Imperial College London

Lecture 16: Sampling

Recommended reading:
Bishop: Chapter 11
MacKay: Chapter 29

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Monte Carlo Methods—Motivation

- Monte Carlo methods are computational techniques that make use of random numbers
- Two typical problems:
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▶▶ Example: Means/variances of distributions, marginal likelihood

Complication: Integral cannot be evaluated analytically

Monte Carlo Estimation

- Statistical sampling can be applied to compute expectations

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$$\approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})$$

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- Example: Making predictions (e.g., Bayesian linear regression with a training set $\mathcal{D} = \{\boldsymbol{X}, \boldsymbol{y}\}$ at test input $\boldsymbol{x}_*$)

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- If we can sample from $p(\boldsymbol{x})$ (or $p(\boldsymbol{\theta})$) we can approximate these integrals

Properties of Monte Carlo Sampling

$$\begin{aligned}\mathbb{E}[f(\boldsymbol{x})] &= \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x} \\ &\approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})\end{aligned}$$

- Estimator is unbiased
- Variance shrinks $\propto 1/S$, regardless of the dimensionality of $\boldsymbol{x}$

Alternatives to Monte Carlo

$$\mathbb{E}[f(\boldsymbol{x})] = \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x}$$

To evaluate these expectations we can use other methods than Monte Carlo:

- Numerical integration (low-dimensional problems)
- Deterministic approximations, e.g., Variational Bayes, Expectation Propagation

Back to Monte Carlo Estimation

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$$\approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)}), \quad \boldsymbol{x}^{(s)} \sim p(\boldsymbol{x})$$

- How do we get these samples?

Need to solve Problem 1

- Sampling from simple distributions
- Sampling from complicated distributions

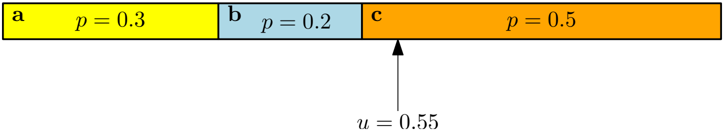
Important Example

- By specifying the model, we know the prior $p(\boldsymbol{\theta})$ and the likelihood $p(\mathcal{D}|\boldsymbol{\theta})$
- The unnormalized posterior is

$$p(\boldsymbol{\theta}|\mathcal{D}) \propto p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

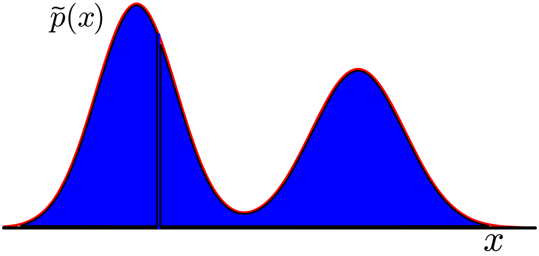
  and there is often no hope to compute the normalization constant
- Samples are a good way to characterize this posterior (important for model comparison, Bayesian predictions, ...)

Sampling Discrete Values



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

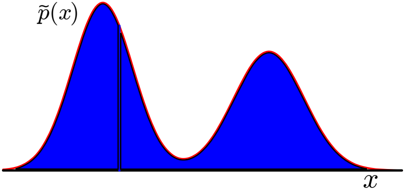
Continuous Variables



More complicated.
Geometrically, sample uniformly from the area under the curve

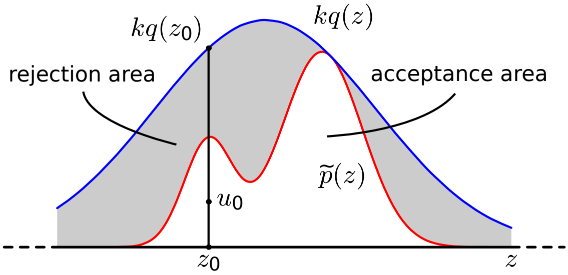
Rejection Sampling

Rejection Sampling: Setting



- 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)
- Find an upper bound $kq(z) \geqslant \tilde{p}(z)$

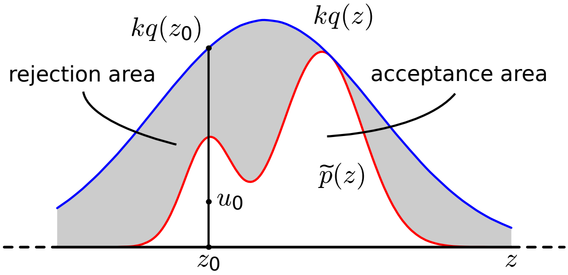
Algorithm



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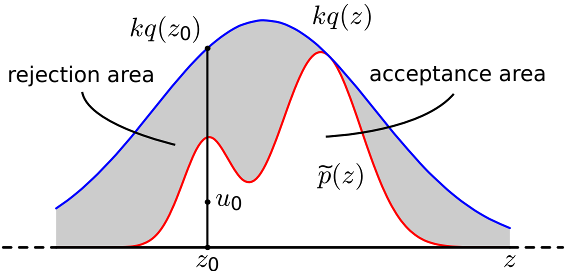
- Accepted pairs (z, u) are uniformly distributed under the curve of $\tilde{p}(z)$
- Probability density of the z-coordiantes of accepted points must be proportional to $\tilde{p}(z)$
- Samples are independent samples from $p(z)$

Shortcomings



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- Finding k is tricky

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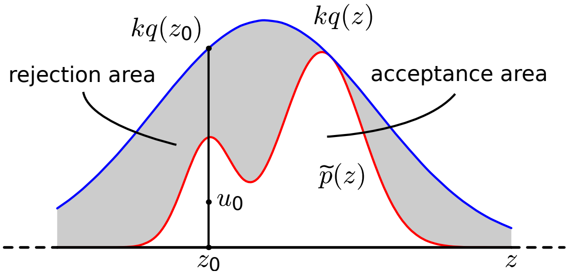

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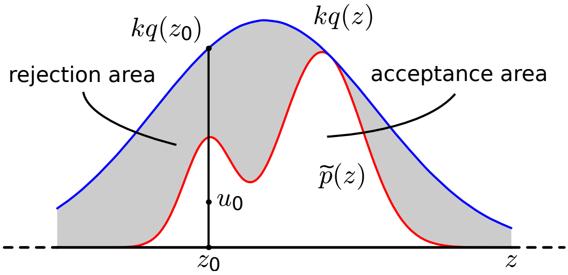

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- Finding k is tricky
- In high dimensions the factor k is probably huge
- **Low acceptance rate**

Importance Sampling

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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 Chains

Objective

Generate samples from an unknown target distribution.

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- **Markov property:** $p(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(t)}) = T(\boldsymbol{x}^{(t+1)}|\boldsymbol{x}^{(t)})$ only depends on the previous setting/state of the chain
- 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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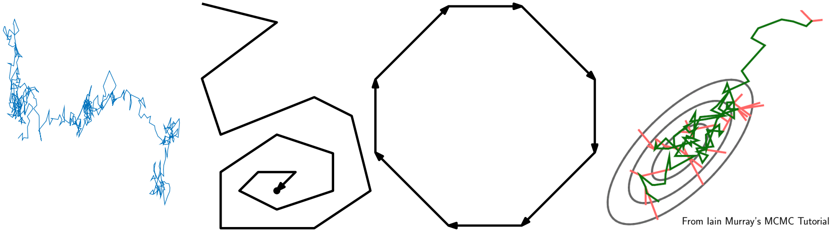
- Samples $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(t)}$ form a **Markov chain**
- Samples $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(t)}$ are no longer independent, but unbiased
  ▸▸ We can still average them

Behavior of Markov Chains



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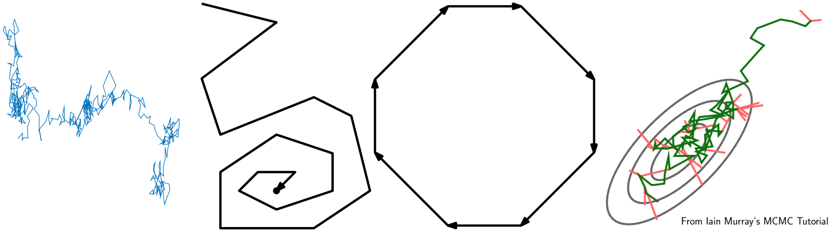

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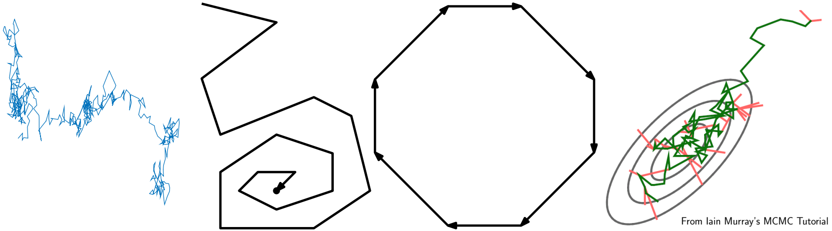

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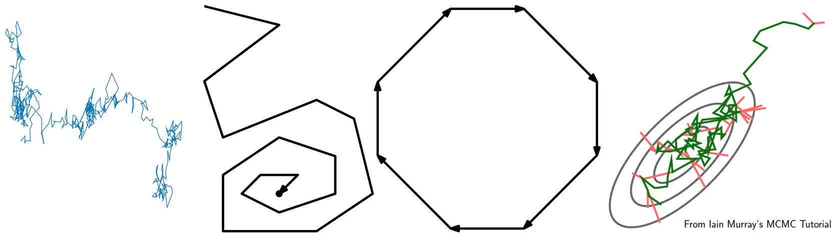

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- Converge to an equilibrium distribution p^*: Markov chain remains in a region, bouncing around in a random way

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  ▶▶ Bouncing around in an equilibrium distribution is a good thing
- Design the Markov chain such that the equilibrium distribution is the desired posterior
- We know the equilibrium distribution (the one we want to sample from)

  ▶▶ 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

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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- 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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- Assume that $\tilde{p} = Zp$ can be evaluated easily (in practice: $\log \tilde{p}$)
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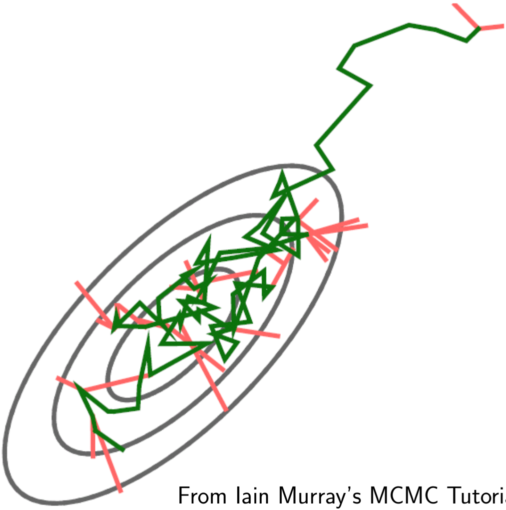
- If proposal distribution is symmetric: Metropolis Algorithm (Metropolis et al., 1953); Otherwise Metropolis-Hastings Algorithm (Hastings, 1970)

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 $-2, 2$.

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- Theoretical results: in 1D 44%, in higher dimensions about 25% acceptance rate for good mixing properties
- Tune the step size

Properties

- 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

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- Assumption: $p(\boldsymbol{x})$ is too complicated to draw samples from directly, but its conditionals $p(x_i|\boldsymbol{x}_{\setminus i})$ are tractable to work with
- Example:

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

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

Then

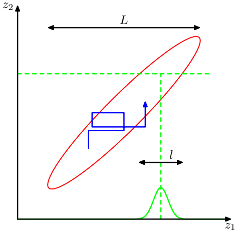
$$p(y, \mu, \tau) = \prod_{i=1}^{n} p(y_i|\mu, \tau)p(\mu)p(\tau)$$

$$\propto \tau^{n/2} \exp(-\frac{\tau}{2}\sum_i (y_i - \mu)^2) \exp(-\tfrac{1}{2}\mu^2)\tau \exp(-\tau)$$

$$p(\mu|\tau) = \mathcal{N}\left(\tfrac{\tau \sum_i y_i}{1+n\tau}, (1+n\tau)^{-1}\right)$$

$$p(\tau|\mu) = \text{Gamma}(2 + \tfrac{n}{2}, 1 + \tfrac{1}{2}\sum (y_i - \mu)^2)$$

Algorithm

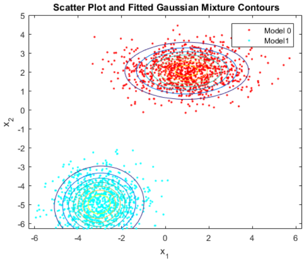


From PRML (Bishop, 2006)

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. $x_n^{(t+1)} \sim p(x_n | x_1^{(t+1)}, \ldots, x_{n-1}^{(t+1)}$

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.

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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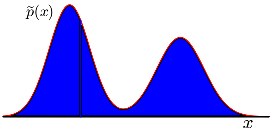
Slice Sampling

Key Idea behind Slice Sampling



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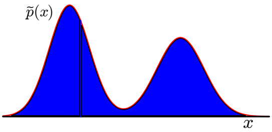

- **Idea:** Sample point (random walk) uniformly under the curve $\tilde{p}(x)$

- 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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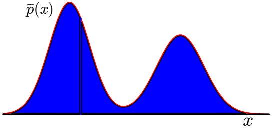

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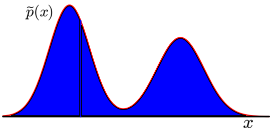

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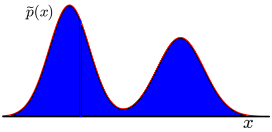

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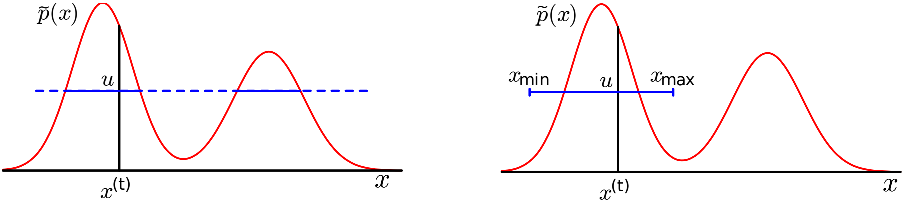
- Gibbs sampling: Update one variable at a time

Slice Sampling Algorithm



Adapted from PRML (Bishop, 2006)

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

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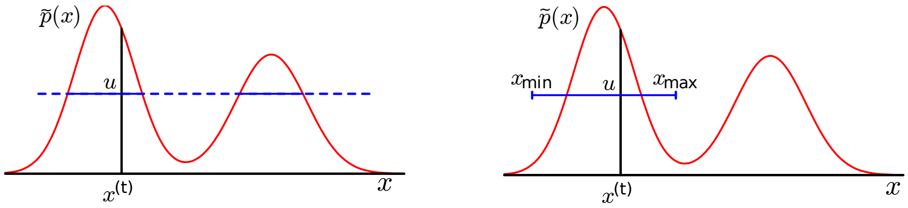

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- In practice, we sample $x^{(t+1)}|u$ uniformly from an interval $[x_{\text{min}}, x_{\text{max}}]$ around $x^{(t)}$.
- The interval is found adaptively (see Neal (2003) for details)

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 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

- Slice sampling can be applied to multivariate distributions by repeatedly sampling each variable 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.
- No rejections
- Adaptive step sizes
- Easy to implement
- Broadly applicable

Discussion MCMC

- Asymptotic guarantee to converge to the equilibrium distribution for any kind of model
- General-purpose method to draw samples in any kind of probabilistic model ⏩ Probabilistic Programming
- Convergence difficult to assess
- Long chains required in high dimensions
- Choice of proposal distribution is hard
- Need to store all samples (subsequent computations require to work with these samples)

References I

[1] C. M. Bishop. *Pattern Recognition and Machine Learning*. Information Science and Statistics. Springer-Verlag, 2006.

[2] D. J. C. MacKay. *Information Theory, Inference, and Learning Algorithms*. Cambridge University Press, The Edinburgh Building, Cambridge CB2 2RU, UK, 2003.