Imperial College London

Approximate Inference: Sampling

Recommended reading:
Bishop, Chapter 11
Iain Murray's tutorial: `http://tinyurl.com/jxb6t7f`
Murphy, Chapters 23–24

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Monte Carlo Methods—Motivation

- Monte Carlo methods are computational techniques that make use of random numbers
- Two typical problems:
  1. **Problem 1:** Generate samples $\{\boldsymbol{x}^{(s)}\}$ from a given probability distribution $p(\boldsymbol{x})$, e.g., for simulation (generative models) or representations of distributions

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  ▶▶ Example: Means/variances of distributions, marginal likelihood

  Complication: Integral cannot be evaluated analytically

Approximate Integration

- Numerical integration (low-dimensional problems)
- Bayesian quadrature, e.g., O'Hagan (1987, 1991); Rasmussen & Ghahramani (2003)
- Variational Bayes, e.g., Jordan et al. (1999)
- Expectation Propagation, Opper & Winther (2001); Minka (2001)
- **Monte-Carlo Methods**, e.g., Gilks et al. (1996), Robert & Casella (2004), Bishop (2006)

Problem 2: Monte Carlo Estimation

- Computing expectations via statistical sampling:

$$\mathbb{E}[f(\boldsymbol{x})] = \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x}$$
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- Making predictions (e.g., Bayesian regression with inputs $\boldsymbol{x}$ and targets $\boldsymbol{y}$)

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- **Key problem:** Generating samples from $p(\boldsymbol{x})$ or $p(\boldsymbol{\theta})$
  ▸▸ Need to solve **Problem 1**

Properties of Monte Carlo Sampling

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\end{aligned}
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- Estimator is asymptotically consistent, i.e.,

$$
\lim_{S\to\infty} \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}) = \mathbb{E}[f(\boldsymbol{x})] + \epsilon
$$

- Error ϵ is normal (Gaussian) and its variance shrinks $\propto 1/S$, independent of the dimensionality
- Estimator is unbiased

Monte Carlo Estimation

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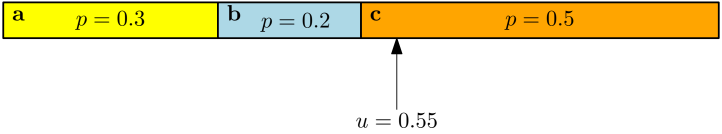
▶▶ Need to solve Problem 1

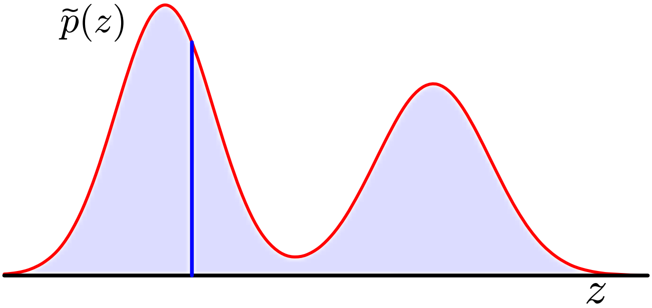
- Sampling from simple distributions
- Sampling from complicated distributions

Sampling Discrete Values



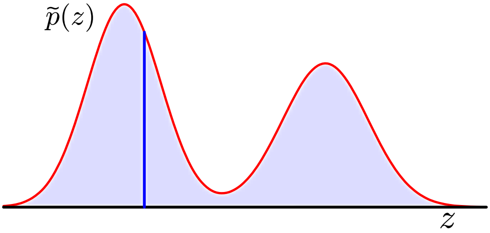
- $u \sim \mathcal{U}[0, 1]$, where $\mathcal{U}$ is the uniform distribution
- $u = 0.55 \Rightarrow x = c$

Continuous Variables



More complicated.
Geometric intuition: sample uniformly from the area under the curve

Rejection Sampling: Setting



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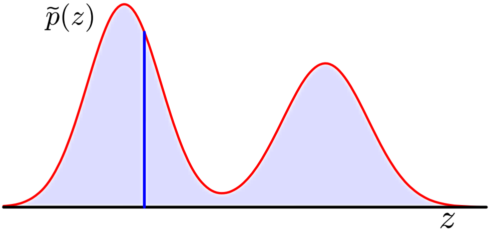
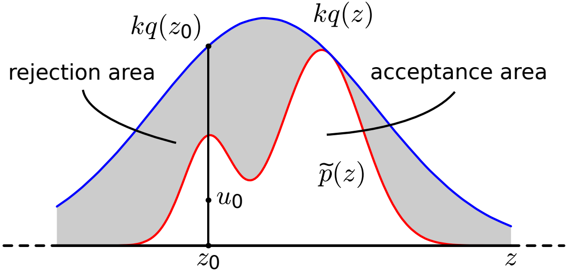


- Assume:
  - Sampling from $p(z)$ is difficult
  - Evaluating $\tilde{p}(z) = Zp(z)$ is easy (and Z may be unknown)
- Find a simpler distribution (proposal distribution) $q(z)$ from which we can easily draw samples (e.g., Gaussian, Laplace)
- Find an upper bound $kq(z) \geqslant \tilde{p}(z)$

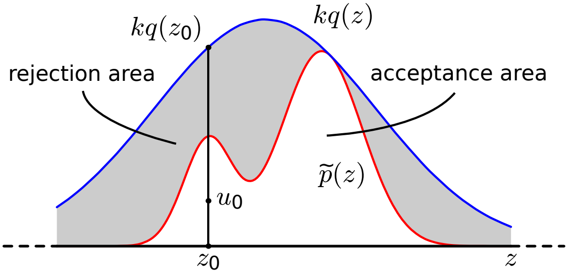
Rejection Sampling: Algorithm



Adapted from PRML (Bishop, 2006)

1. Generate $z_0 \sim q(z)$
2. Generate $u_0 \sim \mathcal{U}[0, kq(z_0)]$
3. If $u_0 > \tilde{p}(z_0)$, reject the sample. Otherwise, retain z_0

Properties



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- Accepted pairs (z, u) are uniformly distributed under the curve of $\tilde{p}(z)$
- Marginal probability density of the z-coordiantes of accepted points must be proportional to $\tilde{p}(z)$
- Samples are independent samples from $p(z)$

Sampling in High Dimensions

Example:

- $p(\boldsymbol{x}) = \mathcal{N}\big(\boldsymbol{0},\, \sigma_p^2 \boldsymbol{I}\big), \quad q(\boldsymbol{x}) = \mathcal{N}\big(\boldsymbol{0},\, \sigma_q^2 \boldsymbol{I}\big)$ where $\sigma_q = 1.01\sigma_p$
- What is the value of k if $\boldsymbol{x} \in \mathbb{R}^{1000}$?

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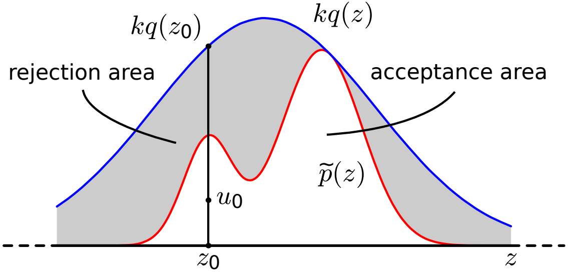
- What is the value of k if $\boldsymbol{x} \in \mathbb{R}^{1000}$?
- $q(0) = 1/(2\pi\sigma_q^2)^{500}$ ⏩ For $kq \geqslant p$ we need to set

$$k \geqslant \frac{p(0)}{q(0)} = \frac{(\sigma_q^2)^{500}}{(\sigma_p^2)^{500}} = \exp\left(1000 \ln \frac{\sigma_q}{\sigma_p}\right) = \exp(1000 \ln 1.01) \approx 20,000$$

- Acceptance rate is the ratio of the volume under p to the volume under kq. In our example: $1/k = 1/20,000$.
- In high dimensions the factor k is probably huge
  ⏩ **Low acceptance rate**
- Finding k is tricky

Shortcomings



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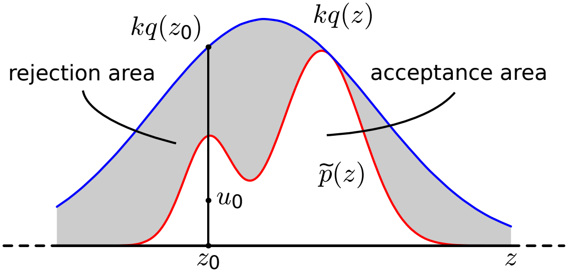

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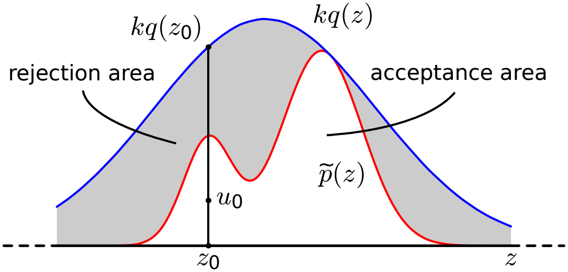

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- In high dimensions the factor k is probably huge
- **Low acceptance rate/high rejection rate** of samples

Importance Sampling

Key idea: Do not throw away all rejected samples, but give them lower weight by rewriting the integral as an expectation under a simpler distribution q (proposal distribution):

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▶▶ Different approach to sample from complicated (high-dimensional) distributions

Markov Chain Monte Carlo

Objective

Generate samples from an unknown target distribution.

Markov Chains

Key idea: Instead of generating independent samples $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots,$ use a proposal density q that depends on the previous sample (state) $\boldsymbol{x}^{(t)}$

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- T is called a **transition operator**
- Example: $T(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(t)}) = \mathcal{N}\big(\boldsymbol{x}^{(t+1)} \,|\, \boldsymbol{x}^{(t)},\, \sigma^2 \boldsymbol{I}\big)$

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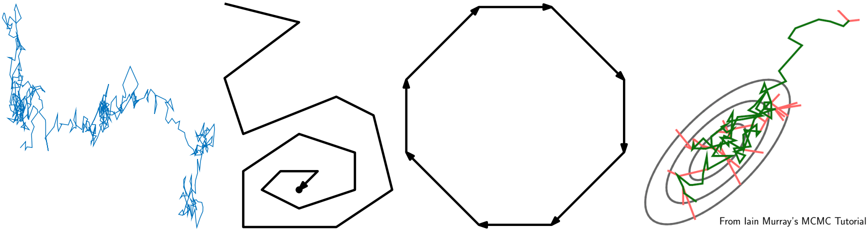
- Samples $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(t)}$ form a **Markov chain**
- Samples $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(t)}$ are no longer independent, but unbiased
  ▶▶ We can still average them

Behavior of Markov Chains



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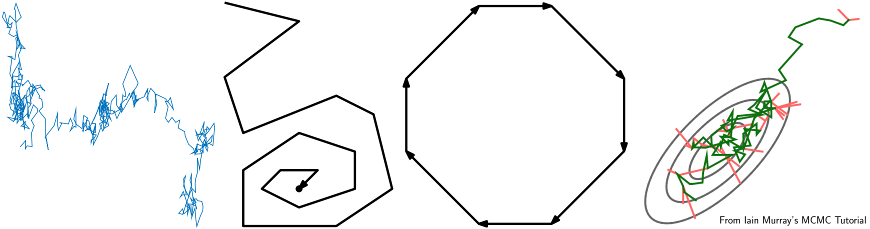

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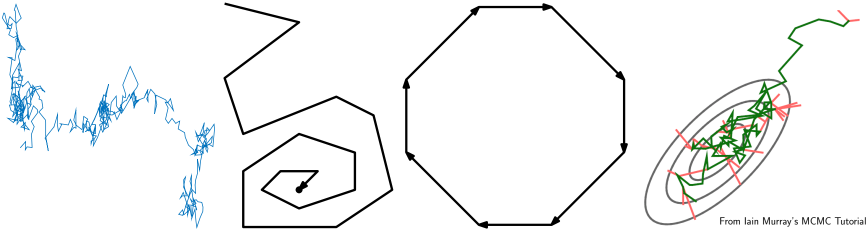

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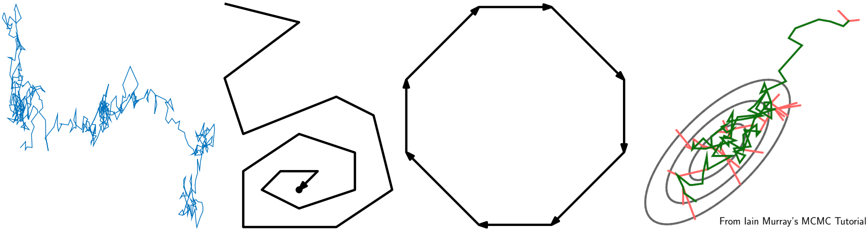

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- Converge to an equilibrium distribution p^*: Markov chain remains in a region, bouncing around in a random way

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- Generate a Markov chain that converges to that equilibrium distribution (independent of start state)
- Although successive samples are dependent we can effectively generate independent samples by running the Markov chain long enough: Discard most of the samples, retain only every Mth sample

Conditions for Converging to an Equilibrium Distribution

2 Markov chain conditions:

- **Invariance/Stationarity:** If you run the chain for a long time and you are in the equilibrium distribution, you stay in equilibrium if you take another step.

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▶▶ Use ergodic and stationary Markov chains to generate samples from the equilibrium distribution

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- Invariance: Each step leaves the distribution p^* invariant (we stay in p^*):

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- Sufficient condition for p^* being invariant:
  Detailed balance:

$$p^*(\boldsymbol{x})T(\boldsymbol{x}'|\boldsymbol{x}) = p^*(\boldsymbol{x}')T(\boldsymbol{x}|\boldsymbol{x}')$$

  ▶▶ Also ensures that the Markov chain is reversible

Metropolis-Hastings

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- Proposal density $q(\boldsymbol{x}'|\boldsymbol{x}^{(t)})$ depends on last sample $\boldsymbol{x}^{(t)}$.
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Metropolis-Hastings Algorithm

1. Generate proposal $\boldsymbol{x}' \sim q(\boldsymbol{x}'|\boldsymbol{x}^{(t)})$
2. If

$$\frac{q(\boldsymbol{x}^{(t)}|\boldsymbol{x}')\tilde{p}(\boldsymbol{x}')}{q(\boldsymbol{x}'|\boldsymbol{x}^{(t)})\tilde{p}(\boldsymbol{x}^{(t)})} \geqslant u\,, \qquad u \sim U[0,1]$$

   accept the sample $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}'$. Otherwise set $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)}$.

Metropolis-Hastings

- Assume that $\tilde{p} = Zp$ can be evaluated easily (in practice: $\log \tilde{p}$)
- Proposal density $q(\boldsymbol{x}'|\boldsymbol{x}^{(t)})$ depends on last sample $\boldsymbol{x}^{(t)}$.
  Example: Gaussian with mean $\boldsymbol{x}^{(t)}$: $q(\boldsymbol{x}'|\boldsymbol{x}^{(t)}) = \mathcal{N}\left(\boldsymbol{x}^{(t)}, \boldsymbol{\Sigma}\right)$

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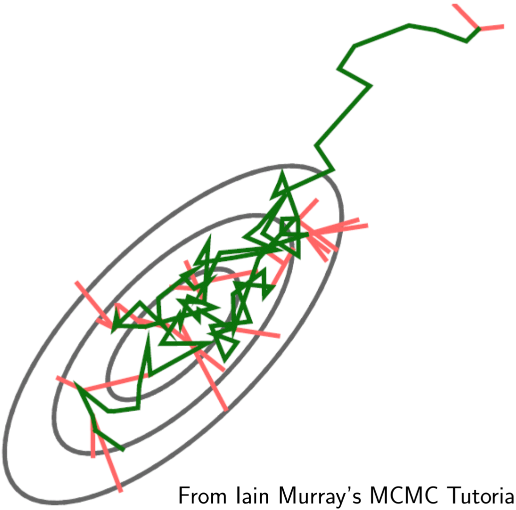
- If proposal distribution is symmetric: Metropolis Algorithm (Metropolis et al., 1953); Otherwise Metropolis-Hastings Algorithm (Hastings, 1970)

Example



From Iain Murray's MCMC Tutorial

Step-Size Demo

- Explore $p(x) = \mathcal{N}\big(x \,|\, 0,\, 1\big)$ for different step sizes σ.
- We can only evaluate $\log \tilde{p}(x) = -x^2/2$
- Proposal distribution q: Gaussian $\mathcal{N}\big(x^{(t+1)} \,|\, x^{(t)},\, \sigma^2\big)$ centered at the current state for various step sizes σ
- Expect to explore the space between $-2, 2$ with high probability

Step-Size Demo: Discussion

- Acceptance rate depends on the step size of the proposal distribution

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- Unlike rejection sampling, the previous sample is used to reset the chain (if a sample was discarded)
- If $q > 0$, we will end up in the equilibrium distribution: $p^{(t)}(\boldsymbol{x}) \xrightarrow{t\to\infty} p^*(\boldsymbol{x})$
- Explore the state space by random walk
  ⏩ May take a while in high dimensions
- No further catastrophic problems in high dimensions

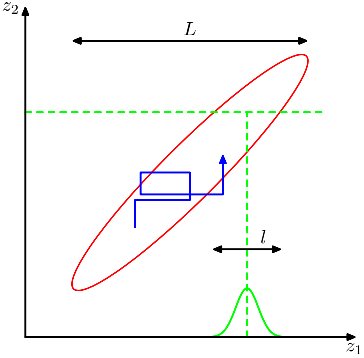
Gibbs Sampling (Geman & Geman, 1984)

- Assumption: $p(\boldsymbol{x}) = p(x_1, \ldots, x_n)$ is too complicated to draw samples from directly, but its conditionals $p(x_i|\boldsymbol{x}_{\setminus i})$ are tractable to work with
- Any distribution "with a name" (Gaussian, Laplace, Bernoulli, Gamma, Wishart, ...) is easy to sample from (standard libraries)

Algorithm

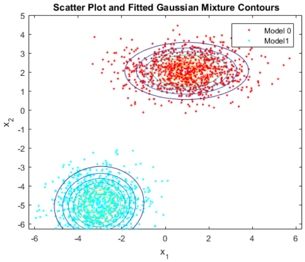
Assuming n parameters $x_1, \ldots, x_n$, Gibbs sampling samples individual variables conditioned on all others:

1. $x_1^{(t+1)} \sim p(x_1 | x_2^{(t)}, \ldots, x_n^{(t)})$
2. $x_2^{(t+1)} \sim p(x_2 | x_1^{(t+1)}, x_3^{(t)}, \ldots, x_n^{(t)})$
3. $\vdots$
4. $x_n^{(t+1)} \sim p(x_n | x_1^{(t+1)}, \ldots, x_{n-1}^{(t+1)})$



From PRML (Bishop, 2006)

Gibbs Sampling: Ergodicity



- $p(\boldsymbol{x})$ is invariant
- Ergodicity: Sufficient to show that all conditionals are greater than 0.

  ▶▶ Then any point in x-space can be reached from any other point (potentially with low probability) in a finite number of steps involving one update of each of the component variables.

Finding the Conditionals

1. Write down the (log-) joint distribution $p(x_1, \ldots, x_n)$
2. For each x_i
   2.1 Throw away all terms that do not depend on the current sampling variable
   2.2 Pretend this is the density for your variable of interest and all other variables are fixed. What distribution does the log-density remind you of?
   2.3 That is your conditional sampling density $p(x_i | \boldsymbol{x}_{\setminus i})$

Example

- Model:

$$y_i \sim \mathcal{N}\left(\mu,\, \tau^{-1}\right), \qquad \mu \sim \mathcal{N}\left(0,\, 1\right), \qquad \tau \sim \text{Gamma}(2, 1)$$

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- Then

$$\begin{aligned} p(\boldsymbol{y}, \mu, \tau) &= \prod_{i=1}^{n} p(y_i|\mu, \tau) p(\mu) p(\tau) \\ &\propto \tau^{n/2} \exp(-\frac{\tau}{2} \textstyle\sum_i (y_i - \mu)^2) \exp(-\frac{1}{2}\mu^2) \tau \exp(-\tau) \end{aligned}$$

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p(\mu|\tau, \boldsymbol{y}) &= \mathcal{N}\big(\tfrac{\tau \sum_i y_i}{1+n\tau},\, (1 + n\tau)^{-1}\big) \\
p(\tau|\mu, \boldsymbol{y}) &= \mathrm{Gamma}(2 + \tfrac{n}{2}, 1 + \tfrac{1}{2} \textstyle\sum_i (y_i - \mu)^2)
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Gibbs Sampling: Properties

- Gibbs is Metropolis-Hastings with acceptance probability 1: Sequence of proposal distributions q is defined in terms of conditional distributions of the joint $p(\boldsymbol{x})$

  ⏩ Converge to equilibrium distribution: $p^{(t)}(\boldsymbol{x}) \xrightarrow{t\to\infty} p(\boldsymbol{x})$

  ⏩ Exploration by random walk behavior can be slow

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- Statistical software derives the conditionals of the model, and it works out how to do the updates: STAN[1], WinBUGS[2], JAGS[3]

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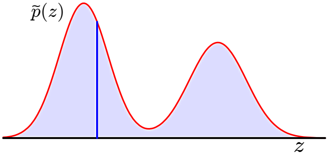
Flavors of Gibbs Sampling

- Collapsed Gibbs sampler: Analytically integrate out some parameters and sample the rest.
  ▶▶ Tends to be much more efficient with smaller variance (see Rao-Blackwellization in the state estimation literature)
- Block-Gibbs sampler: Sample groups of variables at a time instead of single-site updating

Slice Sampling (Neal, 2003)



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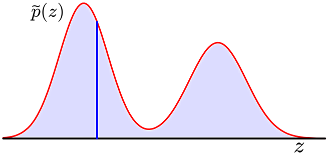

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- Introduce additional variable u, define joint $\hat{p}(x, u)$:

$$\hat{p}(x,u) = \begin{cases} 1/Z_p & \text{if } 0 \leqslant u \leqslant \tilde{p}(x) \\ 0 & \text{otherwise} \end{cases}, \qquad Z_p = \int \tilde{p}(x)dx$$

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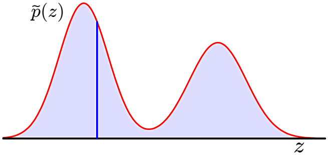

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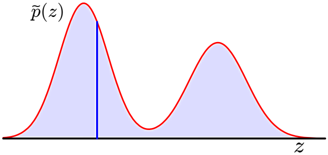

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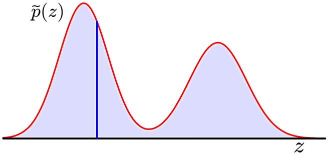

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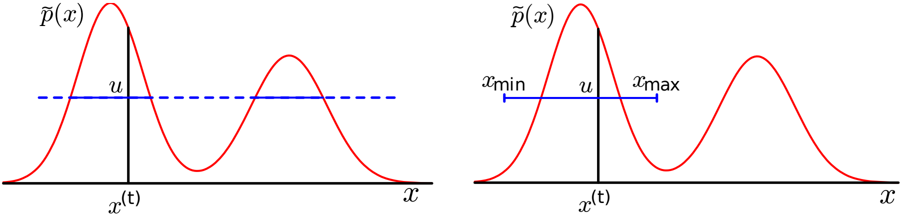
- Gibbs sampling: Update one variable at a time

Slice Sampling Algorithm



Adapted from PRML (Bishop, 2006)

- Repeat the following steps:
  1. Draw $u|x^{(t)} \sim \mathcal{U}[0, \tilde{p}(x)]$
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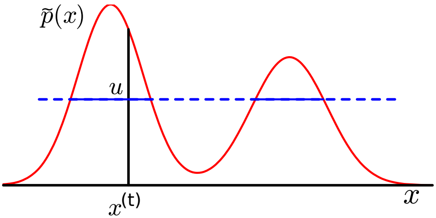

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- In practice, we sample $x^{(t+1)}|u$ uniformly from an interval $[x_{\min}, x_{\max}]$ around $x^{(t)}$.
- The interval is found adaptively (see Neal (2003) for details)

Relation to other Sampling Methods

Similar to:

- Metropolis: Just need to be able to evaluate $\tilde{p}(\boldsymbol{x})$
  More robust to the choice of parameters (e.g., step size is automatically adapted)
- Gibbs: 1-dimensional transitions in state space
  No longer required that we can easily sample from 1-D conditionals
- Rejection: Asymptotically draw samples from the volume under the curve described by $\tilde{p}$
  No upper-bounding of $\tilde{p}$ required

Properties

- Slice sampling can be applied to multivariate distributions by repeatedly sampling each variable/dimension in turn (similar to Gibbs sampling).

  ▶▶ See (Neal, 2003; Murray et al., 2010) for more details
- This requires to compute a function that is proportional to $p(x_i|\boldsymbol{x}_{\setminus i})$ for all variables x_i.

Properties

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- This requires to compute a function that is proportional to $p(x_i|\boldsymbol{x}_{\setminus i})$ for all variables x_i.
- No rejections
- Adaptive step sizes
- Easy to implement
- Broadly applicable

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- Autocorrelation is an indicator for choosing K

MCMC Diagnostics: Trace Plots

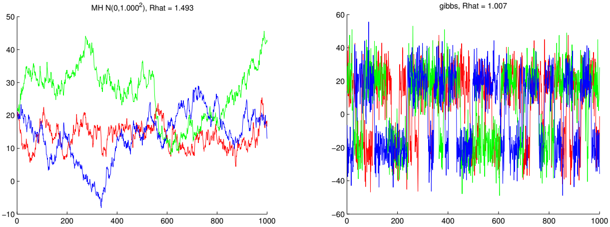

Figure from Murphy (2012)

- Mixing time: Amount of time it takes the Markov chain to converge to the stationary distribution and forget its initial state.
- Trace plots: Run multiple chains from very different starting points, plot the samples of the variables of interest. If the chain has mixed, the trace plots should converge to the same distribution.

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