Markov chain Monte Carlo

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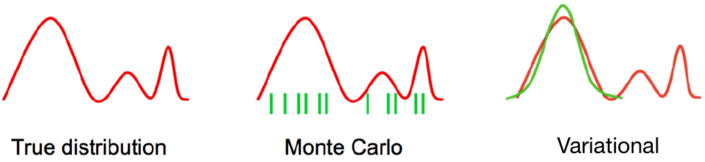
Previously, in MBML...

- Representation (Weeks 1-4)
- Modelling toolbox (Weeks 5-8, 13)
- Inference (Weeks 9-11)
  - Exact inference
    - Analytical (Bayes' rule)
    - Variable elimination
    - Belief propagation
  - Approximate inference
    - Stochastic methods - Markov chain Monte Carlo (MCMC)
    - Deterministic methods - Variational inference (VI)



Learning objectives

- Explain the concept of stochastic approximate inference.
- Explain and apply rejection sampling.
- Explain and apply importance sampling.
- Explain and apply the Metropolis-Hastings algorithm, including Gibbs sampling.
- Explain the concept of Hamiltonian Monte Carlo.

Outline

- Introduction
- Rejection sampling
- Importance sampling
- Metropolis-Hastings
- Hamiltonian Monte Carlo
- Gibbs sampling

Approximate inference

- Suppose we wish to compute the posterior distribution of the latent variables $\mathbf{z}$ given some observed data $\mathbf{x}$: $p(\mathbf{z}|\mathbf{x})$
- So far, we discussed various **exact** algorithms for posterior inference
- But, for many problems of interest exact posterior inference is **intractable**
  - Cannot determine the posterior distribution analytically
  - Cannot even compute expectations with respect to the posterior

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- But, for many problems of interest exact posterior inference is **intractable**
  - Cannot determine the posterior distribution analytically
  - Cannot even compute expectations with respect to the posterior
- Reasons for intractability:
  - Dimensionality of the latent space is too high to work with directly
  - Posterior distribution has a highly complex form for which expectations are not analytically tractable
- We must resort to **approximate inference** methods!

Monte Carlo methods

- In most situations, the posterior distribution $p(\mathbf{z}|\mathbf{x})$ is required only for evaluating **expectations** of some function $f(\mathbf{z})$ (e.g. to make predictions)

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

- (Note: we are using $\mathbf{z}$ to denote the variables whose posterior we wish to infer!)
- For example, the mean of $\mathbf{z}$ is given by

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- The idea behind sampling methods is to obtain a set of **samples** $\mathbf{z}^{(s)}$, for $s \in \{1, \dots, S\}$, drawn independently from the distribution $p(\mathbf{z}|\mathbf{x})$
- Allows to approximate expectations as **finite sums**!

$$\mathbb{E}_{p(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})] \approx \frac{1}{S} \sum_{s=1}^{S} f(\mathbf{z}^{(s)})$$

Example: making predictions

- Let $\mathbf{z}$ denote the parameters of our model (e.g. Bayesian logistic regression)
- Suppose we wish to make a prediction y_* for a new observation $\mathbf{x}_*$

$$\begin{aligned}\mathbb{E}_{p(\mathbf{z}|\mathbf{x})}[y_*|\mathbf{x}_*] &= \int p(y_*|\mathbf{x}_*, \mathbf{z})\, p(\mathbf{z}|\mathbf{x})\, d\mathbf{z} \\ &\approx \frac{1}{S}\sum_{s=1}^{S} p(y_*|\mathbf{x}_*, \mathbf{z}^{(s)})\end{aligned}$$

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where $\mathbf{z}^{(s)} \sim p(\mathbf{z}|\mathbf{x})$

- Notice that

$$\frac{1}{S}\sum_{s=1}^{S} p(y_*|\mathbf{x}_*, \mathbf{z}^{(s)}) \neq p\left(y_* \middle| \mathbf{x}_*, \frac{1}{S}\sum_{s=1}^{S} \mathbf{z}^{(s)}\right)$$

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- Even if the posterior $p(\mathbf{z}|\mathbf{x})$ is intractable to compute, we can still make predictions as long as we can obtain samples from the posterior!
- But if $p(\mathbf{z}|\mathbf{x})$ is intractable, how can we sample from it?

Properties of Monte Carlo

- Monte Carlo estimator:

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

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- Estimator is unbiased:

$$\mathbb{E}_{p(\{\mathbf{z}^{(s)}\}|\mathbf{x})}[\hat{f}] = \frac{1}{S} \sum_{s=1}^{S} \mathbb{E}_{p(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})] = \mathbb{E}_{p(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})]$$

- Variance shrinks proportionally to $1/S$:

$$\mathbb{V}_{p(\{\mathbf{z}^{(s)}\}|\mathbf{x})}[\hat{f}] = \frac{1}{S^2} \sum_{s=1}^{S} \mathbb{V}_{p(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})] = \frac{1}{S} \mathbb{V}_{p(\mathbf{z}|\mathbf{x})}[f(\mathbf{z})]$$

Sampling from distributions

- Draw mass to the left of point: $u \sim \text{Uniform}(0,1)$
- Use inverse CDF to obtain sample $y(u) = h^{-1}(u)$

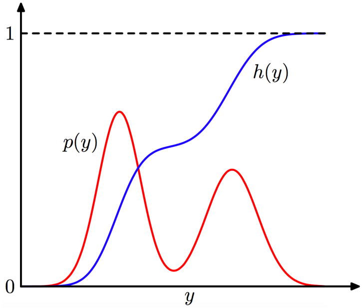

Figure: from PRML book, Bishop (2006)

- However, keep in mind that we can't always compute and invert $h(y)$

Sampling from posterior distributions

- In the context of Bayesian inference, we want to compute

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})\,p(\mathbf{z})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{z})\,p(\mathbf{z})}{\int p(\mathbf{x}|\mathbf{z})\,p(\mathbf{z})\,d\mathbf{z}}$$

  which is intractable...

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  which is intractable...

- But we have easy access to the unnormalized version

$$p(\mathbf{z}|\mathbf{x}) \propto p(\mathbf{x}|\mathbf{z})\, p(\mathbf{z}) \triangleq \tilde{p}(\mathbf{z}|\mathbf{x})$$

- How can we use $\tilde{p}(\mathbf{z}|\mathbf{x})$ (or $\log \tilde{p}(\mathbf{z}|\mathbf{x})$) to sample from $p(\mathbf{z}|\mathbf{x})$?

Rejection sampling

- Suppose we wish to sample from the unnormalized density $\tilde{p}(z) \propto p(z)$
- Construct **proposal distribution** $kq(z) \geq \tilde{p}(z)$

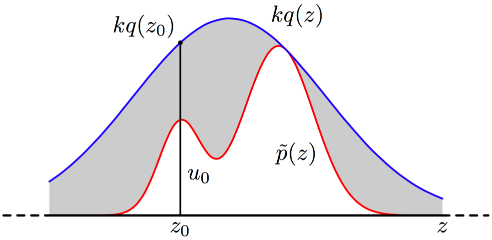

Figure: from PRML book, Bishop (2006)

- Draw sample $z \sim q(z)$
- Draw height $u \sim \text{Uniform}(0, kq(z))$
- **Reject** sample z if $u > \tilde{p}(z)$

Playtime!

- Rejection sampling
    - See “Part 1” of “11 - Markov chain Monte Carlo methods.ipynb" notebook
    - Expected duration: 30 minutes

Importance sampling

- As previously mentioned, the posterior distribution $p(z)$ is often required only for evaluating **expectations** of some function $f(z)$

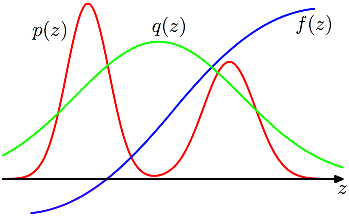

Figure: from PRML book, Bishop (2006)

- Importance sampling allows for just that!
- It does **not** provide a mechanism for drawing samples from the posterior $p(z)$, but it allows to compute expectations with respect to it:

$$\mathbb{E}_{p(z)}[f(z)] \approx \frac{1}{S} \sum_{s=1}^{S} f(z^{(s)}), \quad z^{(s)} \sim p(z)$$

Importance sampling

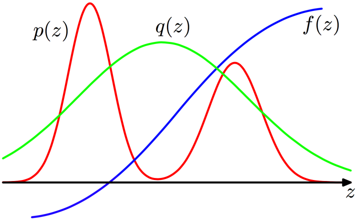

Figure: from PRML book, Bishop (2006)

- Rewrite the integral as an expectation under q:

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

$$\approx \frac{1}{S} \sum_{s=1}^{S} f(z^{(s)}) \frac{p(z^{(s)})}{q(z^{(s)})}, \qquad z^{(s)} \sim q(z)$$

- The ratio $\frac{p(z^{(s)})}{q(z^{(s)})}$ is the **importance/weights** of each sample!
- But, what if we cannot evaluate $p(z)$ but only $\tilde{p}(z) \propto p(z)$?

Importance sampling

- But, what if we cannot evaluate $p(z)$ but only $\tilde{p}(z) \propto p(z)$?
- Let $p(z) = \frac{1}{Z_p}\tilde{p}(z)$ and $q(z) = \frac{1}{Z_q}\tilde{q}(z)$

$$\mathbb{E}_{p(z)}[f(z)] = \int f(z)\, p(z)\, dz \approx \frac{Z_q}{Z_p}\frac{1}{S}\sum_{s=1}^{S} f(z^{(s)})\, \underbrace{\frac{\tilde{p}(z^{(s)})}{\tilde{q}(z^{(s)})}}_{\tilde{r}^{(s)}}, \qquad z^{(s)} \sim q(z)$$

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$$\approx \frac{1}{\cancel{S}}\sum_{s=1}^{S} f(z^{(s)}) \underbrace{\frac{\tilde{r}^{(s)}}{\frac{1}{\cancel{S}}\sum_{j=1}^{S}\tilde{r}^{(j)}}}_{w^{(s)}} = \sum_{s=1}^{S} f(z^{(s)})\, w^{(s)}$$

since $\frac{Z_p}{Z_q} \approx \frac{1}{S}\sum_s \tilde{r}^{(s)}$.

- All we need to do is compute the importance/weight $w^{(s)}$ of each sample s as the normalized ratio $\tilde{r}^{(s)} = \frac{\tilde{p}(z^{(s)})}{\tilde{q}(z^{(s)})}$

Playtime!

- Importance sampling
  - See “Part 2’ of “11 - Markov chain Monte Carlo methods.ipynb" notebook
  - Expected duration: 30 minutes

Importance sampling

- Rejection and importance sampling scale badly with dimensionality
- Also, the whole procedure still feels naive... A 2-dimensional example:

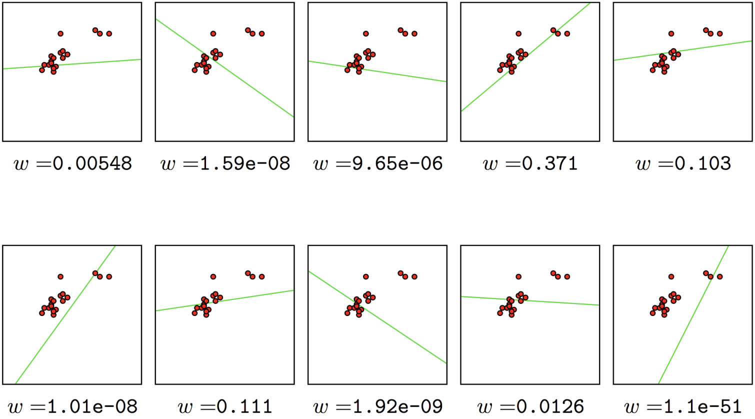

Figure: Samples from posterior over linear regression coefficients $\boldsymbol{\beta} = (\beta_0, \beta_1)^T$ using importance sampling. Figure from Iain Murray (2009)

Metropolis algorithm

- Start with some initial state $\mathbf{z}$ and iterate the following steps:
- Perturb variables using proposal distribution $q(\mathbf{z}'|\mathbf{z})$, e.g. $q(\mathbf{z}'|\mathbf{z}) = \mathcal{N}(\mathbf{z}'|\mathbf{z}, \sigma^2\mathbf{I})$
- Accept proposal with probability: $\min\left(1, \frac{\tilde{p}(\mathbf{z}')}{\tilde{p}(\mathbf{z})}\right)$
- In other words: always accept if new state $\mathbf{z}'$ has higher probability, otherwise go to new state $\mathbf{z}'$ anyway with probability $\frac{\tilde{p}(\mathbf{z}')}{\tilde{p}(\mathbf{z})}$

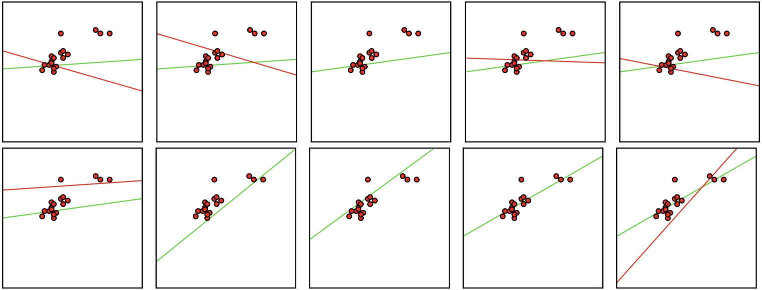

Figure: Samples from posterior over linear regression coefficients $\boldsymbol{\beta} = (\beta_0, \beta_1)^T$ using the Metropolis algorithm. Figure from Iain Murray (2009)

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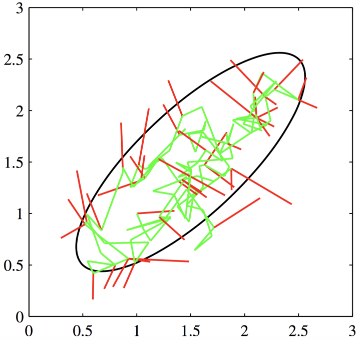

Figure: from PRML book, Bishop (2006)

- Green = accepted steps, Red = rejected steps

Markov chain Monte Carlo

- Construct a **biased** random walk that explores the posterior distribution $\tilde{p}(\mathbf{z})$
- Markov steps at each time step t: $\mathbf{z}^{(t)} \sim p(\mathbf{z}^{(t)}|\mathbf{z}^{(t-1)})$

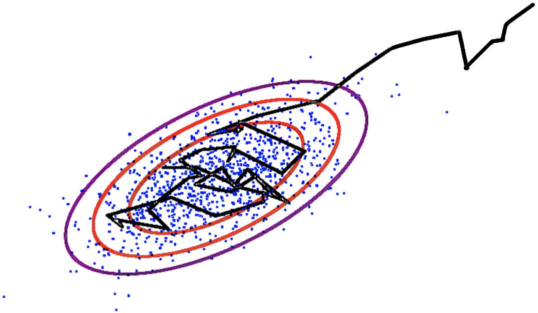

Figure: from Iain Murray (2009)

- MCMC gives approximate (but **correlated!**) samples from $\tilde{p}(\mathbf{z})$
- Can we choose any **transition operator** $T(\mathbf{z}^{(t)} \leftarrow \mathbf{z}^{(t-1)}) \triangleq p(\mathbf{z}^{(t)}|\mathbf{z}^{(t-1)})$?

Some definitions...

- Consider a Markov chain with transition probabilities: $T_t(\mathbf{z}^{(t)} \leftarrow \mathbf{z}^{(t-1)})$
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- In MCMC, the goal is to construct a Markov chain having a stationary distribution $p^*(\mathbf{z})$ from which we can sample from
- A distribution $p^*(\mathbf{z})$ is said to be **invariant**, or **stationary**, with respect to a Markov chain if each step in the chain leaves that distribution invariant
- For a homogeneous Markov chain with transition probabilities $T(\mathbf{z} \leftarrow \mathbf{z}')$, the distribution $p^*(\mathbf{z})$ is invariant if

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

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- Our goal is to use Markov chains to sample from a given distribution
- We can achieve this if we set up a Markov chain such that the desired distribution is invariant!

MCMC properties

- A sufficient (but not necessary) condition for ensuring that the required distribution $p(\mathbf{z})$ is invariant is to choose the transition probabilities to satisfy the property of **detailed balance**, defined by

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

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- A Markov chain that respects detailed balance is said to be **reversible**
- Lastly, we must also require that for $t \to \infty$, $p(\mathbf{z}^{(t)})$ converges to the required invariant distribution $p^*(\mathbf{z})$, irrespective of the choice of initial distribution $p(\mathbf{z}^{(0)})$
- This property is called **ergodicity**
- The invariant distribution is then called the **equilibrium distribution**

Metropolis-Hastings

- A more general version of the Metropolis algorithm:
  - Propose a move from the current state: $\mathbf{z}' \sim q(\mathbf{z}'|\mathbf{z})$
  - Accept proposal with probability:

$$\min\left(1, \frac{\tilde{p}(\mathbf{z}')\, q(\mathbf{z}|\mathbf{z}')}{\tilde{p}(\mathbf{z})\, q(\mathbf{z}'|\mathbf{z})}\right)$$

- Satisfies detailed balance! (see Bishop (2006) for proof)
- Since the Gaussian is a symmetric function, i.e. $\mathcal{N}(\mathbf{z}'|\mathbf{z}, \sigma^2) = \mathcal{N}(\mathbf{z}|\mathbf{z}', \sigma^2)$, when $q(\mathbf{z}'|\mathbf{z}) = \mathcal{N}(\mathbf{z}'|\mathbf{z}, \sigma^2\mathbf{I})$ we get back the Metropolis algorithm:

$$\min\left(1, \frac{\tilde{p}(\mathbf{z}')\, \cancel{q(\mathbf{z}|\mathbf{z}')}}{\tilde{p}(\mathbf{z})\, \cancel{q(\mathbf{z}'|\mathbf{z})}}\right) = \min\left(1, \frac{\tilde{p}(\mathbf{z}')}{\tilde{p}(\mathbf{z})}\right)$$

Metropolis-Hastings

- Be careful how you choose the step size σ^2

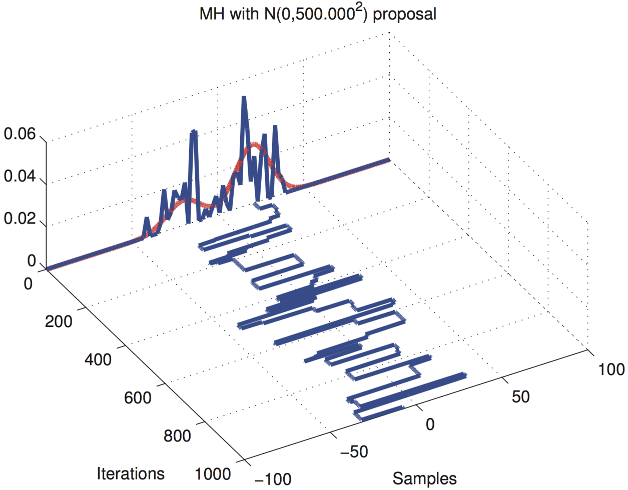

Figure: from ML: A prob. perspective book, Murphy (2011)

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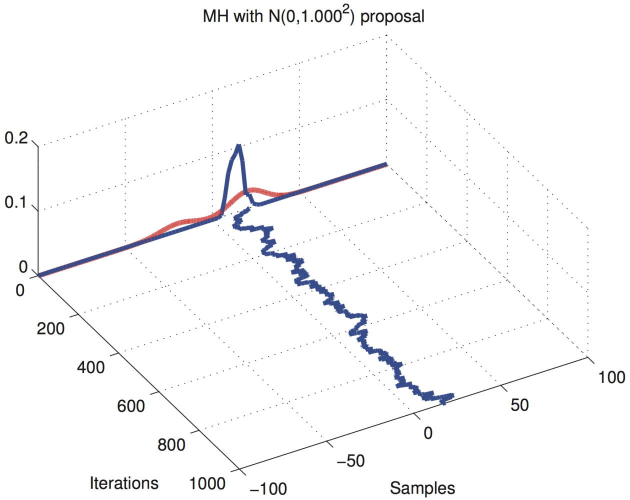

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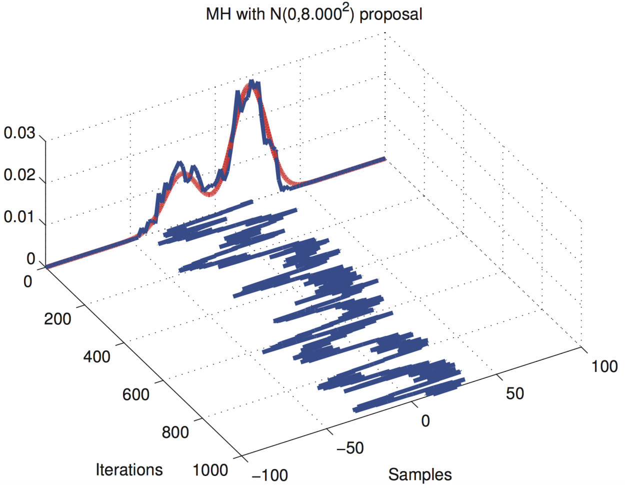

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MCMC in practice

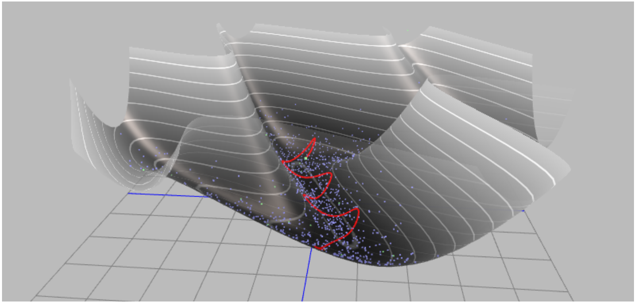
- The samples are correlated! We should **thin** - only keep every n^{th} sample
- Arbitrary initialization means early samples are bad - discard a **burn-in** period
- A good idea is to run **multiple chains** (e.g. in parallel - multicore)
- How do you know when to stop?
- Make sure to check diagnostics!
  (e.g. "Rhat" and number of effective samples in STAN)

Playtime!

- Metropolis-Hastings
  - See “Part 3’ of “11 - Markov chain Monte Carlo methods.ipynb" notebook
  - Expected duration: 30 minutes

Hamiltonian Monte Carlo: basic idea

- Include **Hamiltonian dynamics**
  - Construct a landscape with gravitational potential energy $E(\mathbf{z}) = -\log p^*(\mathbf{z})$
  - Introduce velocity v (auxiliary variable) carrying kinetic energy $K(v)$
- Define joint distribution: $p(\mathbf{z}, v) \propto e^{-E(\mathbf{z})}\, e^{-K(v)} = e^{-H(\mathbf{z},v)}$
- Velocity v is independent of position and Gaussian distributed



Hamiltonian Monte Carlo: basic idea

- Procedure:
  - Gibbs sample velocity v (we will see Gibbs sampling next!)
  - Simulate Hamiltonian dynamics then flip sign of velocity
  - Accept new position with probability: $\min[1, e^{H(\mathbf{z},v)-H(\mathbf{z}',v')}]$
- Hamiltonian dynamics are simulated approximately

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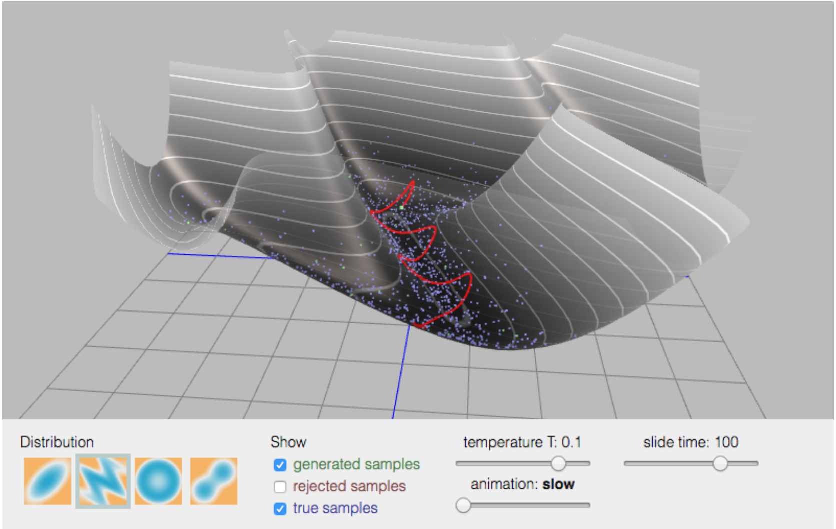
  - Accept new position with probability: $\min[1, e^{H(\mathbf{z},v)-H(\mathbf{z}',v')}]$
- Hamiltonian dynamics are simulated approximately
- Distances between successive generated points are typically large, so we need less iterations to get representative sampling!
- Each iteration is more computationally expensive, but sampling is more efficient
- For a detailed explanation, see: `http://arogozhnikov.github.io/2016/12/19/markov_chain_monte_carlo.html`

Hamiltonian Monte Carlo: basic idea



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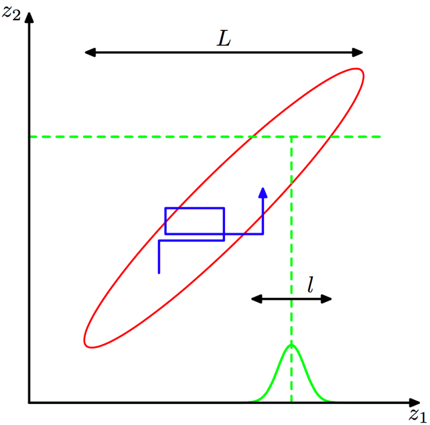
Gibbs sampling



- Suppose we wish to sample from the posterior $p(\mathbf{z}) = p(z_1, \ldots, z_M)$
- Start with initial state $\mathbf{z}^{(0)}$
- Pick each variable z_m in turn (or randomly) and resample it from the conditional:

$$z_m \sim p(z_m | \mathbf{z}_{i \neq m})$$

Gibbs sampling

- Simple and widely applicable MCMC algorithm
- Gibbs sampling has no rejection! (see next slide)
- Must be able to sample from conditional distributions $p(z_m|\mathbf{z}_{i\neq m})$
  - Discrete conditionals with a few possible settings can be explicitly normalized

$$p(z_m|\mathbf{z}_{i\neq m}) = \frac{p(z_m, \mathbf{z}_{i\neq m})}{\sum_{z_m} p(z_m, \mathbf{z}_{i\neq m})}$$

  - Continuous conditionals require either:
    - Conjugacy - to allow for analytical solutions
    - Or efficient approximate solutions (e.g. standard sampling methods)

Gibbs sampling

- Gibbs sampling satisfies detailed balance (see e.g. Bishop (2006) for proof)
- It is a particular instance of the Metropolis-Hastings algorithm where $q(\mathbf{z}'|\mathbf{z}) = p(z'_m|\mathbf{z}_{i \neq m})$

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- It is a particular instance of the Metropolis-Hastings algorithm where $q(\mathbf{z}'|\mathbf{z}) = p(z'_m|\mathbf{z}_{i\neq m})$
- Probability of acceptance:

$$\min\left(1, \frac{p(\mathbf{z}')\,q(\mathbf{z}|\mathbf{z}')}{p(\mathbf{z})\,q(\mathbf{z}'|\mathbf{z})}\right) = \min\left(1, \underbrace{\frac{p(z'_m|\mathbf{z}'_{i\neq m})\,p(\mathbf{z}'_{i\neq m})\,p(z_m|\mathbf{z}'_{i\neq m})}{p(z_m|\mathbf{z}_{i\neq m})\,p(\mathbf{z}_{i\neq m})\,p(z'_m|\mathbf{z}_{i\neq m})}}_{=1}\right) = 1$$

  where we used the fact that $p(\mathbf{z}) = p(z_m|\mathbf{z}_{i\neq m})\,p(\mathbf{z}_{i\neq m})$ and $\mathbf{z}'_{i\neq m} = \mathbf{z}_{i\neq m}$ (because they were left unchanged!)

- Gibbs sampling has **no rejection**!
- A practical example (discrete variables): see slides 18-25 from David Sontag (`http://people.csail.mit.edu/dsontag/courses/pgm13/slides/lecture9.pdf`)

Summary

- We need approximate methods to compute posteriors (sums/integrals)
- Monte Carlo does not explicitly depend on dimension, but simple methods work only in low dimensions
- MCMC methods can make local moves - important for higher dimensions!
- General and often easy to implement (simple computations), but hard to diagnose

Playtime!

- Gibbs sampling
  - See “Part 4’ of “11 - Markov chain Monte Carlo methods.ipynb" notebook
  - Expected duration: 30 minutes