Foundations of Machine Learning
African Masters in Machine Intelligence

Sampling

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Learning Material

- Bishop: Pattern Recognition and Machine Learning, Chapter 11
- MacKay: Information Theory, Inference and Learning Algorithms, Chapter 29
  `http://www.inference.org.uk/itprnn/book.html`
- Iain Murray's MCMC Tutorial:
  `http://videolectures.net/mlss09uk_murray_mcmc/`

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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⏩ Examples: Means/variances of distributions, marginal likelihood, predictions in a Bayesian model

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:

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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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- 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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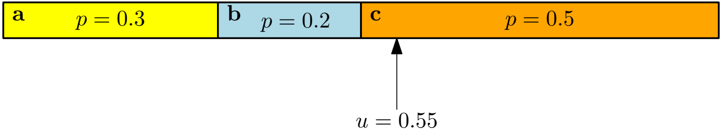
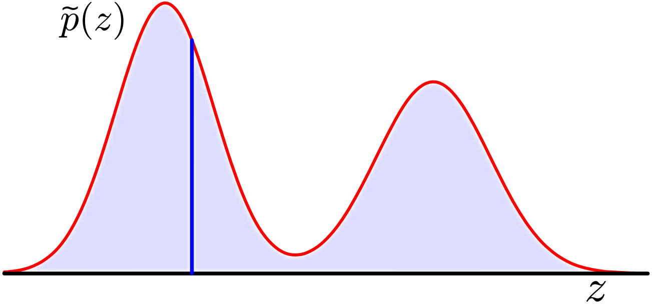
- Sampling from simple distributions
- Sampling from complicated distributions

Sampling Discrete Values



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

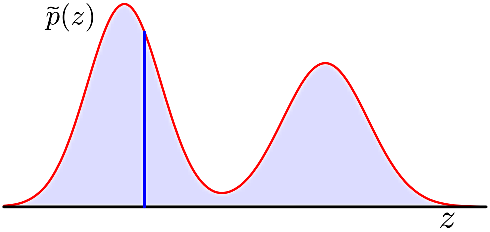
Continuous Variables



More complicated.

Geometric intuition: sample uniformly from the area under the curve

Rejection Sampling: Setting



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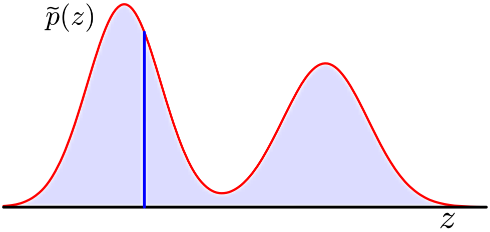
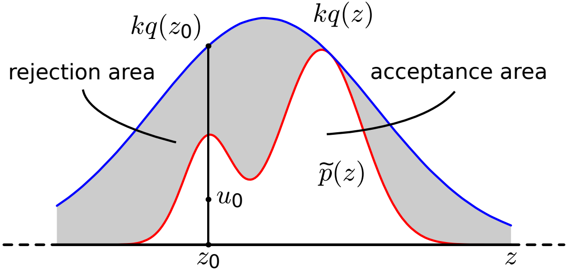


- Assume:
  - Sampling from $p(z)$ is difficult
  - Evaluating $\tilde{p}(z) = Zp(z)$ is easy (and Z may be unknown)
- Find a simpler distribution (proposal distribution) $q(z)$ from which we can easily draw samples (e.g., Gaussian, Laplace)
- Find an upper bound $kq(z) \geqslant \tilde{p}(z)$

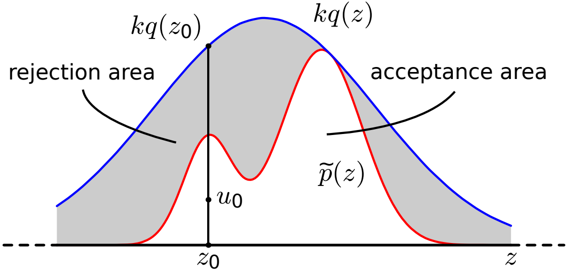
Rejection Sampling: Algorithm



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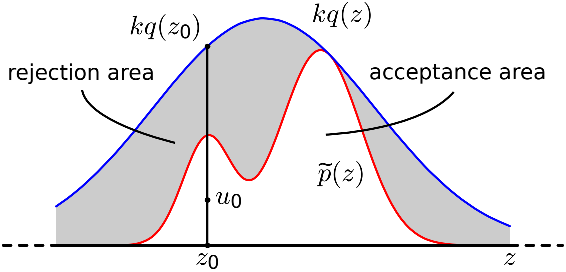
- What is the value of k if $\boldsymbol{x} \in \mathbb{R}^{1000}$?
- $q(0) = 1/(2\pi\sigma_q^2)^{500}$ ⏩ For $kq \geqslant p$ we need to set

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

- 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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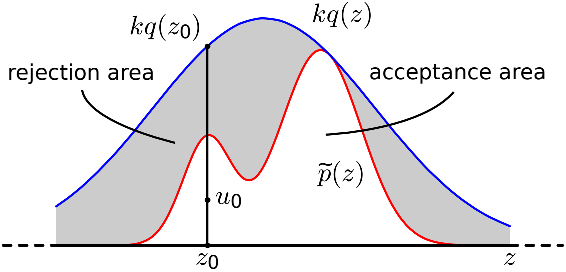

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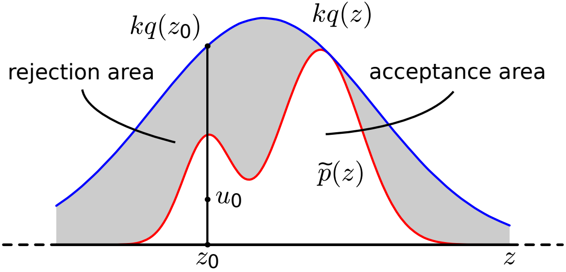

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- Finding the upper bound k is tricky
- In high dimensions the factor k is probably huge
- **Low acceptance rate/high rejection rate** of samples

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.

Target distribution: the distribution we are interested in (e.g., posterior)

Markov Chains

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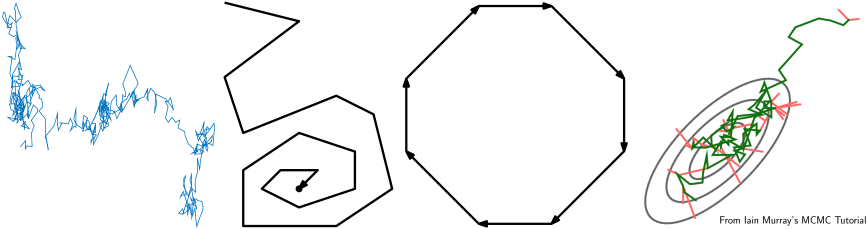
- Samples $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}$ form a **Markov chain**
- Samples $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}$ are no longer independent, but unbiased
  ⏩ We can still average them

Behavior of Markov Chains



From Iain Murray's MCMC Tutorial

Four different behaviors of Markov chains:

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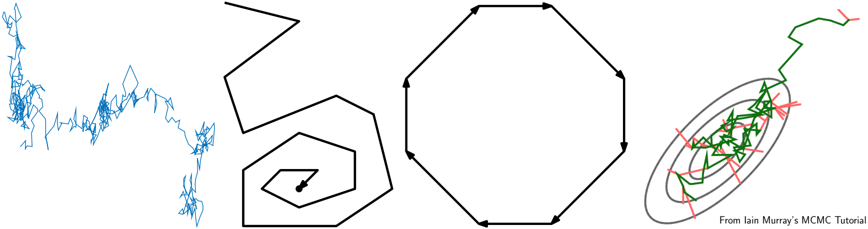

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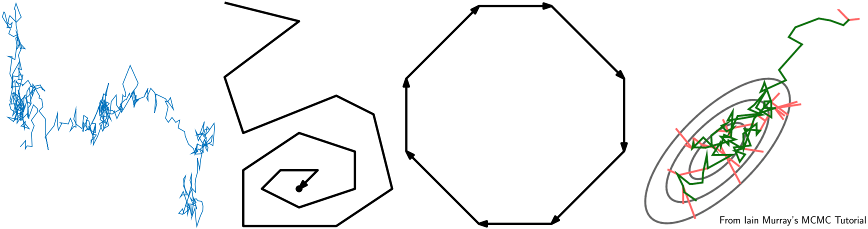

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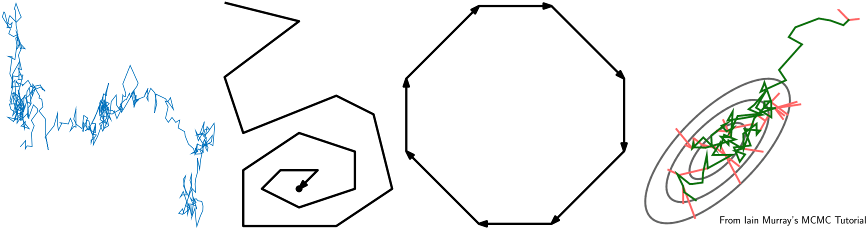

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- Converge to an equilibrium distribution p^*: Markov chain remains in a region, bouncing around in a random way

Converging to an Equilibrium Distribution

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- 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

Invariance and Detailed Balance

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

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  Once we sample from p^*, the transition operator will not change this, i.e., we do not fall back to some funny distribution $p \neq p^*$

- 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

- Assume that $\tilde{p} = Zp$ can be evaluated easily (in practice: $\log \tilde{p}$)
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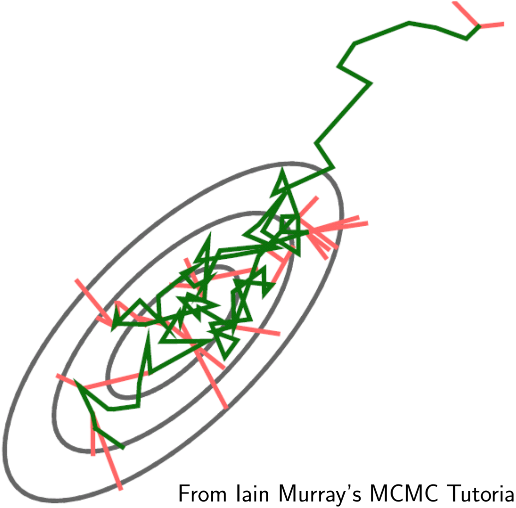
- $p(\boldsymbol{x}^{(t)}) \xrightarrow{t\to\infty} p^*(\boldsymbol{x})$ ⏩ Converge to equilibrium distribution
- If proposal distribution is symmetric: Metropolis Algorithm (Metropolis et al., 1953); Otherwise Metropolis-Hastings

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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- Tune the step size

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- If $q > 0$, we will end up in the equilibrium distribution: $p(\boldsymbol{x}^{(t)}) \xrightarrow{t\to\infty} p^*(\boldsymbol{x})$
- Explore the state space by random walk
  ⏩ May take a while in high dimensions
- No further catastrophic problems in high dimensions

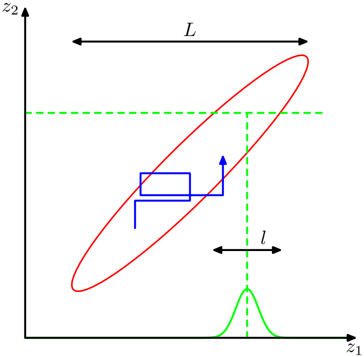
Gibbs Sampling (Geman & Geman, 1984)

- 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

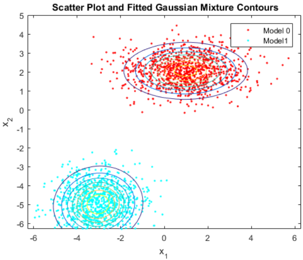
Assuming n parameters $x_1, \dots, x_n$, Gibbs sampling samples individual variables conditioned on all others:

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



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:

$$y_i \sim \mathcal{N}\big(\mu,\, \tau^{-1}\big)\,, \quad \mu \sim \mathcal{N}\big(\mu \,|\, 0,\, 1\big)\,, \quad \tau \sim \text{Gamma}(\tau|2, 1)$$

$$\text{Gamma}(\tau|2, 1) = \frac{1}{\Gamma(2)}\tau \exp(-\tau)$$

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$$p(\boldsymbol{y},\mu,\tau) = \prod\nolimits_{i=1}^{N} p(y_i|\mu,\tau)p(\mu)p(\tau)$$
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$$p(\mu|\tau,\boldsymbol{y}) = \mathcal{N}\big(\tfrac{\tau\sum_i y_i}{1+N\tau},\, (1+N\tau)^{-1}\big)$$

$$p(\tau|\mu,\boldsymbol{y}) = \text{Gamma}(2+\tfrac{N}{2}, 1+\tfrac{1}{2}\textstyle\sum_i(y_i-\mu)^2)$$

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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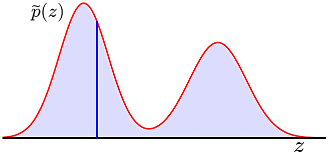
Flavors of Gibbs Sampling

- 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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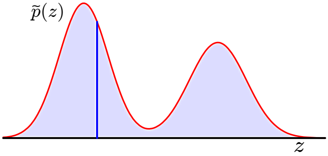

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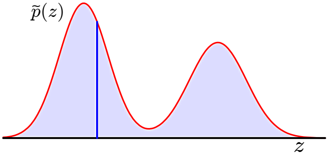

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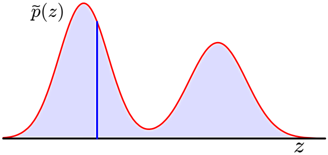

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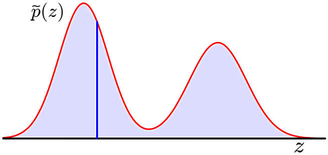

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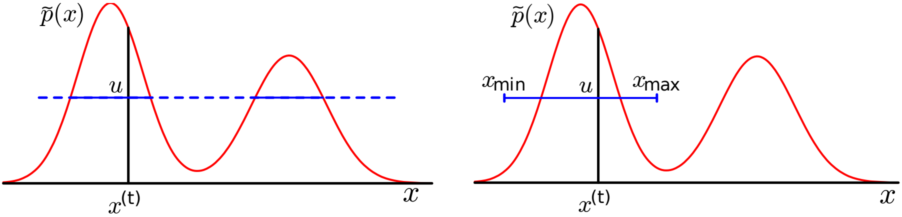
- Gibbs sampling: Update one variable at a time

Slice Sampling Algorithm



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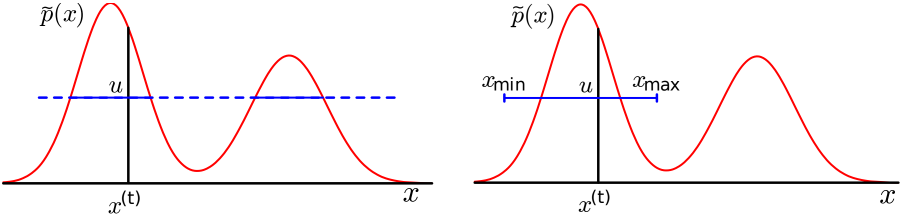

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- In practice, we sample $x^{(t+1)}|u$ uniformly from an interval $[x_{\text{min}}, x_{\text{max}}]$ around $x^{(t)}$.
- The interval is found adaptively (see Neal (2003) for details)

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.

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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

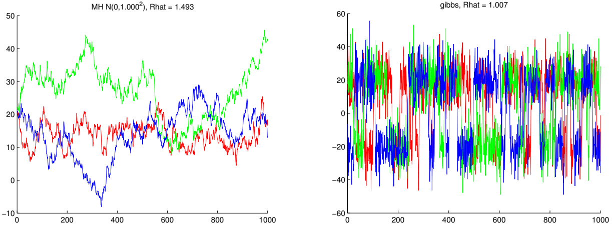

Figure from Murphy (2012)

- 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.

Summary

- Solving integrals, computing expectations
- Monte Carlo methods use random numbers
- Rejection and importance sampling do not work well in high dimensions
- MCMC generates a Markov chain of dependent samples that allow us to generate samples from the target distribution
- Metropolis Hastings, Gibbs, Slice sampling

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