

Introduction to Random Numbers, Sampling, and MCMC Methods

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What is Sampling and why is it useful?

- ▶ Sampling is the practice of generating observations from a population
- ▶ Monte Carlo methods are algorithms that rely on repeated random sampling to obtain approximations where it is difficult or impossible to use deterministic approaches
 - ▶ Optimization
 - ▶ Numerical Integration
 - ▶ Sampling distributions

Application: Approximating π

Algorithm 1 Approximating π

Input: Batch Size N

1: Sample $u_1 \sim \text{Uniform}(0, 1)$ N times

2: Sample $u_2 \sim \text{Uniform}(0, 1)$ N times

3: $\tilde{\pi} = \frac{4}{N} \cdot \left| \left\{ (u_1, u_2) \mid \sqrt{u_1^2 + u_2^2} < 1 \right\} \right|$

Output: $\tilde{\pi}$

Application: Approximating π

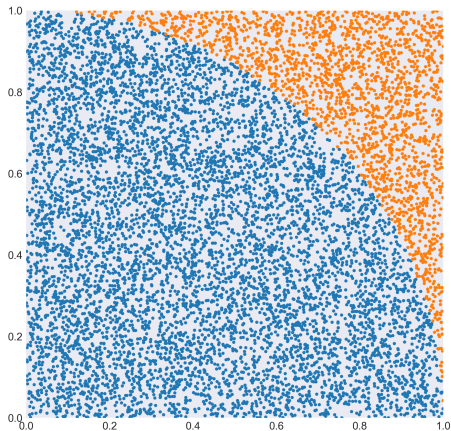
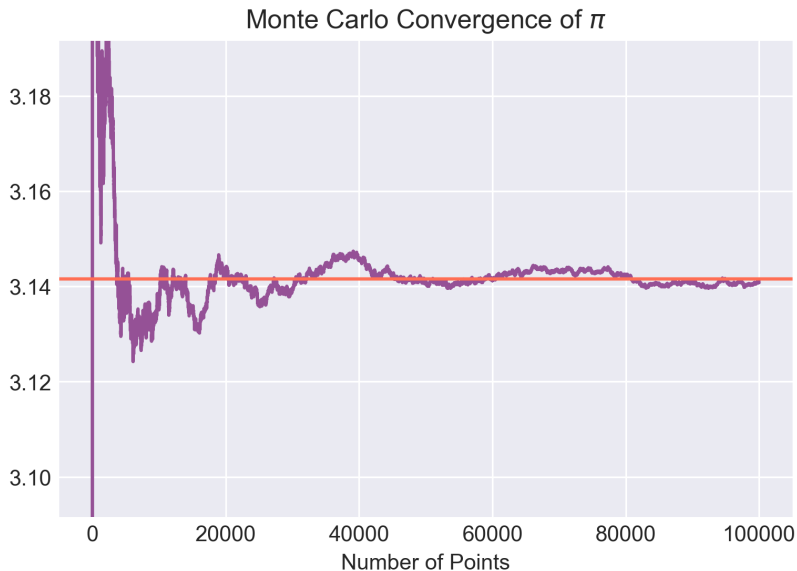


Figure: The ratio of points inside the unit circle approximates $\frac{\pi}{4}$

Application: Approximating π



What can we do with our samples?

- ▶ Integration: $\int p(x) f(x) dx \approx \frac{1}{n} \sum_{x_i \sim P} f(x_i)$
- ▶ Expectation: $\mu \approx \frac{1}{n} \sum_{x_i \sim P} x_i$
- ▶ Variance: $\sigma^2 \approx \frac{1}{n} \sum_{x_i \sim P} (x_i - \mu)^2$
- ▶ Median: $\text{median} \approx \text{median}(x_1, x_2, \dots, x_n)$
- ▶ Entropy: $\mathbb{H}(P) \approx -\frac{1}{n} \sum_{x_i \sim P} \log p(x_i)$
- ▶ CDF: $p(c) \approx \frac{1}{n} |\{x_i \mid x_i \leq c\}|$
- ▶ Conditional Distributions: $\{x_i \mid \Phi(x_i)\}$

Pseudo-Random Number Generators

Pseudo-Random Number Generators

- ▶ If we need random numbers, then how do we generate them?
- ▶ One solution: Pseudo-Random Number Generators
- ▶ Pseudo since they cannot simulate "true" randomness
- ▶ But can be replicated via "seeds"

Pseudo-Random Number Generators: LCG

Algorithm 2 General Linear Congruential Generator

Input: Modulus m , Multiplier a , Increment c , State x_i

1: $x_{i+1} = (a \cdot x_i + c) \bmod m$

2: $u_{i+1} = x_{i+1} / m$

Output: u_{i+1}

- ▶ m should be a large prime
- ▶ $2^{31} - 1$ is the largest 32-bit integer and a Mersenne prime
- ▶ Care should be taken to choose a and c such that the generator has full period

Pseudo-Random Number Generators

- ▶ LCGs are of low quality
- ▶ Not cryptographically secure
- ▶ Mersenne Twister (1998) improves upon many of the flaws of LCGs, and is the default for many modern-day languages
- ▶ Other PRNGs:
 - ▶ Multiple Recursive Generator
 - ▶ Lagged Fibonacci Generator
 - ▶ Inversive Congruential Generator

Inverse Transform Sampling

Generating a Normal from the CDF

- ▶ We can use the cumulative distribution function to sample any distribution
- ▶ For instance, a normal's CDF is:

$$F(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sigma\sqrt{2}} \right) \right]$$

- ▶ With an Inverse CDF as:

$$F^{-1}(p) = \mu + \sigma\sqrt{2} \cdot \operatorname{erf}^{-1}(2p - 1)$$

- ▶ $\operatorname{erf}(x)$ is the error function, defined as:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

Inverse Transform Sampling

- ▶ It's easy to generalize this method to any distribution with a closed-form inverse CDF

Algorithm 3 Inverse Transform Sampling

Input: Inverse CDF F^{-1}

- 1: Sample $u \sim \text{Uniform}(0, 1)$
- 2: $X = F^{-1}(u)$

Output: X

Inverse Transform Sampling: Intuition

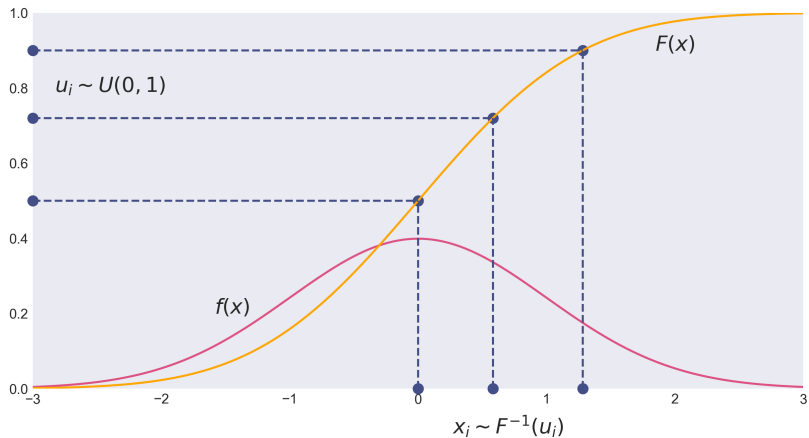


Table of Inverse CDFs for Common Distributions

Distribution	$F(x)$	$F^{-1}(p)$
$\mathcal{N}(\mu, \sigma)$	$\frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x-\mu}{\sigma\sqrt{2}} \right) \right]$	$\mu + \sigma\sqrt{2} \cdot \operatorname{erf}^{-1}(2p - 1)$
$\mathcal{U}(a, b)$	$\frac{x-a}{b-a}$	$a + p \cdot (b - a)$
$\operatorname{Exp}(\lambda)$	$1 - e^{-\lambda x}$	$\frac{-\ln(1-p)}{\lambda}$
$\operatorname{Logistic}(\mu, s)$	$\frac{1}{1 + e^{-\frac{x-\mu}{s}}}$	$\mu + s \ln \left(\frac{p}{1-p} \right)$

Inverse Transform Sampling: Disadvantages

- ▶ Inverse Transform Sampling fails when we cannot analytically integrate the PDF or invert the CDF!
- ▶ No closed form ICDF
 - ▶ t -distribution (also has a complicated CDF)
 - ▶ F -distribution
 - ▶ χ^2 -distribution
 - ▶ Gamma
 - ▶ Beta
 - ▶ Normal
- ▶ We can still approximate these functions using a Taylor Series Expansion

Rejection Sampling

Rejection Sampling

- ▶ What if we do not have a closed form CDF or ICDF?
- ▶ We can instead use Rejection Sampling!

Rejection Sampling: Algorithm

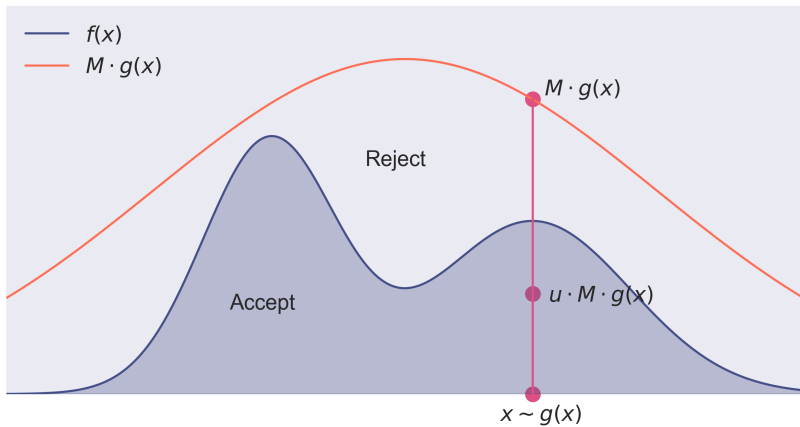
Algorithm 4 Rejection Sampling

Input: Model F , Proposal G , $M > 1$

- 1: Sample $x \sim G$
- 2: Sample $u \sim \text{Uniform}(0, 1)$
- 3: **if** $u < \frac{f(x)}{M \cdot g(x)}$ **then**
- 4: Accept x
- 5: **else**
- 6: Reject x
- 7: **end if**

Output: Accepted Samples

Rejection Sampling: Intuition



Rejection Sampling: Example

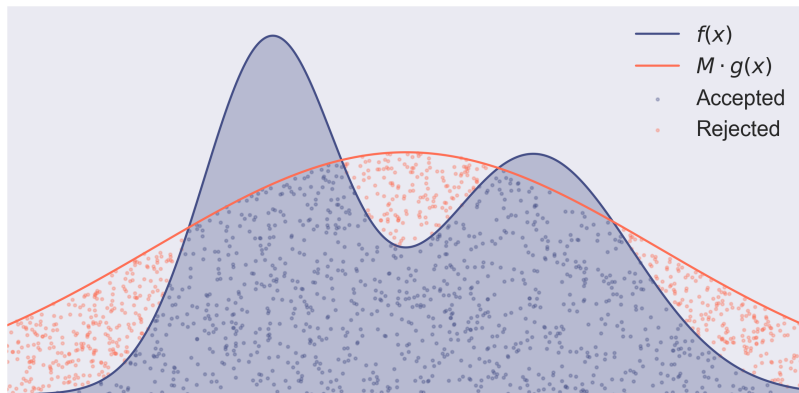


Figure: Rejection Sampling with $M = 1.3$

Rejection Sampling: Example

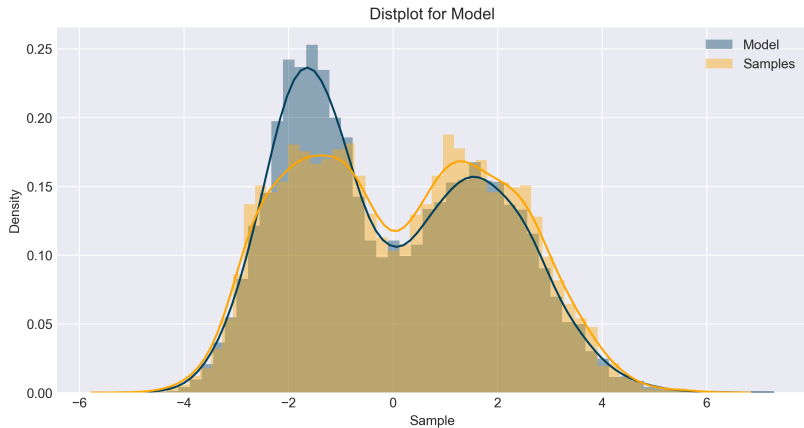


Figure: $M = 1.3$, 6,660 Accepted Samples

Rejection Sampling: Example

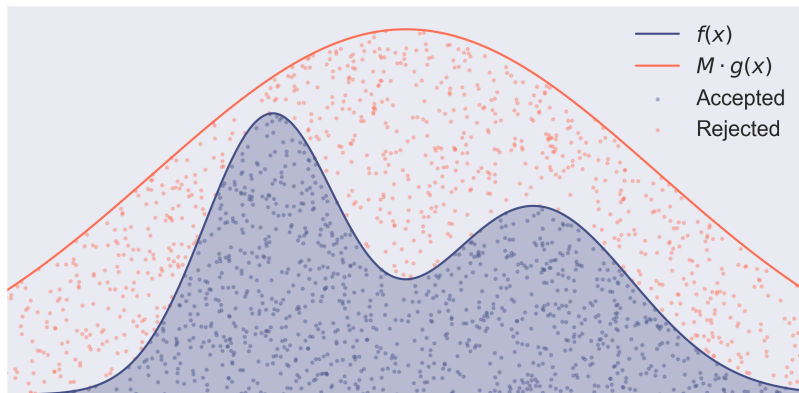


Figure: Rejection Sampling with $M = 2.5$

Rejection Sampling: Example

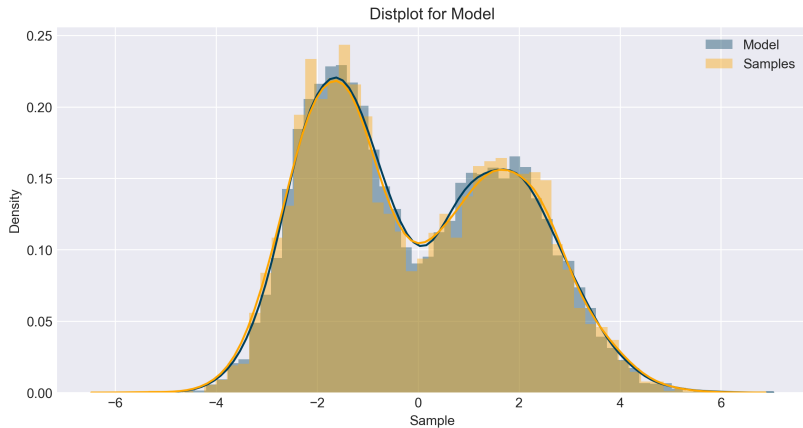


Figure: $M = 2.5$, 4,034 Accepted Samples

Rejection Sampling: Example

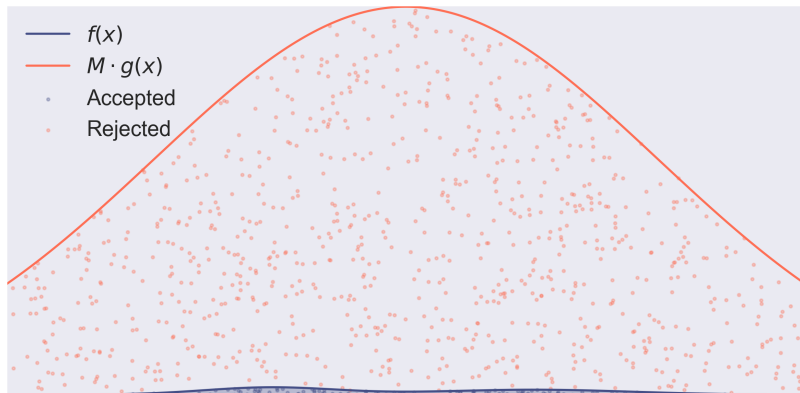


Figure: Rejection Sampling with $M = 100$

Rejection Sampling: Example

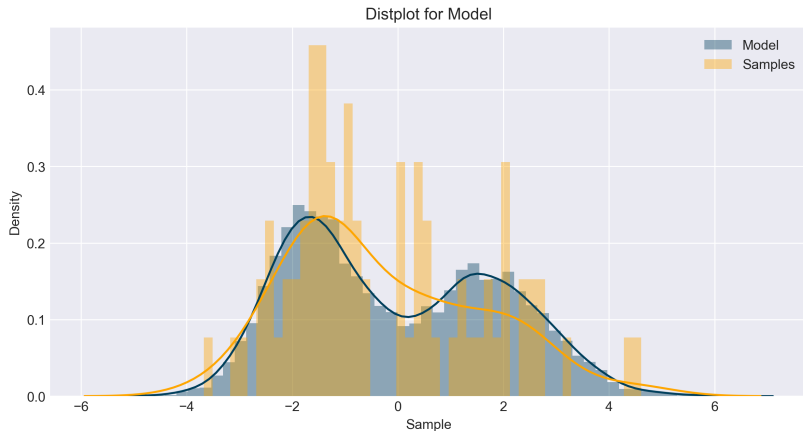


Figure: $M = 100$, 79 Accepted Samples

Rejection Sampling: Pros & Cons

- ▶ Pros:
 - ▶ Can be more efficient if the CDF is intractable
- ▶ Cons:
 - ▶ Tuning M can be difficult. Too high and we reject too many, too low and we under approximate our target
 - ▶ Very inefficient in higher dimensions

Markov Chain Monte Carlo (MCMC)

What is MCMC?

- ▶ Idea: Construct a Markov chain whose stationary distribution is the target density of interest, $f(x)$.
- ▶ The more steps we take in the chain, the better the approximation.
- ▶ This method works well with multi-dimensional continuous variables.

Metropolis-Hastings

Algorithm 5 Metropolis-Hastings Algorithm

Input: Model F , Proposal G

```
1: Initialize  $x_0$ 
2: for  $s = 0, 1, \dots$  do
3:   Sample  $x' \sim g(x'|x_s)$ 
4:   Compute acceptance probability
     
$$r = \min \left( 1, \frac{f(x')}{f(x_s)} \frac{g(x_s|x')}{g(x'|x_s)} \right)$$

5:   Sample  $u \sim \text{Uniform}(0, 1)$ 
6:   if  $u < r$  then
7:     Accept  $x'$ 
8:     Set  $x_{s+1} = x'$ 
9:   else
10:    Reject  $x'$ 
11:    Set  $x_{s+1} = x_s$ 
12:   end if
13: end for
```

Output: Accepted Samples

- ▶ Construct a Markov Chain where we propose a new state x' from the current state x_s with probability $g(x'|x_s)$.
- ▶ After drawing a proposal x' we calculate an acceptance probability, and if accepted, update the state to x' , else stay at state x_s .

Metropolis-Hastings: Example

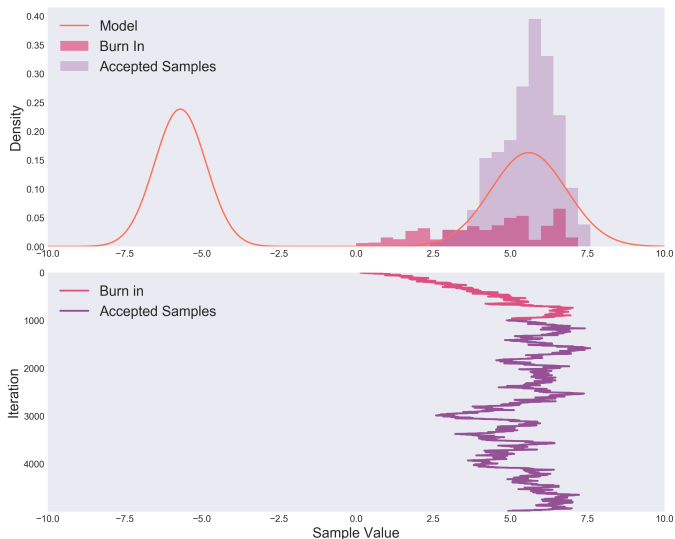


Figure: $\sigma^2 = 0.1$

Metropolis-Hastings: Example

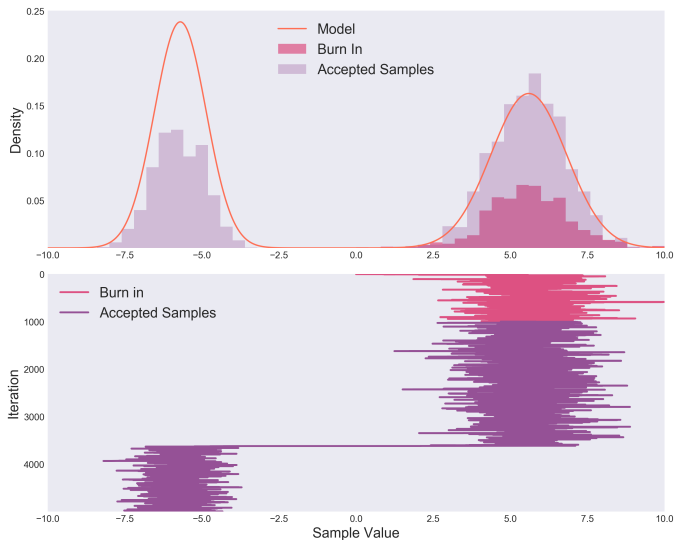


Figure: $\sigma^2 = 3$

Metropolis-Hastings: Example

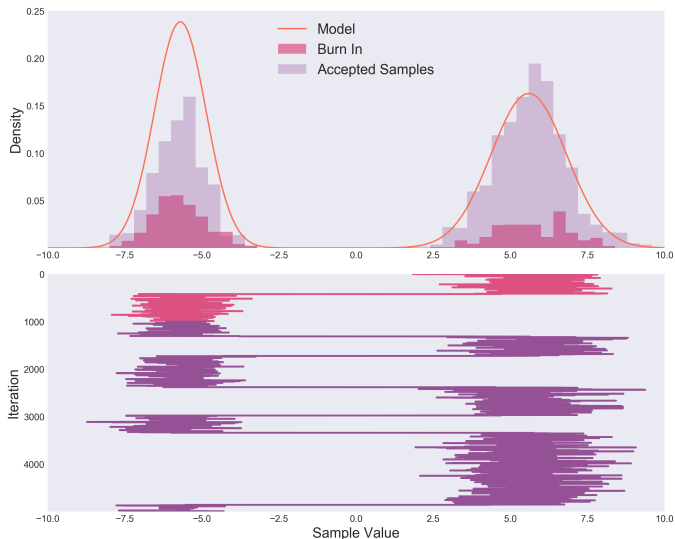


Figure: $\sigma^2 = 10$

Metropolis-Hastings: Example

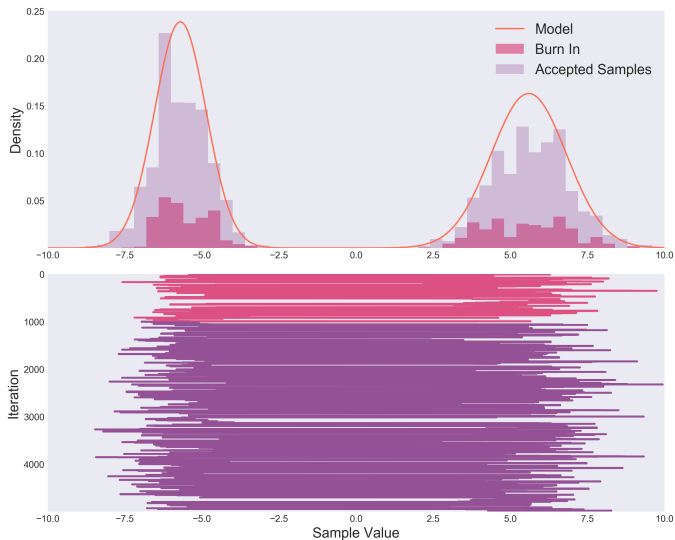


Figure: $\sigma^2 = 100$

Metropolis-Hastings: Key Terms to Know

- ▶ Acceptance Rates
 - ▶ Fraction of draws that are accepted
 - ▶ High acceptance rate \rightarrow bad mixing
 - ▶ Low Acceptance rate \rightarrow inefficient
 - ▶ Theoretical rates: 44% for one dimension, 23.4% as the dimension goes to infinity
- ▶ Chains
- ▶ Burn In
 - ▶ Allows the chain to "forget" its starting values and converge on areas of high probability
- ▶ Mixing
 - ▶ Allowing the chains to fully explore the state space, instead of collapsing in one peak

Variants of Metropolis-Hastings

(Random Walk) Metropolis Algorithm

- ▶ Uses a symmetric proposal distribution G , such that $g(x_s|x') = g(x'|x_s)$
- ▶ Our acceptance probability r is then

$$r = \min \left(1, \frac{f(x')}{f(x_s)} \right)$$

Metropolis Adjusted Langevin Algorithm (MALA)

- ▶ New states are proposed with Langevin dynamics

$$x' = x_s + \tau \nabla \log f(x_s) + \sqrt{2\tau} \xi_k$$

- ▶ Proposal probabilities are normally distributed as

$$g(x'|x_s) \sim \mathcal{N}(x_s + \tau \nabla \log f(x_s), 2\tau I_d)$$

$$g(x_s|x') \sim \mathcal{N}(x' + \tau \nabla \log f(x'), 2\tau I_d)$$

- ▶ Optimal acceptance rate is 57.4%

Metropolis Adjusted Langevin Algorithm: Example

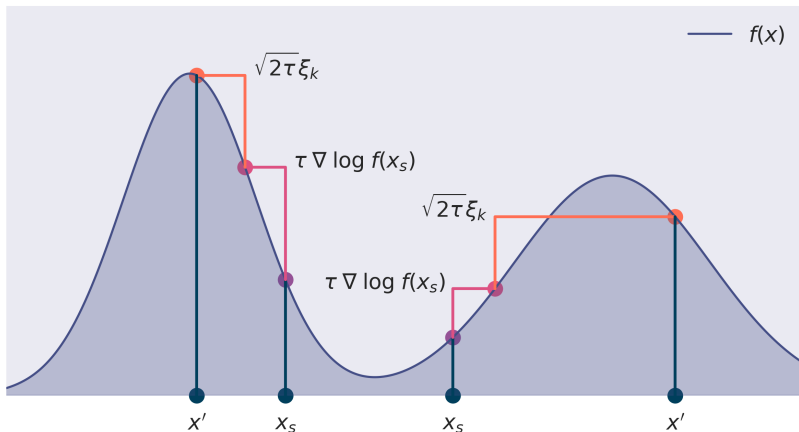


Figure: MALA: $\tau = 0.4$

Hamiltonian Monte Carlo

- ▶ Inspired by using a Hamiltonian dynamics evolution simulated using a time-reversible and volume preserving leapfrog integrator.
- ▶ Purpose was to reduce the correlation between successive sample states by proposing moves to distant states with high probability of acceptance.
- ▶ In simpler terms: flick a puck, wait, stop, then hit it again

Hamiltonian Dynamics

- For a system with state q , momentum p :

$$H(q, p) = U(q) + K(p)$$

$$U(q) = -\log f(q) \qquad K(p) = \sum_i \frac{p_i^2}{2}$$

- The time evolution of the system is defined by:

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\frac{\partial U(q)}{\partial q} \qquad \frac{dq}{dt} = \frac{\partial H}{\partial p} = p$$

- We can update the system coordinates as follows (leapfrog):

$$q_{i+1} = q_i + \epsilon p_i \qquad p_{i+1} = p_i - \epsilon \frac{\partial U(q_{i+1})}{\partial q_{i+1}}$$

- Our acceptance probability for the current state (q_s, p_s) and candidate (q, p) is

$$r = \exp(H(q_s, p_s) - H(q, p))$$

Hamiltonian Monte Carlo: Algorithm

Algorithm 6 HMC, Single Candidate Update

Input: Model F , Stepsize ϵ , Leapfrog Steps L , Current State x_s

```
1: Set  $q = q_s$ ,  $p \sim \mathcal{N}(0, 1)$ ,  $p_s = p$ 
2:  $p = p - \epsilon \frac{\partial U(q)}{\partial q} / 2$ 
3: for  $l = 0, 1, \dots, L$  do
4:    $q = q + \epsilon \cdot p$ 
5:    $p = p - \epsilon \frac{\partial U(q)}{\partial q}$  except at end of trajectory
6: end for
7:  $p = p - \epsilon \frac{\partial U(q)}{\partial q} / 2$ 
8:  $p = -p$  to make proposal symmetric
9: Compute acceptance probability
    $r = \exp(U(q_s) - U(q) + K(p_s) - K(p))$ 
10: Sample  $u \sim \text{Uniform}(0, 1)$ 
11: if  $u < r$  then
12:   return  $q$ 
13: else
14:   return  $q_s$ 
15: end if
```

Hamiltonian Monte Carlo: The Leapfrog Path

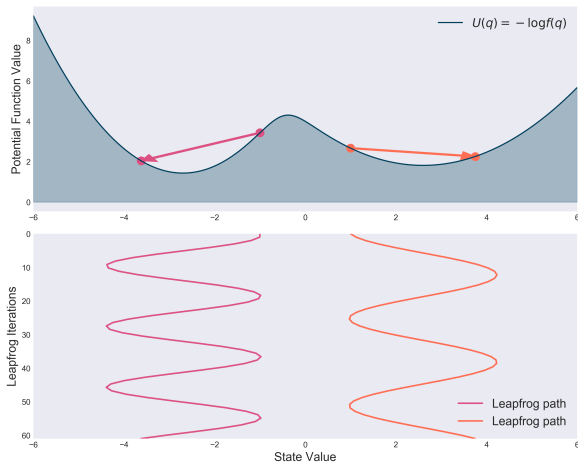


Figure: Leapfrog Paths: $\epsilon = 0.3$, $L = 60$

Hamiltonian Monte Carlo: Tampering to Overcome Energy Barriers

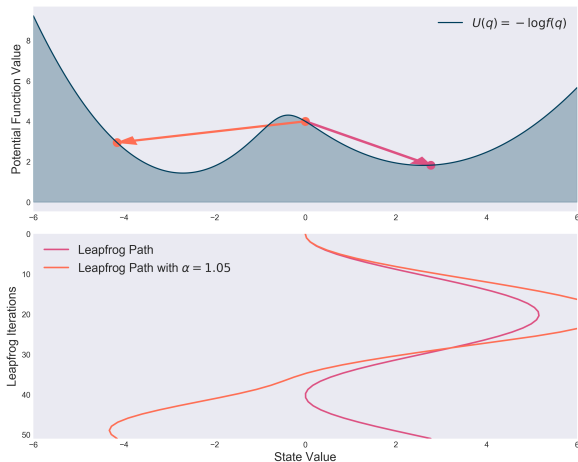


Figure: Leapfrog Paths: $\epsilon = 0.2$, $L = 50$, $\alpha = 1.05$

Hamiltonian Monte Carlo: Example

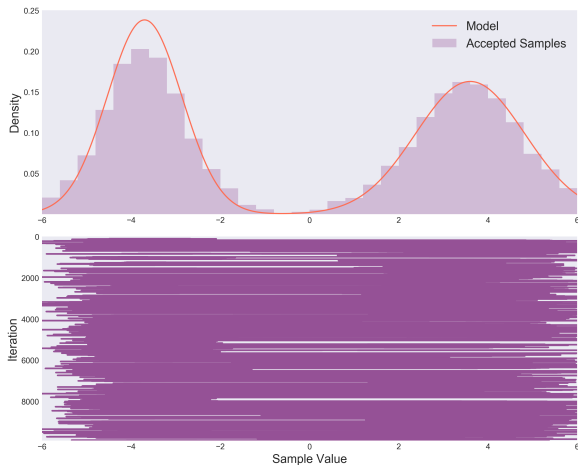


Figure: HMC: $\epsilon = 0.6$, $L = 40$, $\alpha = 1.05$, 100 burn in iterations, 10,000 epochs

Hamiltonian Monte Carlo: Considerations

- ▶ Distances between points are large, thus requiring less iterations
- ▶ Mostly accepts new states, more efficient even with the leapfrog "price"
- ▶ Tuning leapfrog steps can be difficult:
 - ▶ Small $L \rightarrow$ random walk behavior
 - ▶ Large $L \rightarrow$ wasted computation
- ▶ Has trouble sampling from distributions with isolated local minimums (lack of energy to cross the energy barrier)
- ▶ Optimal acceptance rate is 65%
- ▶ HMC Interactive Demo

No-U-Turn Sampler (NUTS)

- ▶ Removes the need to set the leapfrog step L in HMC
- ▶ Uses a recursive algorithm to build a set of likely candidate points
- ▶ As efficient as a well tuned HMC method

General Error Bounds

Analysis of Error

- ▶ How many samples S does it take to approximate the target distribution "well"?
- ▶ Answer: Use the Hoeffding bound

$$\Pr(\hat{p}(x) \notin [p(x) - \epsilon, p(x) + \epsilon]) \leq 2e^{-2S\epsilon^2}$$

- ▶ For the number of samples S , an error bound ϵ with probability $1 - \delta$, we can solve:

$$2e^{-2S\epsilon^2} \leq \delta$$
$$S \geq \frac{\log(2/\delta)}{2\epsilon^2}$$

Analysis of Error

- ▶ We can also use the Chernoff Bound relative to the true value $p(x)$
- ▶ However, this is dependent on $p(x)$, which is not always known.

$$Pr(\hat{p}(x) \notin [p(x)(1 - \epsilon), p(x)(1 + \epsilon)]) \leq 2e^{-Sp(x)\epsilon^2/3}$$

$$S \geq 3 \frac{\log(2/\delta)}{p(x)\epsilon^2}$$

Tools, References, and Further Reading

Libraries and Tools

- ▶ PyMC3
- ▶ TensorFlow Probability
- ▶ Pyro
- ▶ Stan
- ▶ RStan
- ▶ R mcmc

Noteworthy Concepts Not Covered

- ▶ Alternatives to Inverse Transform Sampling for Normal Distributions
 - ▶ Box-Muller Transform
 - ▶ Marsaglia-Bray Polar Method
 - ▶ Ziggurat Algorithm
- ▶ Variance Reduction Techniques for Monte Carlo Methods
 - ▶ Control Variates
 - ▶ Antithetic Variates
 - ▶ Stratified Sampling
 - ▶ Importance Sampling
- ▶ Alternative MCMC Algorithms
 - ▶ Gibbs Sampling
 - ▶ Slice Sampling
 - ▶ Reversible-Jump
 - ▶ Adaptive Metropolis-Hastings
- ▶ Quasi-Monte Carlo Methods

References & Further Reading

- ▶ Machine Learning: A Probabilistic Perspective by Kevin Murphy
- ▶ Monte Carlo Methods in Financial Engineering by Paul Glasserman
- ▶ Probabilistic Graphical Models: Principles and Techniques by Daphne Koller and Nir Friedman
- ▶ Sampling Lecture from my PGM Professor Daniel Malinsky
- ▶ MCMC Using Hamiltonian Dynamics by Radford M. Neal
- ▶ Probabilistic Inference Using Markov Chain Monte Carlo Methods by Radford M. Neal
- ▶ Hamiltonian Monte Carlo Explained by Alex Rogozhnikov
- ▶ The Markov-chain Monte Carlo Interactive Gallery by Chi Feng
- ▶ The No-U-Turn Sampler by Hoffman and Gelman
- ▶ CMU Notes on Probability Inequalities by Larry Wasserman