional independence property holds

$$p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}) = p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)})$$

- *Transition probabilities* $T_m(\mathbf{z}^{(m)}, \mathbf{z}^{(m+1)}) \triangleq p(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)})$
- If T_m are the same for all *m*, it is *Homogeneous* Markov chain
- $p^*(\mathbf{z})$ satisfies the *detailed balance* if

$$p^*(\mathbf{z})T(\mathbf{z}, \mathbf{z}') = p^*(\mathbf{z}')T(\mathbf{z}', \mathbf{z})$$

- If $p^*(\mathbf{z})$ satisfies the detailed balance, then it's *invariant (stationary)*

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

- A chain is *ergodic* if it converges to the invariant distribution, irrespective of the initial distribution

Metropolis-Hasting Algorithm

- A generalization of the Metropolis algorithm to the case where the proposal distribution is no longer symmetric
- Draw sample $\mathbf{z}^* \sim q_k(\mathbf{z}|\mathbf{z}^{(\tau)})$ and accept it with probability

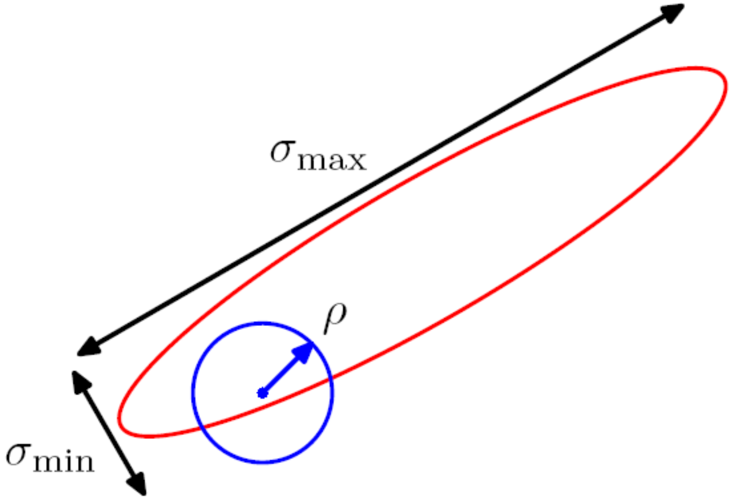
$$A_k(\mathbf{z}^*, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^*)q_k(\mathbf{z}^{(\tau)}|\mathbf{z}^*)}{\tilde{p}(\mathbf{z}^{(\tau)})q_k(\mathbf{z}^*|\mathbf{z}^{(\tau)})}\right)$$

- We can show $p(\mathbf{z})$ is an invariant distribution of MC defined by MH algorithm, by showing the detailed balance

$$\begin{aligned}
p(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})A_k(\mathbf{z}', \mathbf{z}) &= \min\left(p(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z}), p(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')\right) \\
&= \min\left(p(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}'), p(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})\right) \\
&= p(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}') \min\left(1, \frac{p(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})}{p(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')}\right) \\
&= p(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')A_k(\mathbf{z}, \mathbf{z}')
\end{aligned}$$

Issues with Proposal Distribution

- **Proposal**: isotropic Gaussian (blue) centered at current state



  - Small ρ leads to high accept rate, but progress through the state space takes a long time due to random walk
  - Large ρ leads to high rejection rate
  - Roughly best choice: $\rho \approx \sigma_{\min}$

Gibbs Sampling

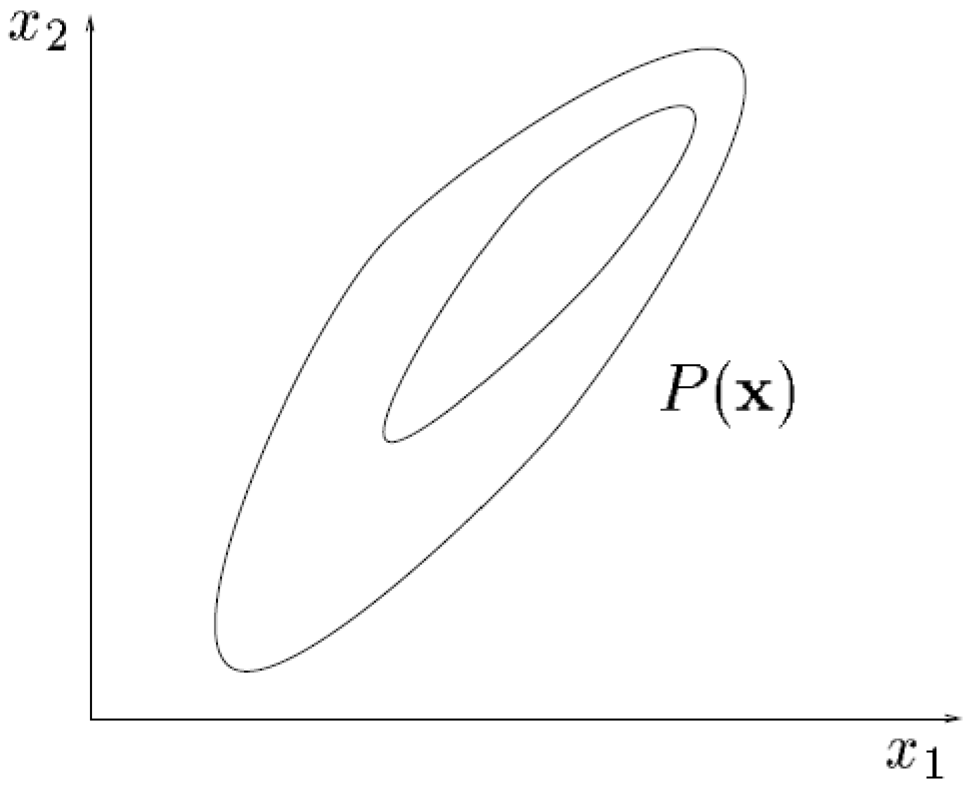
- A special case of Metropolis-Hastings algorithm
- Consider the distribution $p(\mathbf{z}) = p(z_1, \ldots, z_M)$
- Gibbs sampling performs the follows
  - Initialize $\{z_i : i = 1, \ldots, M\}$
  - For $\tau = 1, \ldots, T$
    - Sample $z_1^{(\tau+1)} \sim p(z_1 | z_2^{(\tau)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$

      $\vdots$
    - Sample $z_j^{(\tau+1)} \sim p(z_j | z_1^{(\tau+1)}, \ldots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \ldots, z_M^{(\tau)})$

      $\vdots$
    - Sample $z_M^{(\tau+1)} \sim p(z_j | z_1^{(\tau+1)}, z_2^{(\tau+1)}, \ldots, z_{M-1}^{(\tau+1)})$

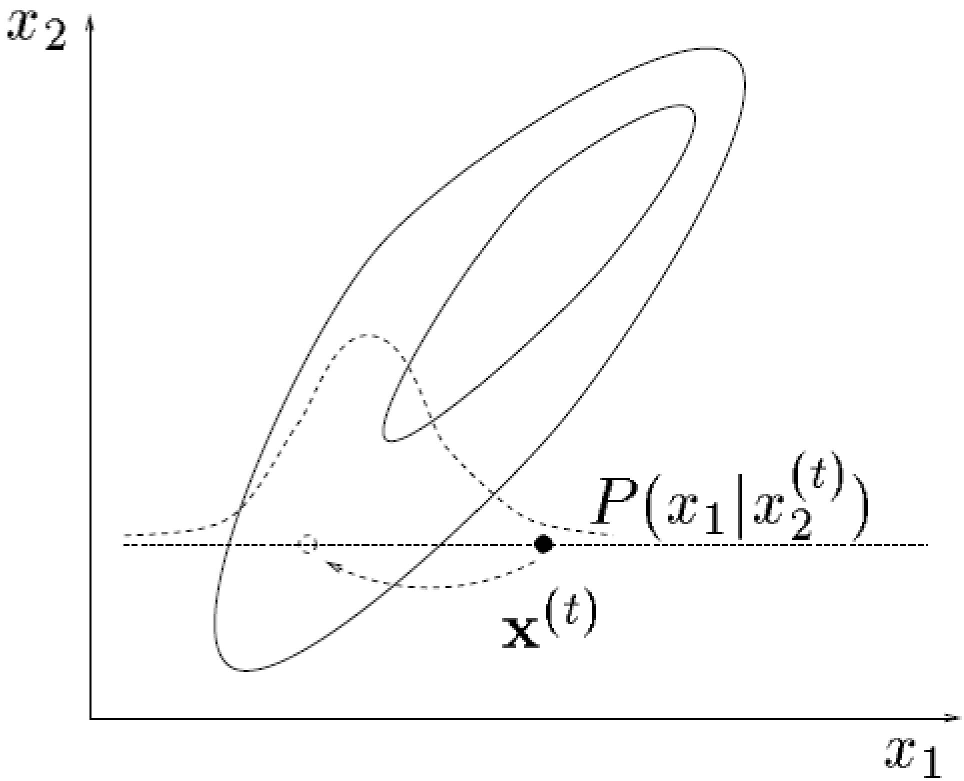
Geometry of Gibbs Sampling

- The target distribution in 2 dimensional space



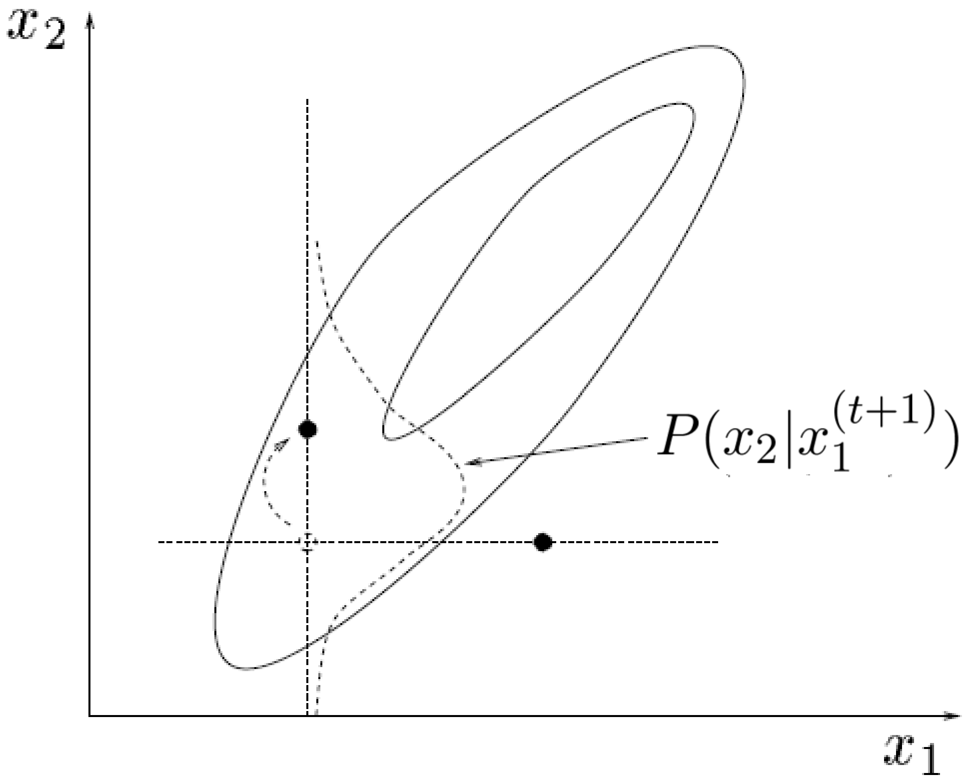
Geometry of Gibbs Sampling

- Starting from a state $\mathbf{x}^{(t)}$, $x_1^{(t+1)}$ is sampled from $P(x_1|x_2^{(t)})$



Geometry of Gibbs Sampling

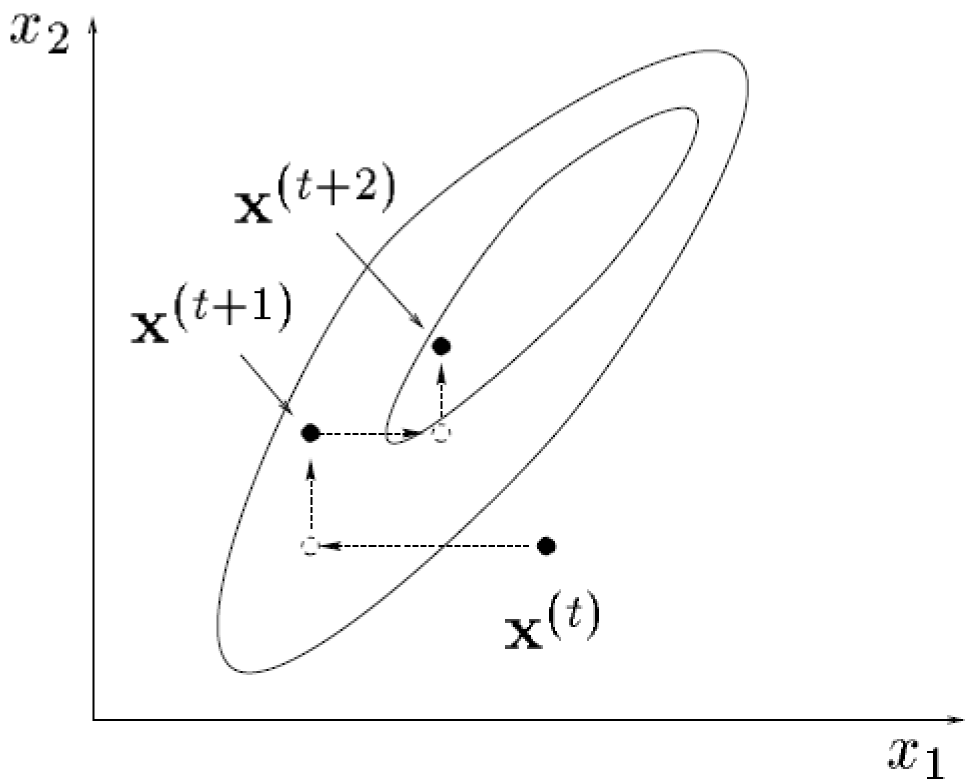
- A sample is drawn from $P(x_2|x_1^{(t+1)})$



this finishes one single iteration.

Geometry of Gibbs Sampling

- After a few iterations



Gibbs Sampling

- How to show Gibbs sampling samples from $p(\mathbf{z})$?
  - show that p(z) is an invariant distribution at each sample steps
    - The marginal $p(\mathbf{z}_{-i})$ is invariant as $\mathbf{z}_{-i}$ is unchanged
    - Also, the conditional $p(z_i|\mathbf{z}_{-i})$ is correct
    - Thus, the joint distribution $p(z_i|\mathbf{z}_{-i})p(\mathbf{z}_{-i})$ is invariant at each step
  - the Markov chain is ergodic
    - A sufficient condition is that none of the conditional distributions be anywhere zero
    - If the requirement is not satisfied (some conditionals have zeros), ergodicity must be proven explicitly

Gibbs Sampling

- a special case of Metropolis-Hastings algorithm
- Consider a MH sampling step involving variable z_k in which other variables $\mathbf{z}_{-k}$ remain fixed
- The transition probability is

$$q_k(\mathbf{z}^*|\mathbf{z}) = p(z_k^*|\mathbf{z}_{-k})$$

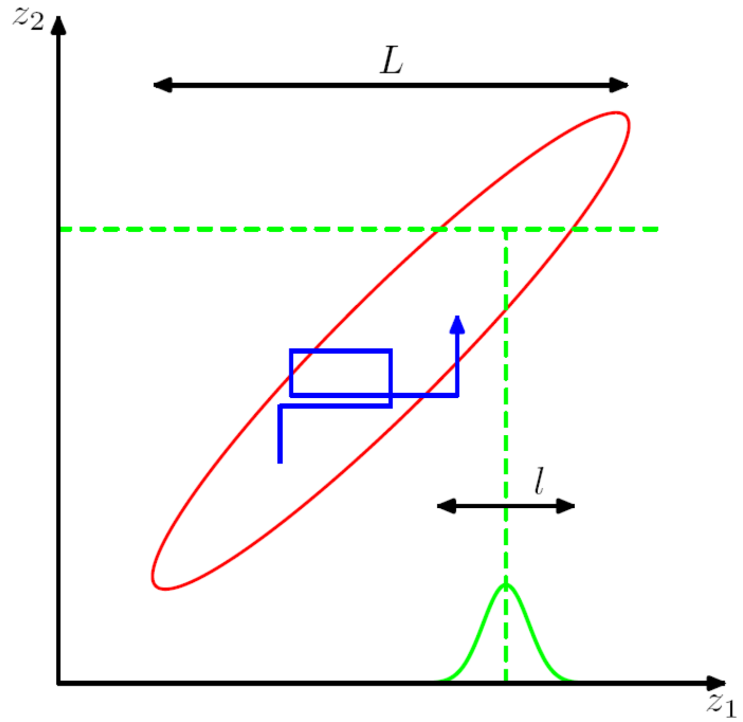
- Note that $\mathbf{z}^*_{-k} = \mathbf{z}_{-k}$ and $p(\mathbf{z}) = p(z_k|\mathbf{z}_{-k})p(\mathbf{z}_{-k})$
- Then, the MH acceptance probability is

$$A(\mathbf{z}^*, \mathbf{z}) = \frac{p(\mathbf{z}^*)q_k(\mathbf{z}|\mathbf{z}^*)}{p(\mathbf{z})q_k(\mathbf{z}^*|\mathbf{z})} = \frac{p(z_k^*|\mathbf{z}^*_{-k})p(\mathbf{z}^*_{-k})p(z_k|\mathbf{z}^*_{-k})}{p(z_k|\mathbf{z}_{-k})p(\mathbf{z}_{-k})p(z_k^*|\mathbf{z}_{-k})} = 1$$

  - always accepted!

Behavior of Gibbs Sampling

- **Correlated Gaussian**: marginal distributions of width L and conditional distributions of width l



Summary

- Monte Carlo methods are power tools that allow one to implement any distribution in the form

$$p(\mathbf{x}) = p^*(\mathbf{x})/Z$$

- Monte Carlo methods can answer virtually any query related to by putting the query in the form

$$\int f(\mathbf{x})p(\mathbf{x})d\mathbf{x} \approx \frac{1}{L}\sum_{l} f(\mathbf{x}^{(l)})$$

- In high-dimensional problems the only satisfactory methods are those based Markov chain Monte Carlo: Metropolis-Hastings and Gibbs sampling
- Simple Metropolis and Gibbs sampling algorithms, although widely used, may suffer from slow random walk. More sophisticated algorithms are needed.

Sampling and EM Algorithm

- General procedure of the EM algorithm
  - E-step: compute the expected complete-data log-likelihood

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

  - M-step: update model parameters

$$\theta^{\text{new}} = \arg\max_{\theta} Q(\theta, \theta^{\text{old}})$$

- Sampling methods can be applied to approximate the integral in E-step
  - called Monte Carlo EM algorithm

$$Q(\theta, \theta^{\text{old}}) \approx \frac{1}{L} \sum_{l=1}^{L} \ln p(\mathbf{X}, \mathbf{Z}^{(l)}|\theta)$$

References

- Chap. 11 of Pattern Recognition and Machine Learning, Bishop, 2006
- Introduction to Monte Carlo Methods. D.J.C. MacKay, 1998