

Day3 : Introduction to Markov Chain Monte Carlo

[FastCampus] AI센터 베이지안 통계과정

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- Monte Carlo Estimation
 - 1d sampling (discrete)
 - 1d sampling (continuous) – rejection sampling
- Markov Chain
- Gibbs Sampling
- Metropolis Hastings
- MCMC examples (with PyMC3)

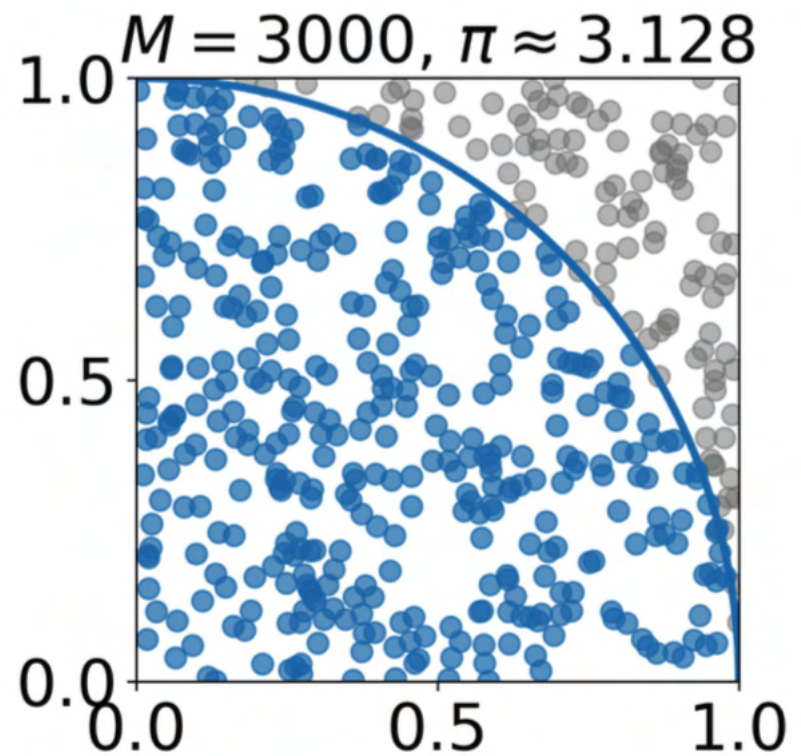
Ch 1. Monte Carlo Estimation

Monte Carlo Markov Chain (MCMC)

- 몬테카를로 기법(Monte Carlo Method)은 난수를 이용하여 함수의 값을 확률적으로 근사하는 알고리즘을 뜻하는 용어다.
- 일반적으로 평균값(expected value)을 근사하기 위해 사용되며, Bayesian Theory에서는 Posterior의 sampling을 얻기 위해 활용된다.
- Two common MCMC approaches:
 - Gibbs sampling – reducing multidimensional sampling to a sequence of 1d
 - Metropolis Hastings – rejection sampling for Markov Chains (gives more freedom)

Monte Carlo

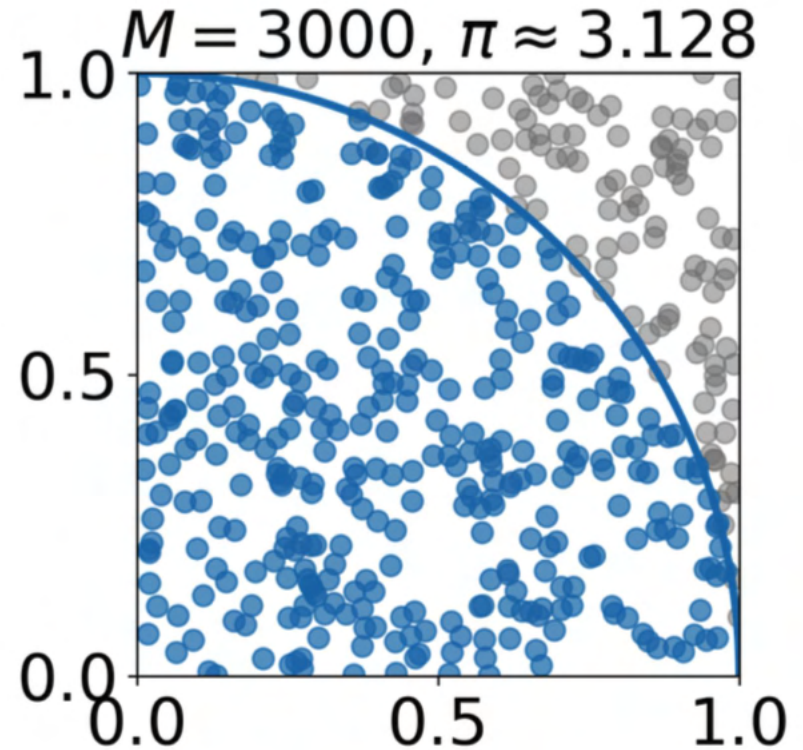
Estimate expected values by sampling



Monte Carlo

Estimate expected values by sampling

$$\frac{\pi}{4} = \mathbb{E} [x^2 + y^2 \leq 1]$$



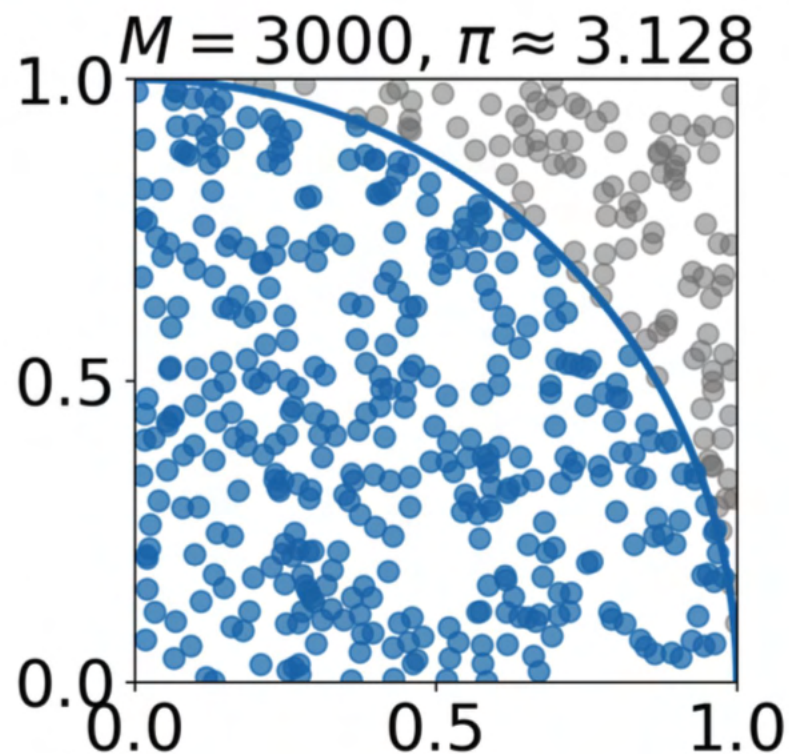
Monte Carlo

Estimate expected values by sampling

$$\frac{\pi}{4} = \mathbb{E} [x^2 + y^2 \leq 1]$$

$$\approx \frac{1}{M} \sum_{s=1}^M [x_s^2 + y_s^2 \leq 1]$$

$$x_s, y_s \sim \mathcal{U}(0, 1)$$



Monte Carlo

Estimate expected values by sampling

$$\mathbb{E}_{p(x)} f(x) \approx \frac{1}{M} \sum_{s=1}^M f(x_s)$$

$$x_s \sim p(x)$$

Monte Carlo Approximation is Unbiased

Monte Carlo

$$\mathbb{E}_{p(x)} f(x) \approx \frac{1}{M} \sum_{s=1}^M f(x_s)$$

$$x_s \sim p(x)$$

Unbiased estimate (larger $M \Rightarrow$ better accuracy)

$$\mathbb{E}_{p(x)} \frac{1}{M} \sum_{s=1}^M f(x_s) = \mathbb{E}_{p(x)} f(x)$$

Monte Carlo

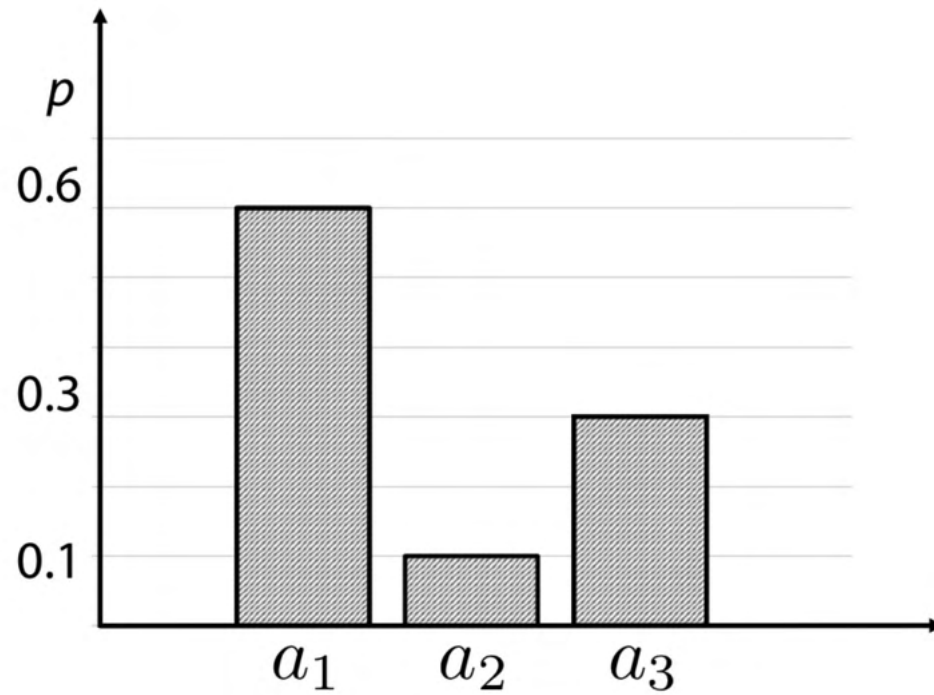
Why do we need to estimate expected values?

- Bayesian Analysis에서는 일반적으로 Sample들을 이용해서, Posterior Distribution을 분석하거나 Predictive Distribution을 계산하는데 활용된다.

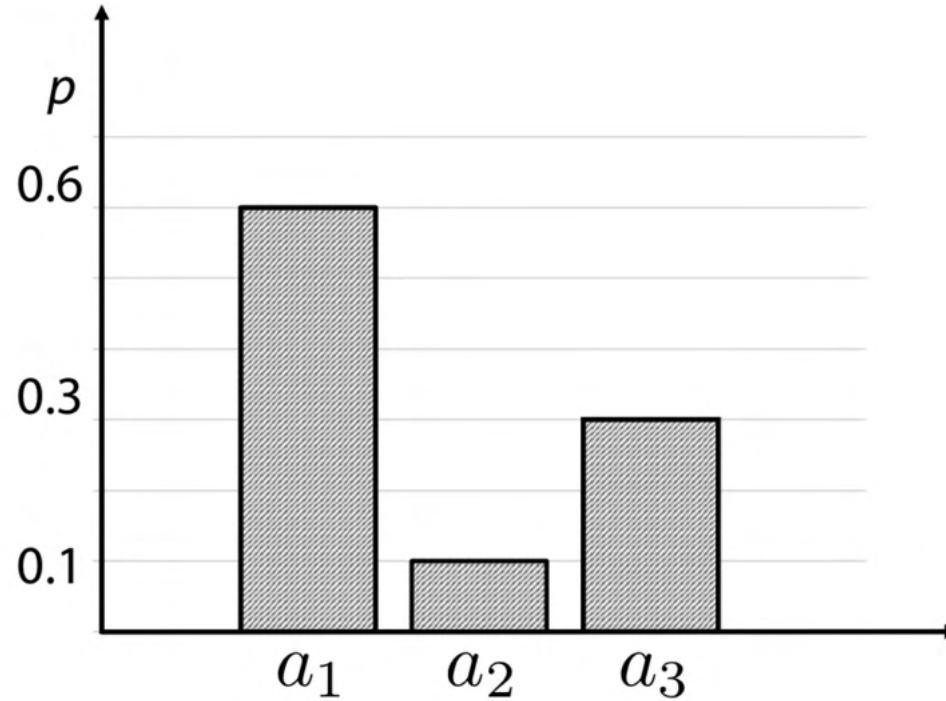
$$\begin{aligned} p(y | x, Y_{\text{train}}, X_{\text{train}}) \\ &= \int p(y | x, w) p(w | Y_{\text{train}}, X_{\text{train}}) dw \\ &= \mathbb{E}_{p(w | Y_{\text{train}}, X_{\text{train}})} p(y | x, w) \end{aligned}$$

$$p(w | Y_{\text{train}}, X_{\text{train}}) = \frac{p(Y_{\text{train}} | X_{\text{train}}, w) p(w)}{Z}$$

1d sampling (discrete)

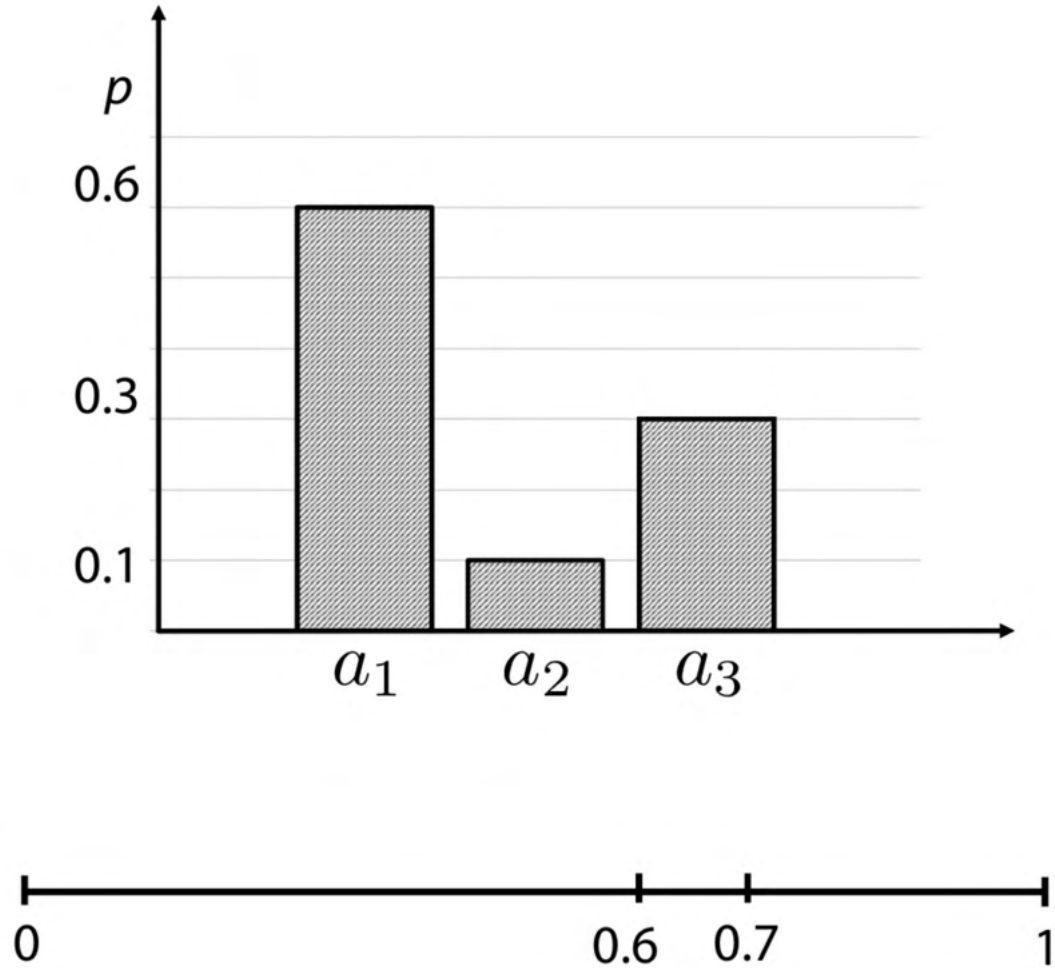


1d sampling (discrete)

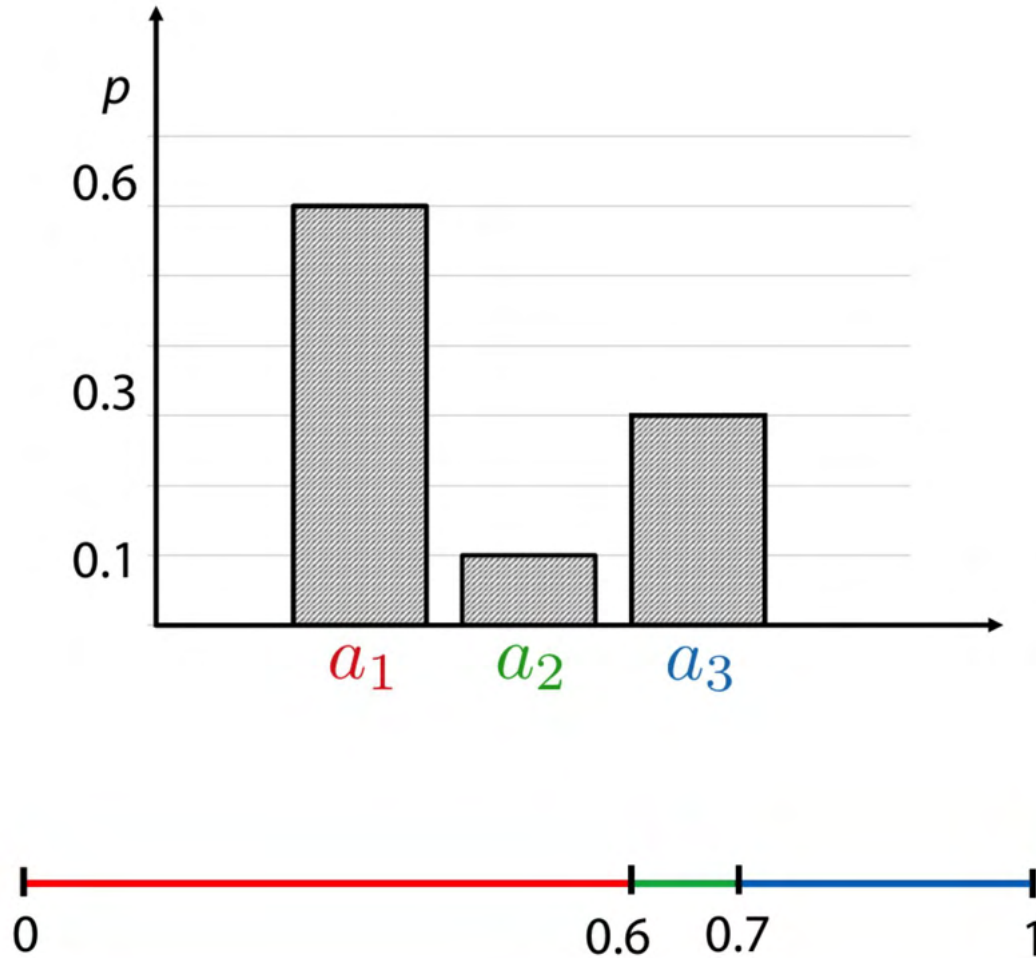


We can always sample from uniform $\mathcal{U}[0, 1]$

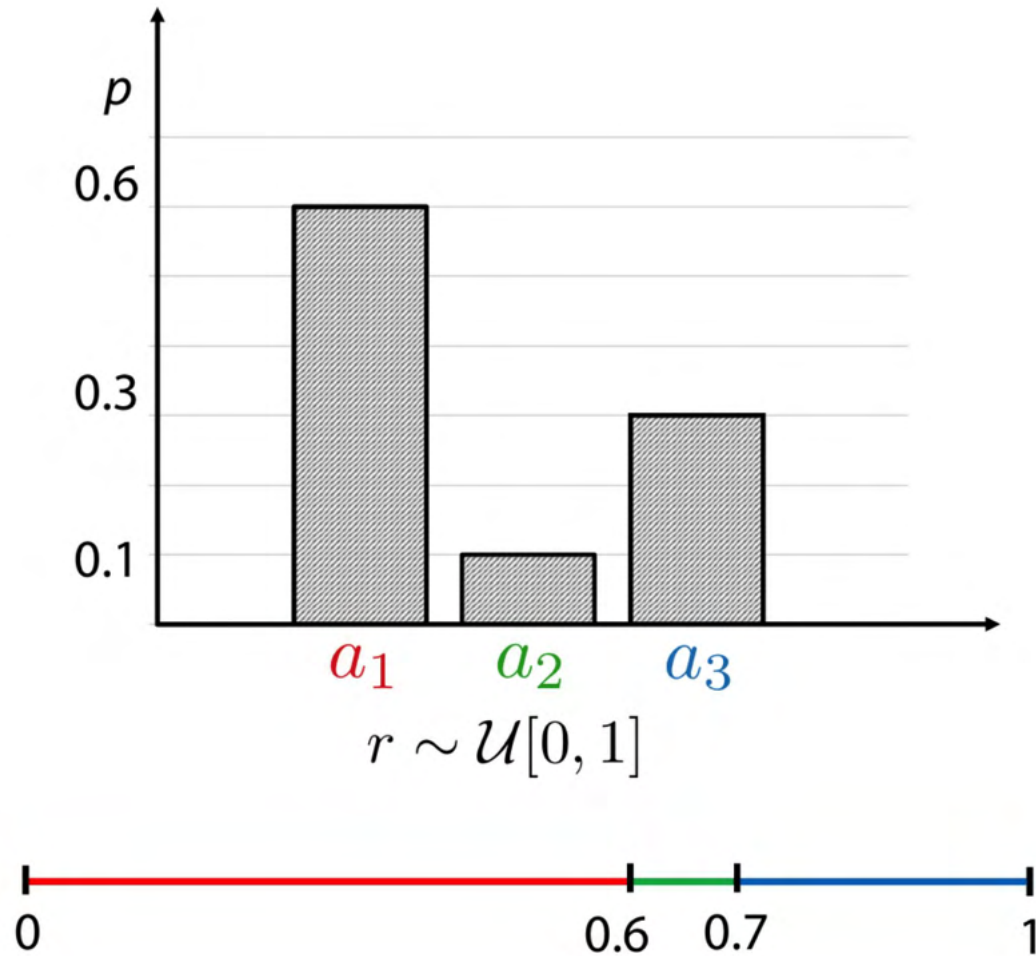
1d sampling (discrete)



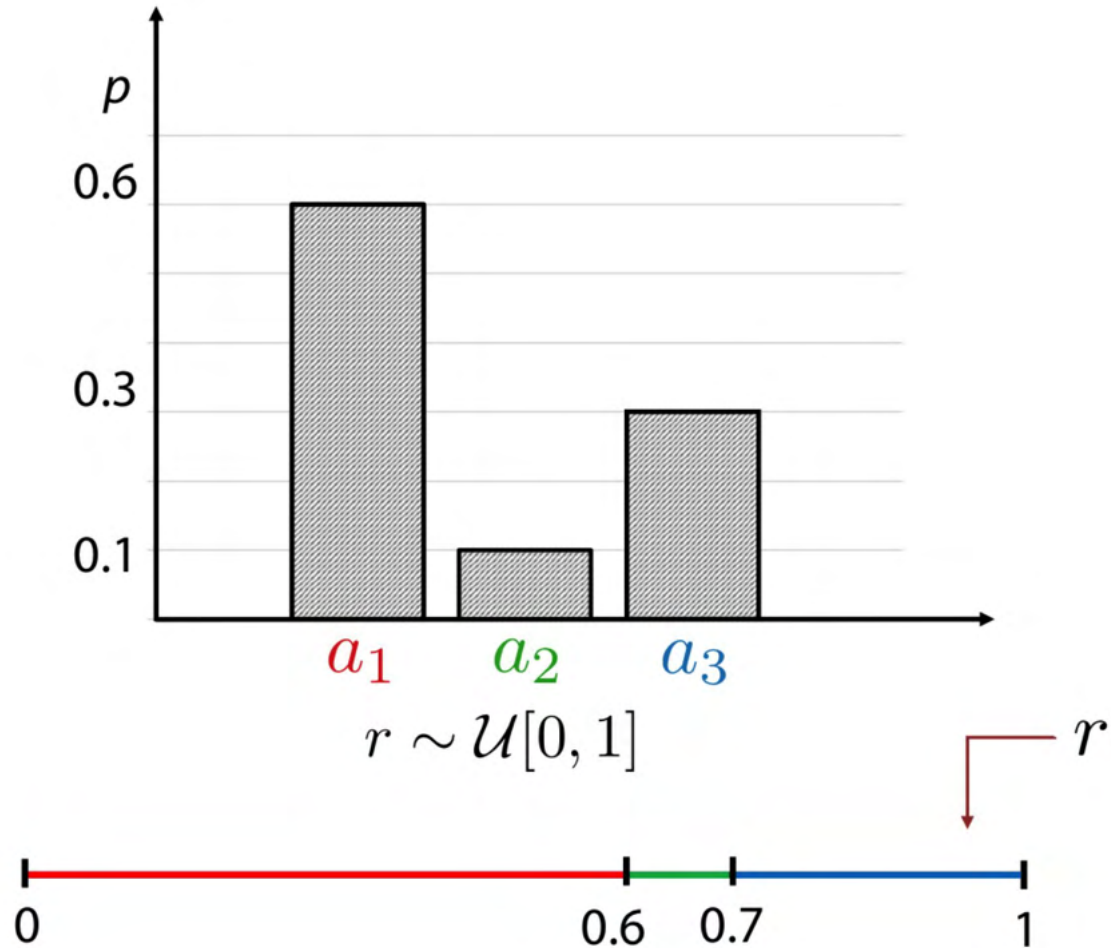
1d sampling (discrete)



1d sampling (discrete)



1d sampling (discrete)

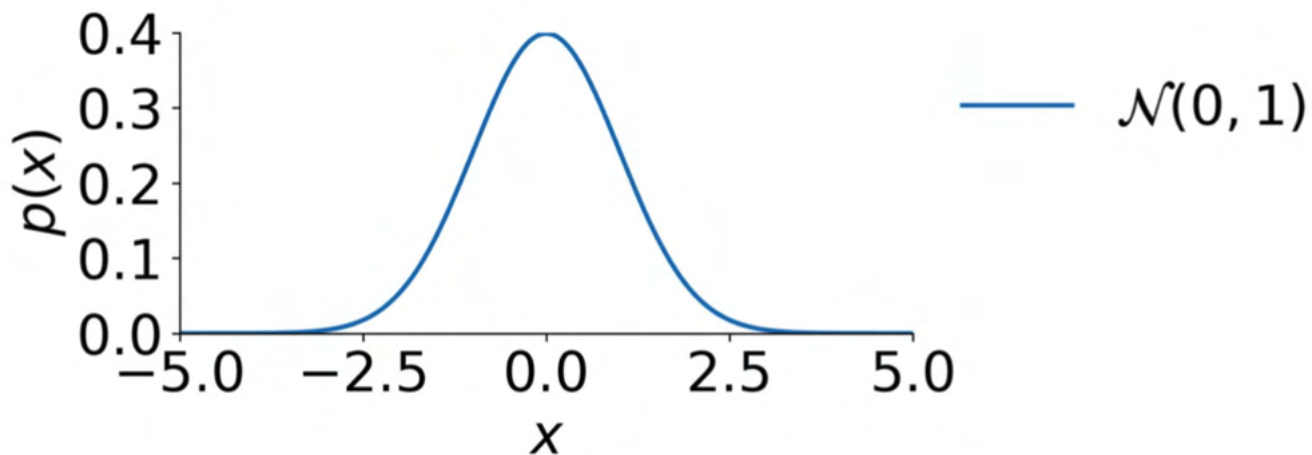


1d sampling (discrete) - Summary

- 차원이 낮은 discrete distribution으로 부터 sampling을 하는 방법은 아주 쉽다
 - At least then number of values is $< 100\ 000$
- 고차원인 경우 훨씬 많은 sample이 필요하다.

1d sampling (continuous) - Gaussian

Sampling from Gaussian distribution

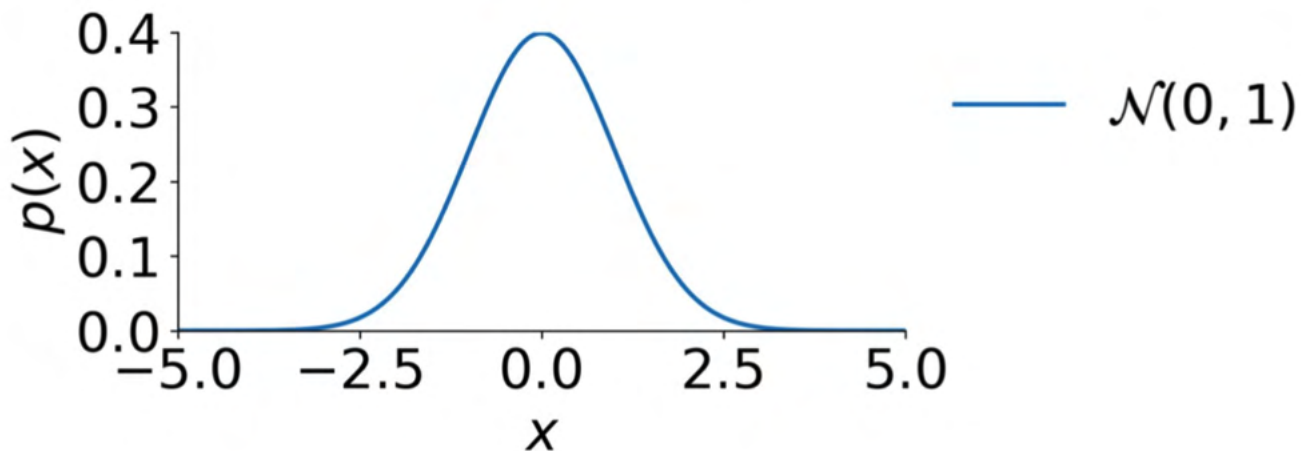


1d sampling (continuous) - Gaussian

Sampling from Gaussian distribution

$$z = \sum_{i=1}^{12} x_i - 6, \quad x_i \sim \mathcal{U}[0, 1]$$

$$p(z) \approx \mathcal{N}(0, 1)$$

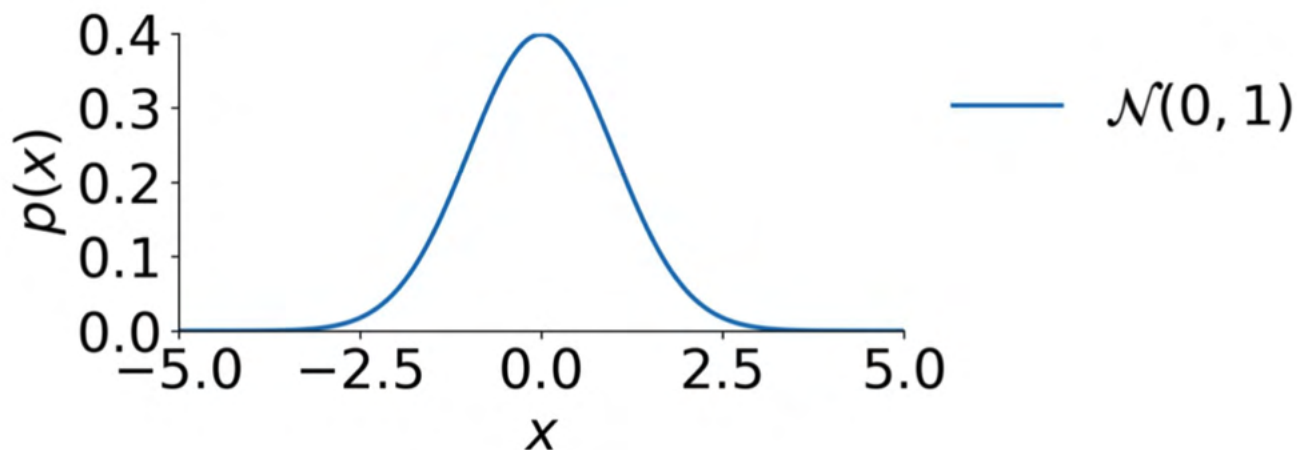


1d sampling (continuous) - Gaussian

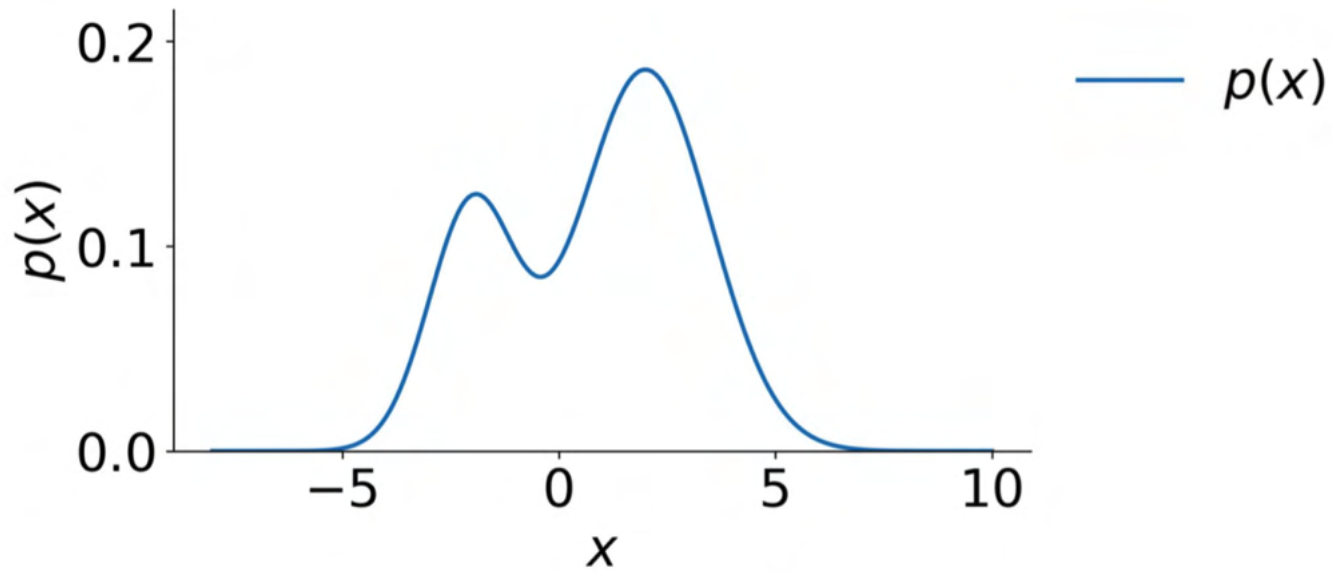
Sampling from Gaussian distribution

Or call library function 😊

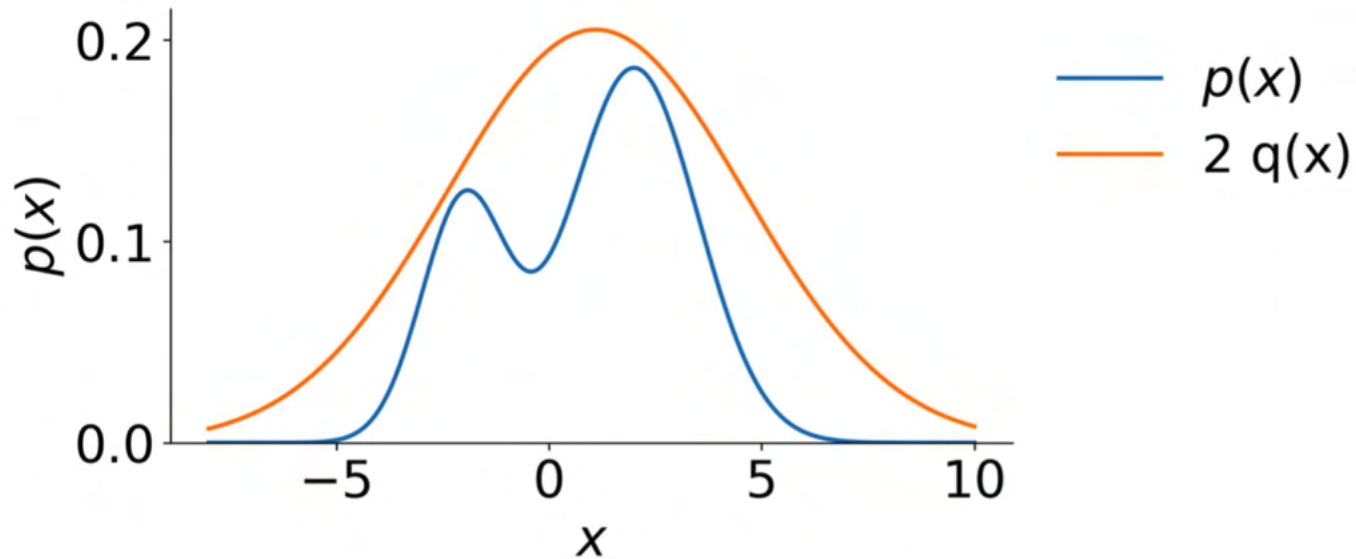
```
z = numpy.random.randn()
```



1d sampling (continuous) - General



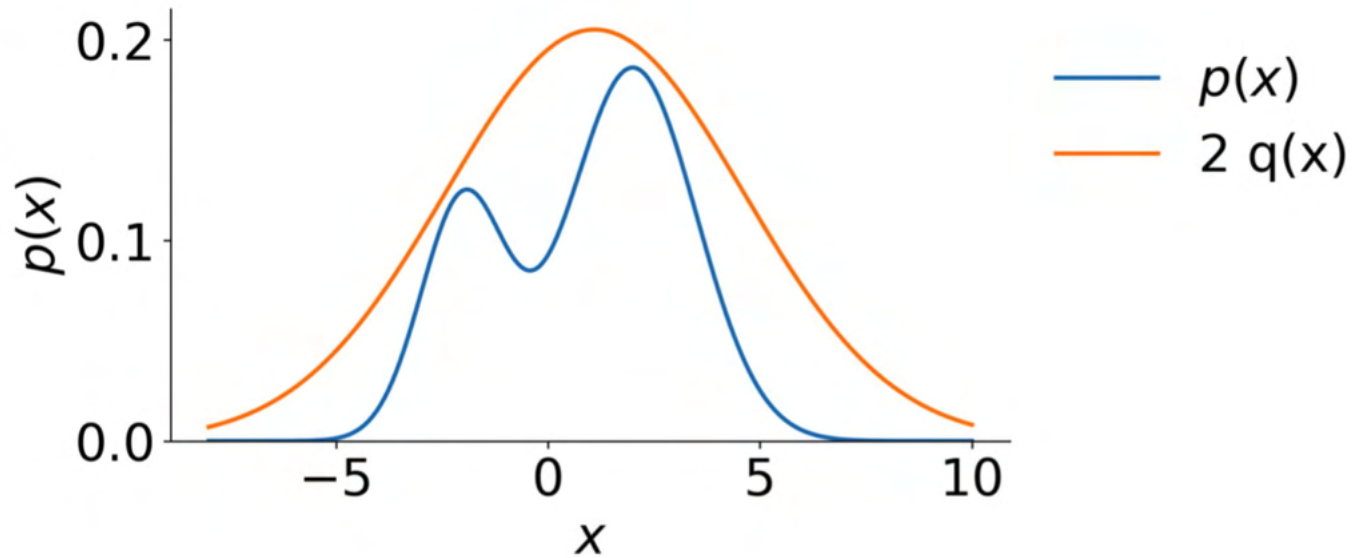
Rejection sampling



$$q(x) = \mathcal{N}(1, 3^2)$$

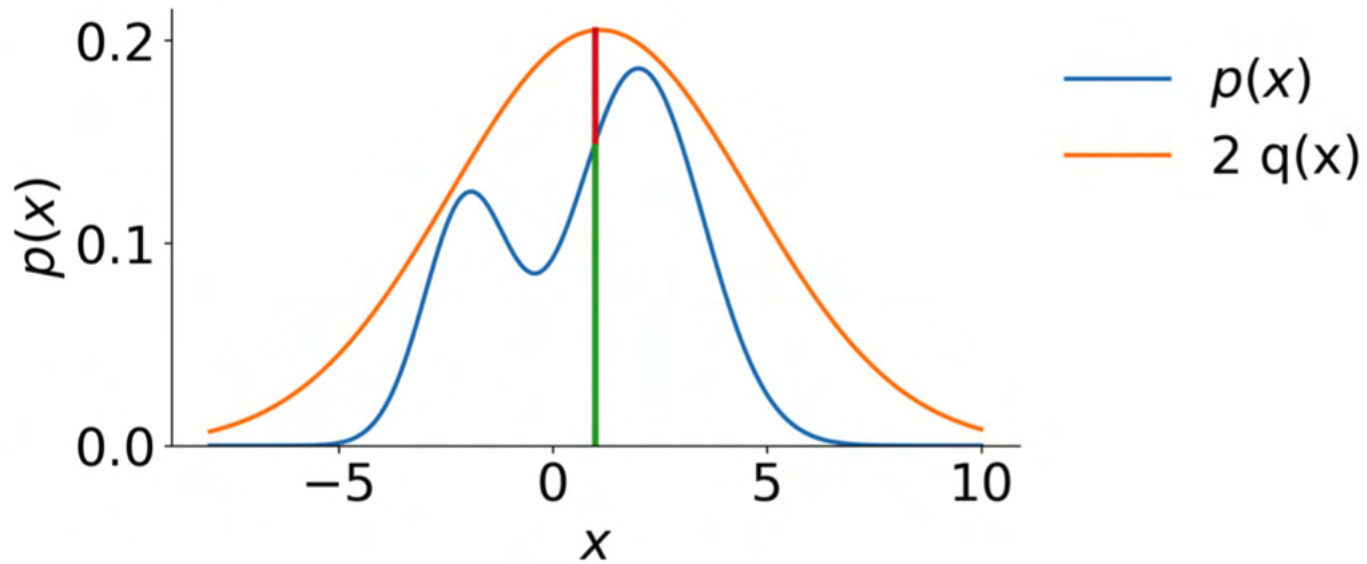
$$p(x) \leq 2q(x)$$

Rejection sampling



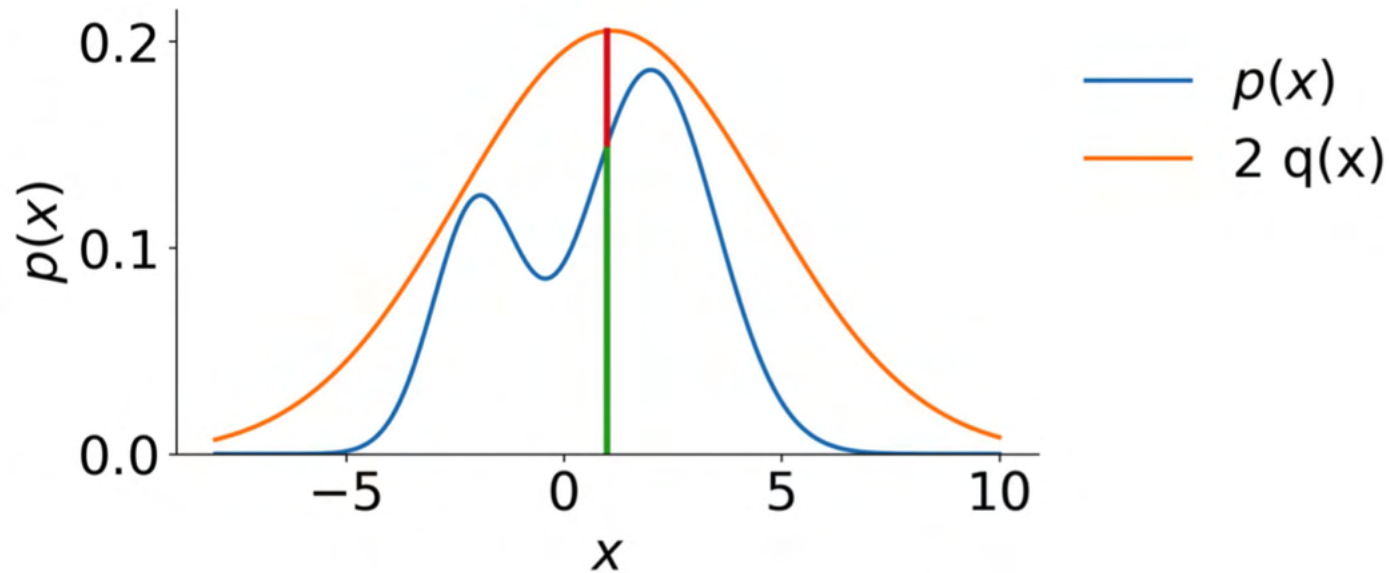
$$\tilde{x} \sim q(x)$$

Rejection sampling



$$\tilde{x} \sim q(x)$$

Rejection sampling

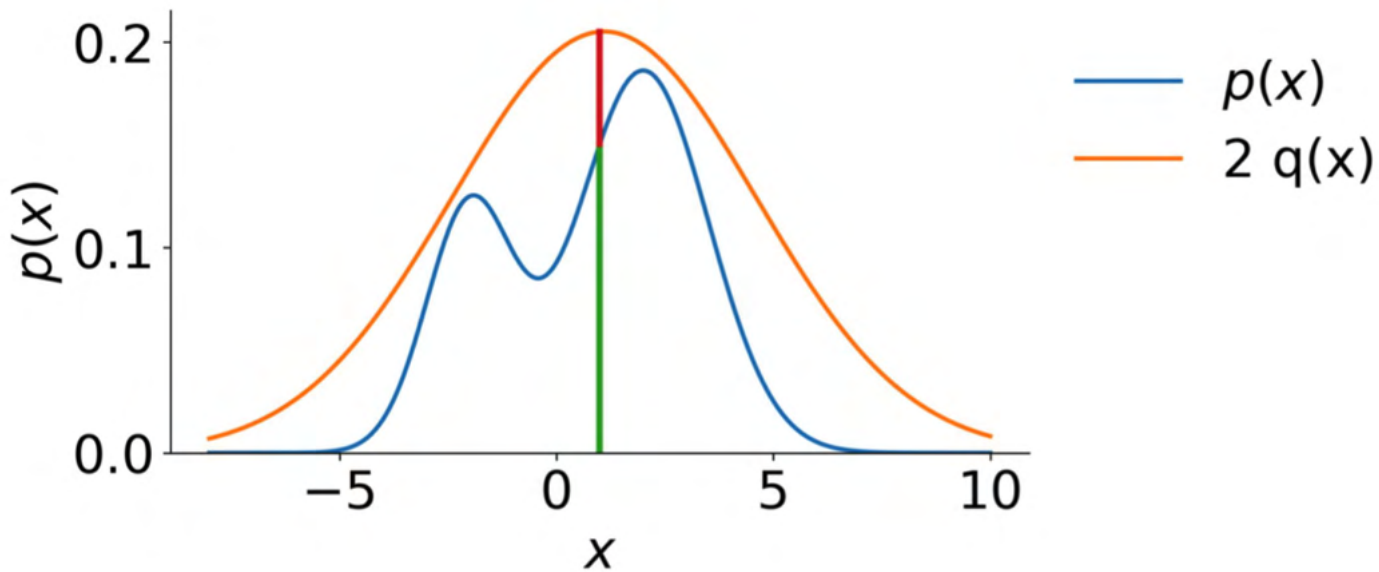


$$\tilde{x} \sim q(x)$$

$$y \sim \mathcal{U}[0, 2q(\tilde{x})]$$

Accept \tilde{x} with probability $\frac{p(x)}{2q(x)}$

Rejection sampling

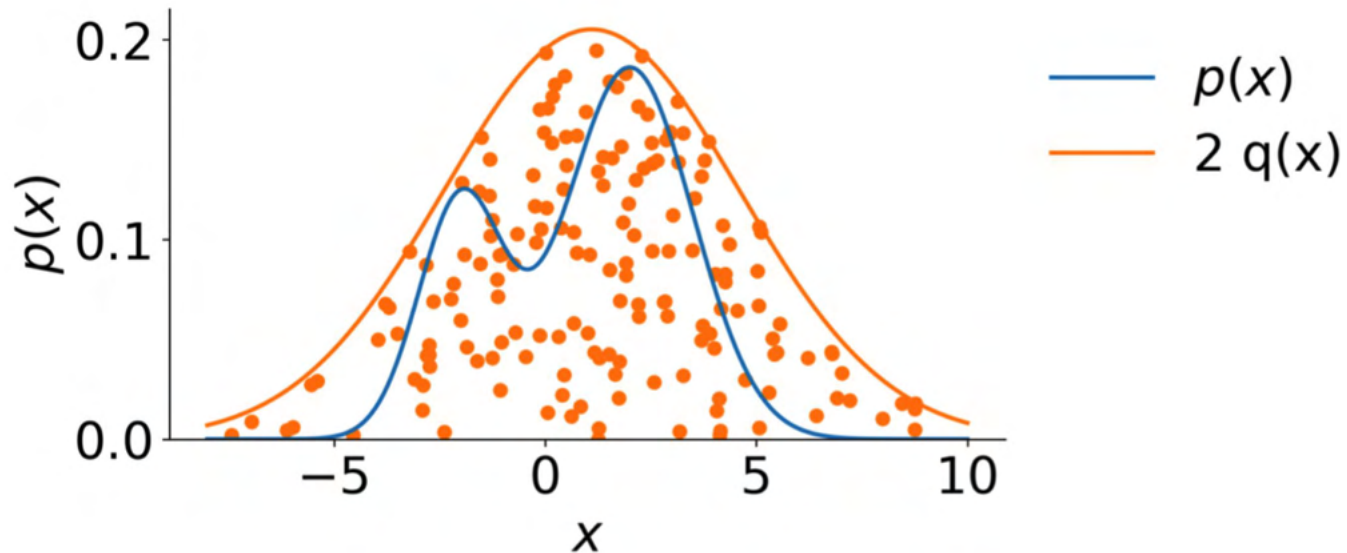


$$\tilde{x} \sim q(x)$$

$$y \sim \mathcal{U}[0, 2q(\tilde{x})]$$

Accept \tilde{x} with probability $\frac{p(x)}{2q(x)}$: if $y \leq p(x)$

Rejection sampling

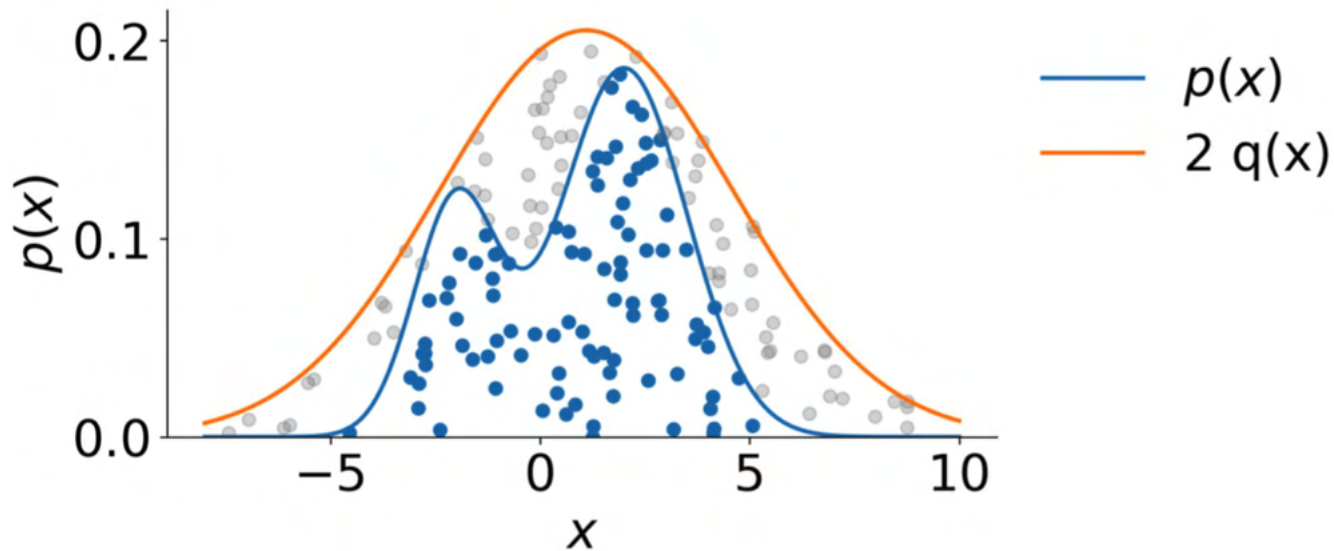


$$\tilde{x} \sim q(x)$$

$$y \sim \mathcal{U}[0, 2q(\tilde{x})]$$

Accept \tilde{x} with probability $\frac{p(x)}{2q(x)}$: if $y \leq p(x)$

Rejection sampling

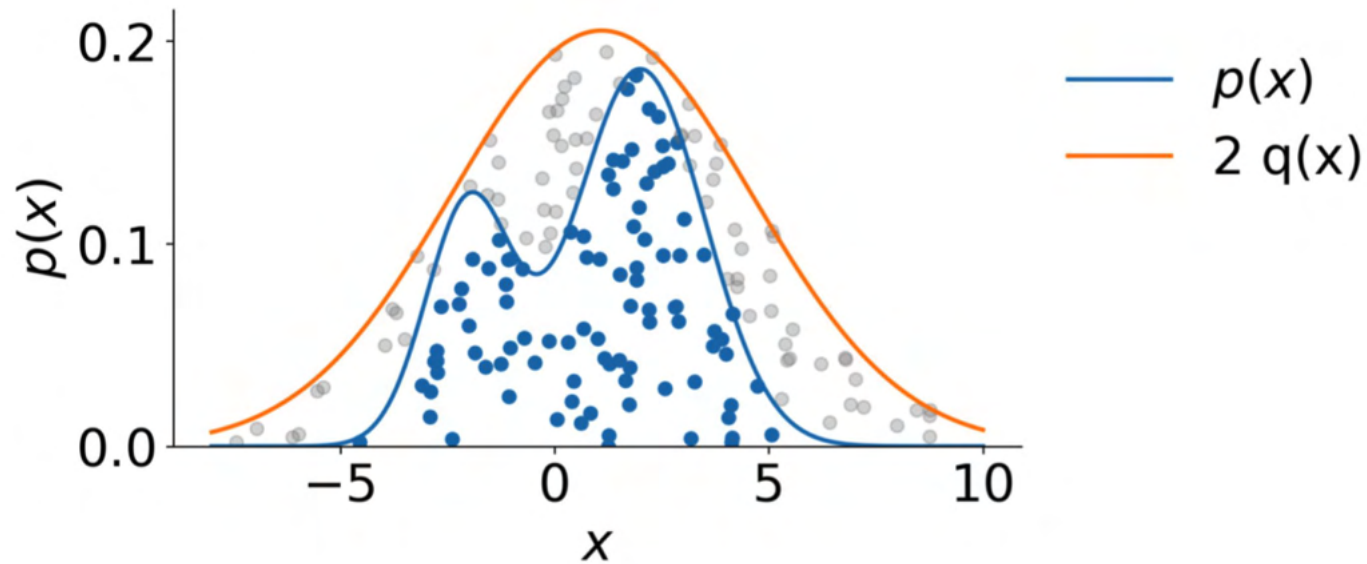


$$\tilde{x} \sim q(x)$$

$$y \sim \mathcal{U}[0, 2q(\tilde{x})]$$

Accept \tilde{x} with probability $\frac{p(x)}{2q(x)}$: if $y \leq p(x)$

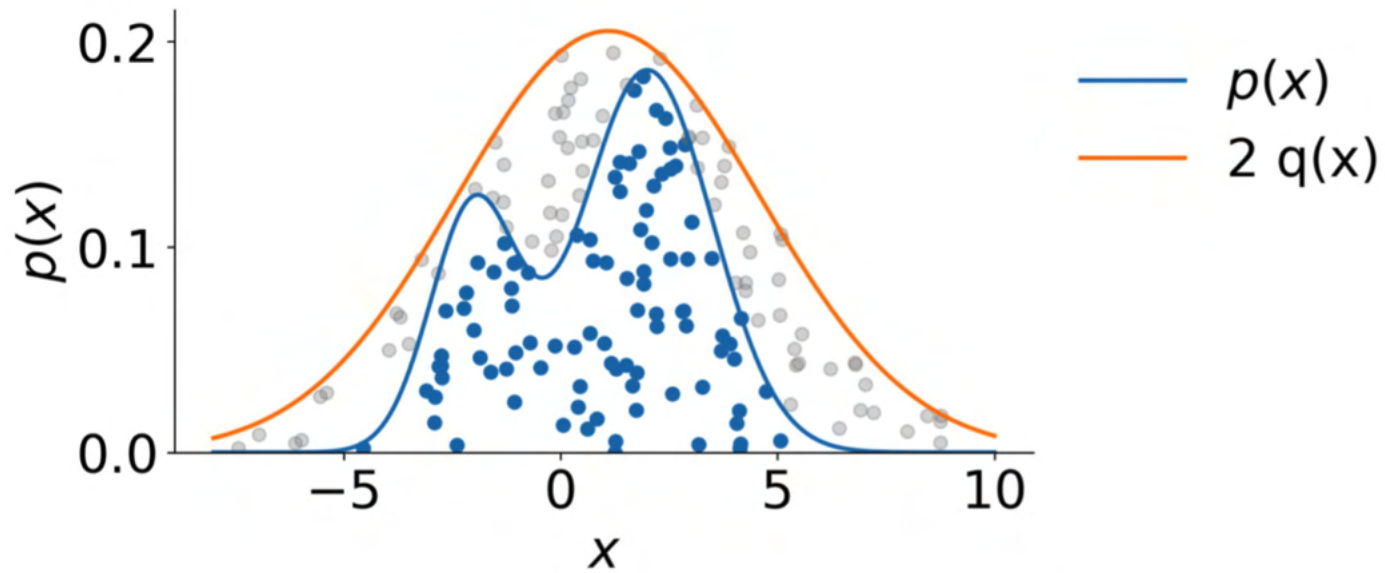
Rejection sampling



$$p(x) \leq Mq(x)$$

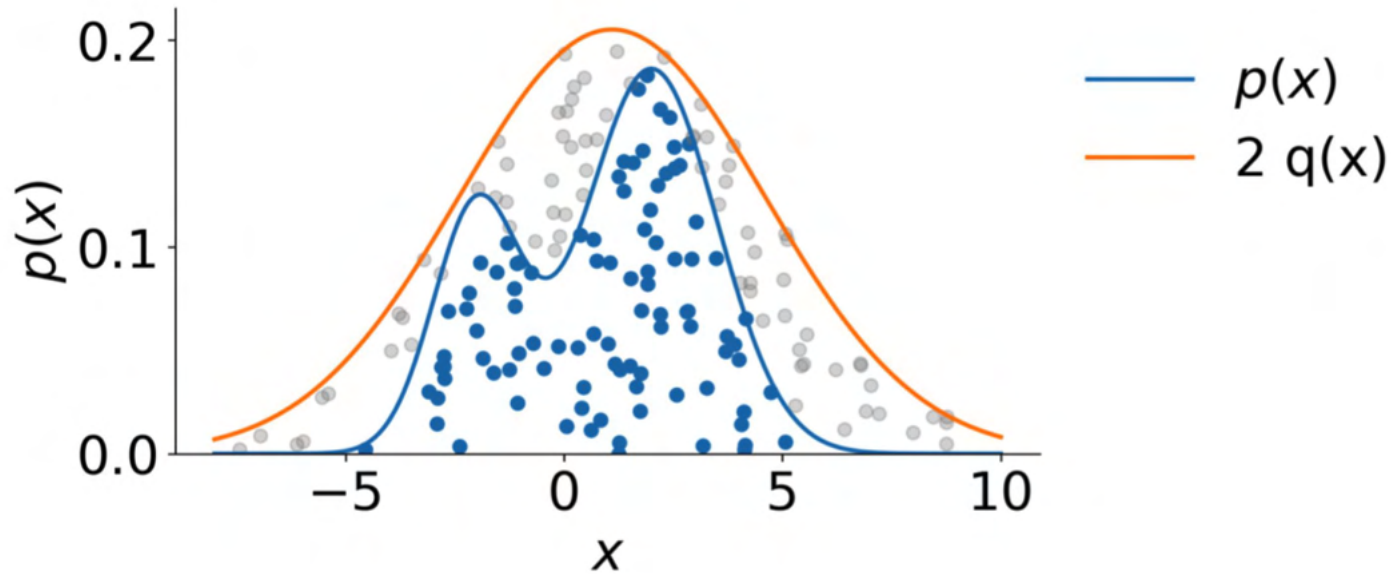
Accepts $\frac{1}{M}$ points on average

Rejection sampling



$$\frac{\hat{p}(x)}{Z} \leq Mq(x)$$

Rejection sampling



$$\hat{p}(x) \leq \underbrace{ZM}_{\tilde{M}} q(x)$$

Monte Carlo Sampling – Summary

Pros:

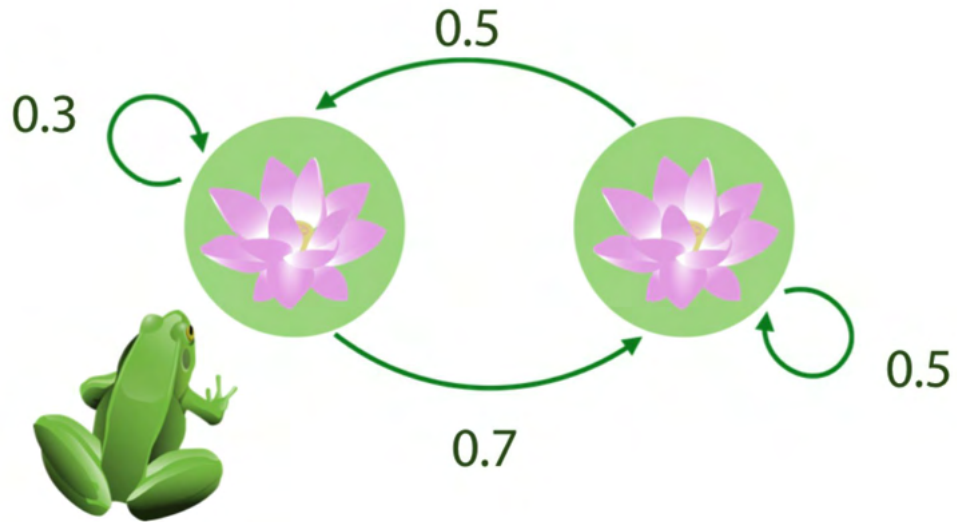
- Works for most distributions (even unnormalized)

Cons:

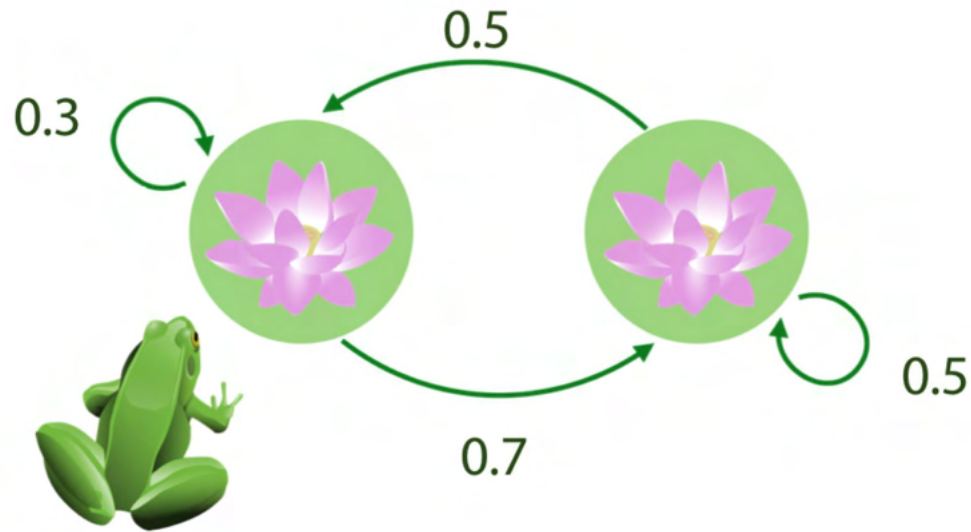
- If q and p are too different (M is large), rejects most of the points
- M is large for d -dimensional distributions

Ch 2. Markov Chain

Markov Chains



Markov Chains



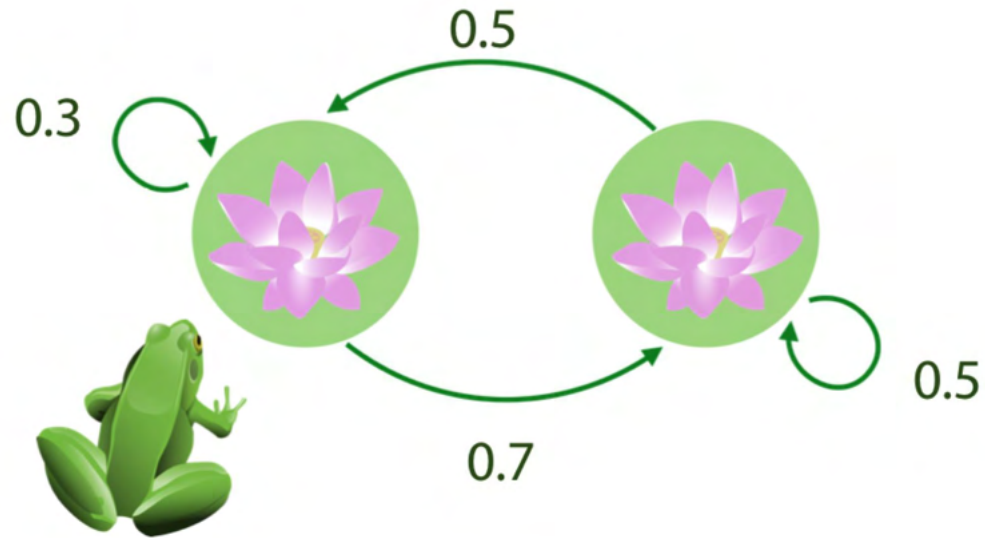
$$T(L \rightarrow L) = 0.3$$

$$T(R \rightarrow L) = 0.5$$

$$T(L \rightarrow R) = 0.7$$

$$T(R \rightarrow R) = 0.5$$

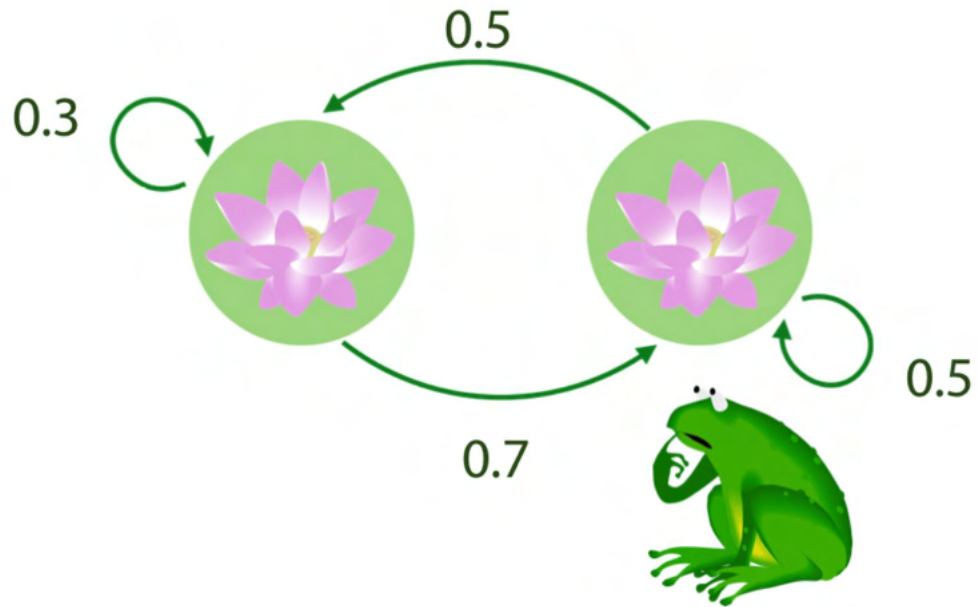
Markov Chains



Timestamp: **1**

Log: **L**

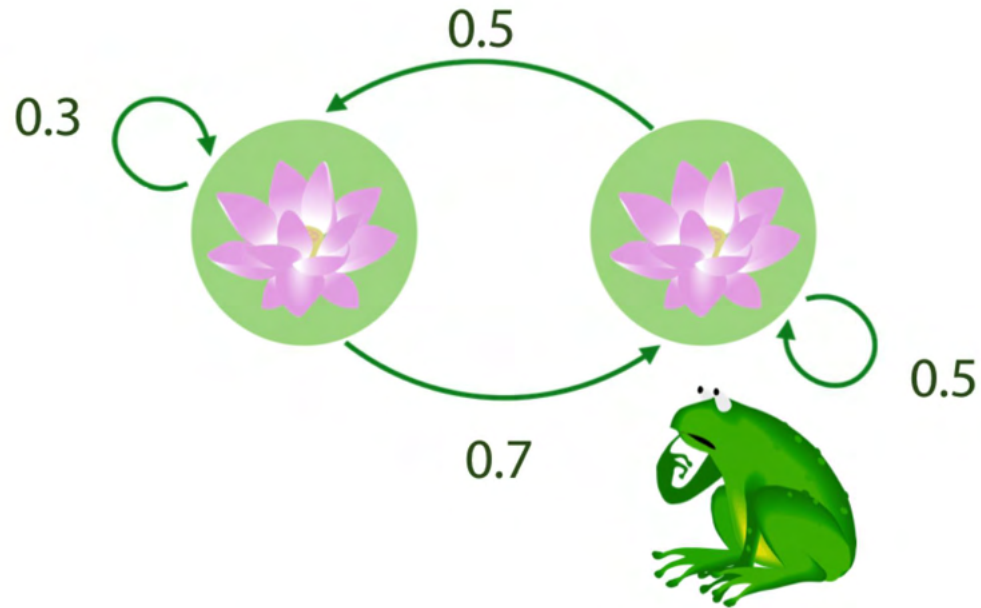
Markov Chains



Timestamp: **2**

Log: **L R**

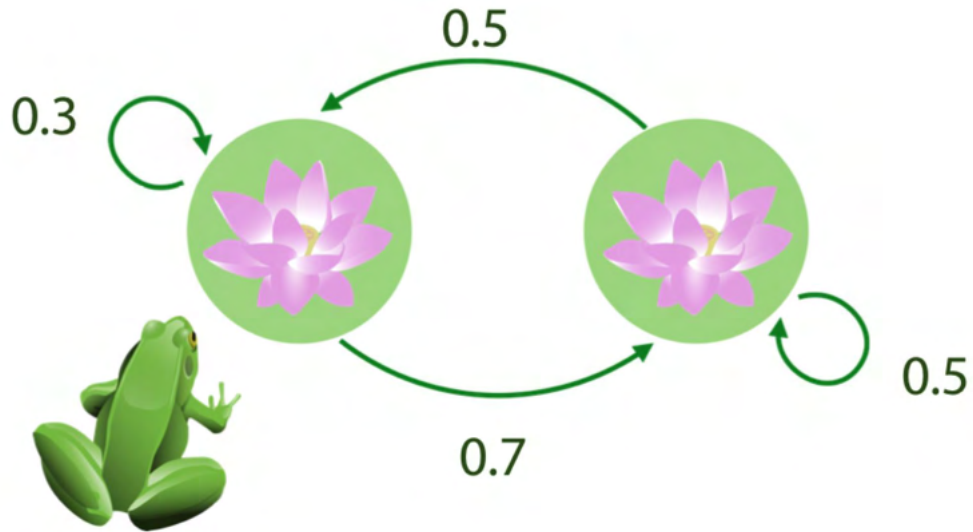
Markov Chains



Timestamp: **3**

Log: **L R R**

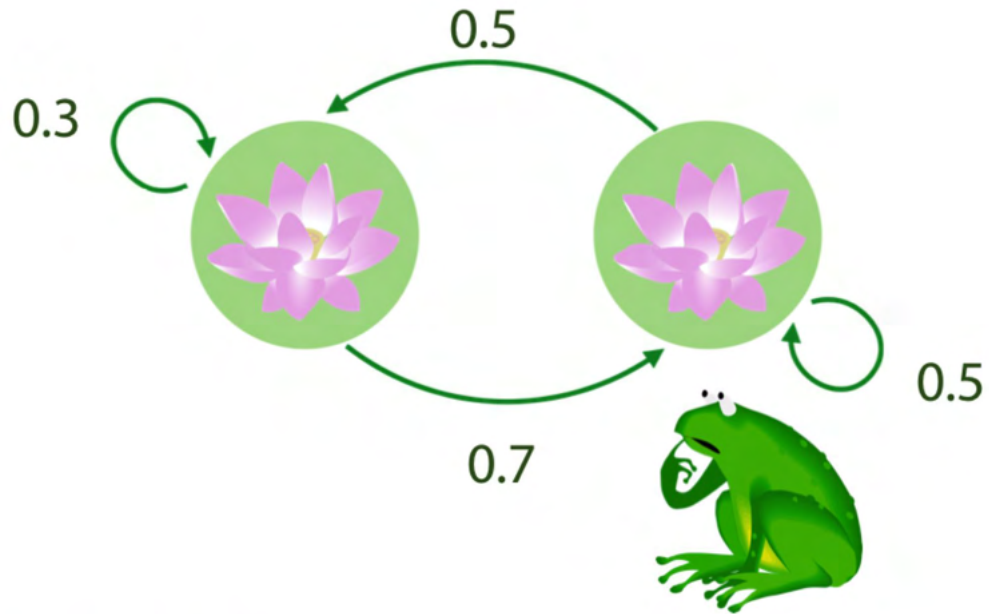
Markov Chains



Timestamp: **4**

Log: **LRRL**

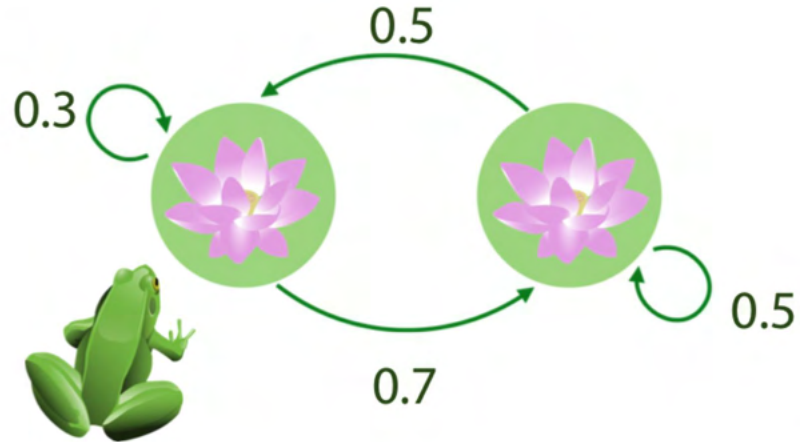
Markov Chains



Timestamp: **5**

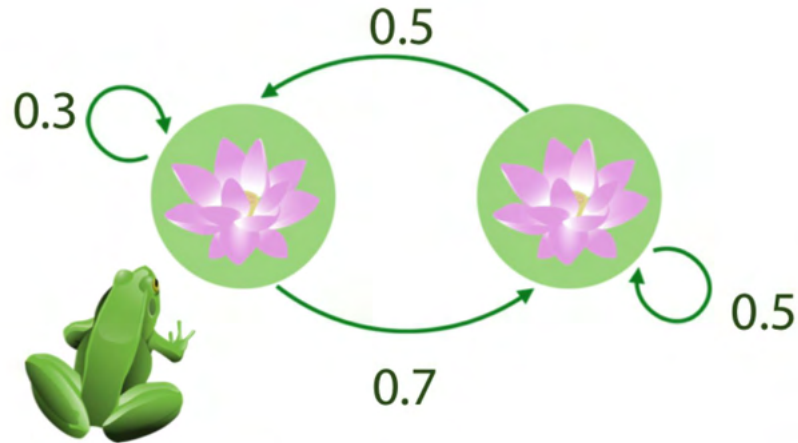
Log: **L R R L R**

Markov Chains



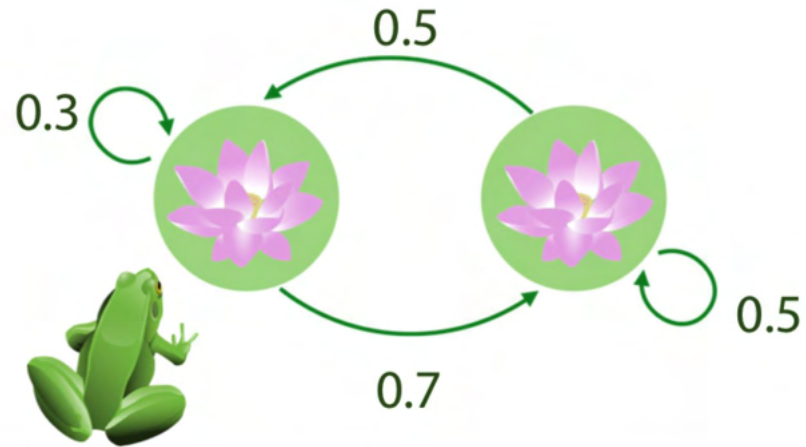
	p(Left)	p(Right)
x^1	1	0

Markov Chains



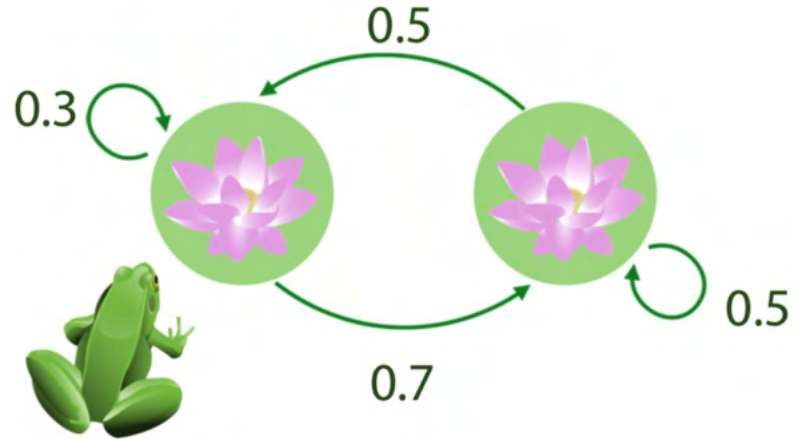
	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7

Markov Chains



	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3		

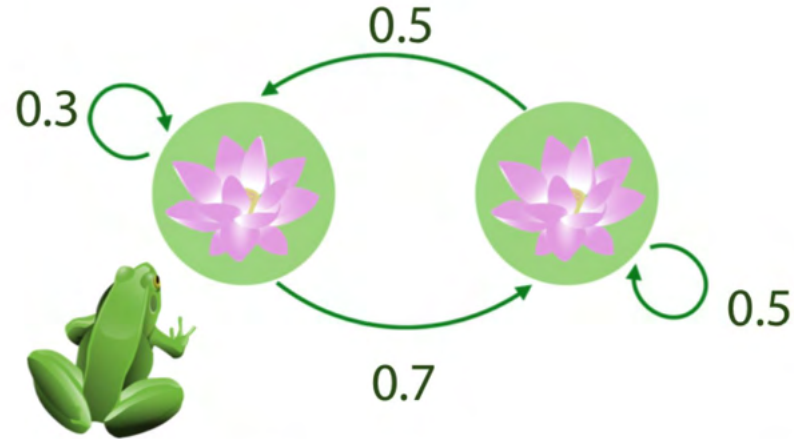
Markov Chains



	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3		

$$p(x^3) = p(x^3 \mid x^2 = \text{L})p(x^2 = \text{L}) \\ + p(x^3 \mid x^2 = \text{R})p(x^2 = \text{R})$$

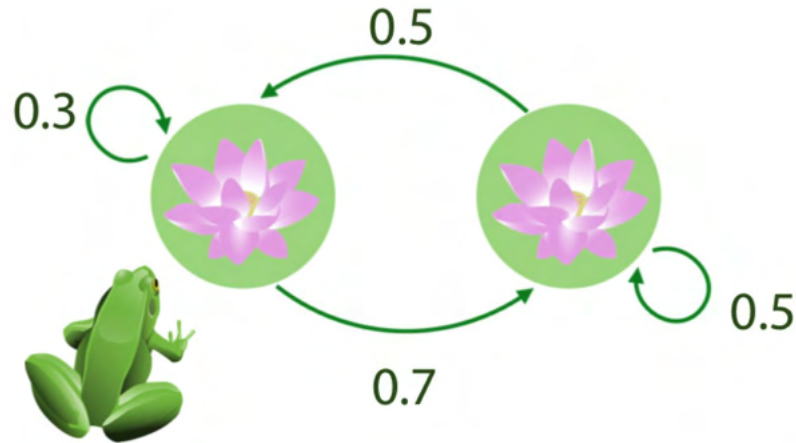
Markov Chains



	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3	$0.3^2 + 0.7 \cdot 0.5$	

$$p(x^3) = p(x^3 | x^2 = \text{L})p(x^2 = \text{L}) + p(x^3 | x^2 = \text{R})p(x^2 = \text{R})$$

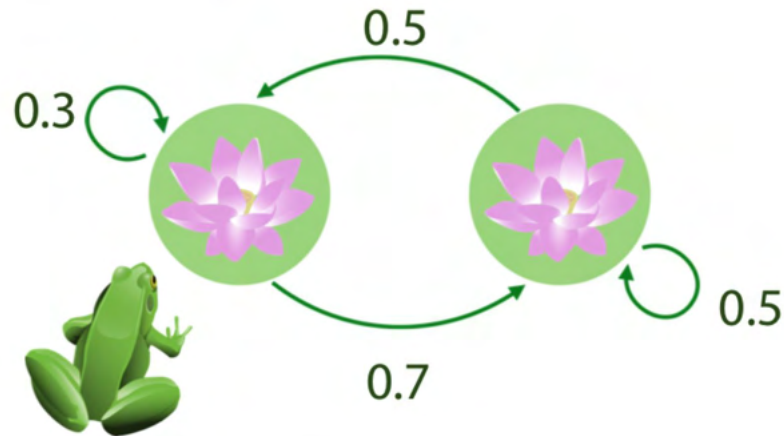
Markov Chains



	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3	$0.3^2 + 0.7 \cdot 0.5$	$0.3 \cdot 0.7 + 0.7 \cdot 0.5$

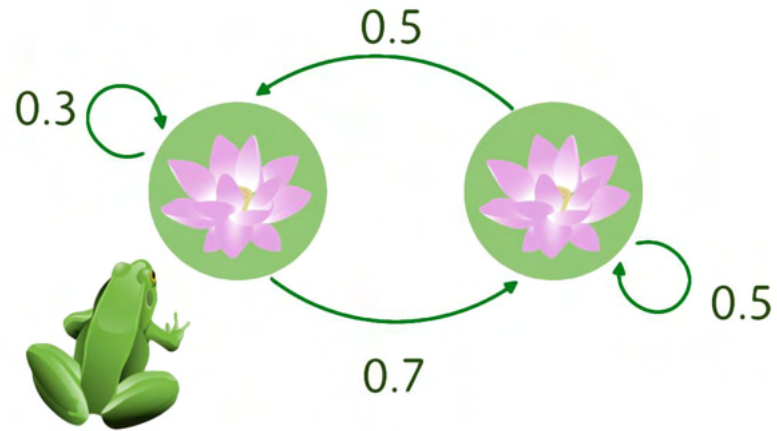
$$p(x^3) = p(x^3 | x^2 = \text{L})p(x^2 = \text{L}) \\ + p(x^3 | x^2 = \text{R})p(x^2 = \text{R})$$

Markov Chains



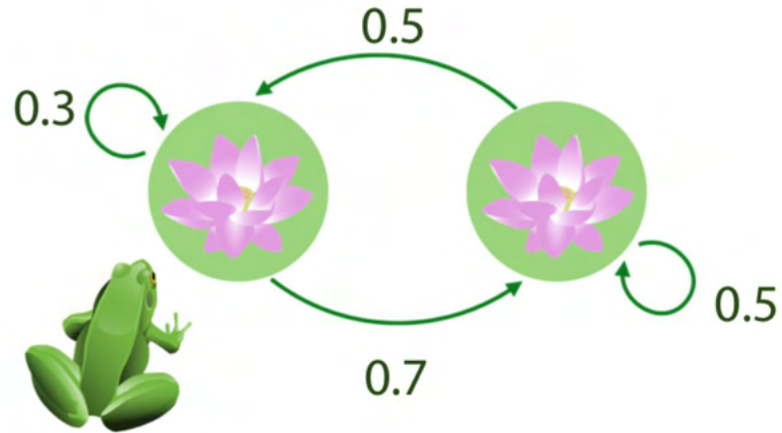
	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3	0.44	0.56

Markov Chains



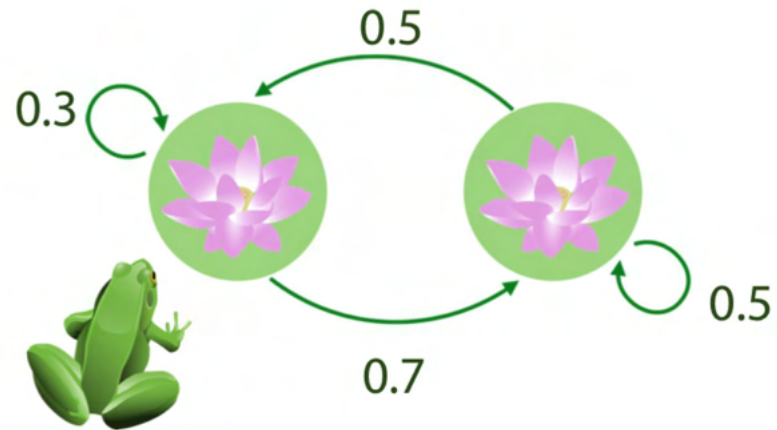
	p(Left)	p(Right)
x^1	1	0
x^2	0.3	0.7
x^3	0.44	0.56
...
	≈ 0.42	≈ 0.58

Markov Chains



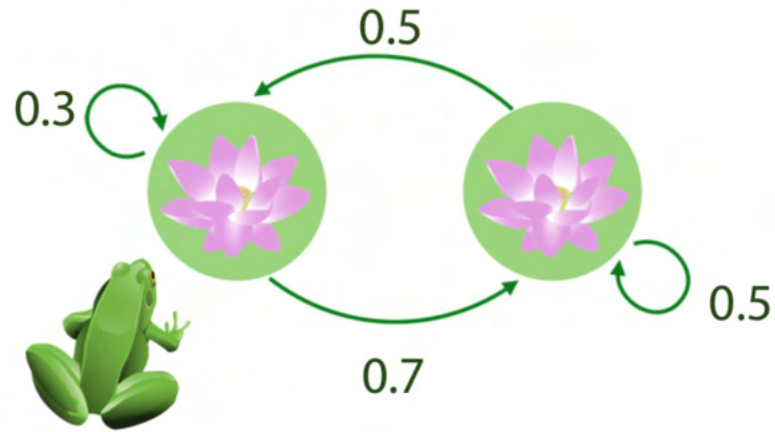
LRRLR...LL

Markov Chains



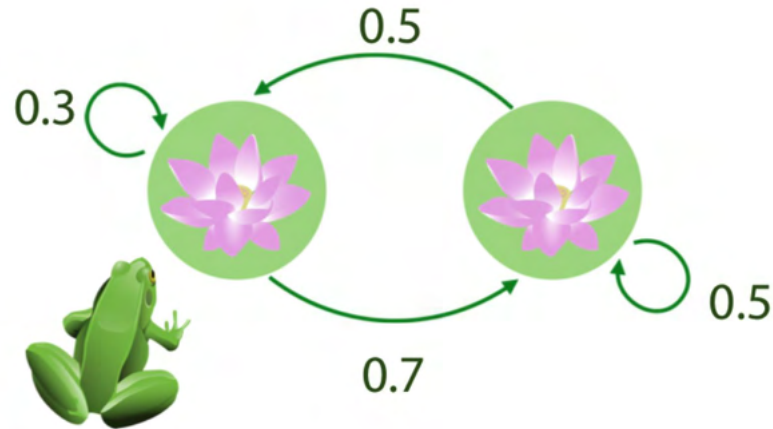
LRRLR... L **L**

Markov Chains



LRRLR... LL
LRRLR... LR

Markov Chains

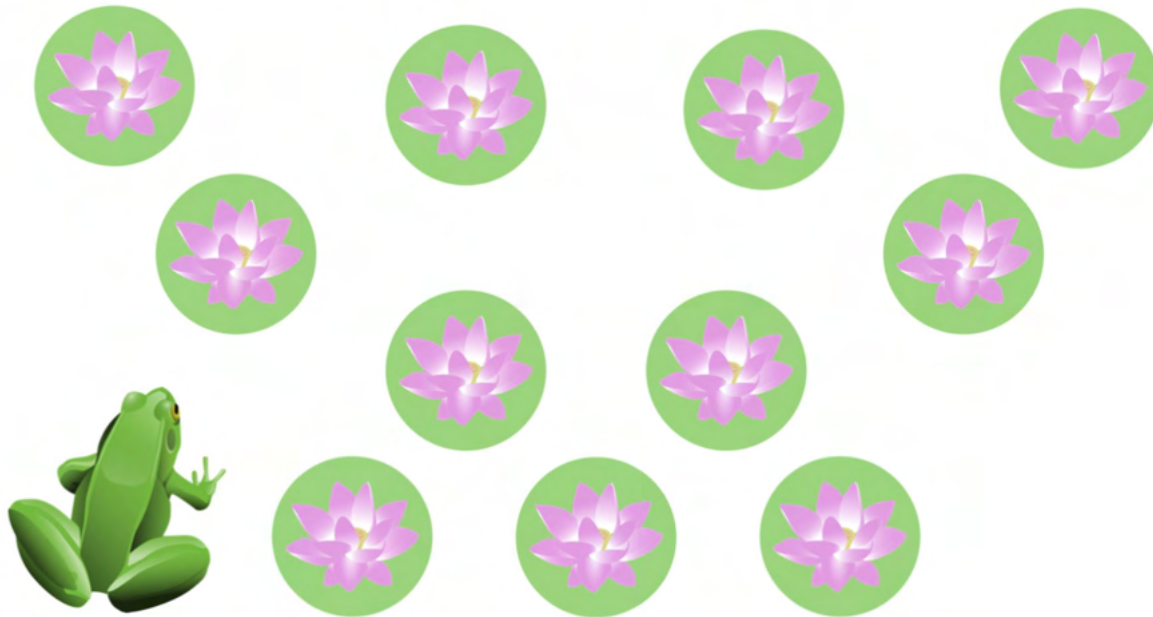


LRRLR... L **L**
LRRLR... L **R**
LRLRR... R **R**
LRRLR... L **R**
LLRLR... R **L**

$$p(L) \approx 0.42$$

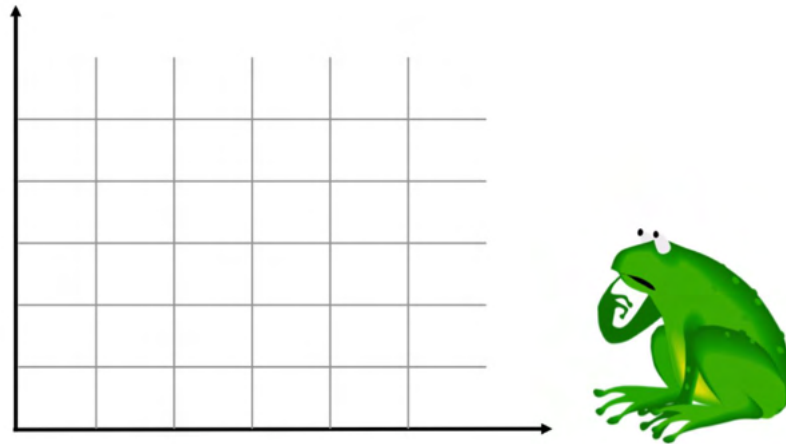
$$p(R) \approx 0.58$$

Markov Chains



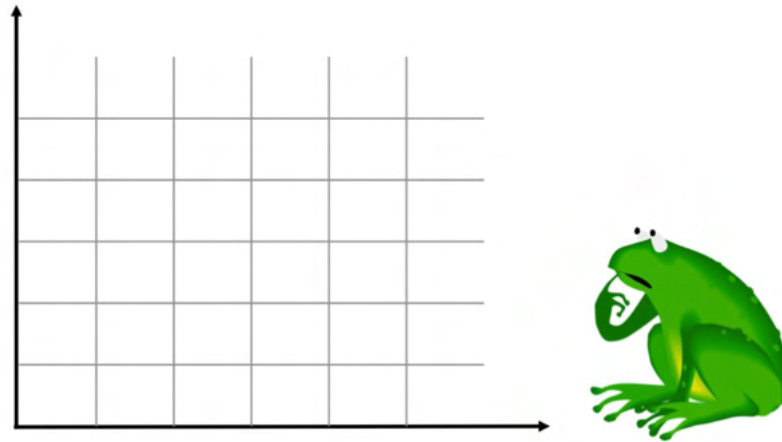
But what if there are 10 lilies? Or a billion?

Markov Chains



But what if there are 10 lilies? Or a billion?
Or maybe frog position is continuous?

Markov Chains



But what if there are 10 lilies? Or a billion?
Or maybe frog position is continuous?
You can still sample!

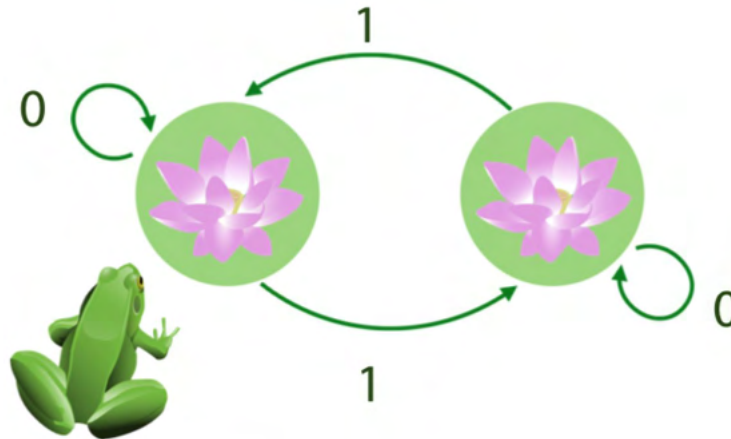
How to use Markov Chains?

- We want to sample from $p(x)$
- Build a Markov chain that converge to $p(x)$
- Start from any x^0
- For $k = 0, 1, \dots$

$$x^{k+1} \sim T(x^k \rightarrow x^{k+1})$$

- Eventually x^k will look like samples from $p(x)$

Do Markov Chains always converge?



	p(Left)	p(Right)
x^1	1	0
x^2	0	1
x^3	1	0
...

Does not converge

Stationary Distribution

Definition:

A distribution π is called stationary if

$$\pi(x') = \sum_x T(x \rightarrow x')\pi(x)$$

Convergence Theorem

Theorem:

If $T(x \rightarrow x') > 0$ for all x, x' then exists unique π :

$$\pi(x') = \sum_x T(x \rightarrow x')\pi(x)$$

And Markov chain converges to π from any starting point

Ch 3. Gibbs Sampling

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

$$x_1^1 \sim p(x_1 \mid x_2 = x_2^0, x_3 = x_3^0)$$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

$$\begin{aligned} x_1^1 &\sim p(x_1 \mid x_2 = x_2^0, x_3 = x_3^0) \\ &= \frac{\hat{p}(x_1, x_2^0, x_3^0)}{Z_1} \end{aligned}$$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

$$x_1^1 \sim p(x_1 \mid x_2 = x_2^0, x_3 = x_3^0)$$

$$x_2^1 \sim p(x_2 \mid x_1 = x_1^1, x_3 = x_3^0)$$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

$$x_1^1 \sim p(x_1 \mid x_2 = x_2^0, x_3 = x_3^0)$$

$$x_2^1 \sim p(x_2 \mid x_1 = x_1^1, x_3 = x_3^0)$$

$$x_3^1 \sim p(x_3 \mid x_1 = x_1^1, x_2 = x_2^1)$$

Gibbs Sampling

$$p(x_1, x_2, x_3) = \frac{\hat{p}(x_1, x_2, x_3)}{Z}$$

Start with (x_1^0, x_2^0, x_3^0) , e. g. $(0, 0, 0)$

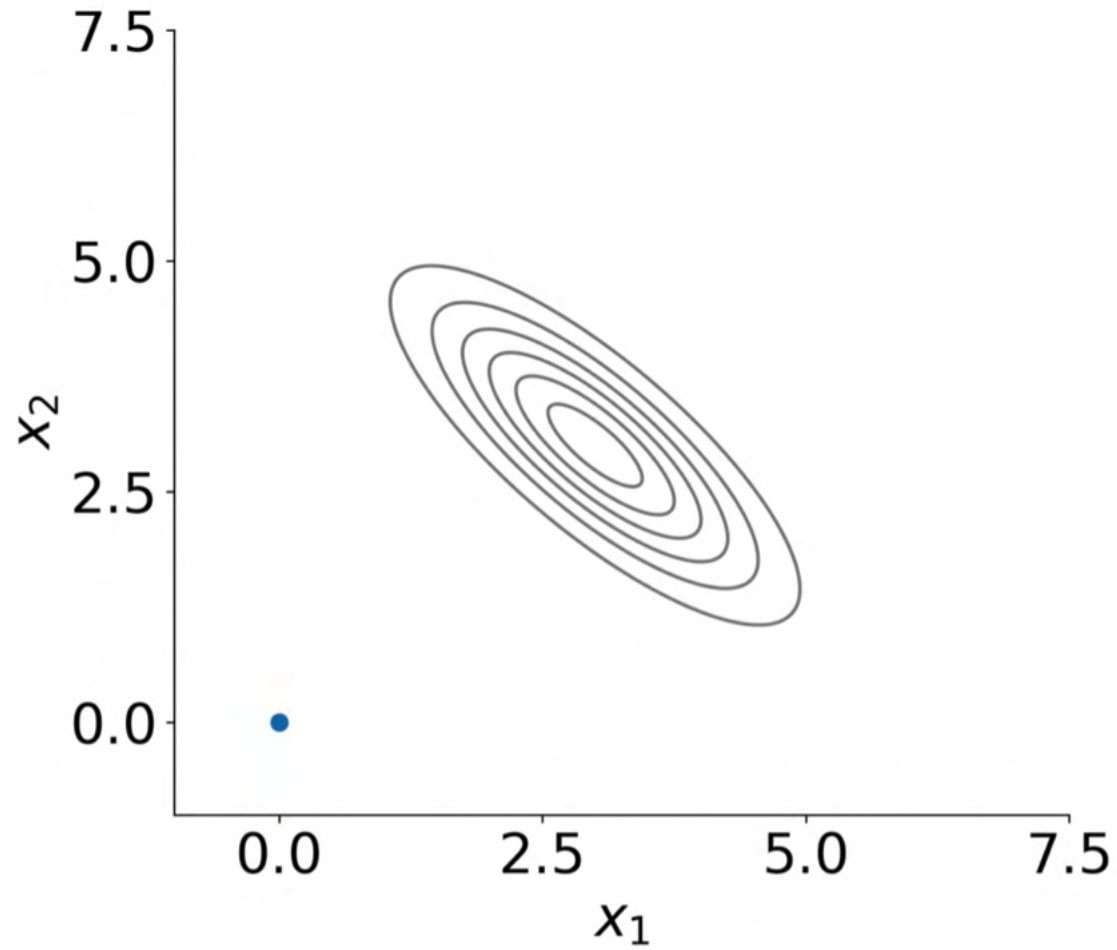
For $k = 0, 1, \dots$

$$x_1^{k+1} \sim p(x_1 \mid x_2 = x_2^k, x_3 = x_3^k)$$

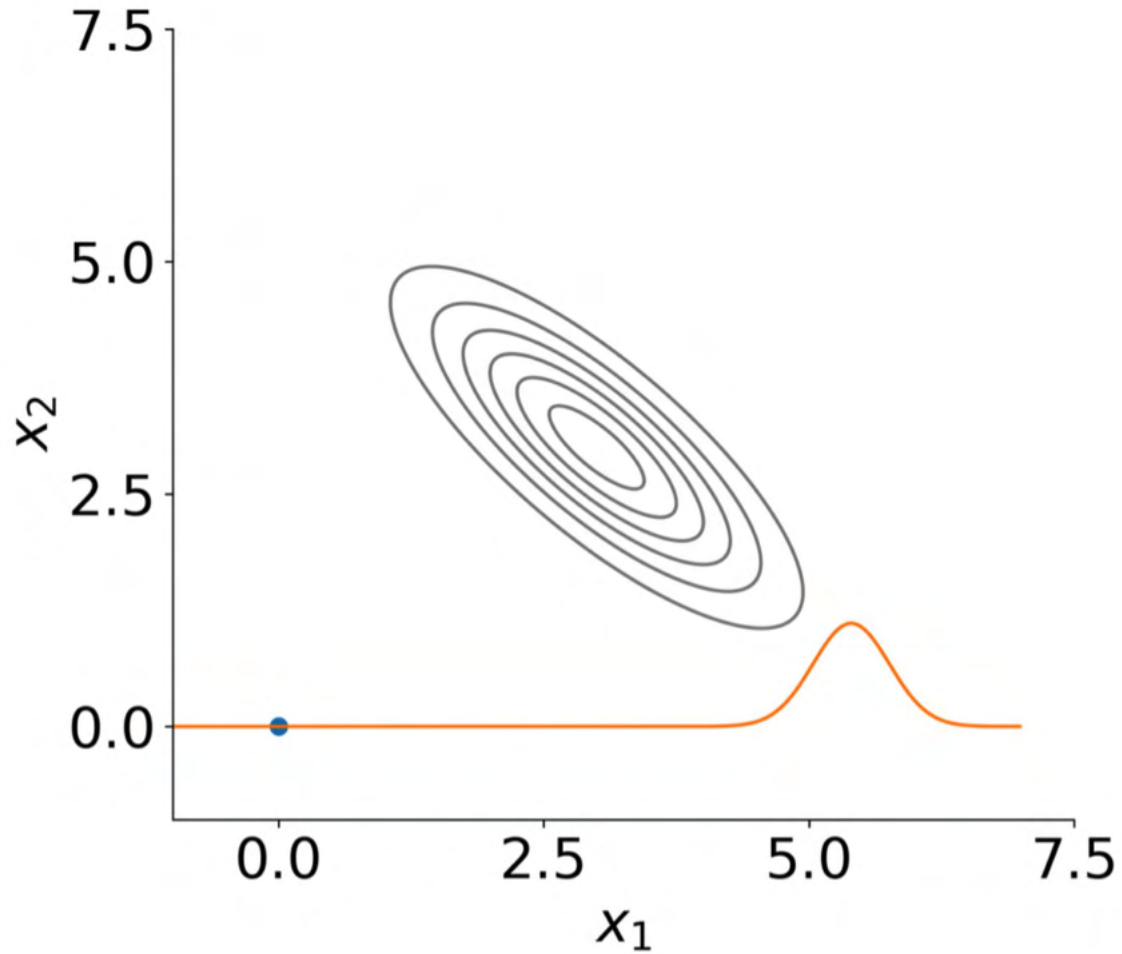
$$x_2^{k+1} \sim p(x_2 \mid x_1 = x_1^{k+1}, x_3 = x_3^k)$$

$$x_3^{k+1} \sim p(x_3 \mid x_1 = x_1^{k+1}, x_2 = x_2^{k+1})$$

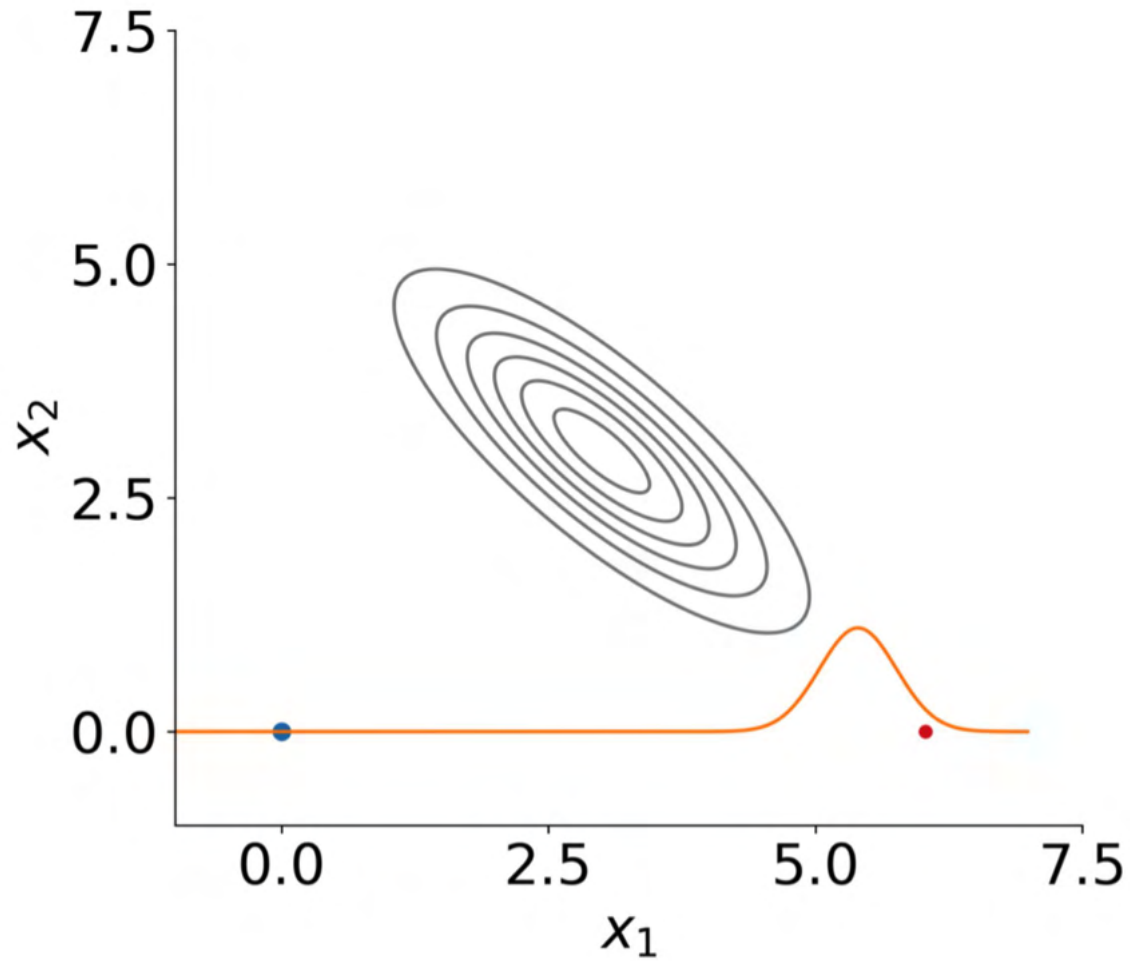
Gibbs Sampling - Demo



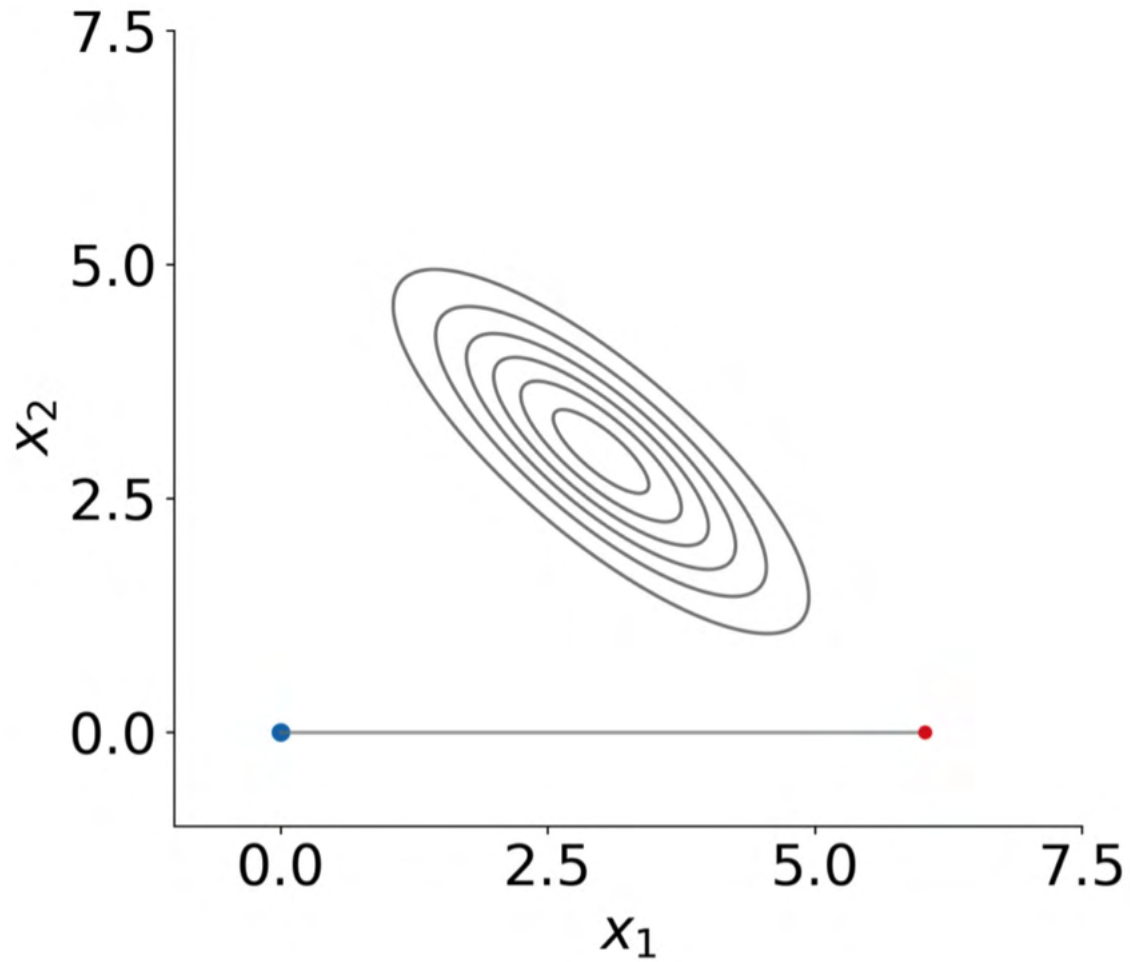
Gibbs Sampling - Demo



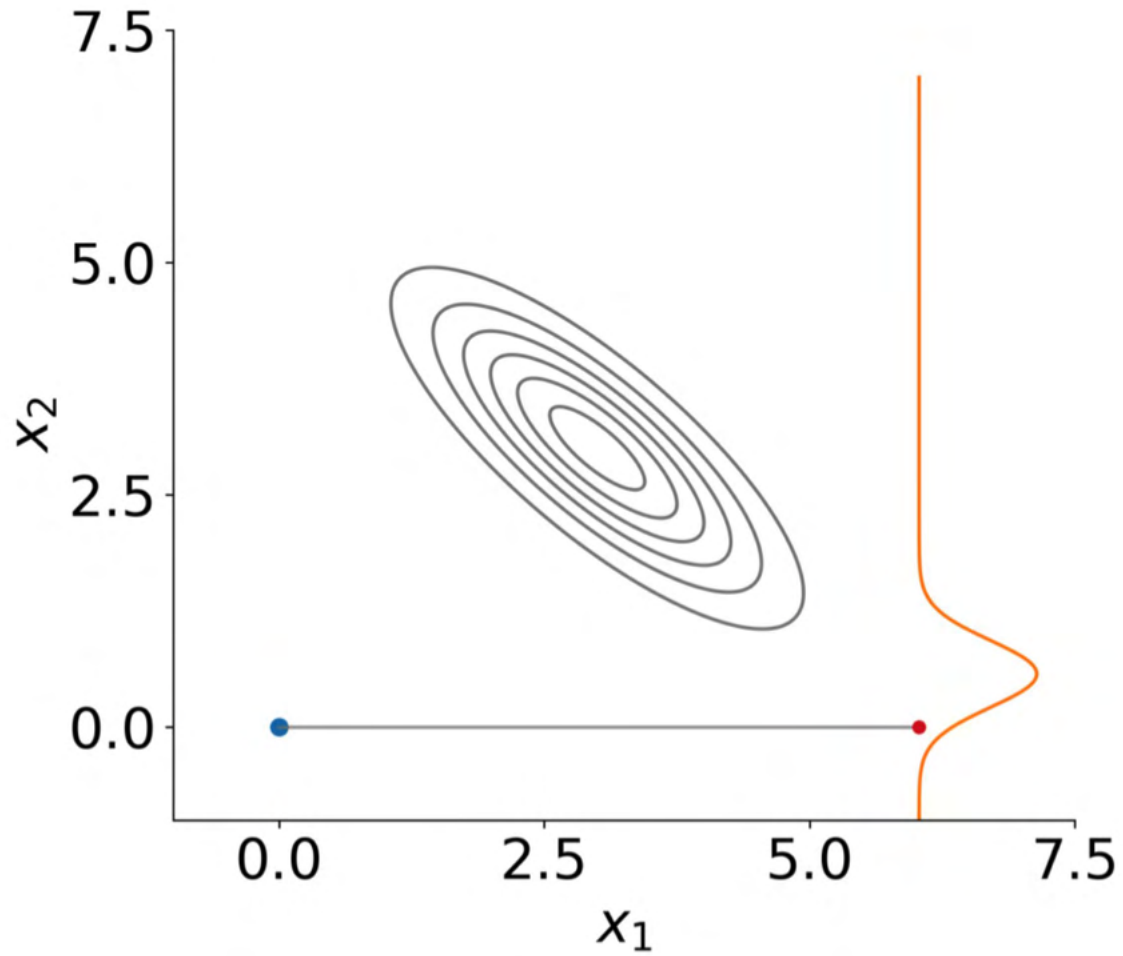
Gibbs Sampling - Demo



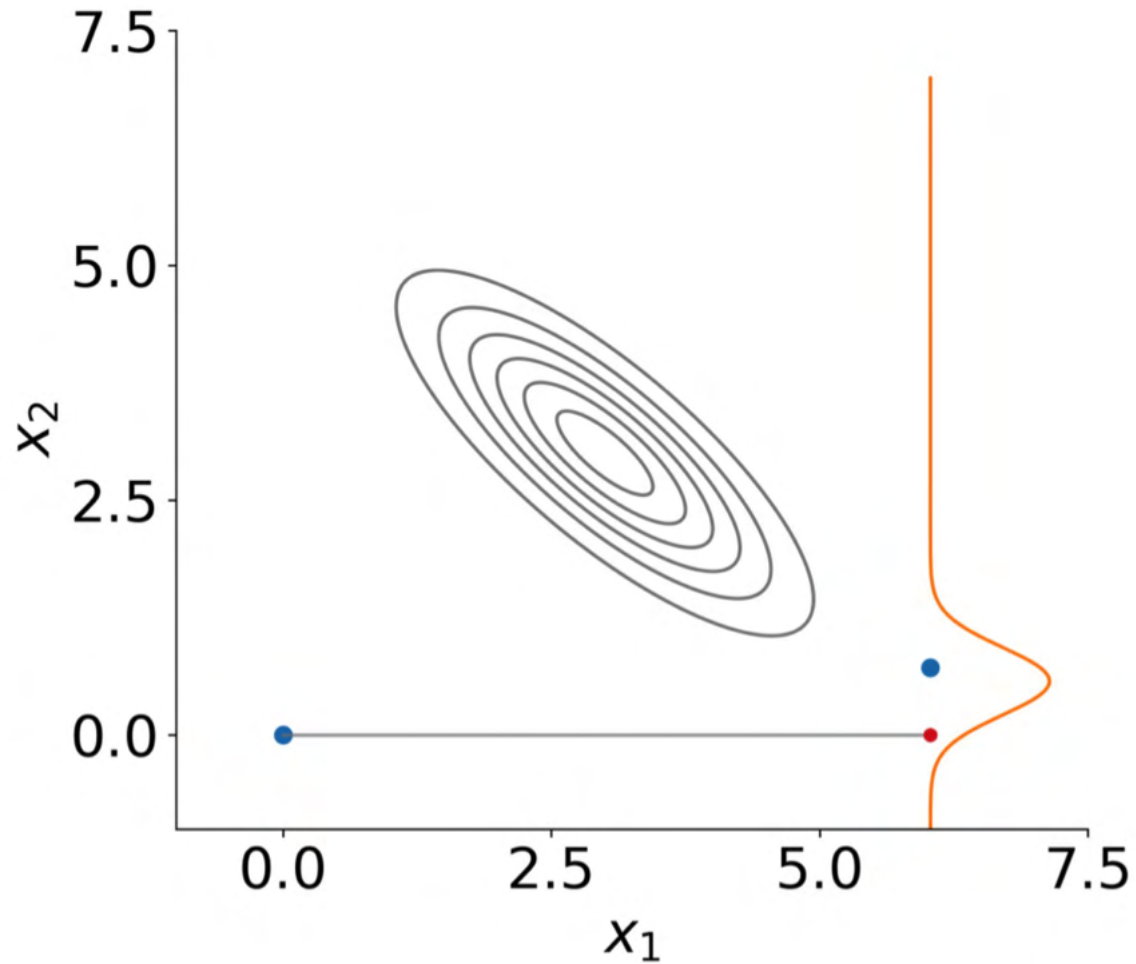
Gibbs Sampling - Demo



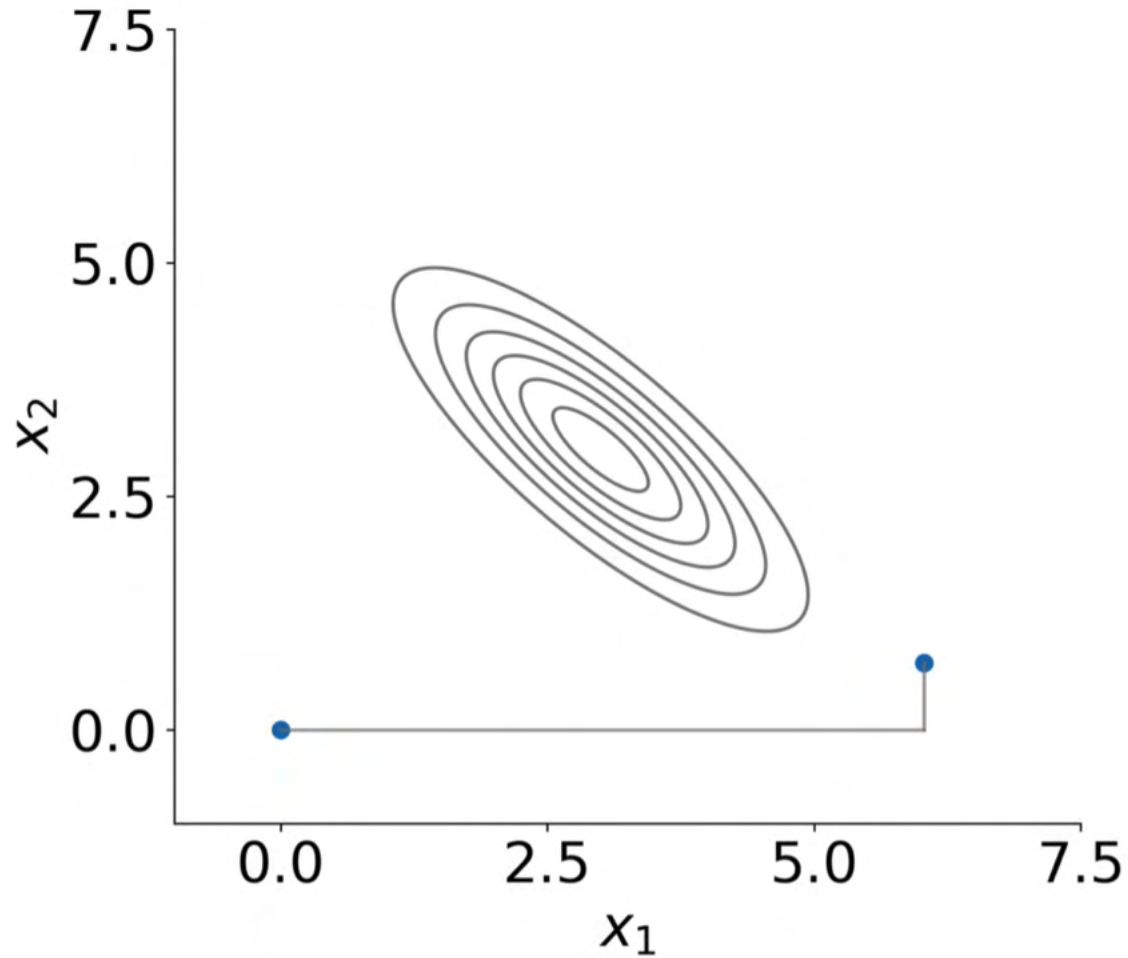
Gibbs Sampling - Demo



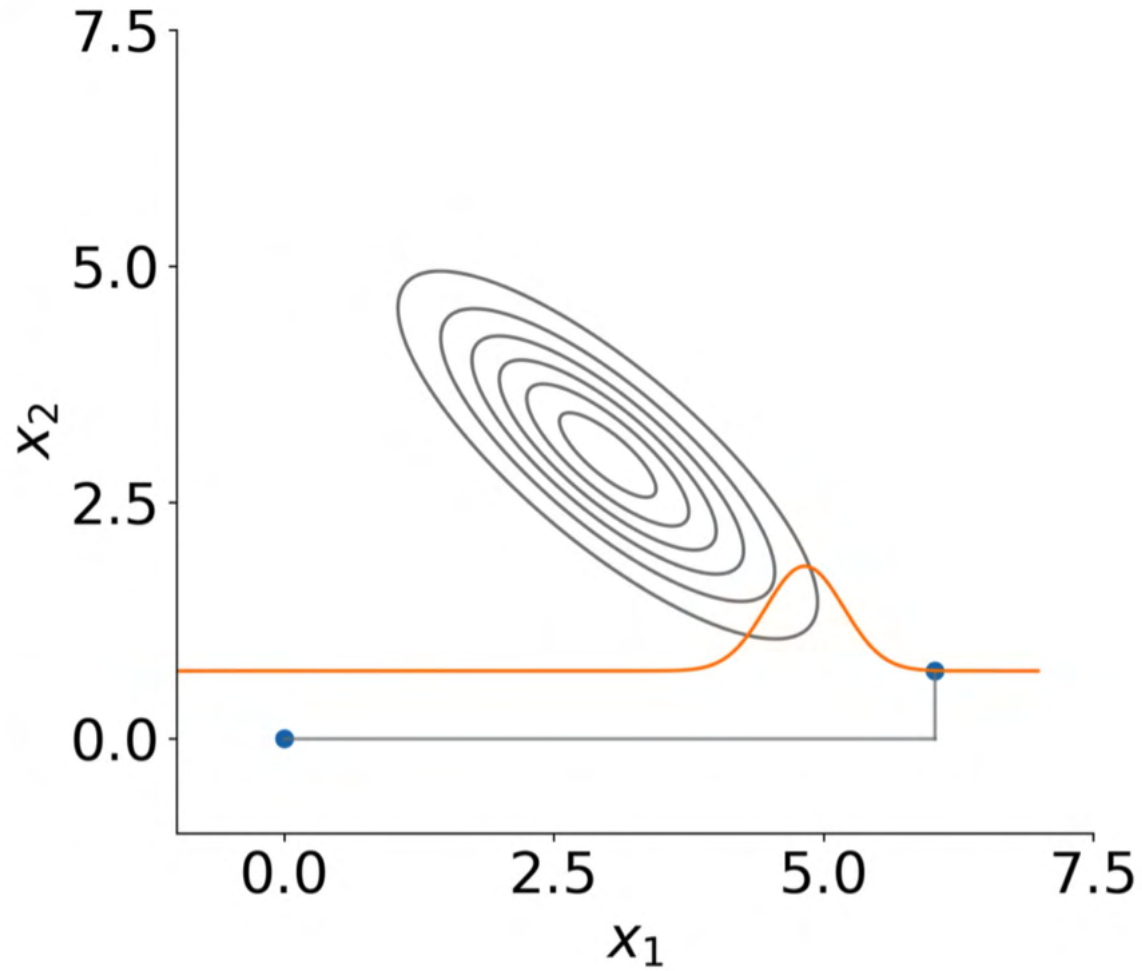
Gibbs Sampling - Demo



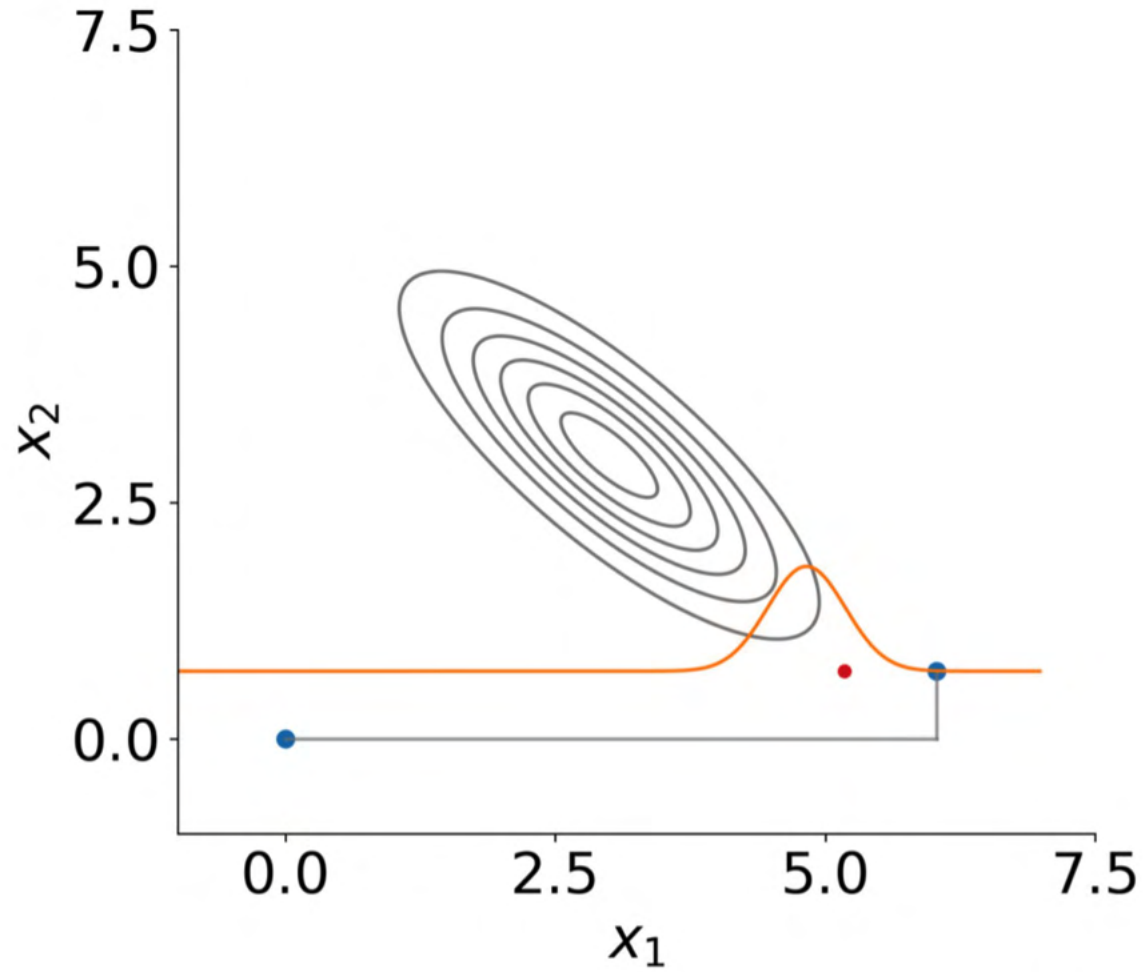
Gibbs Sampling - Demo



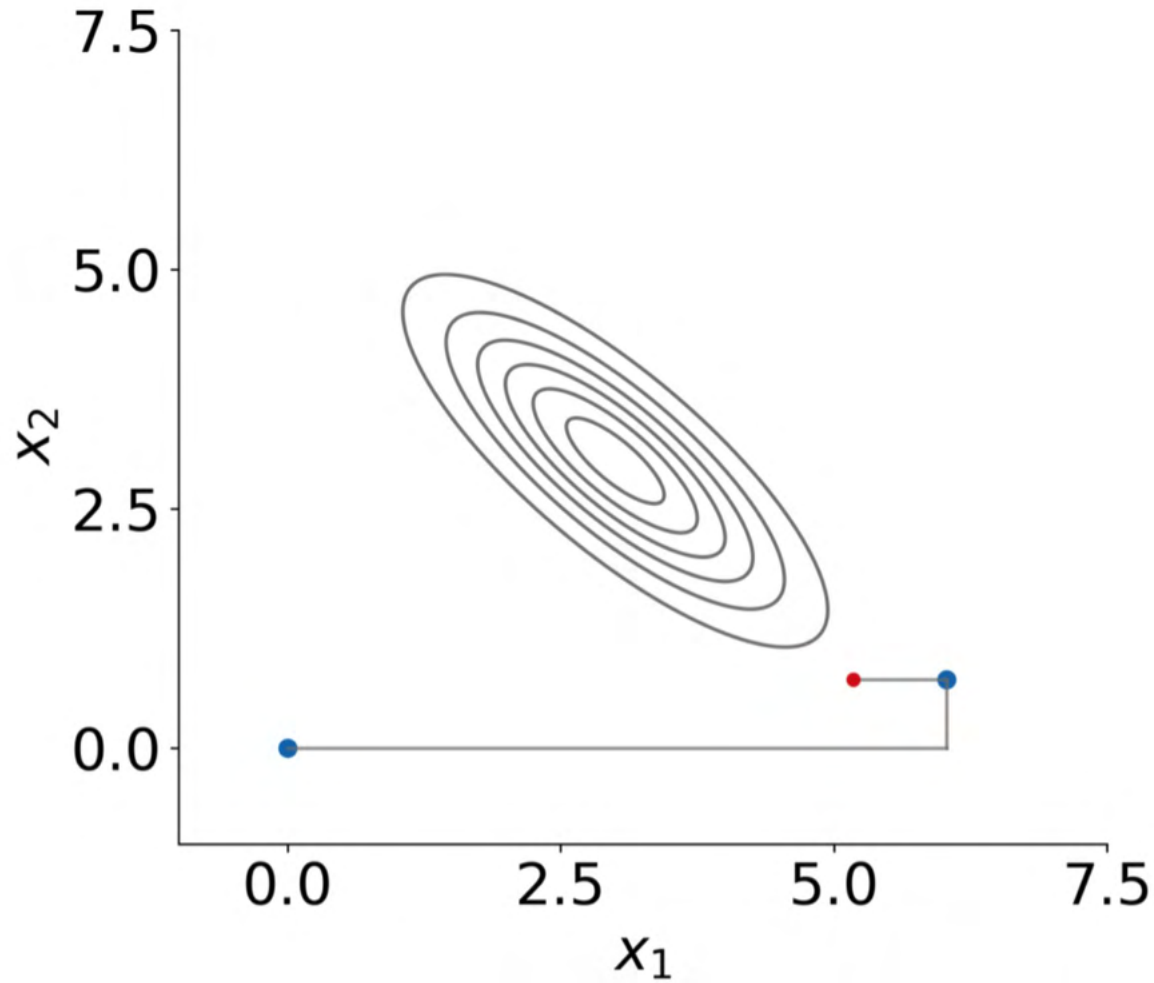
Gibbs Sampling - Demo



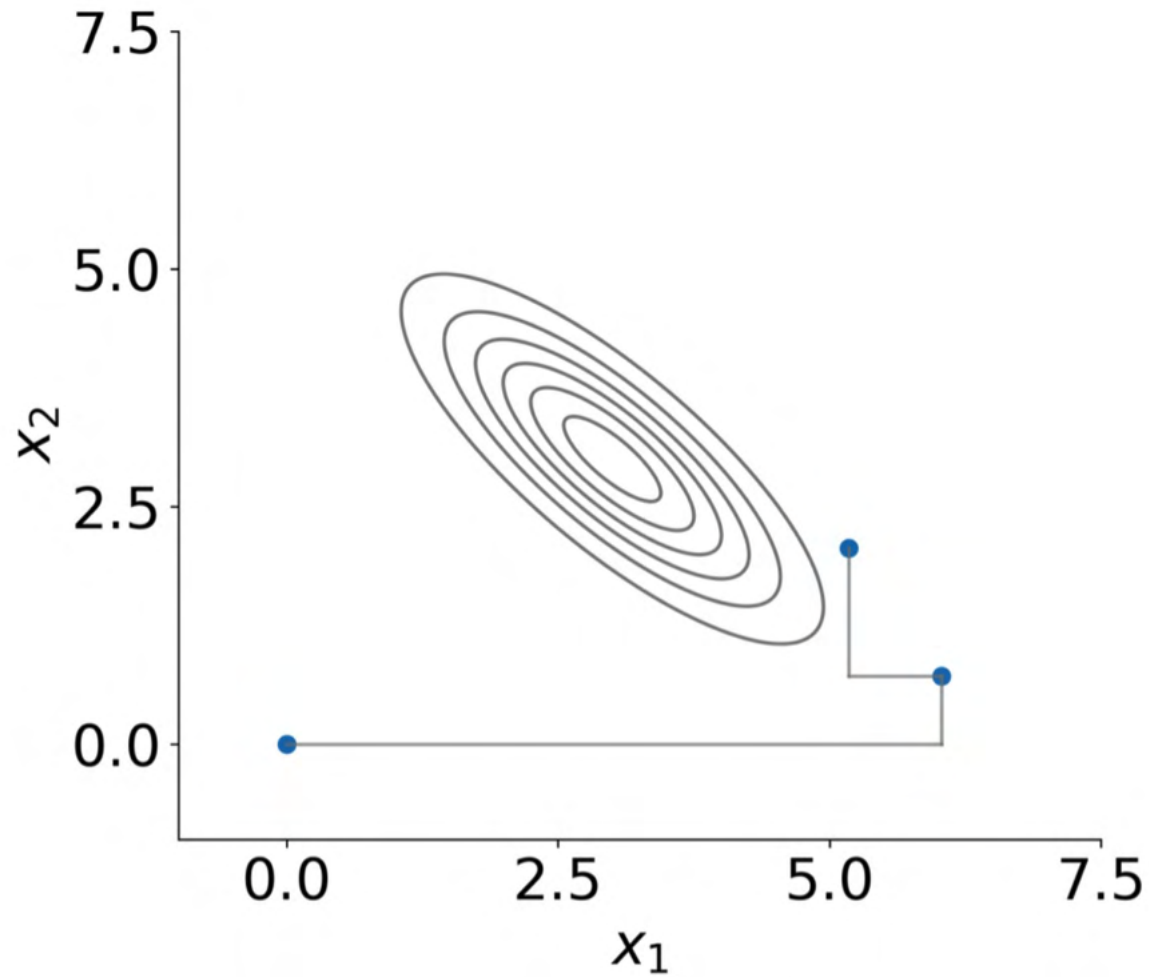
Gibbs Sampling - Demo



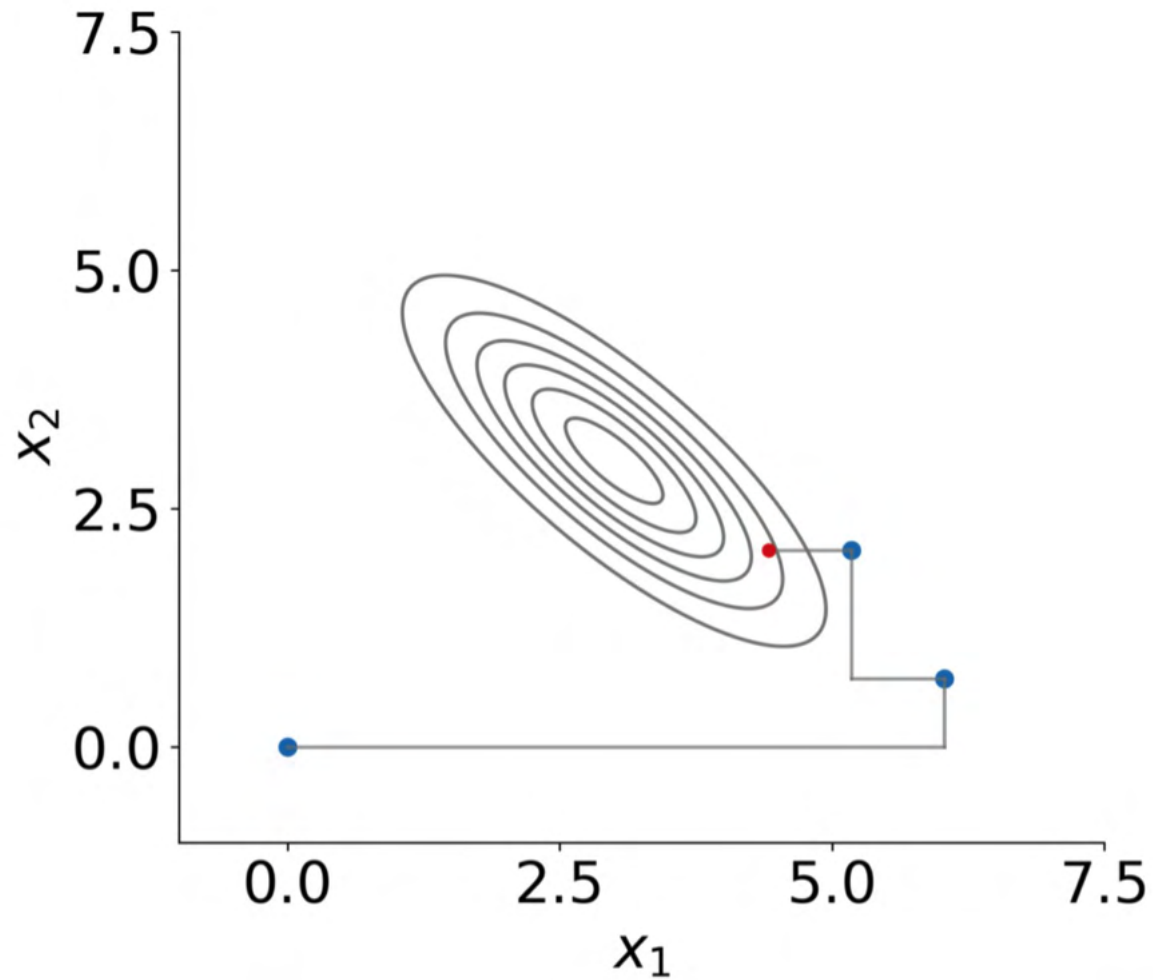
Gibbs Sampling - Demo



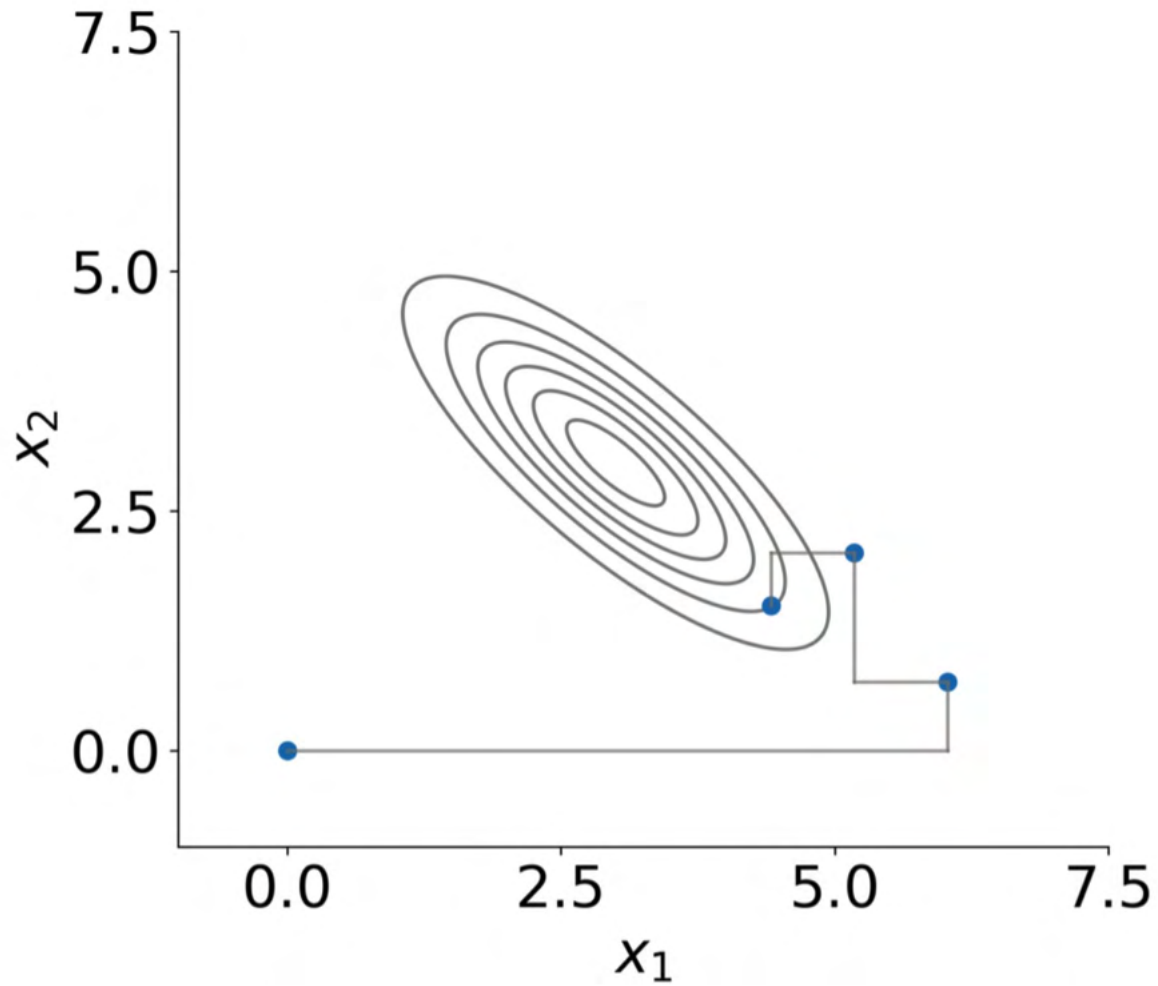
Gibbs Sampling - Demo



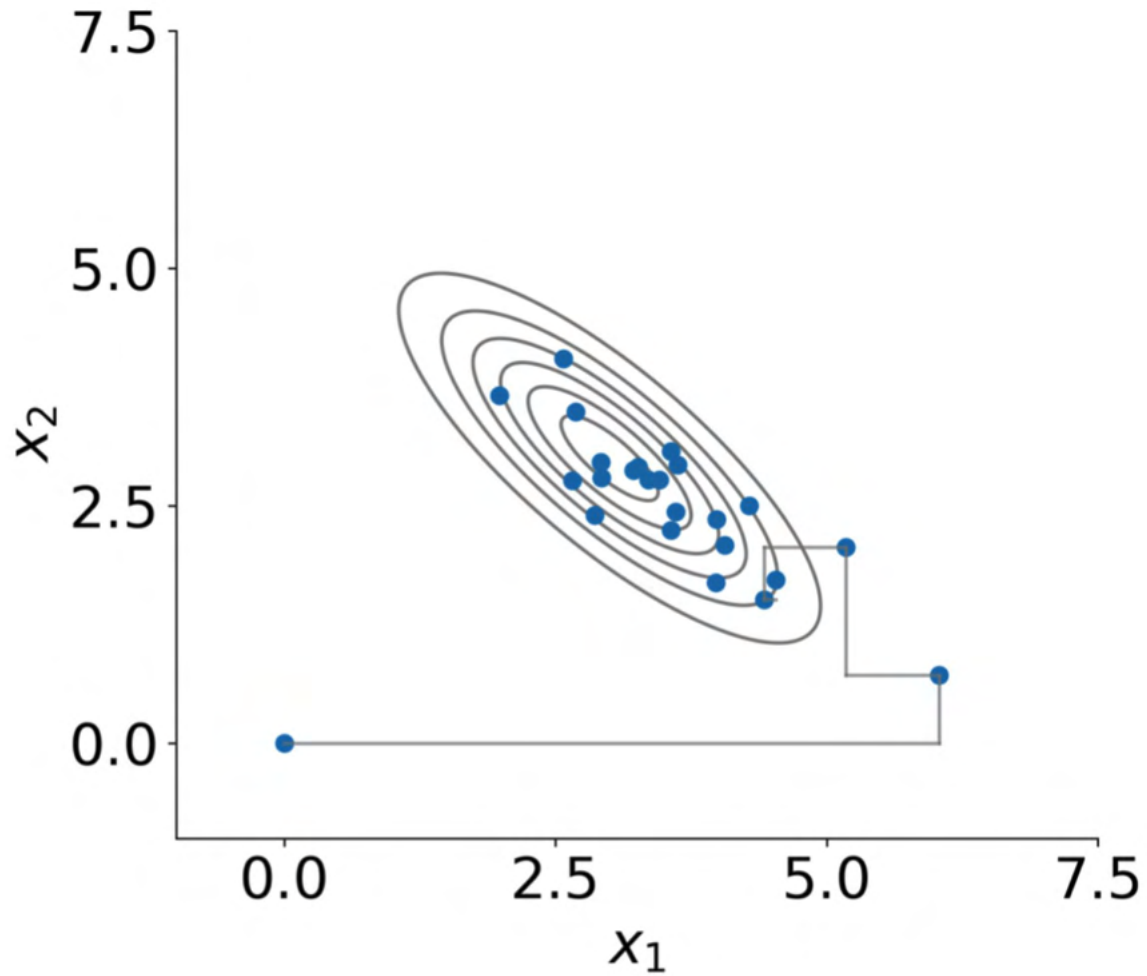
Gibbs Sampling - Demo



Gibbs Sampling - Demo



Gibbs Sampling - Demo



Gibbs Sampling - Summary

Pros:

- Reduce multidimensional sampling to sequence of 1d samplings
- A few lines of code

Cons:

- Highly correlated samples
 - Samples are similar to each others
- Slow Convergence (Mixing)
- Not Parallel

Ch 5. Metropolis-Hastings

Metropolis-Hastings

- Sometimes Gibbs samples are too correlated
- Apply Rejection Sampling to Markov Chains

Metropolis-Hastings

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$

Metropolis-Hastings

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$
- Accept proposal x' with probability $A(x^k \rightarrow x')$
- Otherwise stay at x^k

$$x^{k+1} = x^k$$

Metropolis-Hastings

For $k = 1, 2, \dots$

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$$x^{k+1} = x^k$$

$$T(x \rightarrow x') = Q(x \rightarrow x')A(x \rightarrow x') \quad \text{for all } x \neq x'$$

Metropolis-Hastings

For $k = 1, 2, \dots$

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$$T(x \rightarrow x') = Q(x \rightarrow x')A(x \rightarrow x') \quad \text{for all } x \neq x'$$

$$T(x \rightarrow x) = Q(x \rightarrow x)A(x \rightarrow x)$$

$$+ \sum_{x' \neq x} Q(x \rightarrow x')(1 - A(x \rightarrow x'))$$

Metropolis-Hastings

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$
- Accept proposal x' with probability $A(x^k \rightarrow x')$
- Otherwise stay at x^k

$$x^{k+1} = x^k$$

$$T(x \rightarrow x') = Q(x \rightarrow x')A(x \rightarrow x') \quad \text{for all } x \neq x'$$

$$T(x \rightarrow x) = Q(x \rightarrow x)A(x \rightarrow x)$$

$$+ \sum_{x' \neq x} Q(x \rightarrow x')(1 - A(x \rightarrow x'))$$

How to choose A: $\pi(x') = \sum_x \pi(x)T(x \rightarrow x')$

Detailed Balance

- Sufficient Condition for Stationary Distribution

If $\pi(x)T(x \rightarrow x') = \pi(x')T(x' \rightarrow x)$

Then $\pi(x') = \sum_x \pi(x)T(x \rightarrow x')$

Detailed Balance

- Sufficient Condition for Stationary Distribution

If $\pi(x)T(x \rightarrow x') = \pi(x')T(x' \rightarrow x)$

Then $\pi(x') = \sum_x \pi(x)T(x \rightarrow x')$

Proof
$$\begin{aligned} \sum_x \pi(x)T(x \rightarrow x') &= \sum_x \pi(x')T(x' \rightarrow x) \\ &= \pi(x') \sum_x T(x' \rightarrow x) \\ &= \pi(x') \end{aligned}$$

Choosing a Critic (Accepting Prob.)

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$
- Accept proposal x' with probability $A(x^k \rightarrow x')$
- Otherwise stay at x^k

$$x^{k+1} = x^k$$

$$T(x \rightarrow x') = Q(x \rightarrow x')A(x \rightarrow x') \quad \text{for all } x \neq x'$$

$$T(x' \rightarrow x') = Q(x' \rightarrow x')$$

How to choose A:

$$\pi(x') = \sum_x \pi(x)T(x \rightarrow x')$$

Choosing a Critic (Accepting Prob.)

For $k = 1, 2, \dots$

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$$\pi(x)T(x \rightarrow x') = \pi(x')T(x' \rightarrow x)$$

Metropolis Hastings

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$
- Accept proposal x' with probability $A(x^k \rightarrow x')$
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$$x^{k+1} = x^k$$

$$A(x \rightarrow x') = \min \left(1, \frac{\pi(x')Q(x' \rightarrow x)}{\pi(x)Q(x \rightarrow x')} \right)$$

Metropolis Hastings

For $k = 1, 2, \dots$

- Sample x' from a **wrong** $Q(x^k \rightarrow x')$
- Accept proposal x' with probability $A(x^k \rightarrow x')$
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$$x^{k+1} = x^k$$

$$A(x \rightarrow x') = \min \left(1, \frac{\hat{\pi}(x')Q(x' \rightarrow x)}{\hat{\pi}(x)Q(x \rightarrow x')} \right)$$

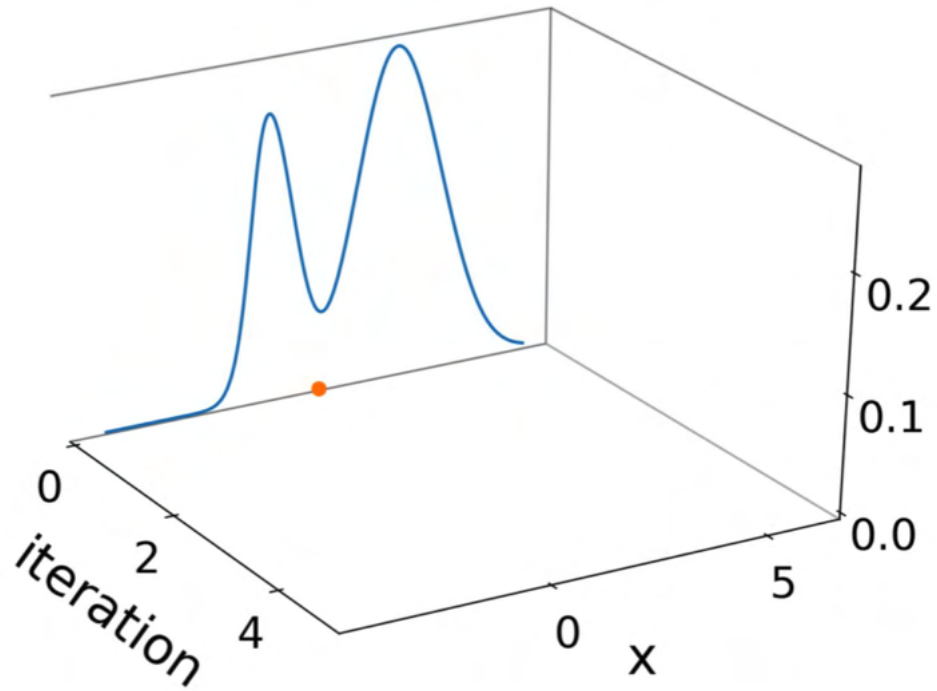
Choice of Q (Proposal Distribution)

$$Q(x \rightarrow x') > 0$$

Opposing forces:

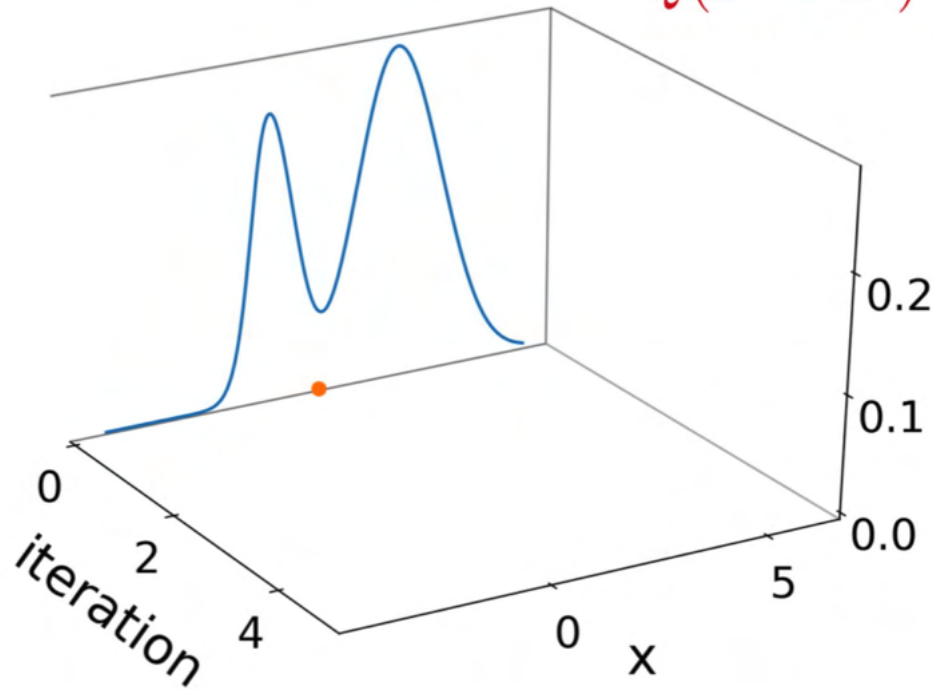
- Q should spread out, to improve mixing and reduce correlation
- But then acceptance probability is often low

Metropolis Hastings - Demo



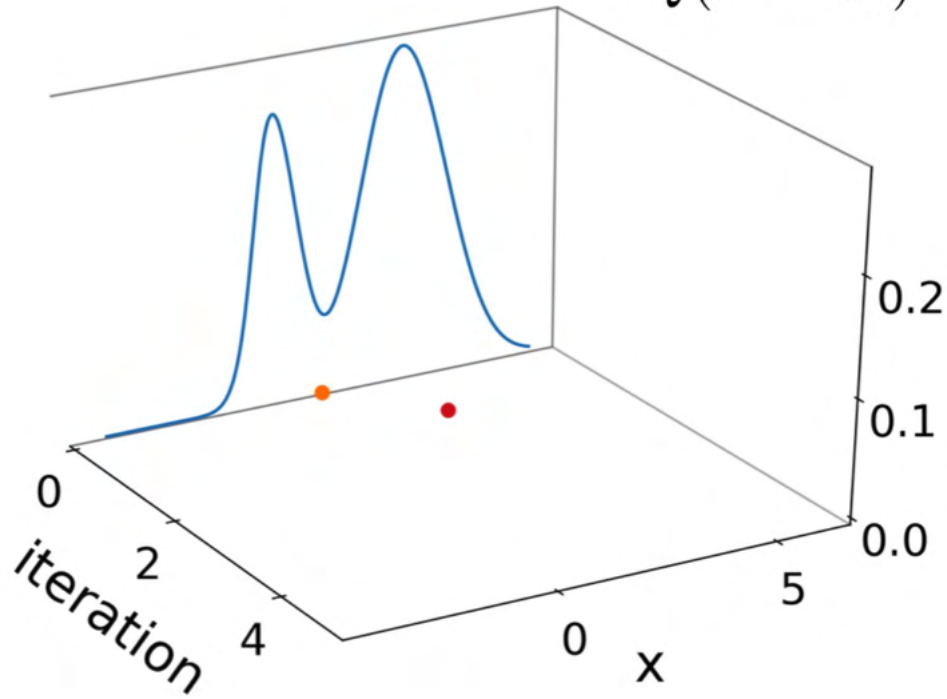
Metropolis Hastings - Demo

$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$

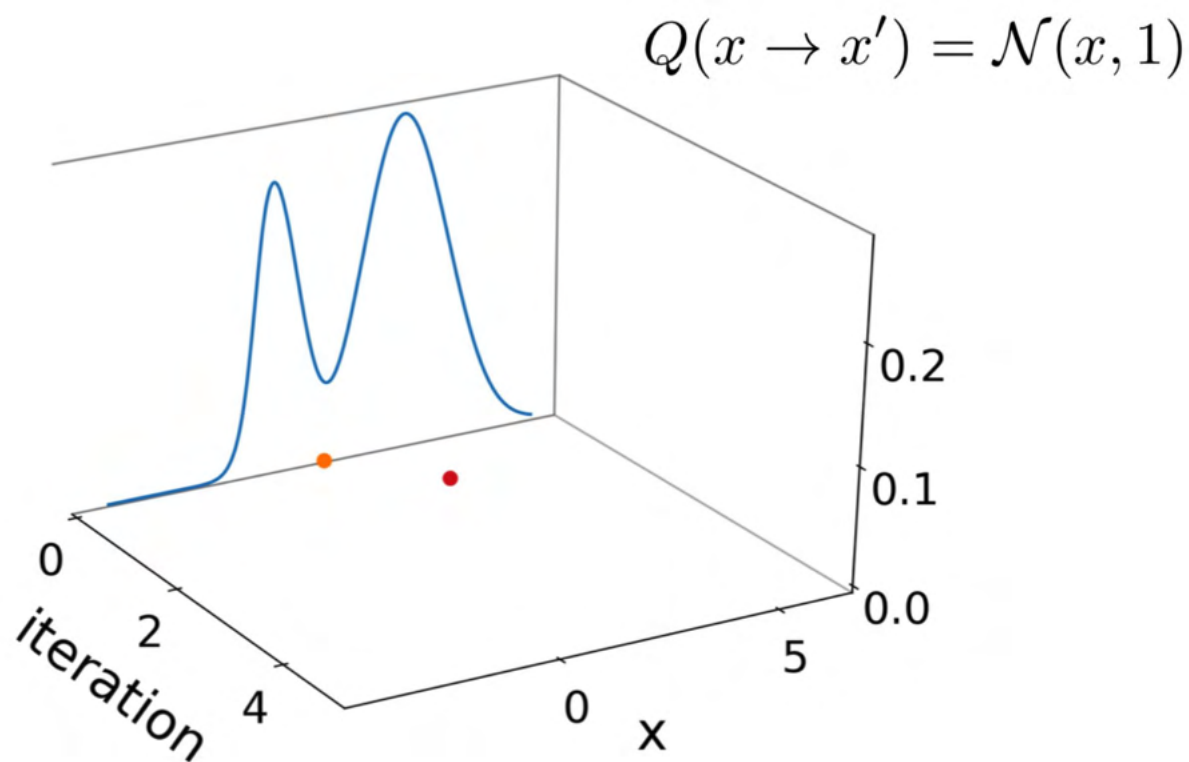


Metropolis Hastings - Demo

$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$

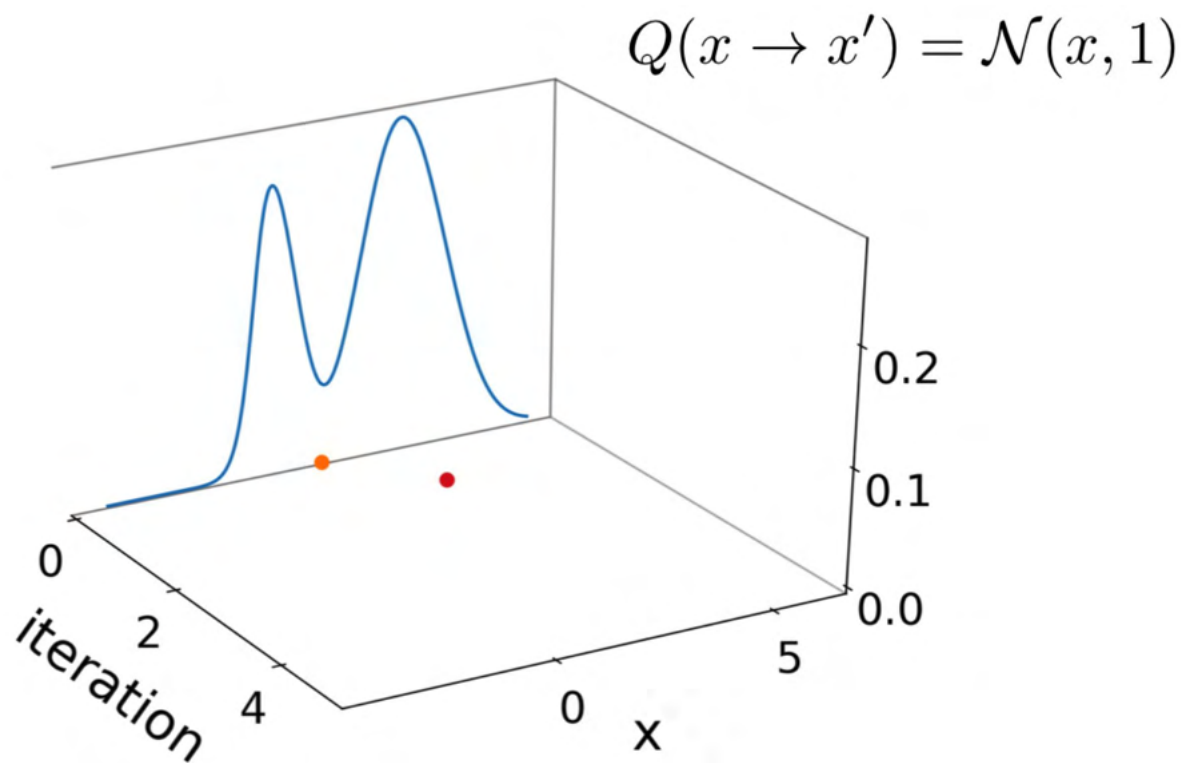


Metropolis Hastings - Demo



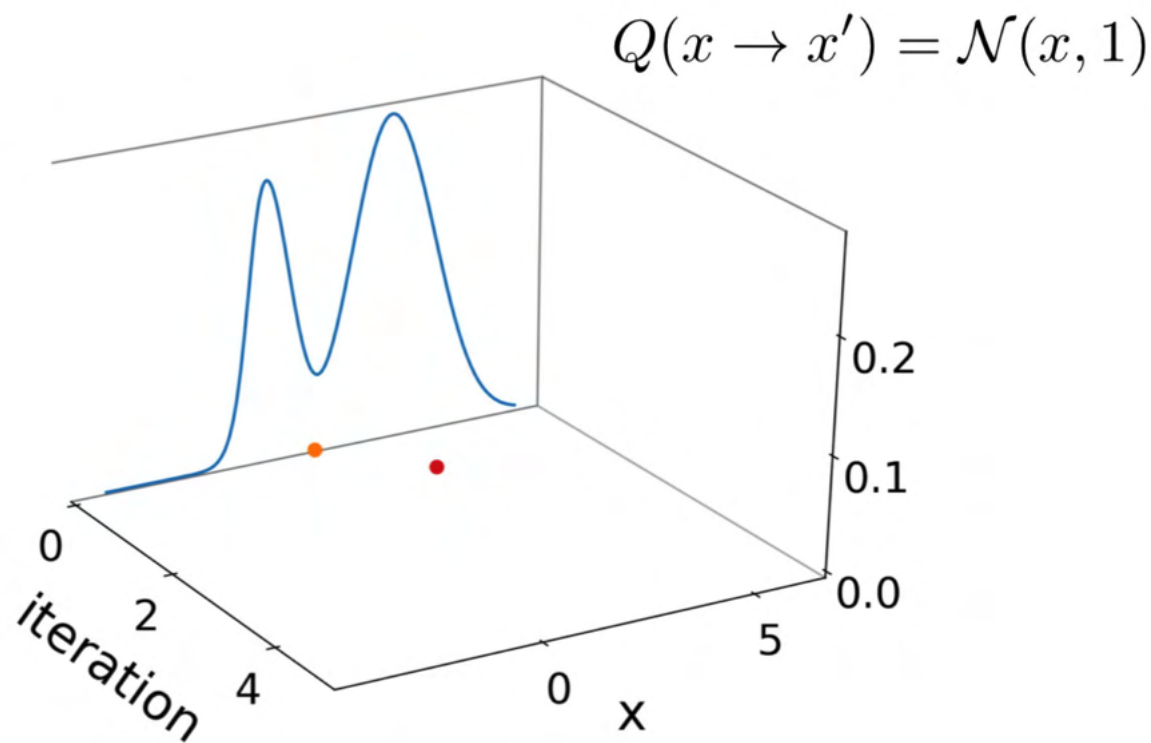
$$A(x \rightarrow x') = \min \left(1, \frac{\pi(x')Q(x' \rightarrow x)}{\pi(x)Q(x \rightarrow x')} \right)$$

Metropolis Hastings - Demo



$$A(x \rightarrow x') = \min \left(1, \frac{\pi(x')Q(x' \rightarrow x)}{\pi(x)Q(x \rightarrow x')} \right) = \min \left(1, \frac{\pi(x')}{\pi(x)} \right)$$

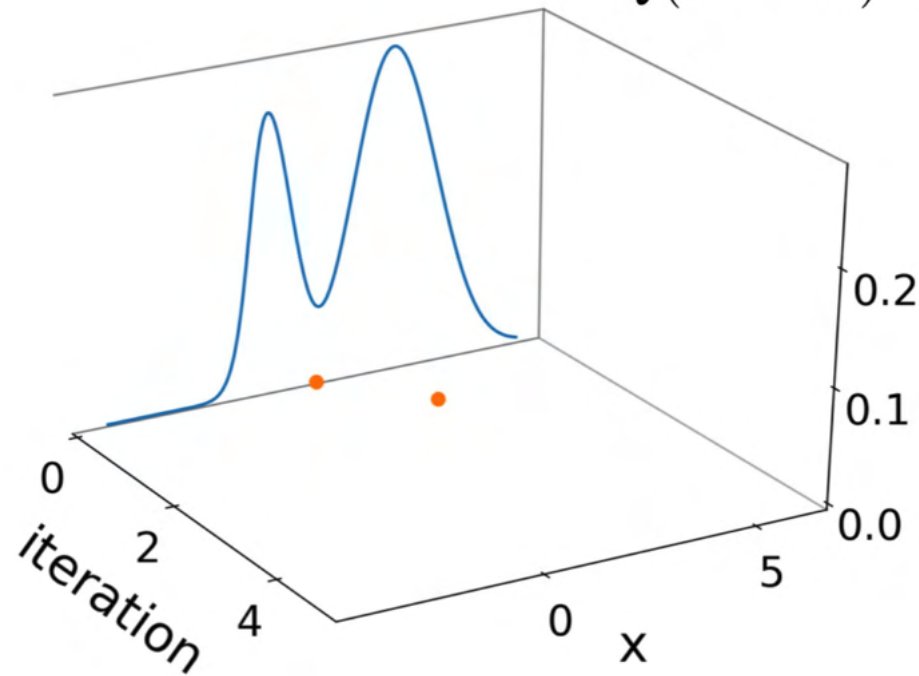
Metropolis Hastings - Demo



$$A(x \rightarrow x') = \min \left(1, \frac{0.27}{0.07} \right) = \min(1, 3.87)$$

Metropolis Hastings - Demo

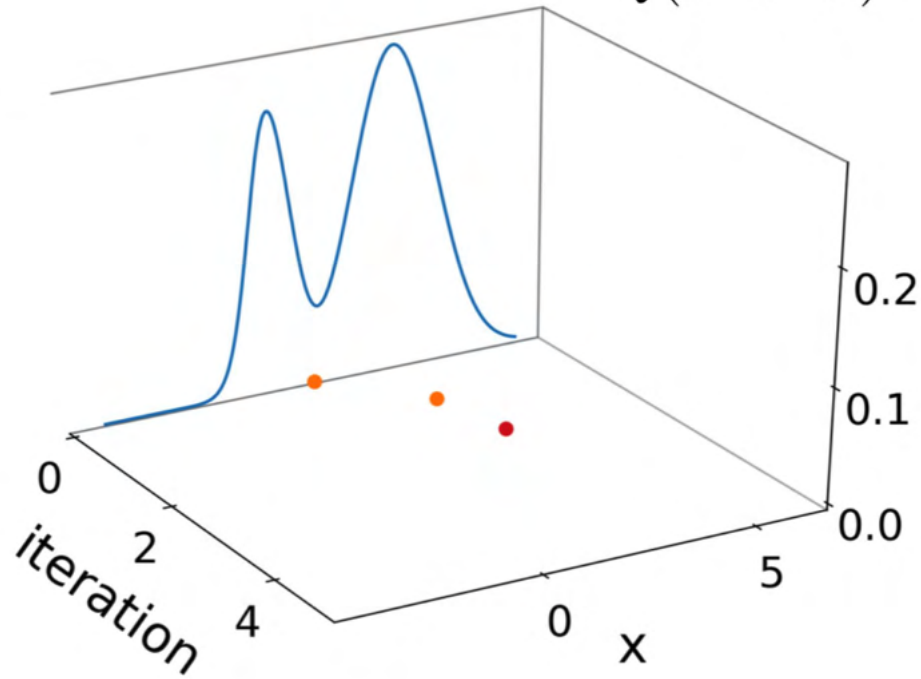
$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



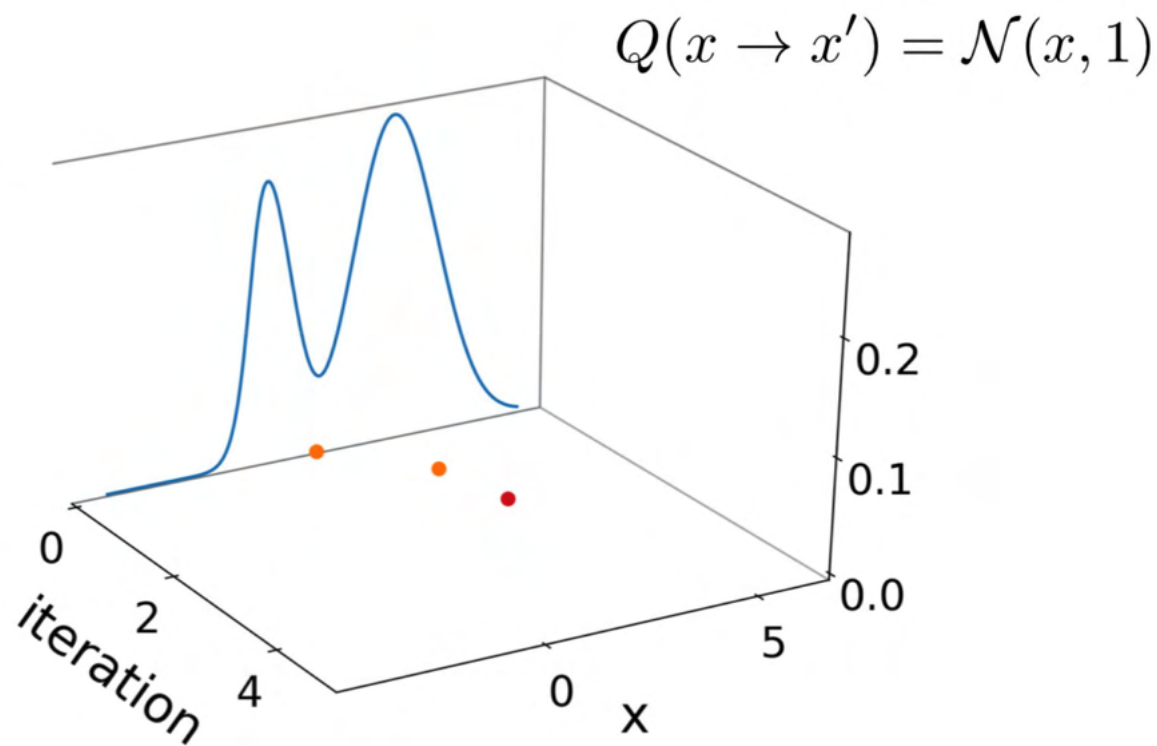
$$A(x \rightarrow x') = \min \left(1, \frac{0.27}{0.07} \right) = \min(1, 3.87)$$

Metropolis Hastings - Demo

$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



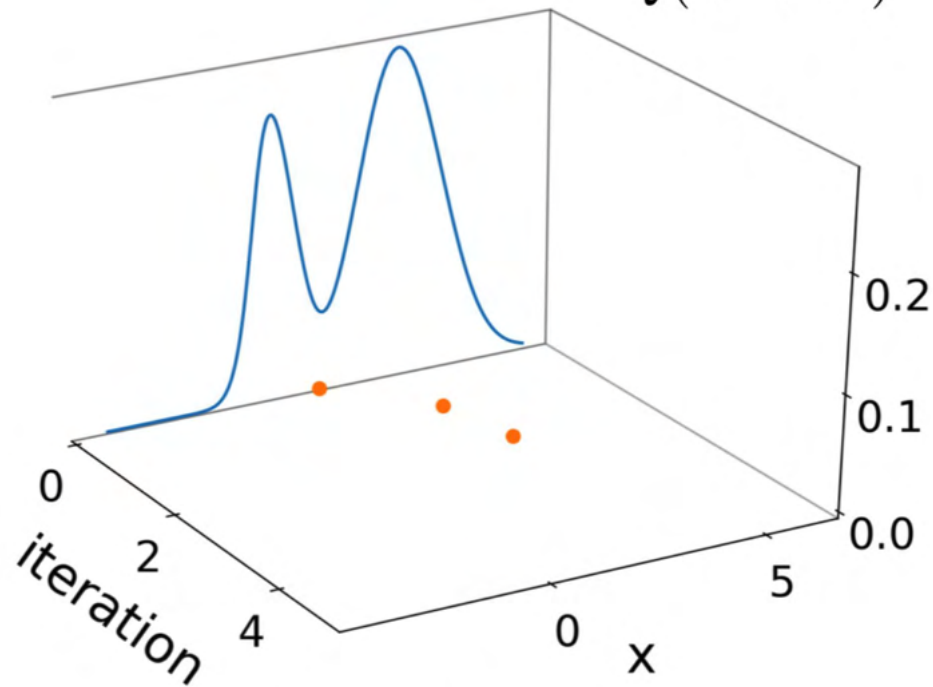
Metropolis Hastings - Demo



$$A(x \rightarrow x') = \min \left(1, \frac{0.28}{0.27} \right) = \min(1, 1.01)$$

Metropolis Hastings - Demo

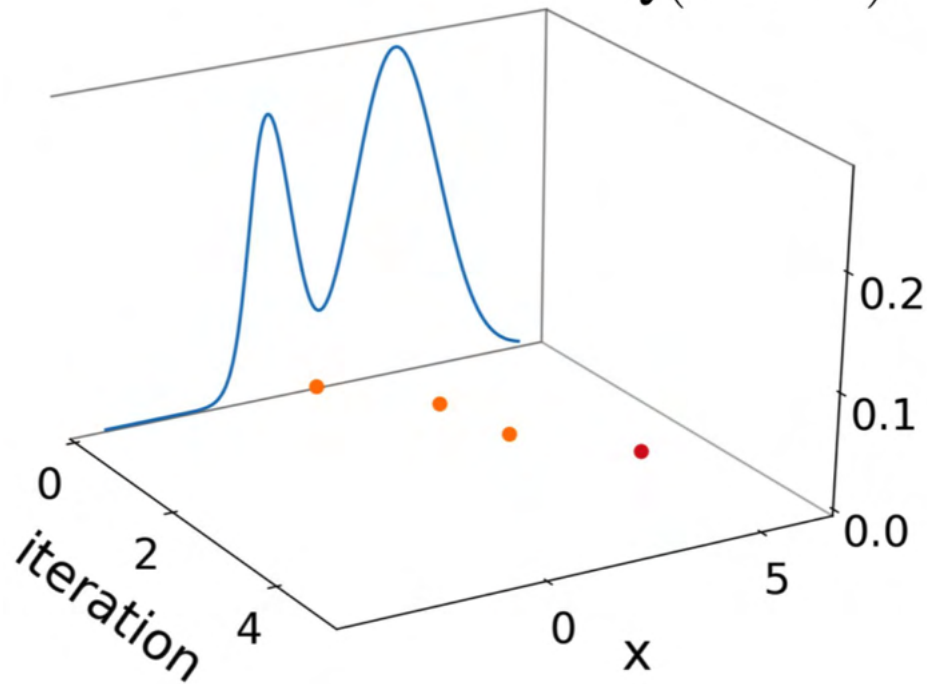
$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



$$A(x \rightarrow x') = \min \left(1, \frac{0.28}{0.27} \right) = \min(1, 1.01)$$

Metropolis Hastings - Demo

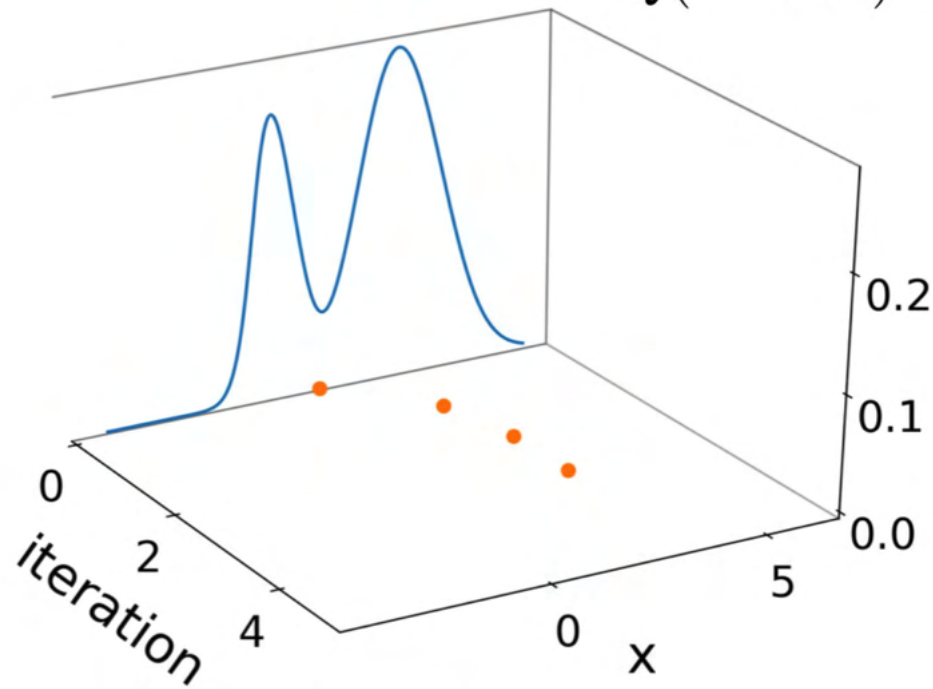
$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



$$A(x \rightarrow x') = \min \left(1, \frac{0.04}{0.28} \right) = \min(1, 0.13)$$

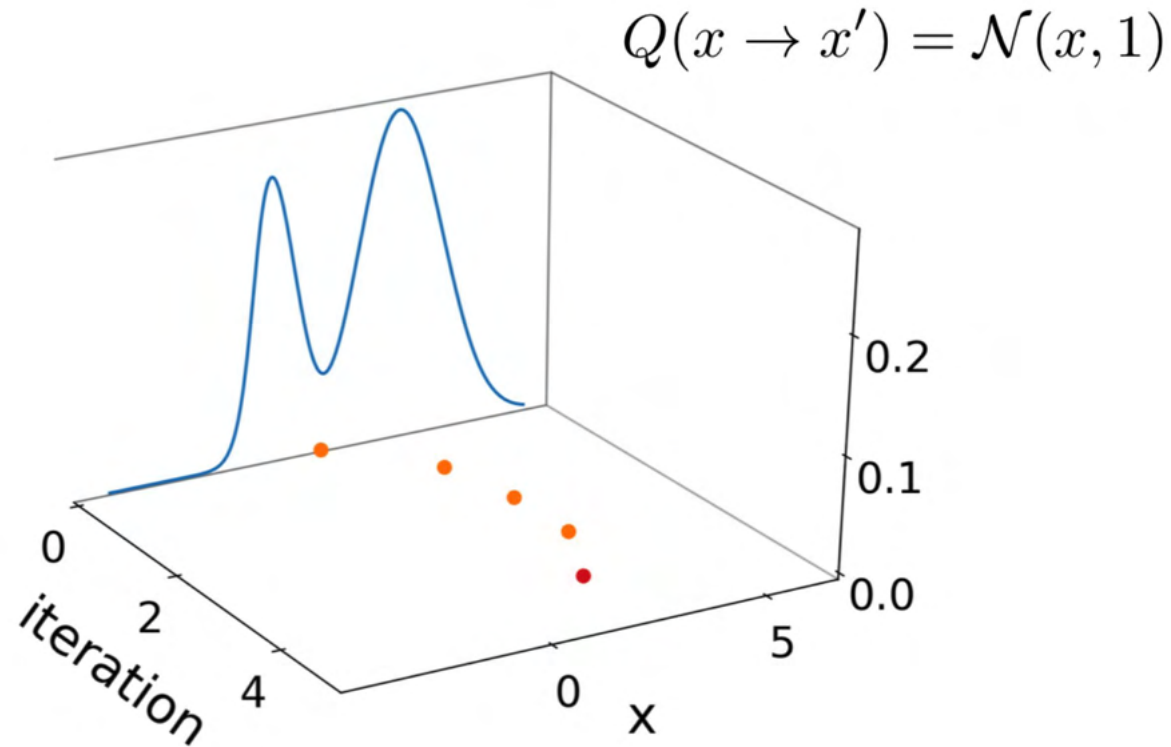
Metropolis Hastings - Demo

$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



$$A(x \rightarrow x') = \min \left(1, \frac{0.04}{0.28} \right) = \min(1, 0.13)$$

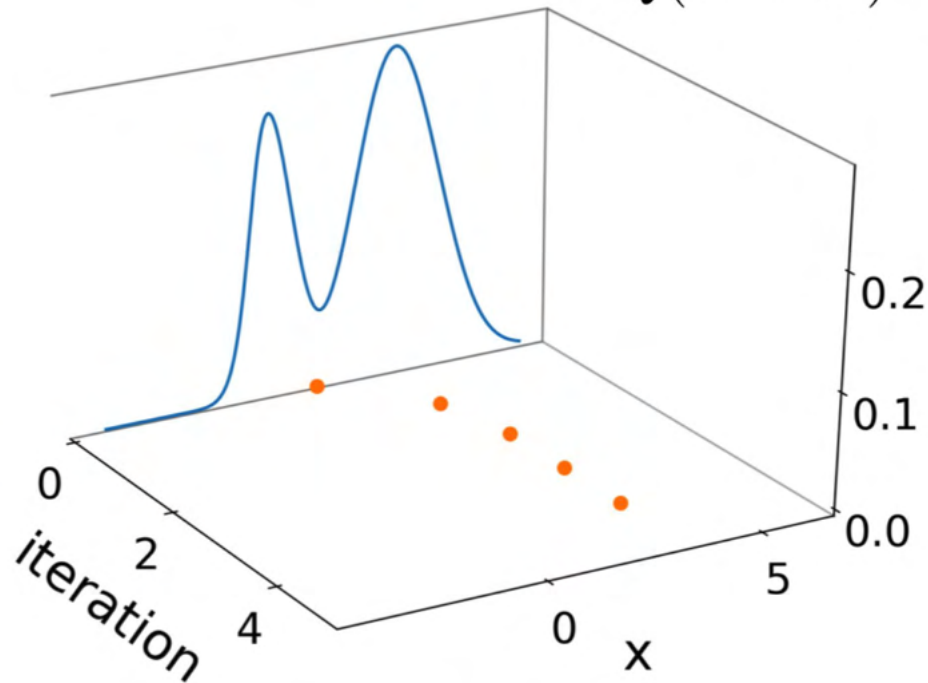
Metropolis Hastings - Demo



$$A(x \rightarrow x') = \min \left(1, \frac{0.20}{0.28} \right) = \min(1, 0.73)$$

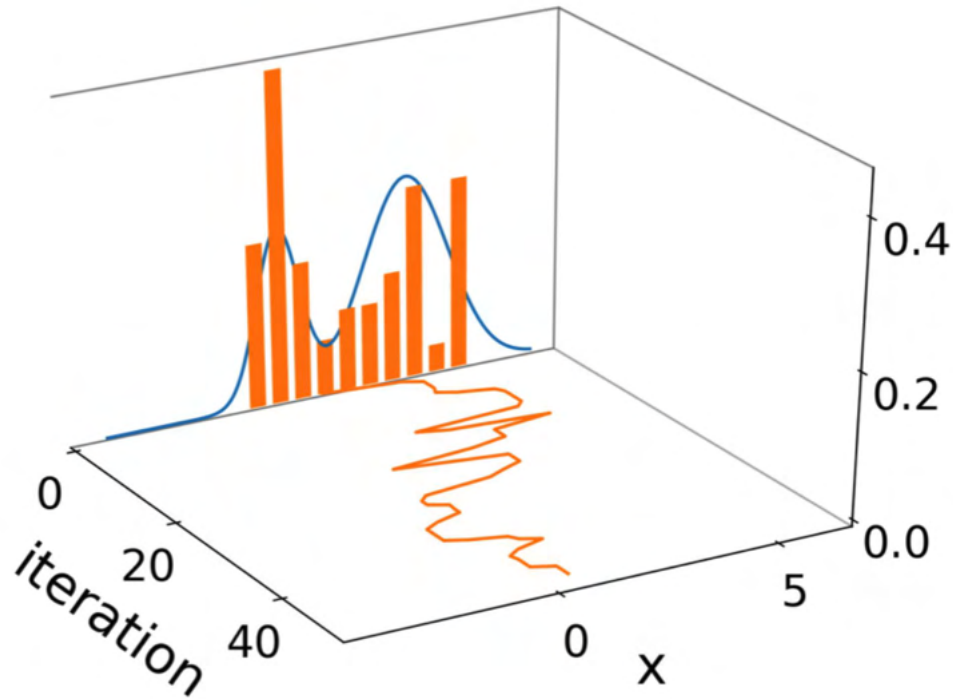
Metropolis Hastings - Demo

$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$



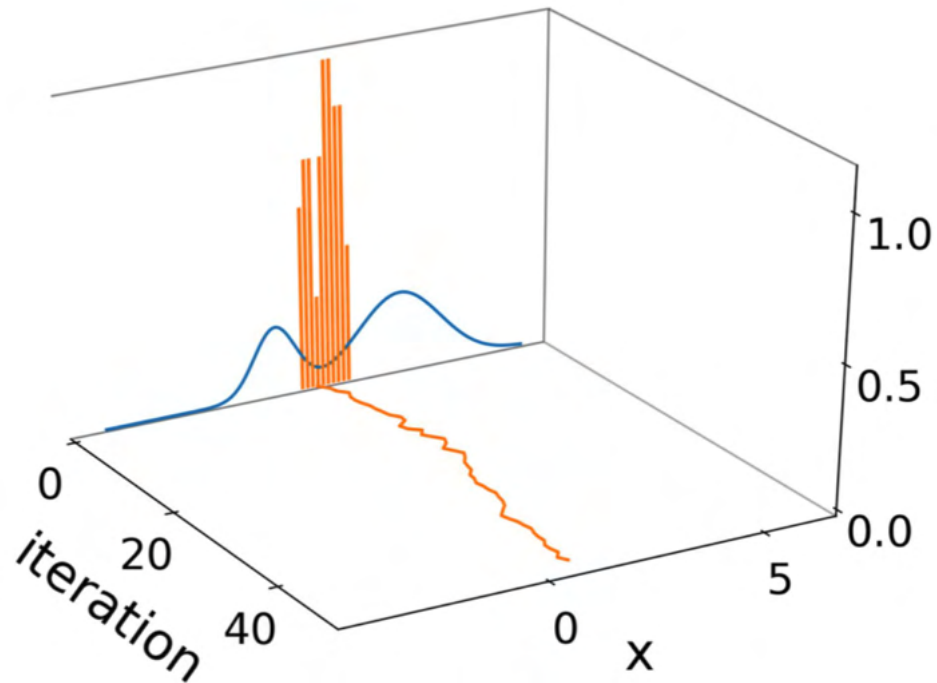
$$A(x \rightarrow x') = \min \left(1, \frac{0.20}{0.28} \right) = \min(1, 0.73)$$

Metropolis Hastings - Demo



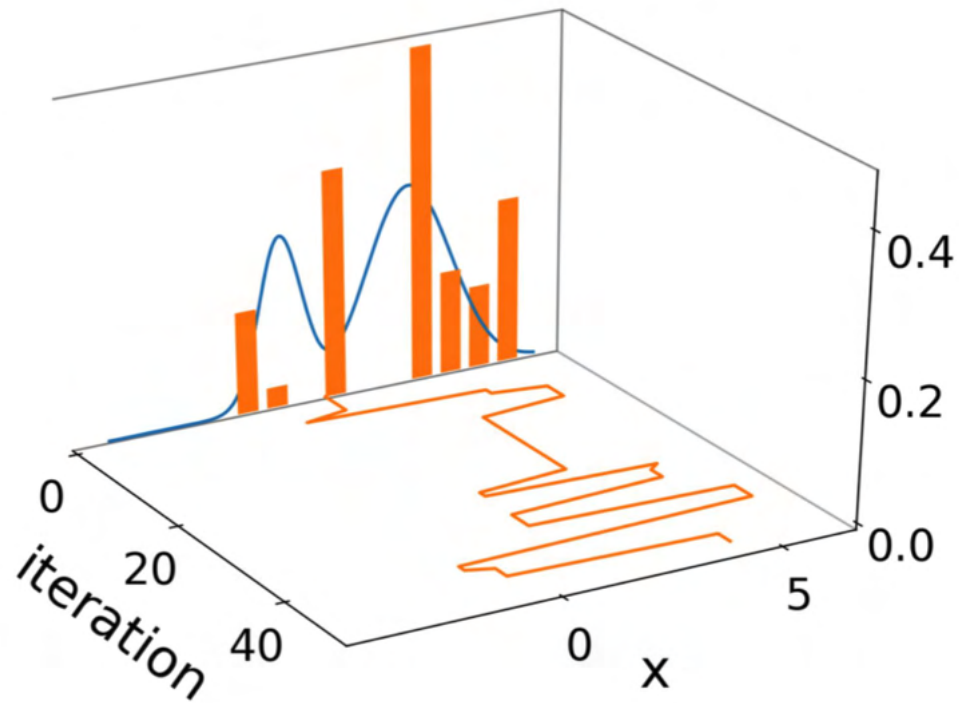
$$Q(x \rightarrow x') = \mathcal{N}(x, 1)$$

Metropolis Hastings - Demo



$$Q(x \rightarrow x') = \mathcal{N}(x, 0.1^2)$$

Metropolis Hastings - Demo



$$Q(x \rightarrow x') = \mathcal{N}(x, 10^2)$$

Metropolis Hastings as correction scheme

- Recall Gibbs sampling

$$x_1^{k+1} \sim p(x_1 \mid x_2 = x_2^k, x_3 = x_3^k)$$

$$x_2^{k+1} \sim p(x_2 \mid x_1 = x_1^{k+1}, x_3 = x_3^k)$$

$$x_3^{k+1} \sim p(x_3 \mid x_1 = x_1^{k+1}, x_2 = x_2^{k+1})$$

Metropolis Hastings as correction scheme

- Recall Gibbs sampling
- Let's make it parallel

$$x_1^{k+1} \sim p(x_1 \mid x_2 = x_2^k, x_3 = x_3^k)$$

$$x_2^{k+1} \sim p(x_2 \mid x_1 = x_1^k, x_3 = x_3^k)$$

$$x_3^{k+1} \sim p(x_3 \mid x_1 = x_1^k, x_2 = x_2^k)$$

Metropolis Hastings as correction scheme

- Recall Gibbs sampling
- Let's make it parallel
- It's wrong now, but can correct with Metropolis Hastings!

$$x_1^{k+1} \sim p(x_1 \mid x_2 = x_2^k, x_3 = x_3^k)$$

$$x_2^{k+1} \sim p(x_2 \mid x_1 = x_1^k, x_3 = x_3^k)$$

$$x_3^{k+1} \sim p(x_3 \mid x_1 = x_1^k, x_2 = x_2^k)$$

Metropolis Hastings - Summary

- Rejection sampling applied to Markov Chains

Pros:

- You can choose among family of Markov Chains • Works for unnormalized densities
- Easy to implement

Cons:

- Samples are still correlated
- Have to choose among family of Markov Chains

Next - MCMC examples with
PyMC3