Markov Chain Monte Carlo (MCMC)

Tim Frasier

What is MCMC?

What Is MCMC?

- Markov Chain Monte Carlo

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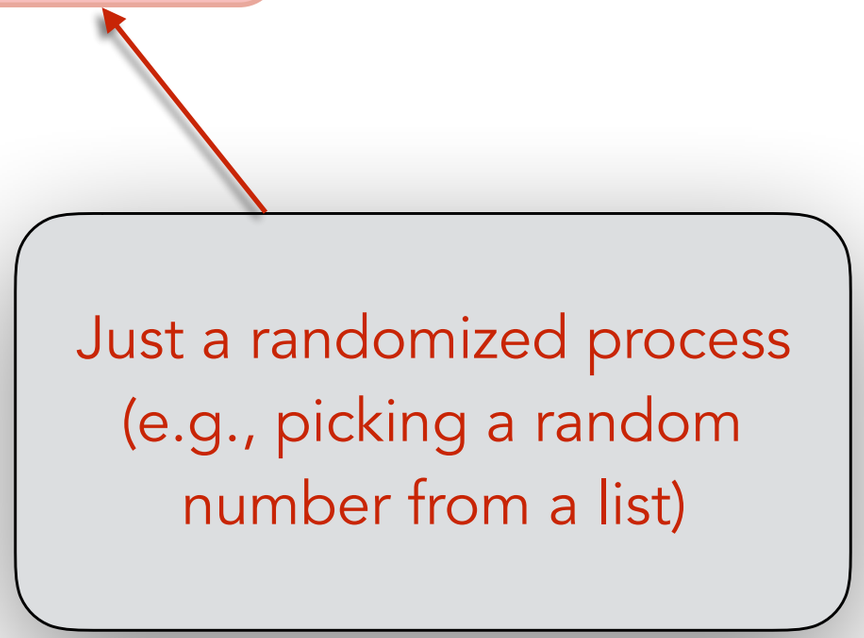
- Markov Chain Monte Carlo



What Is MCMC?

- Markov Chain Monte Carlo

A process where the next step only depends on the current location (this will make more sense in a minute)

What Is MCMC?

Think of a robot walking through a field

- Step 1: Pick a random point along an edge to start at
- Step 2: Randomly select what direction it turns
- Step 3: If step will keep robot in field, take one step in that direction

If steps 2 & 3 repeated enough times, will eventually visit every position in the field even though it is a random process

What Is MCMC?

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The Monte Carlo part

What Is MCMC?

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- Step 2: Randomly select what direction it turns
- Step 3: If step will keep robot in field, take one step in that direction

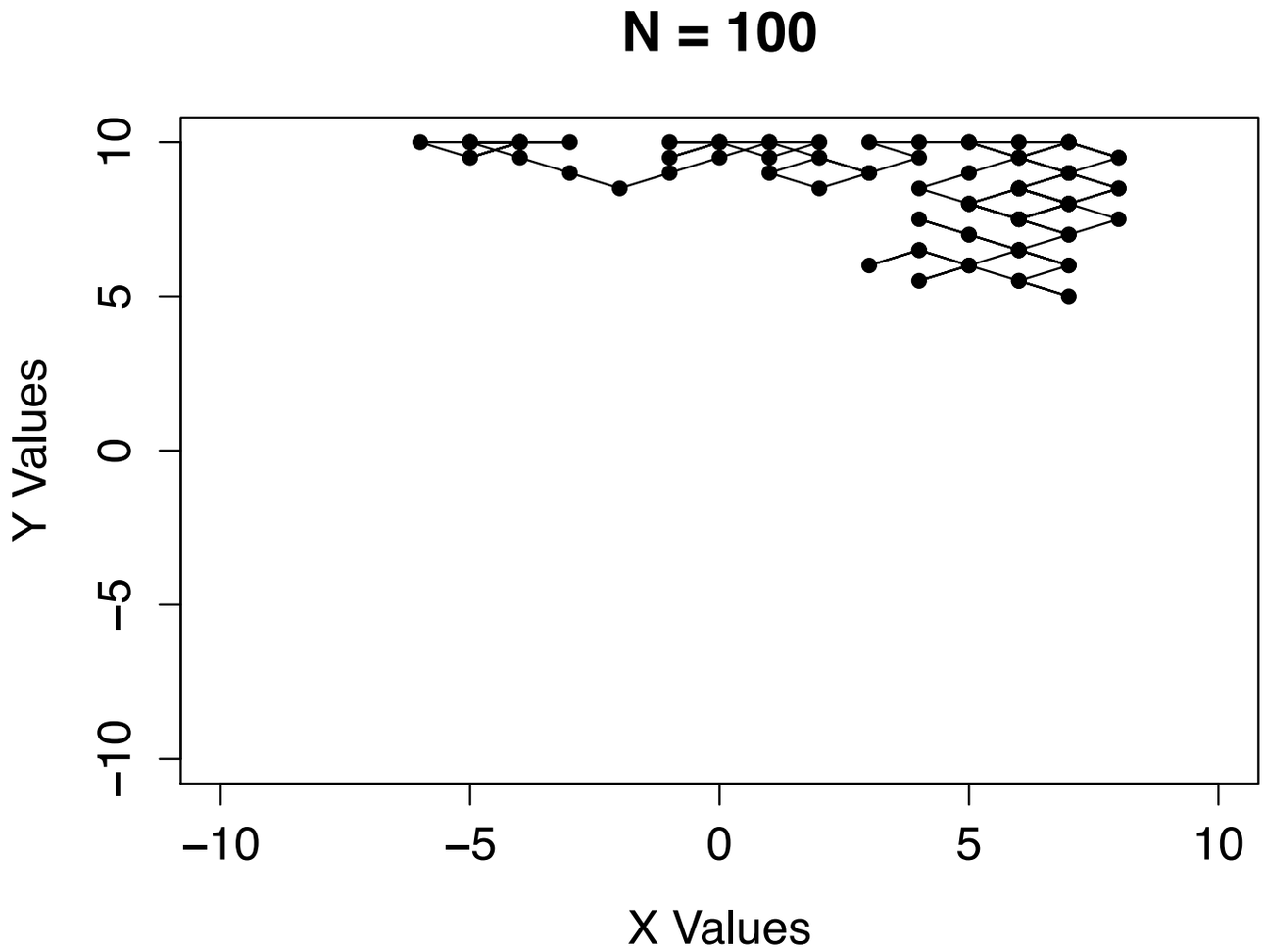
If steps 2 & 3 repeated enough times, will eventually visit every position in the field even though it is a

The Markov Chain part (where it goes next depends on where it is now)

What Is MCMC?

Think of a robot walking through a field

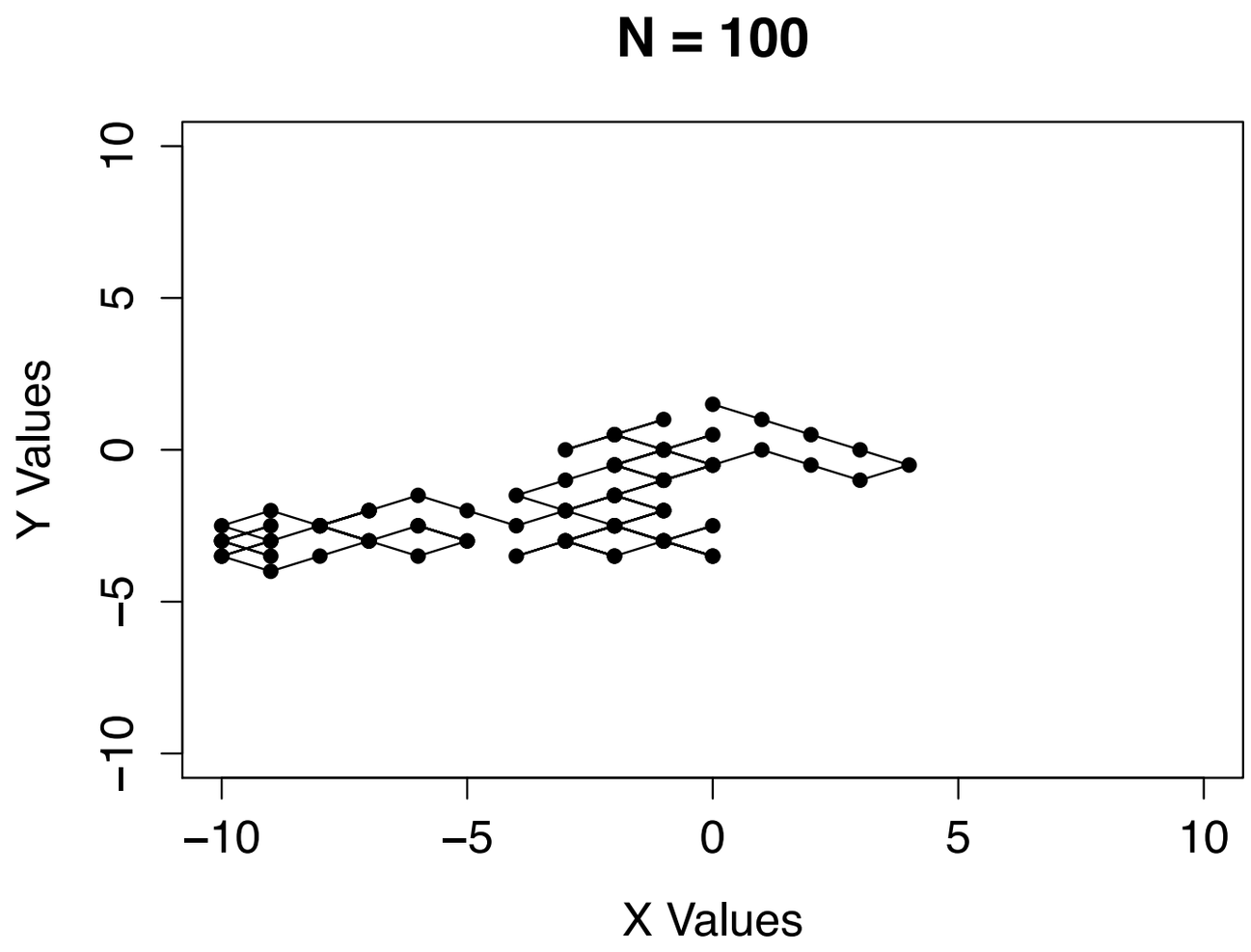
- 100 steps



What Is MCMC?

Think of a robot walking through a field

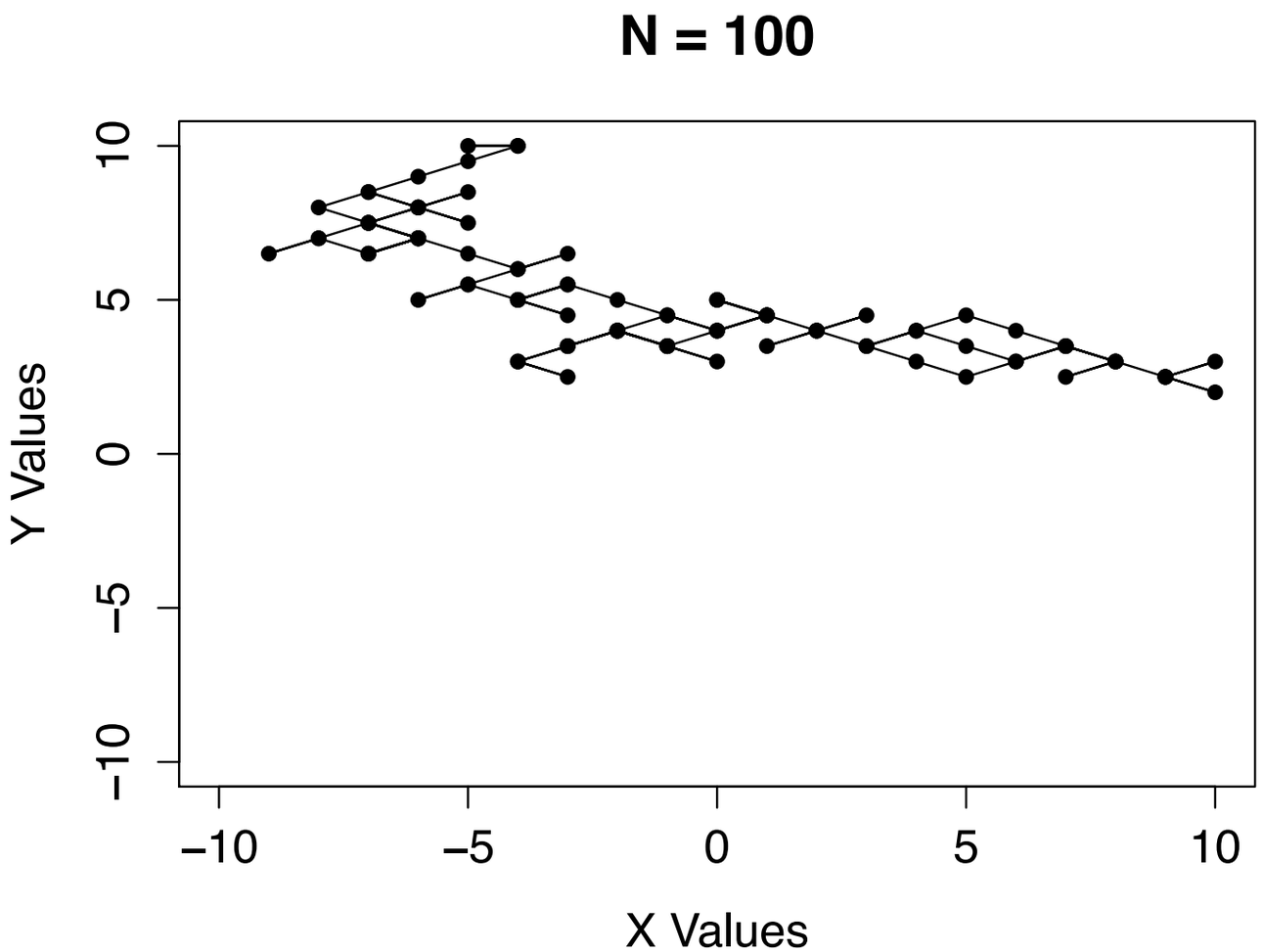
- 100 steps (again)



What Is MCMC?

Think of a robot walking through a field

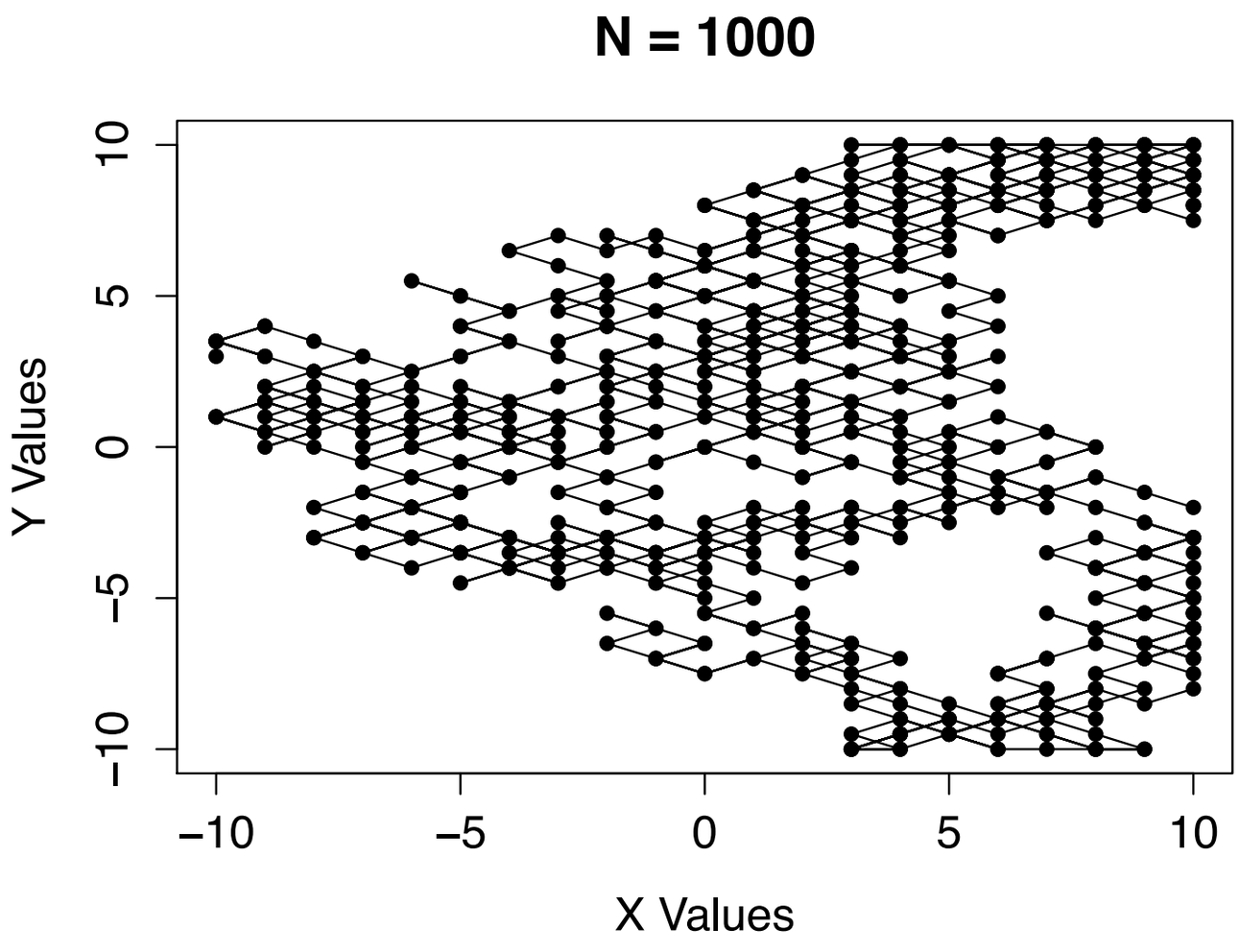
- 100 steps (and again)



What Is MCMC?

Think of a robot walking through a field

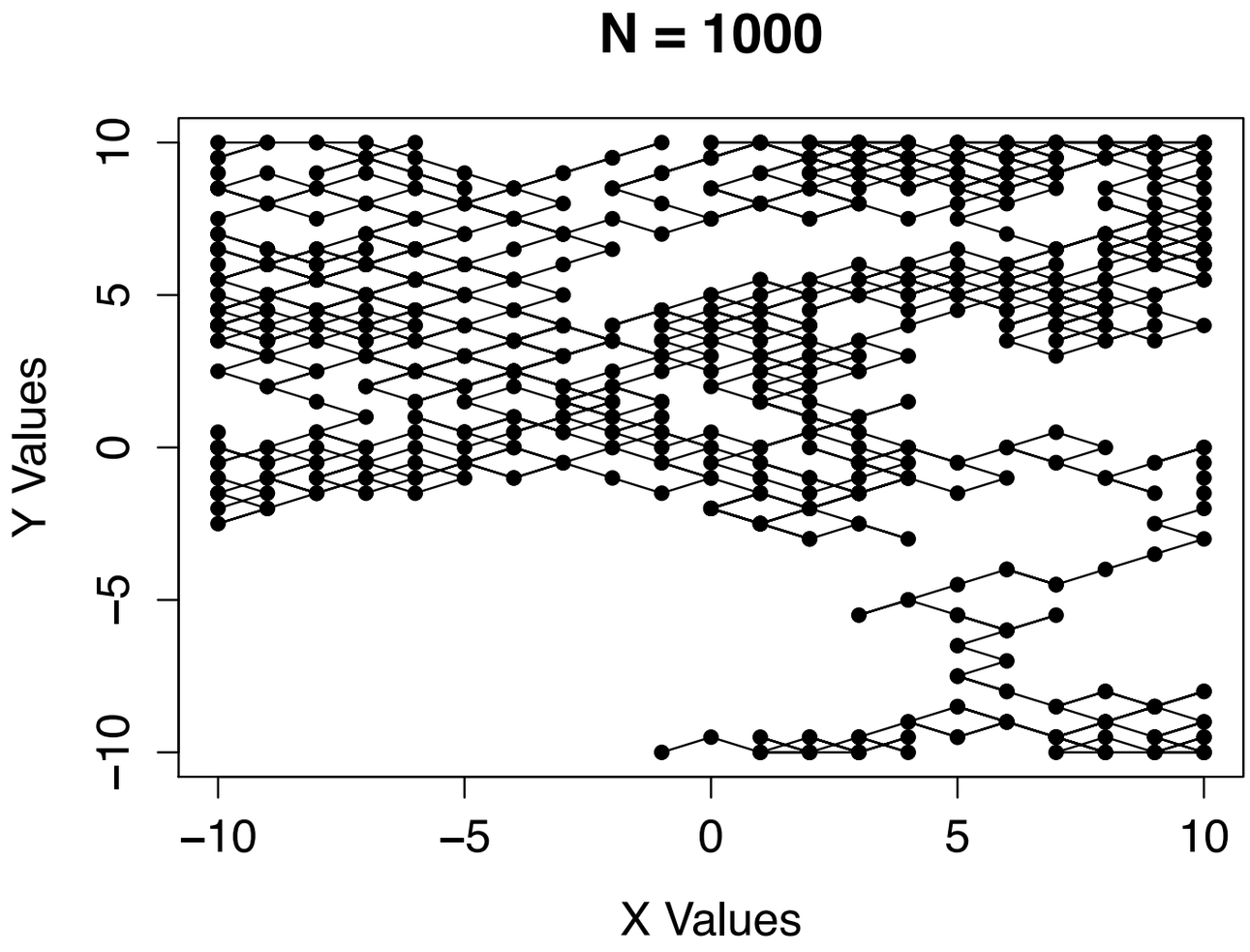
- 1,000 steps



What Is MCMC?

Think of a robot walking through a field

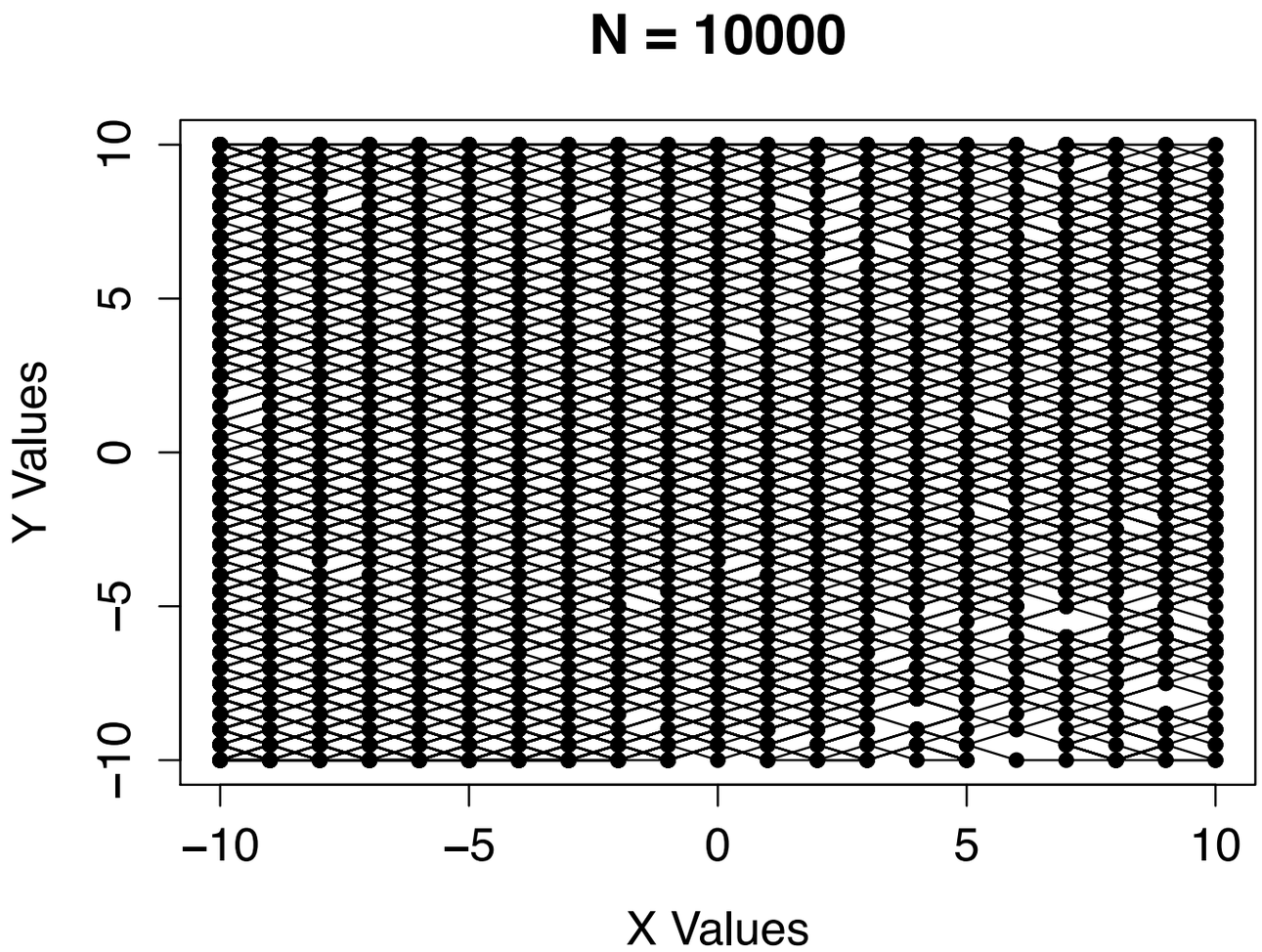
- 1,000 steps (again)



What Is MCMC?

Think of a robot walking through a field

- 10,000 steps



Your Turn!

MCMC Exercise 1

1. Put `basicMCMC.R` file in R's working directory

2. Load it into R

```
source("basicMCMC.R")
```

MCMC Exercise 1

3. Explore how different starting points influence chain. For example, repeat the command below a number of times. (remember the ↑ functionality). Try other chain lengths too!

```
basicMCMC(nSteps = 100)
```

MCMC Exercise 1

4. Explore how different chain lengths influence chain. Some examples are below, but play around yourself!

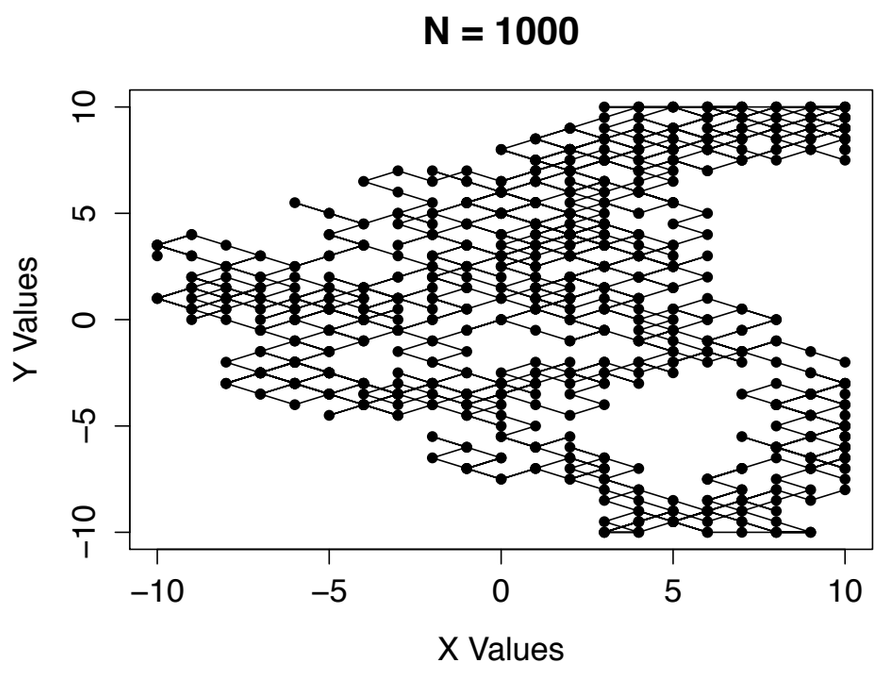
```
basicMCMC(nSteps = 100)
basicMCMC(nSteps = 500)
basicMCMC(nSteps = 1000)
basicMCMC(nSteps = 5000)
```

How Does It Find Values With Highest Probabilities?

How Does It Find High Probabilities?

Clarification

- Instead of a robot walking through a field, is really a model moving through parameter space



How Does It Find High Probabilities?

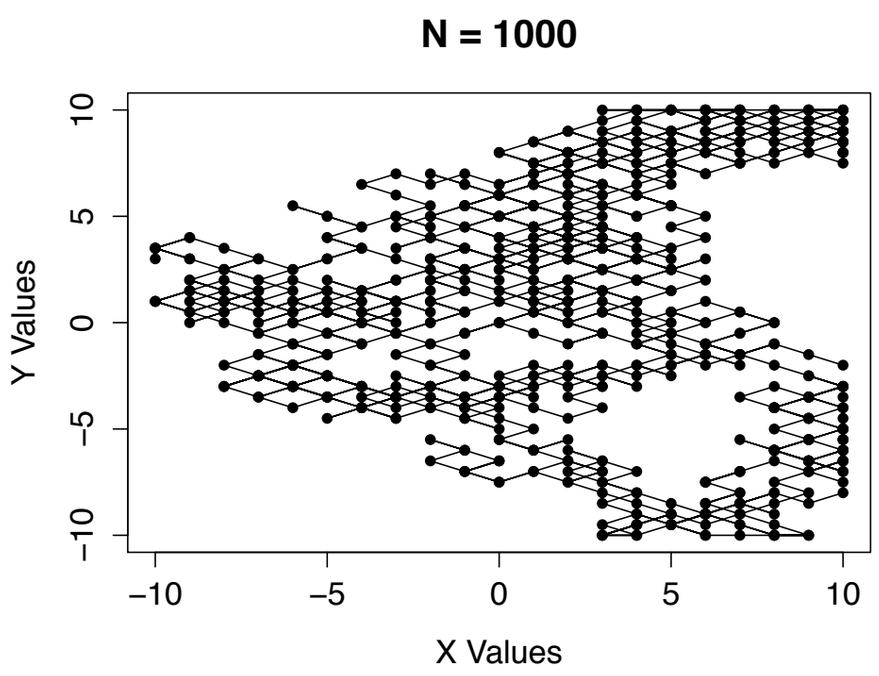
Clarification

- Instead of a robot walking through a field, is really a model moving through parameter space

  - Parameter space:
    possible x and y values

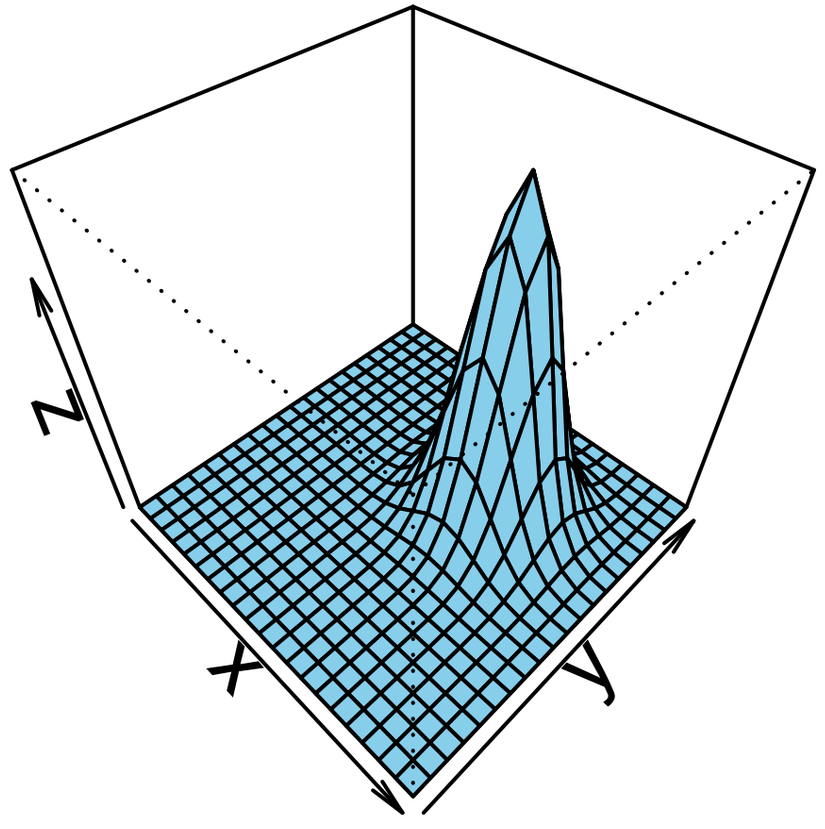
  - Model (simple):
    If proposed value is in
    possible values (-10 to 10 in this case),
    take step

Current parameter space is **flat** (no values have higher likelihood than others)



How Does It Find High Probabilities?

- In real problems, different values will have different likelihoods
- Suppose a simple parameter space with a single peak representing a normal distribution with a mean of 3 and a standard deviation of 2 (in both the x- and y-directions)



How Does It Find High Probabilities?

- The hight of the peak for a given value represents the likelihood of that value

- For all probability distributions, this value is calculable (often ugly, but still calculable)

- For the normal distribution, this equation is:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$\mathbf{x}$ = observed value

μ = mean

$\boldsymbol{\sigma}$ = s.d.

Your Turn!

Peak-Finding Exercise 1

- Explore how different x values result in different likelihoods

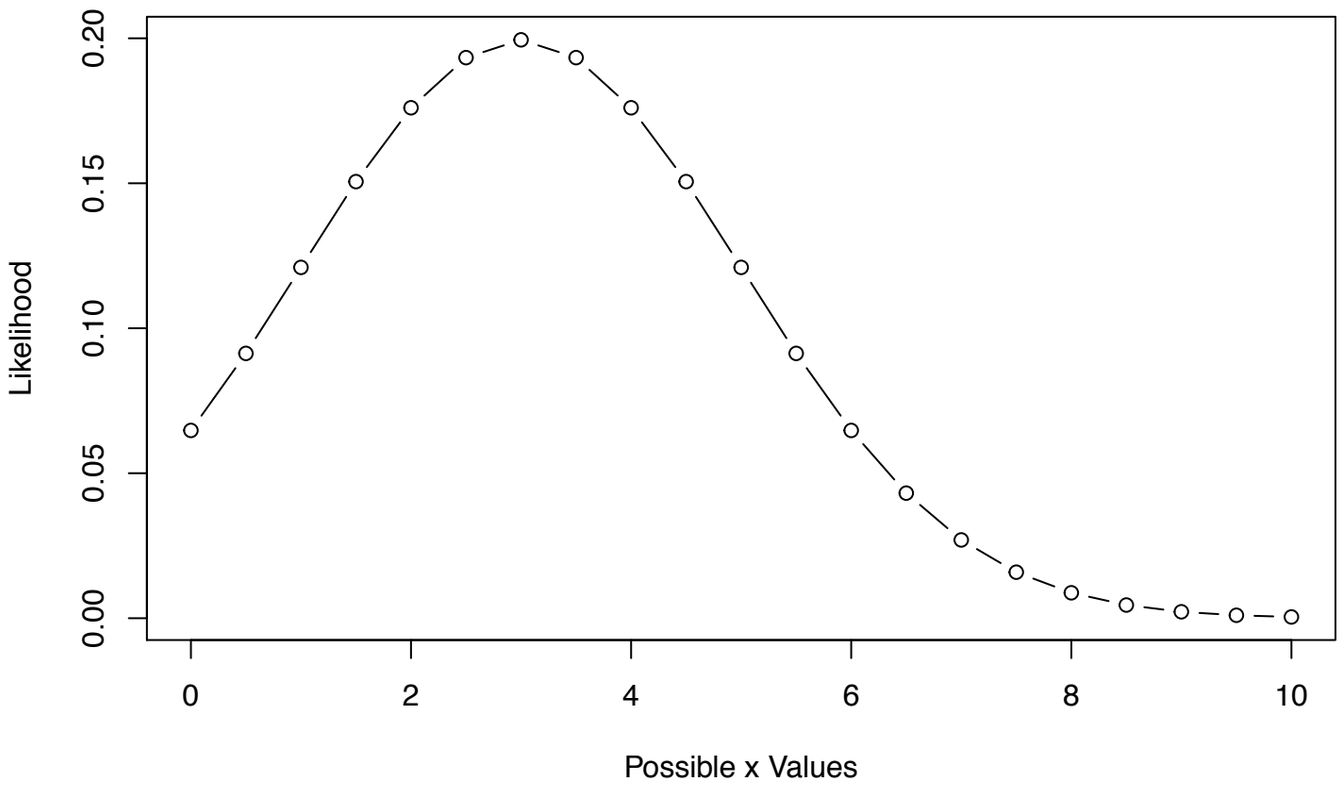
```
dnorm(1, mean = 3, sd = 2)
dnorm(2, mean = 3, sd = 2)
etc.
```

Peak-Finding Exercise 1

- Examine the pattern

```
x = seq(from = 0, to = 10, by = 0.5)
y = dnorm(x, mean = 3, sd = 2)

plot(x, y, type = “b”, xlab = “Possible x values”, ylab = “Likelihood”)
```



How Does It Find High Probabilities?

- Need to set up an algorithm that will cause the model to find peaks (if they exist)

Algorithm

A series of instructions for a computer program to follow (like a recipe, but for a computer)

How Does It Find High Probabilities?

- Need to set up an algorithm that will cause the model to find peaks (if they exist)

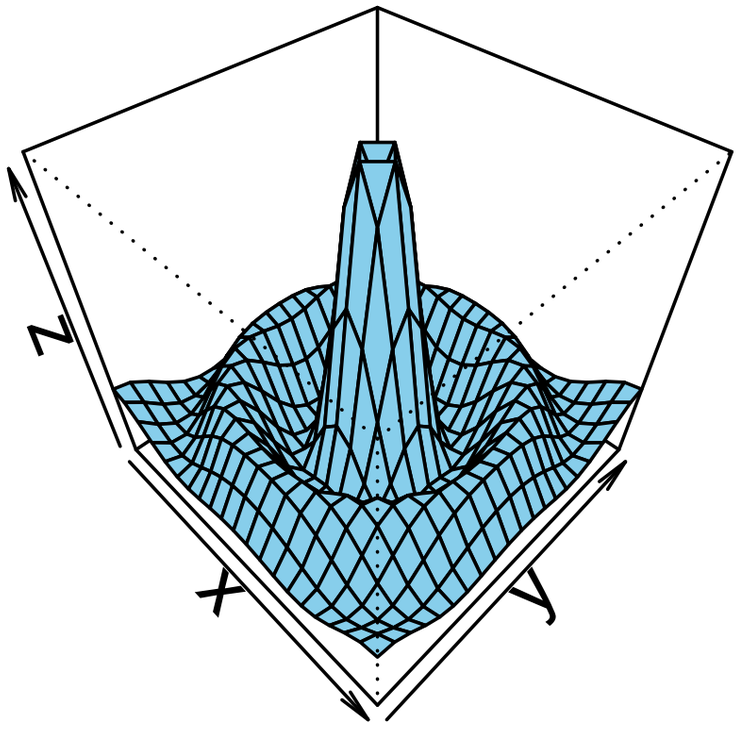
- Example (**algorithm 1**):
  - Step 1: Propose new value (next step)
  - Step 2: Calculate the probability at proposed position
  - Step 3: (a) If proposed probability > probability at current position, take the step
    (b) If not, stay in current position

Repeat steps 1-3 many times

How Does It Find High Probabilities?

- **Algorithm 1** will "work", in that it will climb the first peak it finds and stay there

- However
  - Will get stuck on local peaks (no way to move "downhill")
  - Won't explore parameter space very well



How Does It Find High Probabilities?

- Need an algorithm that preferentially takes steps to values with higher likelihoods, but has some potential to also move to values with lower likelihoods (to walk through valleys)

- **Metropolis-Hastings Algorithm**

How Does It Find High Probabilities?

- **Metropolis-Hastings Algorithm**
  - Step 1: Propose new value (next step)
  - Step 2: Calculate the probability at proposed position
  - Step 3: (a) If proposed probability > probability at current position, take the step

    (b) If not,

    (i) Calculate the ratio of the probabilities at the proposed and current position

    (ii) Draw a random number between 0 and 1 (inclusive)

    (iii) If random number is >= this ratio, take step

    (iv) If not, don't take step

How Does It Find High Probabilities?

- **Metropolis-Hastings Algorithm**
  - Step 1: Propose new value (next
  - Step 2: Calculate the probability at proposed position
  - Step 3: (a) If proposed probability > probability at current position, take the step

    (b) If not,

      (i) Calculate the ratio of the probabilities at the proposed and current position

      (ii) Draw a random number between 0 and 1 (inclusive)

      (iii) If random number is >= this ratio, take step

      (iv) If not, don't take step

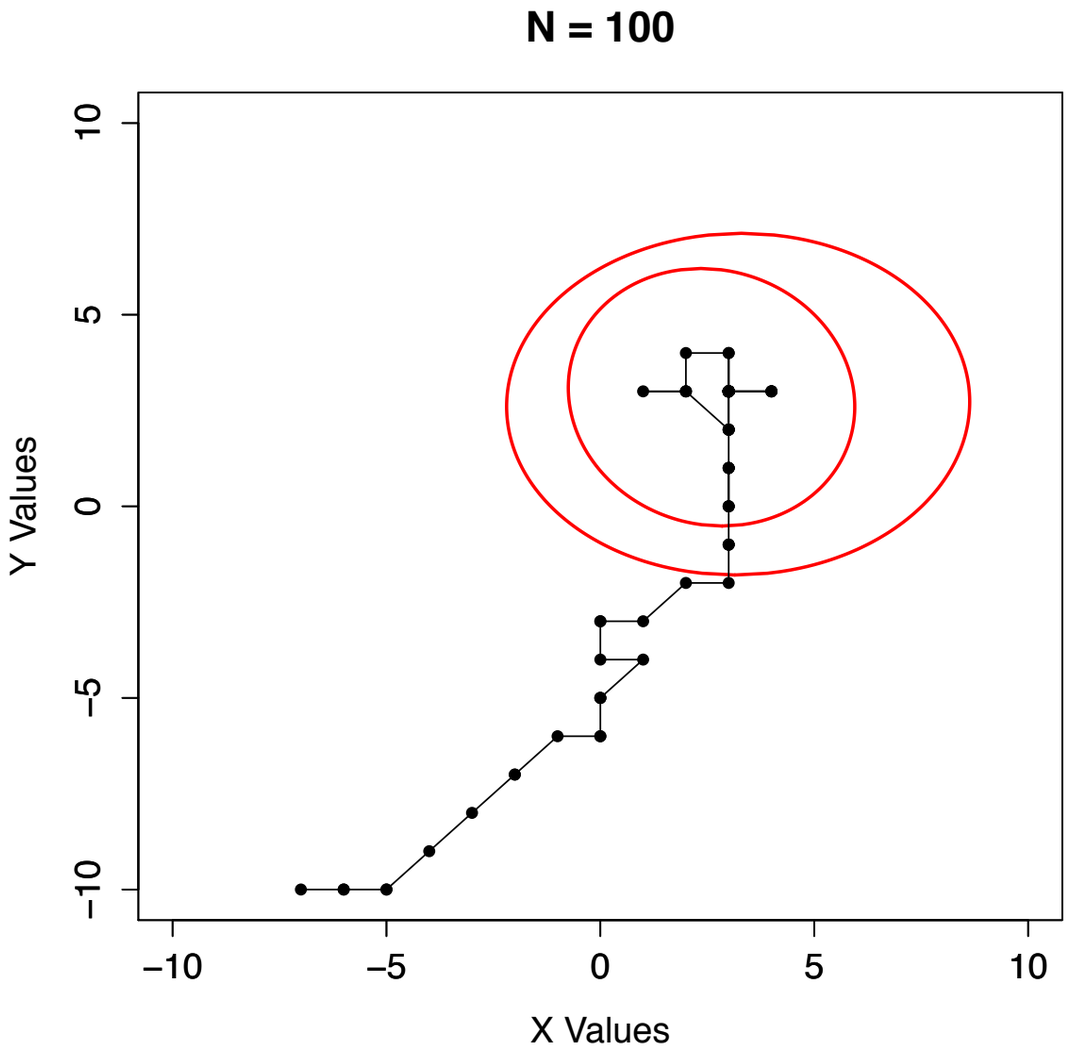
More readily takes small steps down than big steps, but big steps not impossible

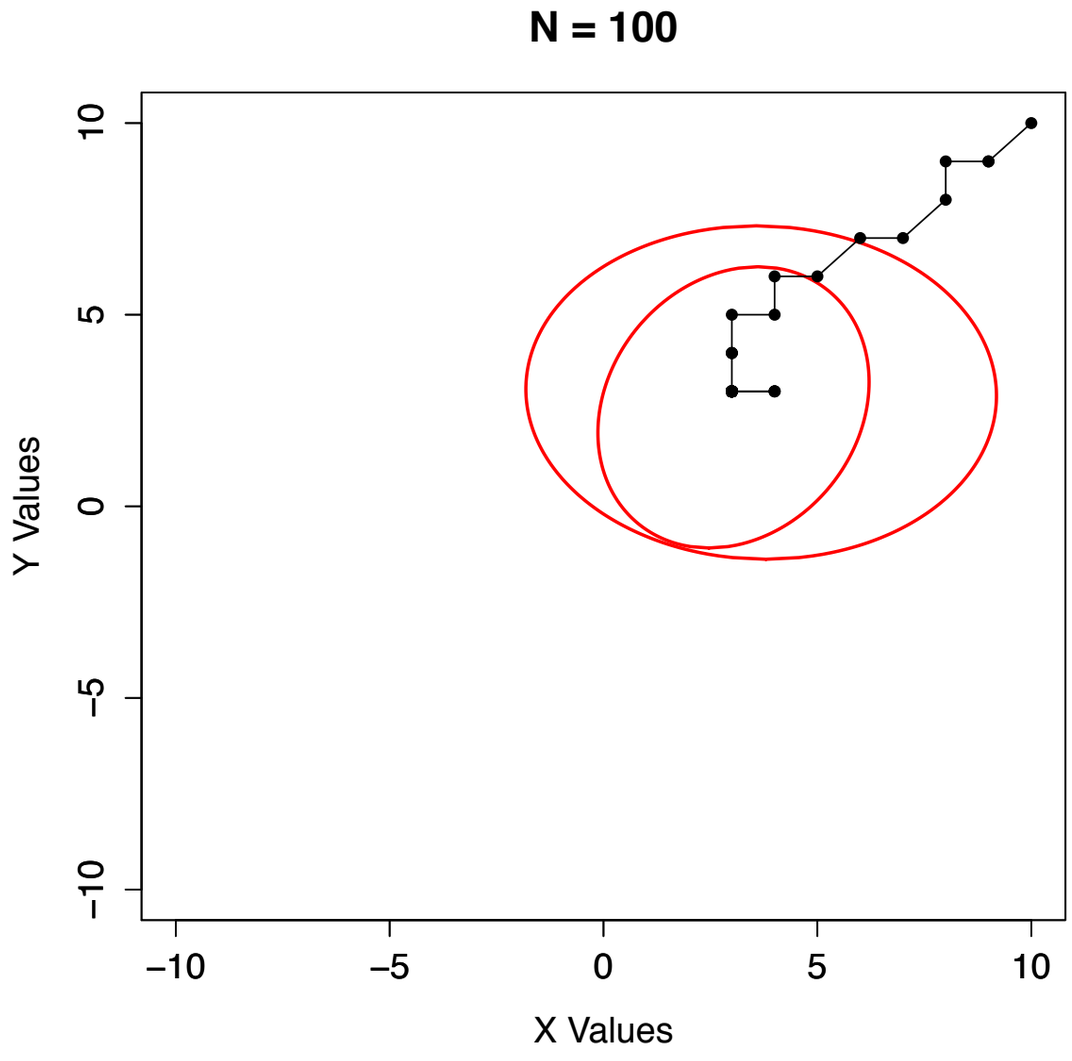
How Does It Find High Probabilities?

- Again, the model doesn't have to "know" where peaks are
- If we follow these rules, it should walk around parameter space until it finds a peak, then it should climb the peak and stay there (with some potential to cross valleys)

How Does It Find High Probabilities?

Some examples





Video

https://chi-feng.github.io/mcmc-demo/

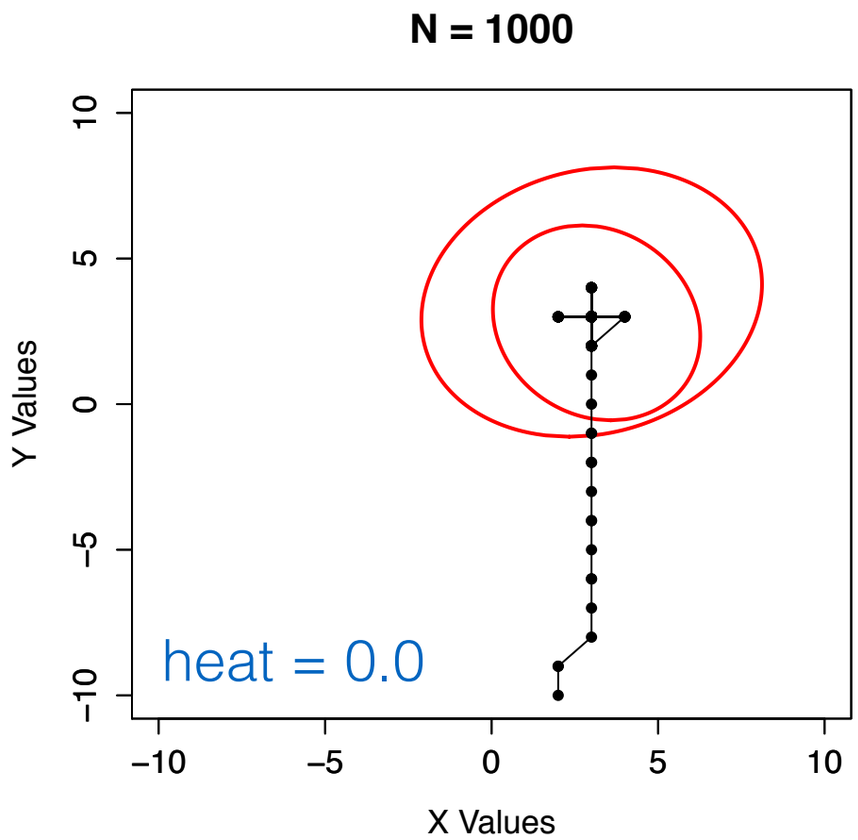
How Does It Find High Probabilities?

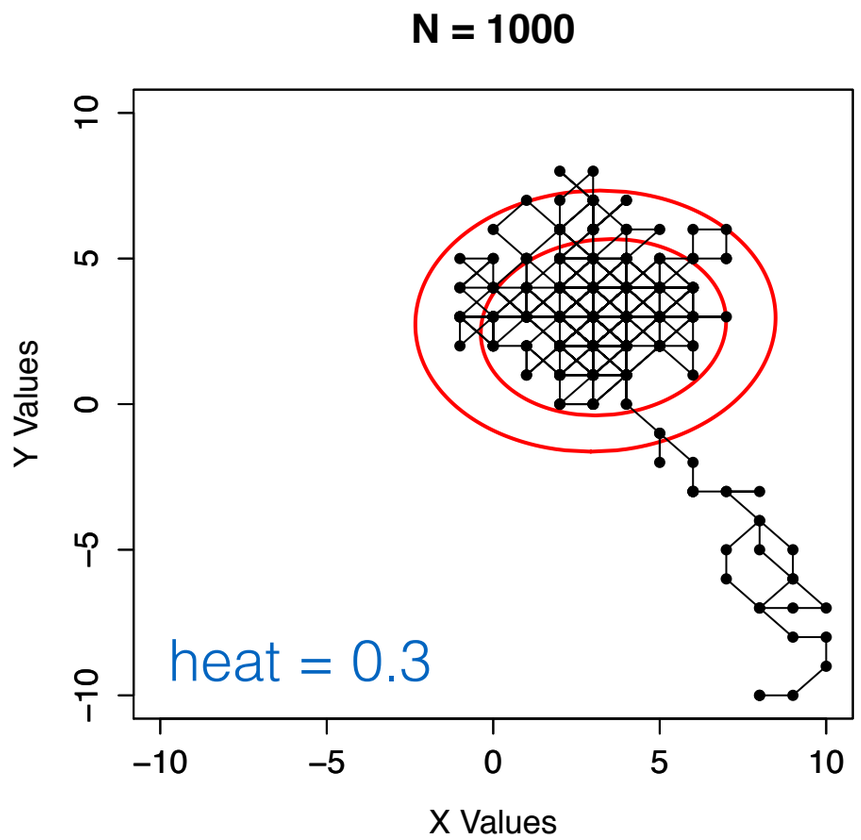
Heating chains

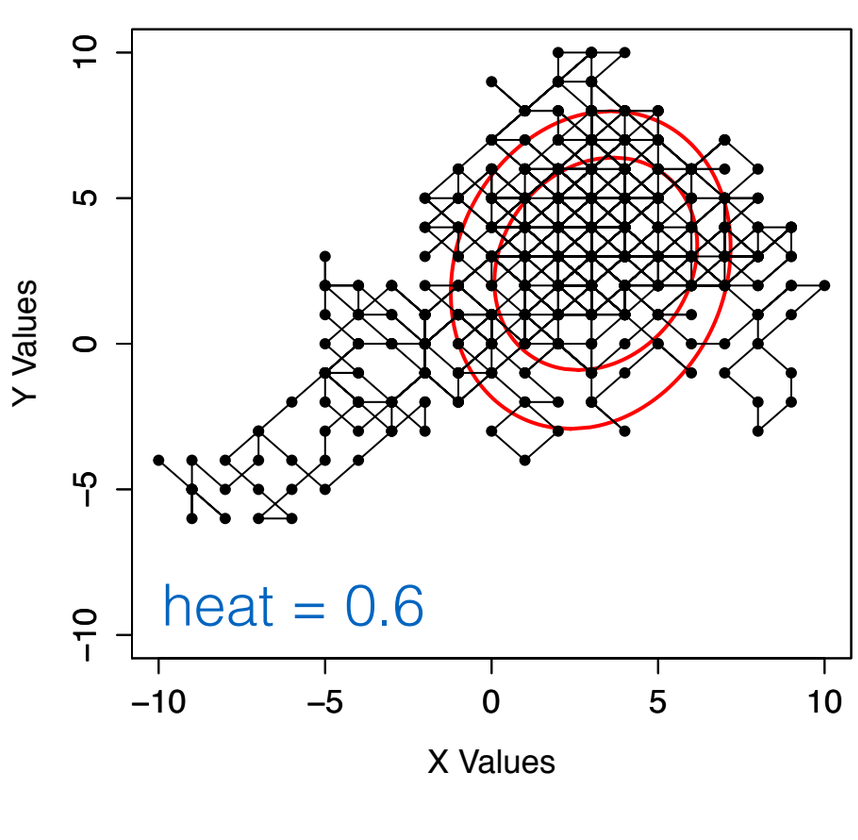
- Can tweak how stringent conditions are for taking a step to a lower likelihood (downhill)

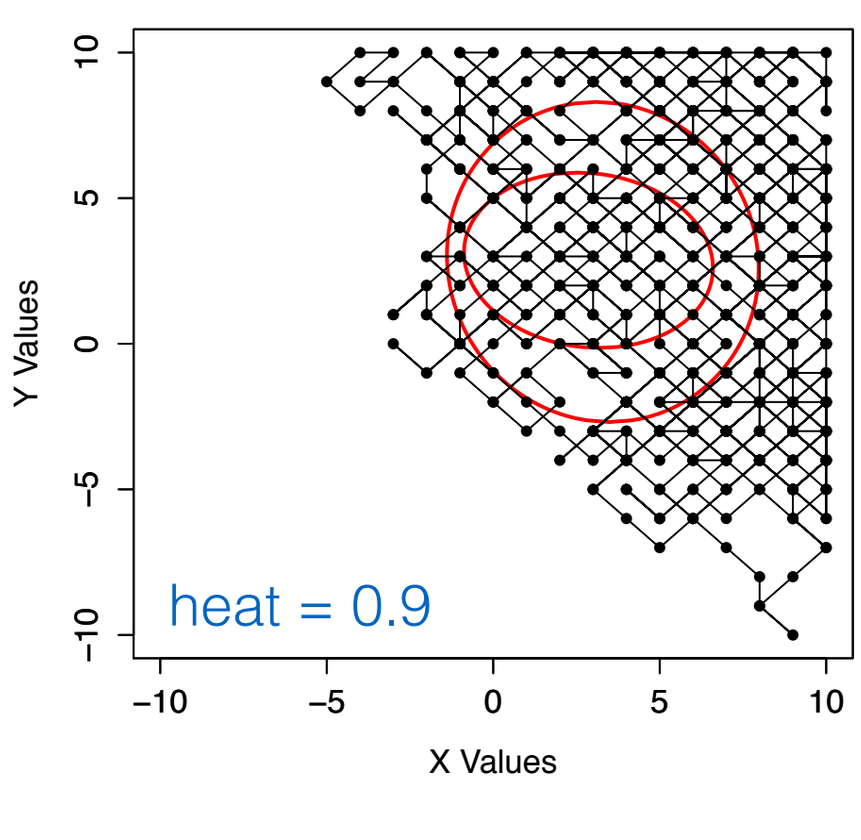
- Chains that more readily take such steps are called “heated”
  - The more heated a chain is, the more readily it will explore parameter space - good
  - The more heated a chain is, the less time it will stay on top of peaks - bad

Need a balance


N = 1000
heat = 0.0
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10


N = 1000
heat = 0.3
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10


N = 1000
heat = 0.6
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10


N = 1000
heat = 0.9
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10

Your Turn!

Peak-Finding Exercise 2

1. Need to install the following libraries
    a. `MASS`
    b. `cluster`

2. Put `onePeakMCMC.R` file in R's working directory

3. Load it into R

```
source("onePeakMCMC.R")
```

Peak-Finding Exercise 2

3. Explore how different starting points influence chain's ability to find peaks. For example, repeat the command below a number of times. (remember the ↑ functionality). Try other chain lengths too!

```
onePeakMCMC(nSteps = 100, heat = 0, burnin = 0)
```

Peak-Finding Exercise 2

4. Explore how different heating strategies influence how readily the chain steps away from the peak. For example:

```
onePeakMCMC(nSteps = 1000, heat = 0.0, burnin = 0)
onePeakMCMC(nSteps = 1000, heat = 0.2, burnin = 0)
onePeakMCMC(nSteps = 1000, heat = 0.4, burnin = 0)
onePeakMCMC(nSteps = 1000, heat = 0.6, burnin = 0)
onePeakMCMC(nSteps = 1000, heat = 0.8, burnin = 0)
onePeakMCMC(nSteps = 1000, heat = 1.0, burnin = 0)
```

Try some of your own!

What does this have to do with Bayesian analysis?

MCMC & Bayesian Analysis

Like peanut butter & chocolate

- Remember Bayes' Rule

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

MCMC & Bayesian Analysis

Like peanut butter & chocolate

- Remember Bayes' Rule

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

Unsolvable for most problems

MCMC & Bayesian Analysis

Like peanut butter & chocolate

- Remember Bayes' Rule

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

- If MCMC model is exploring space well:
  - Proportion of time spent at a value represents the posterior probability of that value

MCMC & Bayesian Analysis

Like peanut butter & chocolate

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

1. Propose new value of (H)

MCMC & Bayesian Analysis

Like peanut butter & chocolate

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

1. Propose new value of (H)
2. Multiply the prior and likelihood for proposed value

MCMC & Bayesian Analysis

Like peanut butter & chocolate

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

1. Propose new value of (H)
2. Multiply the prior and likelihood for proposed value
   a. If this product is >= current value, take step
   b. If this product is <= current value, follow some rules to determine whether or not to take step

MCMC & Bayesian Analysis

Like peanut butter & chocolate

$$P(\mathrm{H}|\mathrm{D}) = \frac{P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}{\int P(\mathrm{H}) \times P(\mathrm{D}|\mathrm{H})}$$

1. Propose new value of H
2. Multiply the prior and likelihood for proposed value
    a. If this product is >= current value, take step
    b. If this product is <= current value, follow some rules to determine whether or not to take step
3. If MCMC model is exploring space well, proportion of time spent at a specific value of H will represent it's posterior probability

MCMC & Bayesian Analysis
Like peanut butter & chocolate

- The benefits of this cannot be overstated
- Allows easy computation of very difficult problems
  - Problems not solvable (or even fathomable) before MCMC & good computing power
- Only downside is that MCMC is computationally “expensive”

MCMC & Bayesian Analysis
Like peanut butter & chocolate

- Can easily accommodate problems dealing with 10s or even 100s of parameters
    - As long as likelihood for each can be calculated…
    - … and model is set up properly

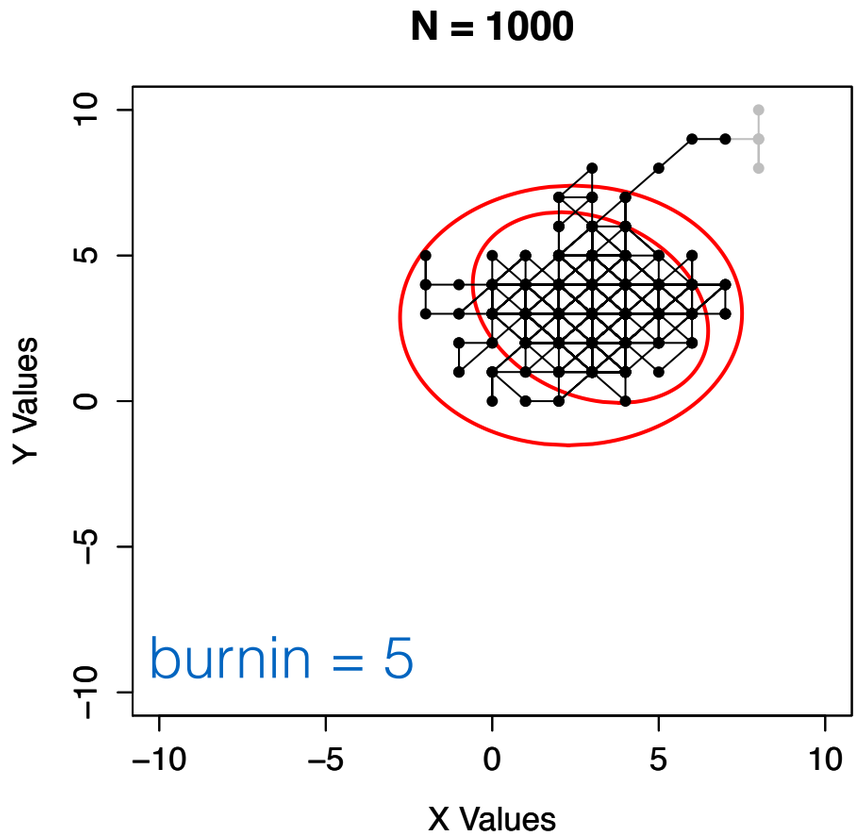
Burn-in

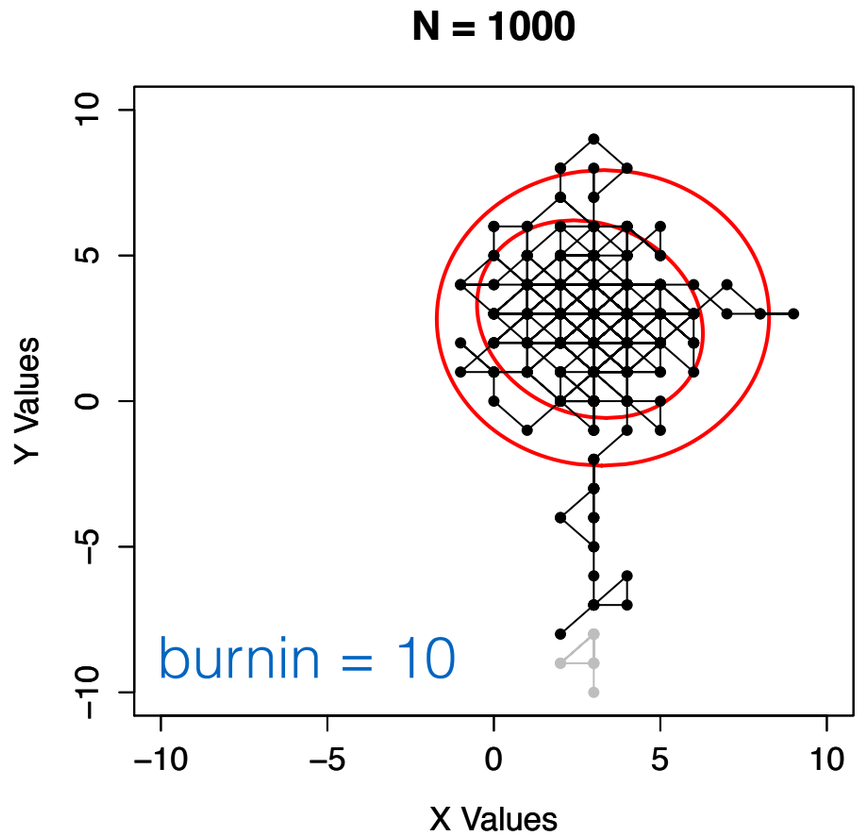
Burn-in

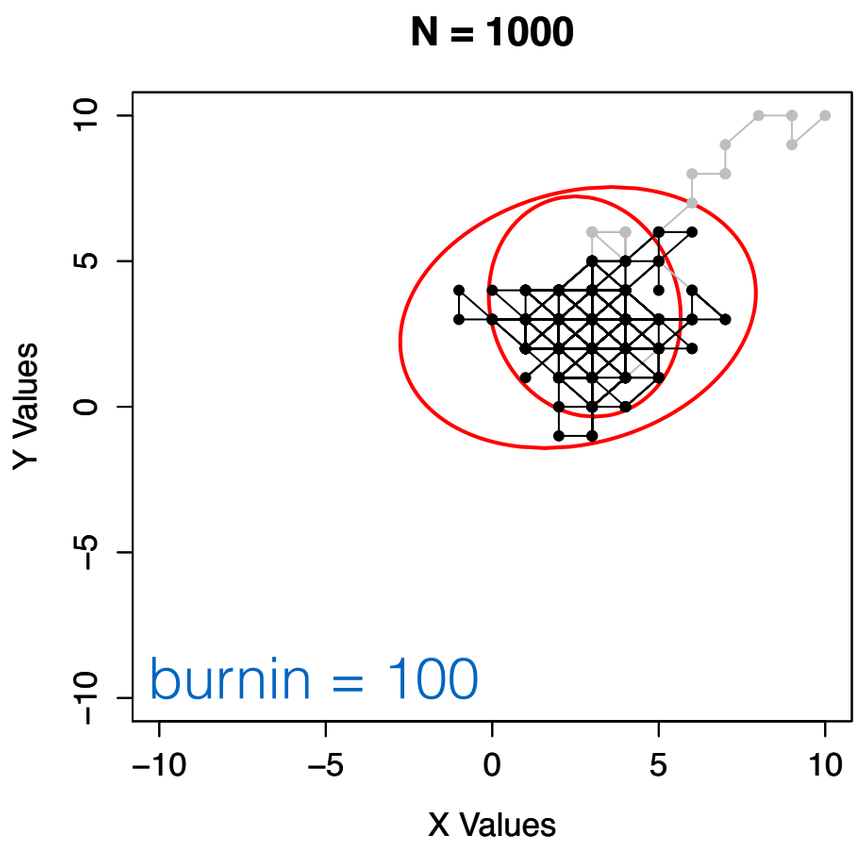
- To be useful in Bayesian analyses, proportion of time spent at a value should be reflective of that value's probability

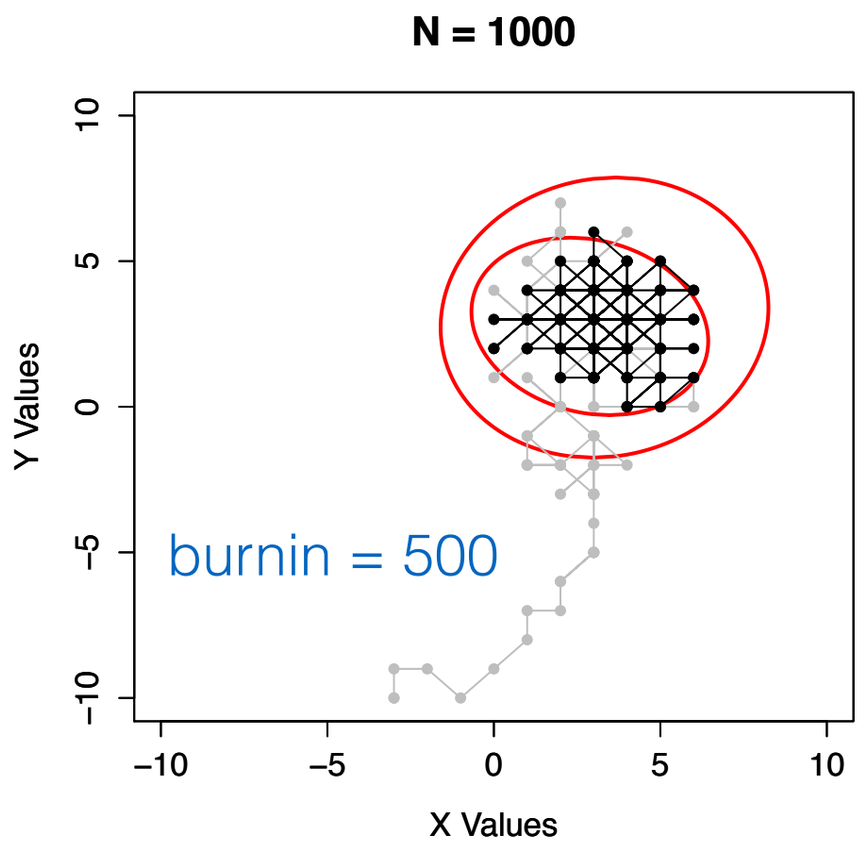
- But, remember that the model wanders aimlessly, and is heavily biased by where it starts, until it actually finds a peak

- Need to ignore these steps when making estimation
  - Number of steps ignored is called the "burn-in"
  - No way to know ahead of time, but better to ignore too many than too few


N = 1000
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10
burnin = 5


N = 1000
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10
burnin = 10


N = 1000
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10
burnin = 100


N = 1000
Y Values
X Values
10
5
0
−5
−10
−10
−5
0
5
10
burnin = 500

Your Turn!

Burn-in Exercise

1. Explore how different burn-in lengths fit with different chain lengths and heating values.

```
onePeakMCMC(nSteps = 1000, heat = 0.5, burnin = 10)
onePeakMCMC(nSteps = 1000, heat = 0.5, burnin = 50)
onePeakMCMC(nSteps = 1000, heat = 0.5, burnin = 100)
etc.
```

Try some of your own!

Burn-in

- Not really possible to have burn-in “too long” (but you need enough steps of data collection to obtain good estimates)

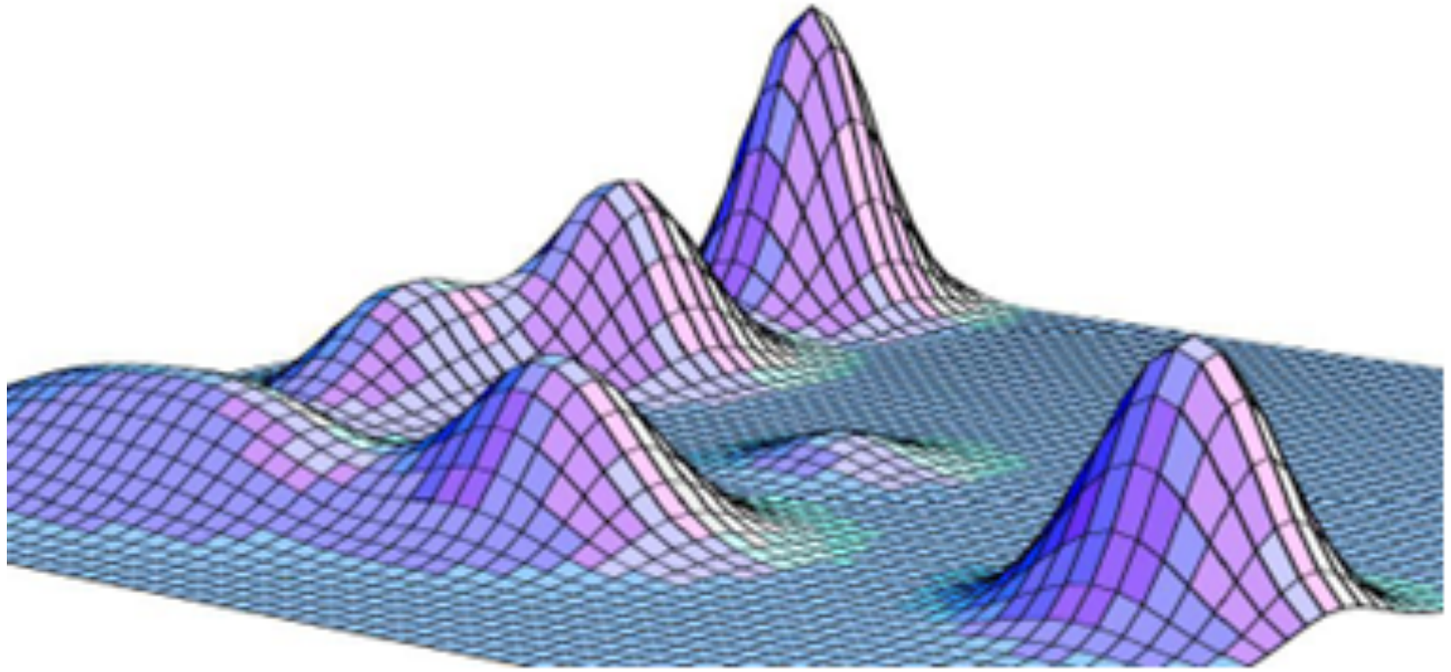
- A burn-in that is too short can cause real problems

We’ll go over some ways to examine this later

Running Multiple Chains

Running Multiple Chains

- We've been talking about very simple examples
- Parameter space for "real" problems are likely quite complex (and unknowingly so)



Running Multiple Chains

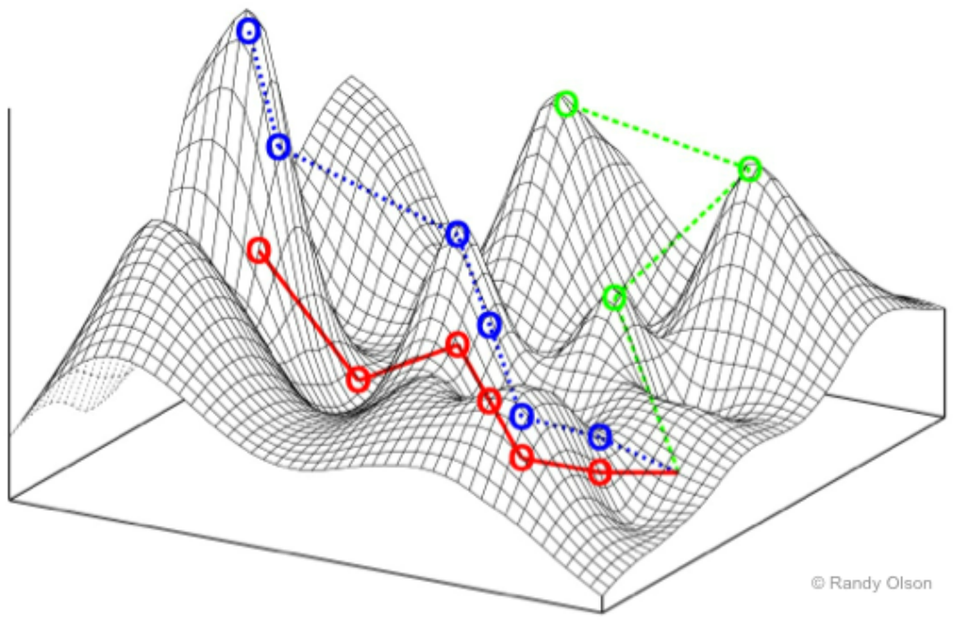
- Often more efficient to run multiple chains
  - Each starting in a different place
  - Each with a different heating value

Will explore parameter space more efficiently than a single chain

Running Multiple Chains

- Have them swap periodically
  - Have one main chain, and the rest “workers”
  - Every so often, compare the probability of positions of each chain
  - If a worker chain has a higher probability than the main chain, switch parameter values between chains

Allows main chain to “jump” to peaks that other chains have found



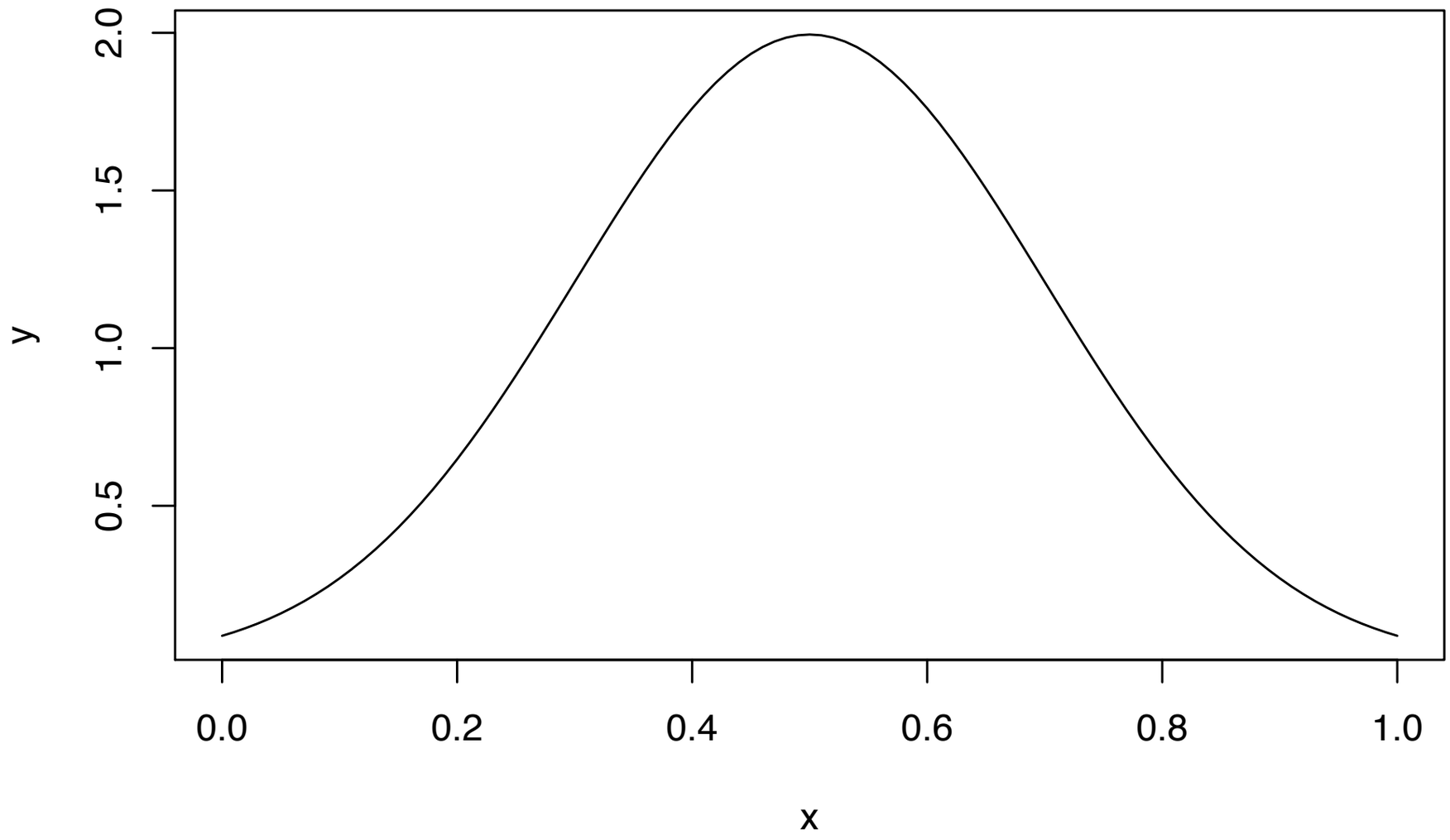
Hamiltonian Monte Carlo

Hamiltonian Monte Carlo

- A physics simulation
- Represent parameter state as a particle in *n*-dimensional space
- Flick particle around frictionless -log-posterior
- Record positions

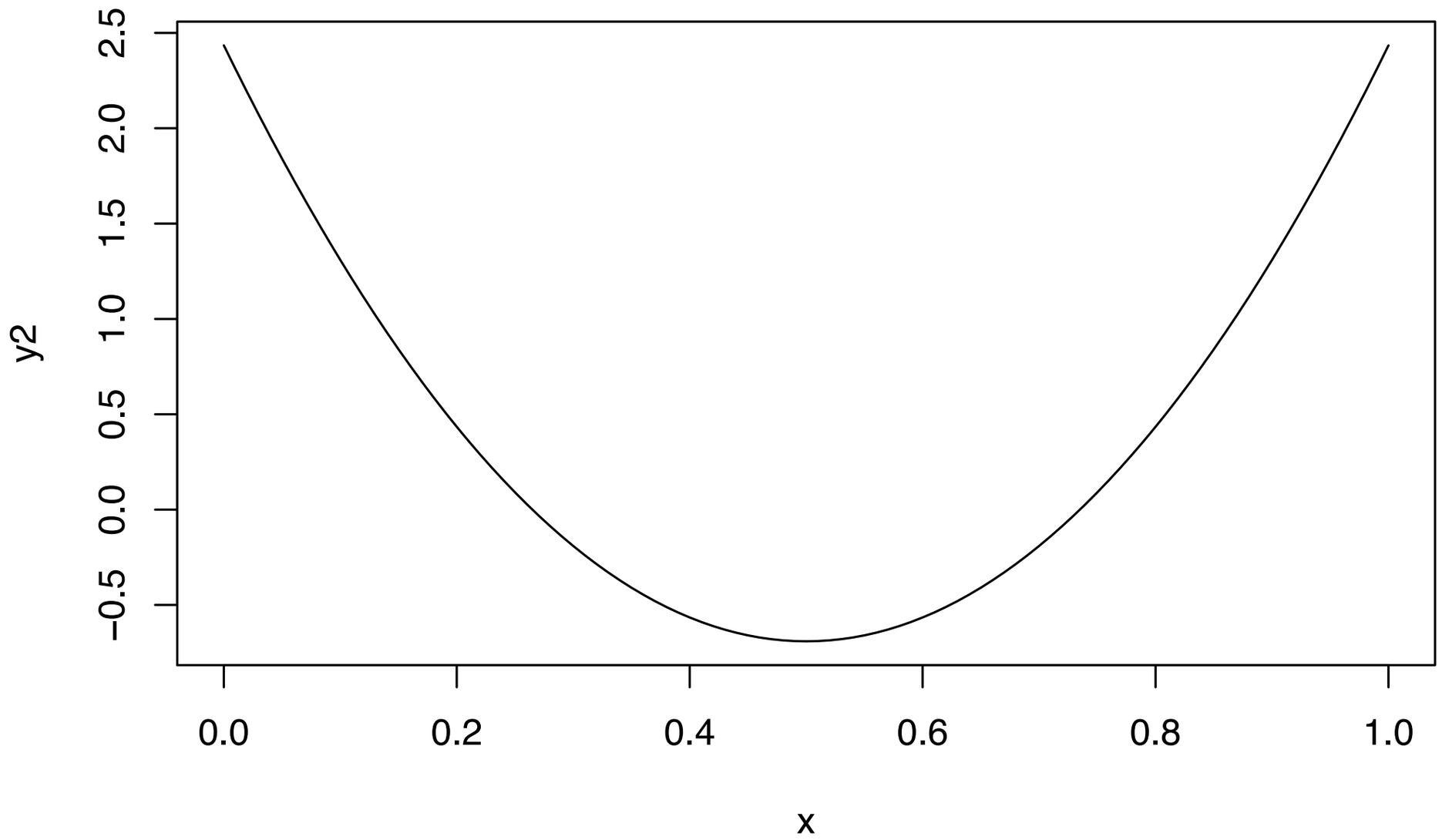
Hamiltonian Monte Carlo

```
x = seq(from = 0, to = 1, by = 0.01)
y = dnorm(x, mean = 0.5, sd = 0.2)
plot(y ~ x, type = “l”)
```

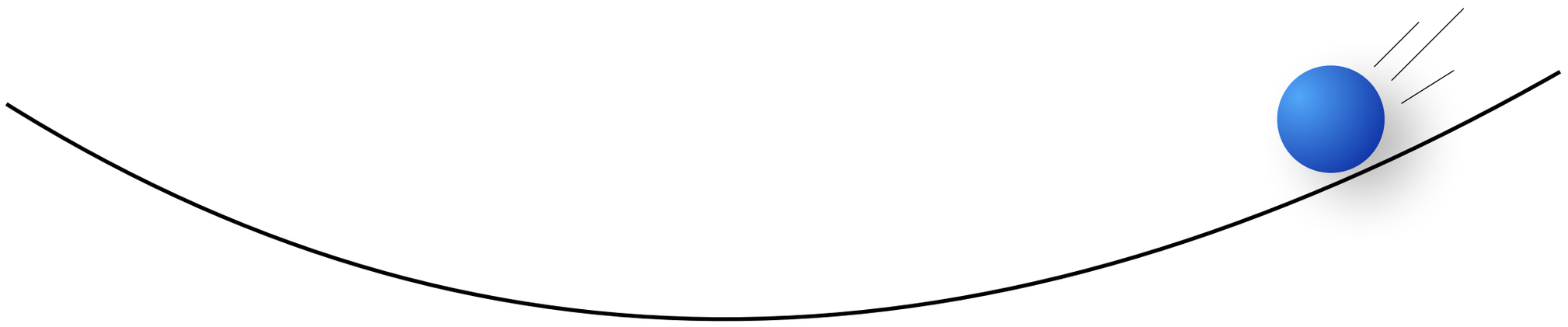


Hamiltonian Monte Carlo

```
y2 = -log(y)
plot(y2 ~ x, type = “l”)
```



Hamiltonian Monte Carlo



- Position
  - Present parameter values
- Speed (momentum of parameter values)
  - Fast when parameter values have low probability (high -log-prob)
  - Slow when parameter values have high probability (low -log-prob)
- Samples of position are samples from posterior

Video
(Naïve HMC)

https://chi-feng.github.io/mcmc-demo/

Hamiltonian Monte Carlo

- When do you take estimate (stop the particle)?

- NUTS: No U-turn sampler
  - Start trajectory in both directions
  - Run until it starts to turn around

Video

https://chi-feng.github.io/mcmc-demo/

Hamiltonian Monte Carlo

- Does not have *burn-in*
- Has *warmup* instead
  - Stan is optimizing model behaviour for your model (step size, mass of particle, etc.)

Questions?