Bayesian approaches to parameter estimation

CSCS 530 - Marisa Eisenberg

Timeline

- Lab 4 & project proposal: due April 14
    - Submit lab 4 on Canvas
    - Upload project proposal to google drive (ADD LINK)
- Project proposal comments: April 21
    - Comment on 2 other proposals
- Final Project writeup: Due April 30

Bayesian approaches to parameter estimation

- Bayes' Theorem, rewritten for inference problems:

$$P(p \mid z) = P(params \mid data) = \frac{P(z \mid p) \cdot P(p)}{P(z)}$$

- Allows one to account for prior information about the parameters
  - E.g. previous studies in a similar population
- Update parameter information based on new data

Bayesian approaches to parameter estimation

Likelihood

Prior distribution

$$P(p \mid z) = P(params \mid data) = \frac{P(z \mid p) \cdot P(p)}{P(z)}$$

Normalizing constant
(can be difficult to calculate!)

$$P(z) = \int_p P(z, p) dp$$

Denominator term - P(z)

- The denominator term:

$$P(z) = \int_p P(z,p)dp$$

- Probability of seeing the data z from the model, over all parameter space
- Often doesn't have a closed form solution—evaluating numerically can also be difficult
    - E.g. if p is a three dimensional, then if we took 1000 grid points in each direction, the grid representing the function to be integrated has $1000^3 = 10^9$ points

Maximum *a posteriori* (MAP) estimation

- Instead of working with the full term, just use the numerator:

$$P(p|z) = \frac{P(z|p) \cdot P(p)}{P(z)}$$

- The denominator is a constant, so the numerator is proportional to the posterior we are trying to estimate

- Then the ***p*** which yields max($P(z|p) \cdot P(p)$) is the same ***p*** that maximizes $P(p|z)$

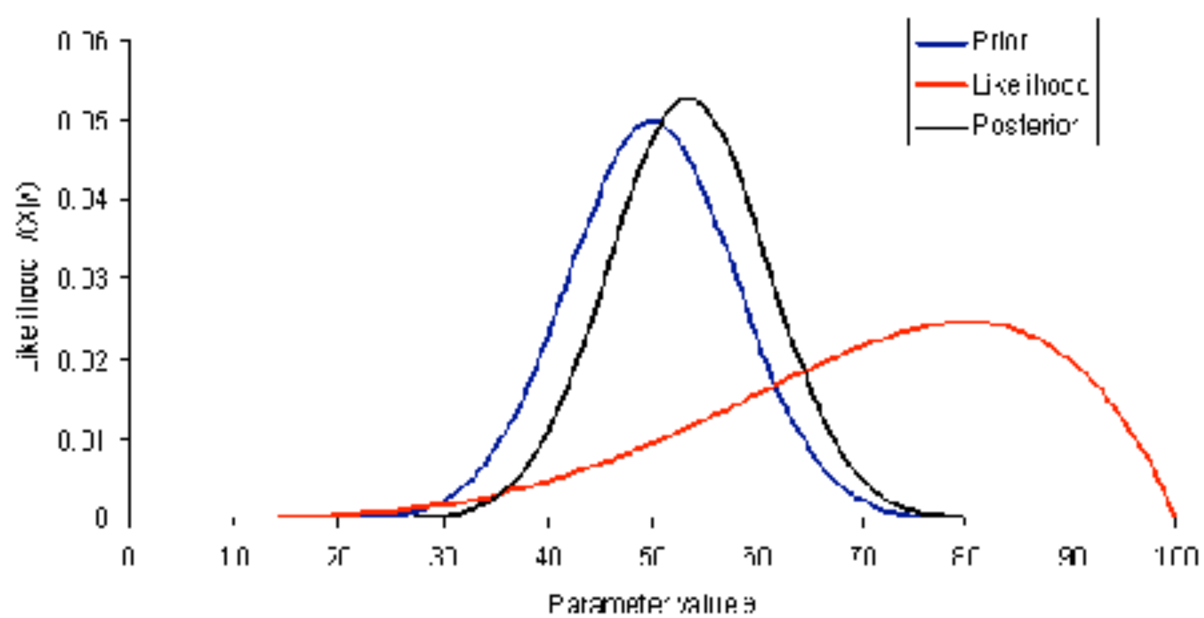
- If we only need a point estimate, MAP gets around needing to estimate $P(z)$

Bayesian Parameter Estimation

- Can think of Bayesian estimation as a map, where we update the prior to a new posterior based on data

$$P(p) \longrightarrow \boxed{\times \frac{P(z|p)}{P(z)}} \longrightarrow P(p|z)$$

Prior   Likelihood/P(z)   Posterior



Conjugate Priors

- For a likelihood distribution, there may be a distribution family for our prior, which makes the posterior and prior come from the same type of distribution

- This is called a **conjugate prior** for that likelihood

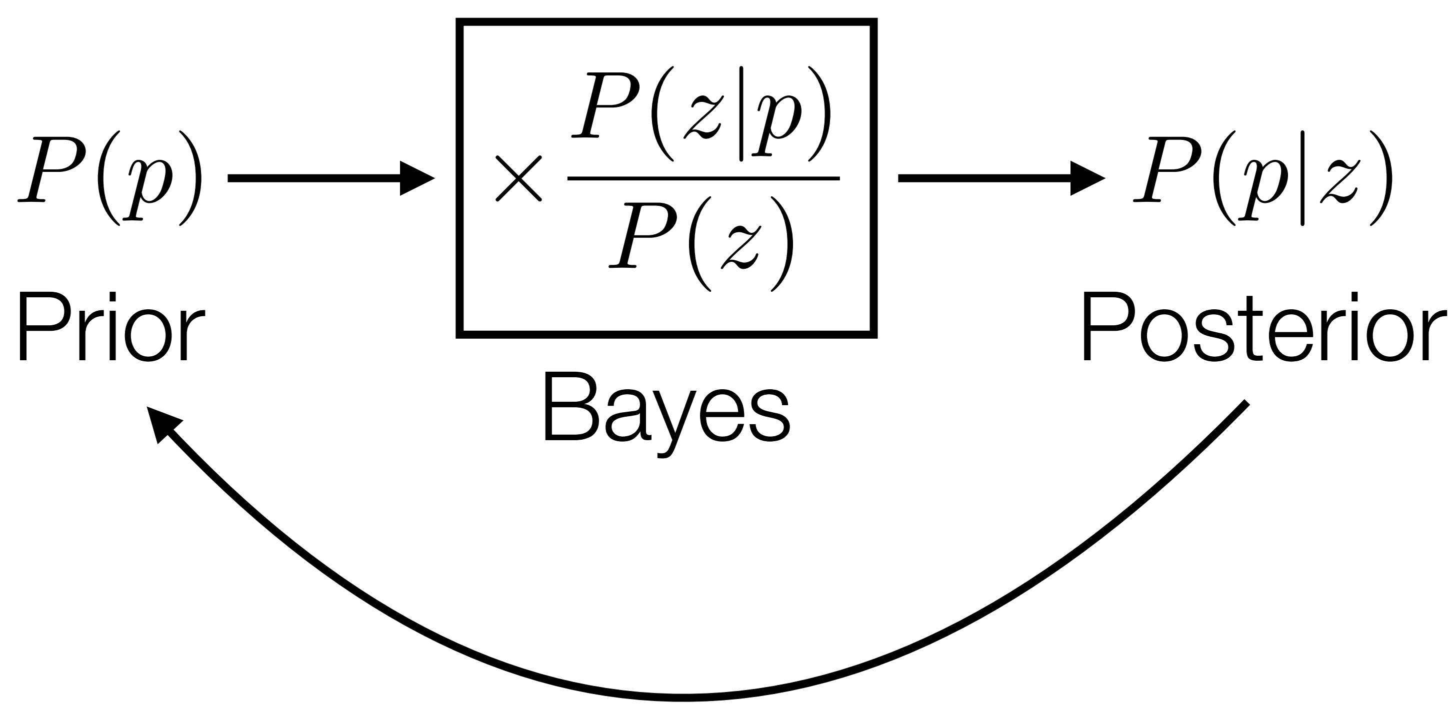
- For example, a gamma distribution is the conjugate prior for a Poisson likelihood.

$$\underbrace{P(p)}_{\text{Gamma}} \longrightarrow \underbrace{\boxed{\times \frac{P(z|p)}{P(z)}}}_{\text{Poisson}} \longrightarrow \underbrace{P(p|z)}_{\text{Gamma}}$$

Why conjugate priors?

- If we have a conjugate prior, we can calculate the posterior directly from the likelihood and the prior—handles the issue with calculating the denominator P(z)

- Also makes it easier to repeat Bayesian estimation—making the posterior the prior and updating as new data comes in



Conjugate prior example: coin flip

- Let z be the data—i.e. the coin flip outcome, z = 1 if it's heads, z = 0 if it's tails
- Let θ be the probability the coin shows heads
- Likelihood: Bernoulli distribution

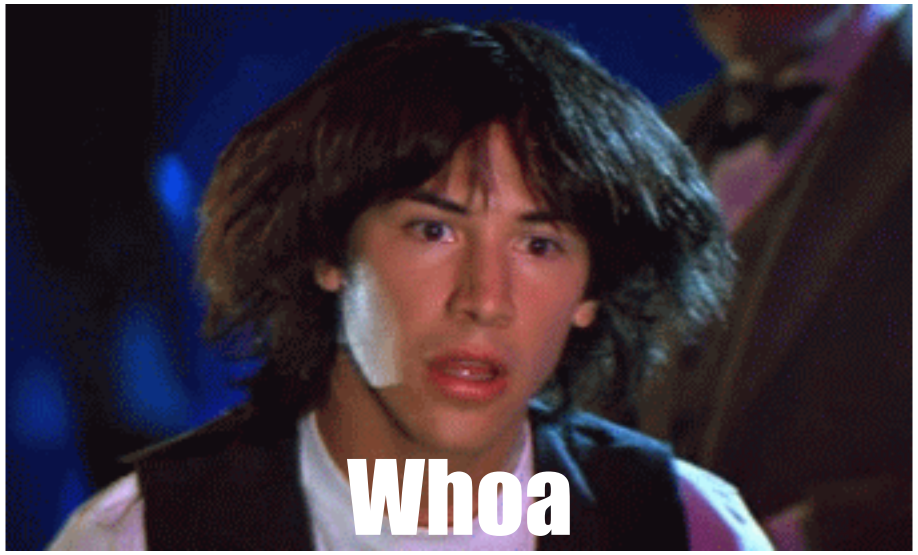
$$P(z|\theta) = \theta^z (1-\theta)^{1-z}$$

Conjugate prior example: coin flip

- **Conjugate prior**: beta distribution

$$P(\theta|\alpha,\beta) = \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1} d\theta}$$

- α and β are **hyperparameters** - shape parameters that describe the distribution of the model parameters



How does the posterior work out to be a beta distribution as well?

$$P(\theta|z) = \frac{P(z|\theta)P(\theta|\alpha,\beta)}{P(z)}$$

$$= \frac{\theta^z(1-\theta)^{1-z}\frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1}d\theta}}{P(z)}$$

$$= \frac{\theta^z(1-\theta)^{1-z}\frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1}d\theta}}{\int_0^1 P(z,\theta)d\theta}$$

$$= \frac{\theta^z(1-\theta)^{1-z}\frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1}d\theta}}{\int_0^1 \theta^z(1-\theta)^{1-z}d\theta}$$

Etc.—but you can see it will work out to be beta distributed

Coin flip example - Posterior

- **Beta distributed** with posterior hyperparameters:

$$\alpha_{post} = \alpha + z \qquad \beta_{post} = \beta + 1 - z$$

- If we take multiple data points, this works out to be:

$$\alpha_{post} = \alpha + \sum_{i=1}^{n} z_i \qquad \beta_{post} = \beta + n - \sum_{i=1}^{n} z_i$$

Sampling methods: approximating a distribution

- What if we want priors that aren't conjugate? Or what if our likelihood is more complicated and it isn't clear what the conjugate prior is?
- Now we need some way to get the posterior, even though the denominator term is annoying
- How to approximate the distribution?

Markov Chain Monte Carlo (MCMC)

- Sampling-based methods—in particular, **Markov chain Monte Carlo (MCMC)**
- Also used for many other things! Can approximate distributions more generally—used in cryptography, calculating neutron diffusion, all sorts of things

Markov Chain Monte Carlo (MCMC)

- **MCMC** is a method for sampling from a distribution
- **Markov chain**: a type of (discrete) Markov process
    - Markov: memoryless, i.e. what happens at the next step only depends on the current step
- **Monte Carlo methods** are a class of algorithms that use sampling/randomness—often used to solve deterministic problems (such as approximating an integral)

Markov Chain Monte Carlo (MCMC)

- **Main idea**: make a Markov chain that converges to the distribution we're trying to sample from (the posterior)
  - The Markov chain will have some transient dynamics (burn-in), and then reach an equilibrium distribution which is the one we're trying to approximate

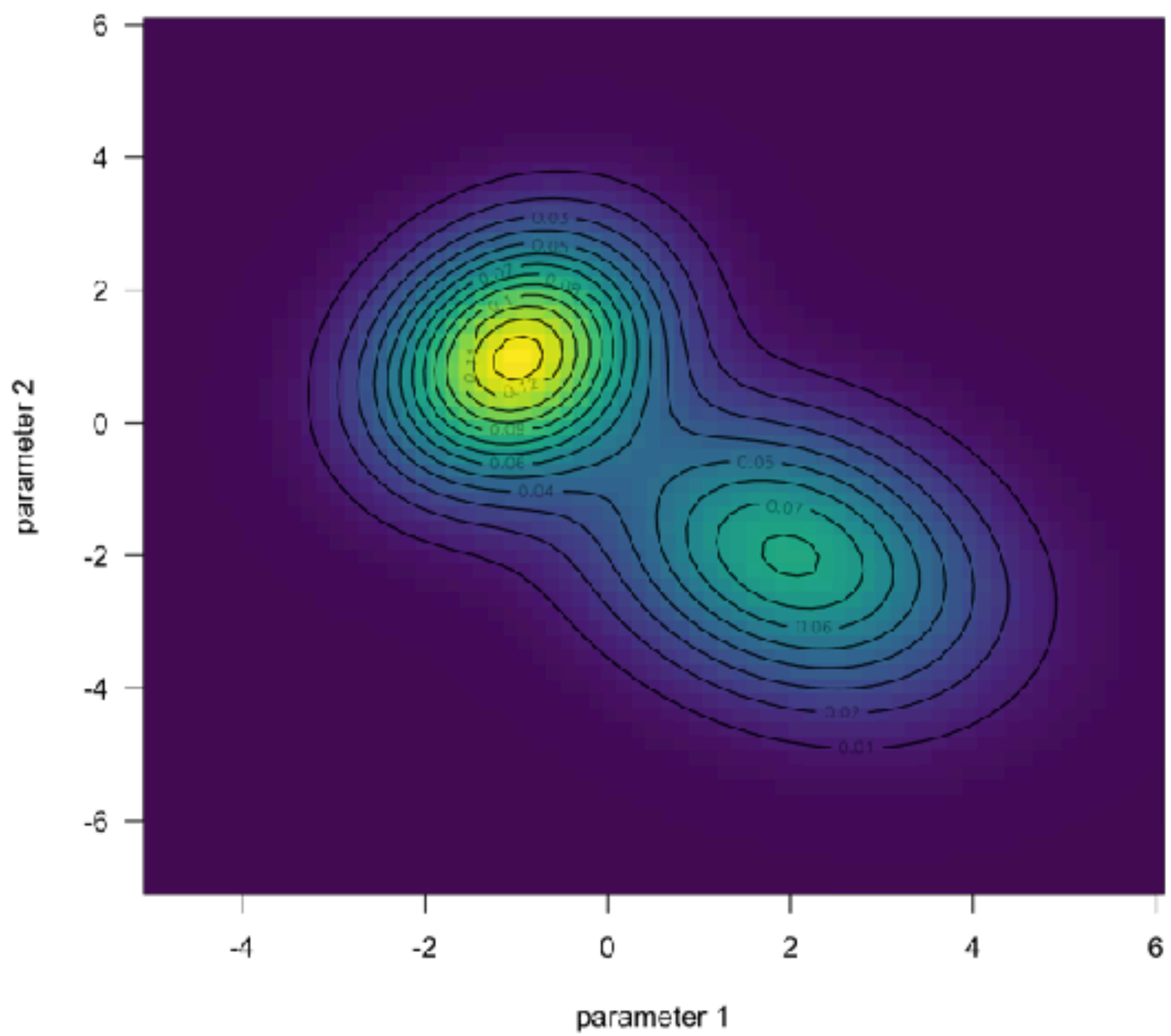
Markov Chain Monte Carlo (MCMC)

- Many MCMC methods are based on random walks
    - Set up walk to spend more time in higher probability regions
- Typically don’t need the actual distribution for this, just something proportional—so we can get the relative probability density at two points
    - So we don’t need to calculate P(z)! We can just use the numerator

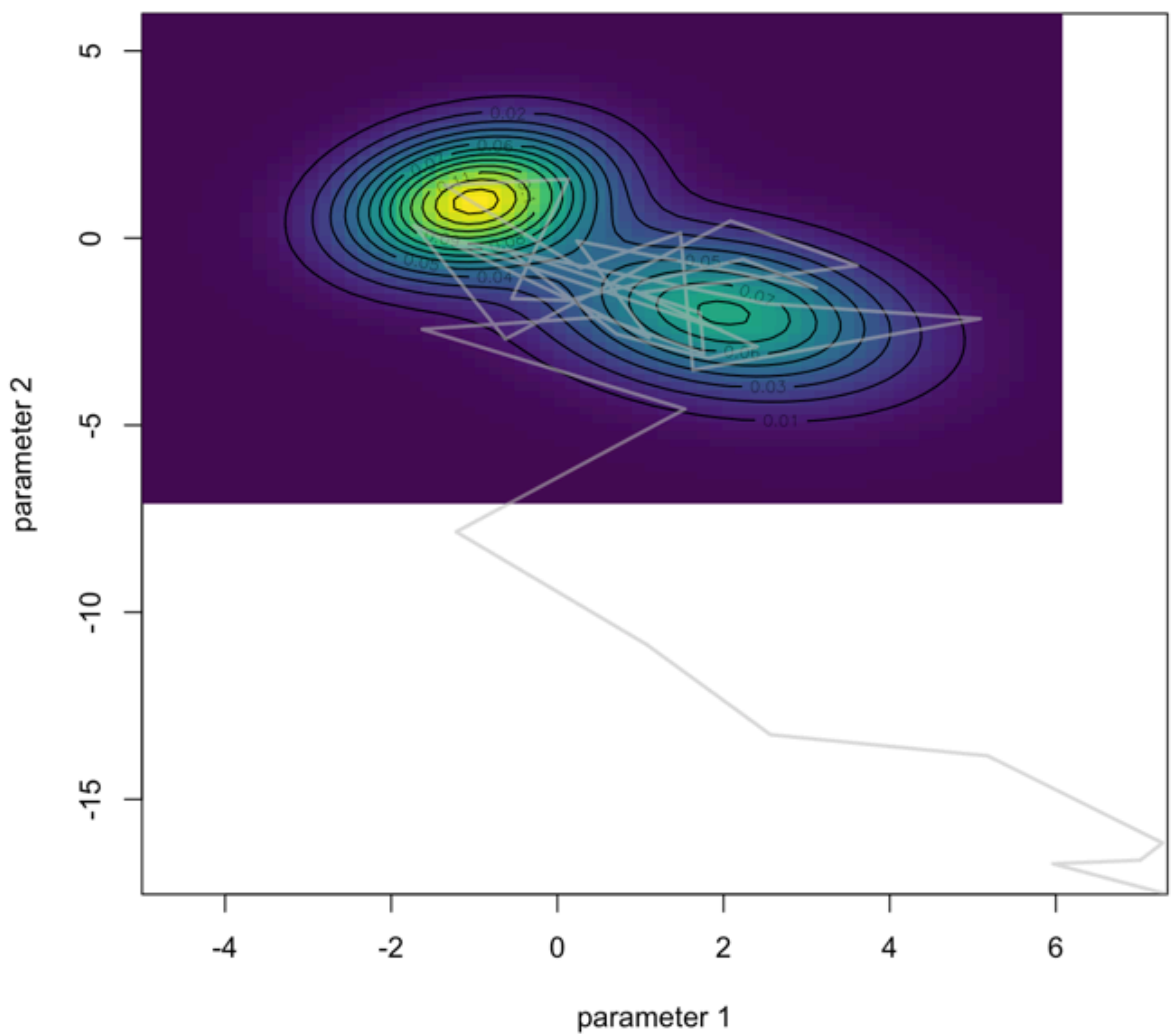
Example adapted from https://nicercode.github.io/guides/mcmc/

Example

- Suppose two parameters, with likelihood x prior:

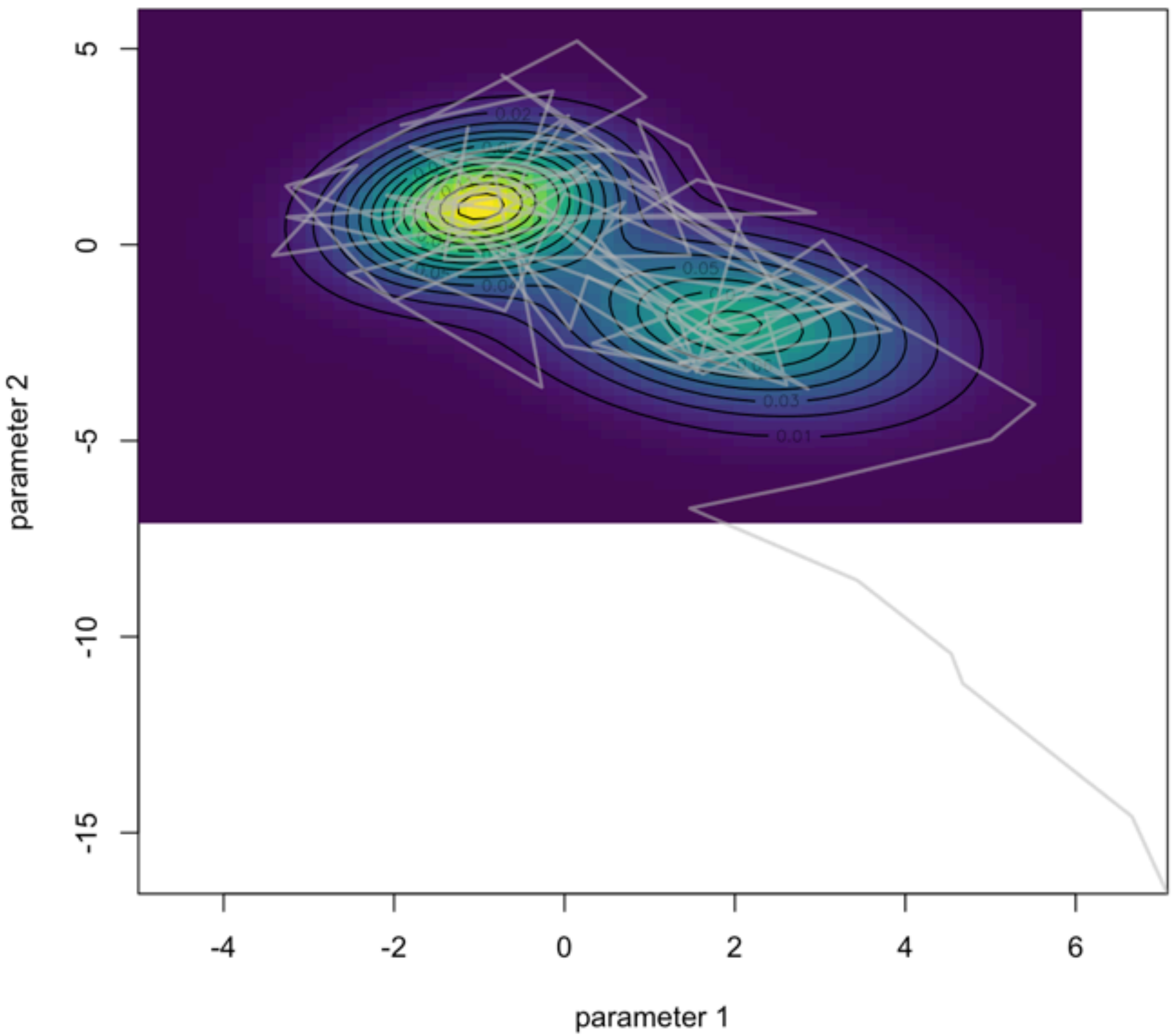


Sample path

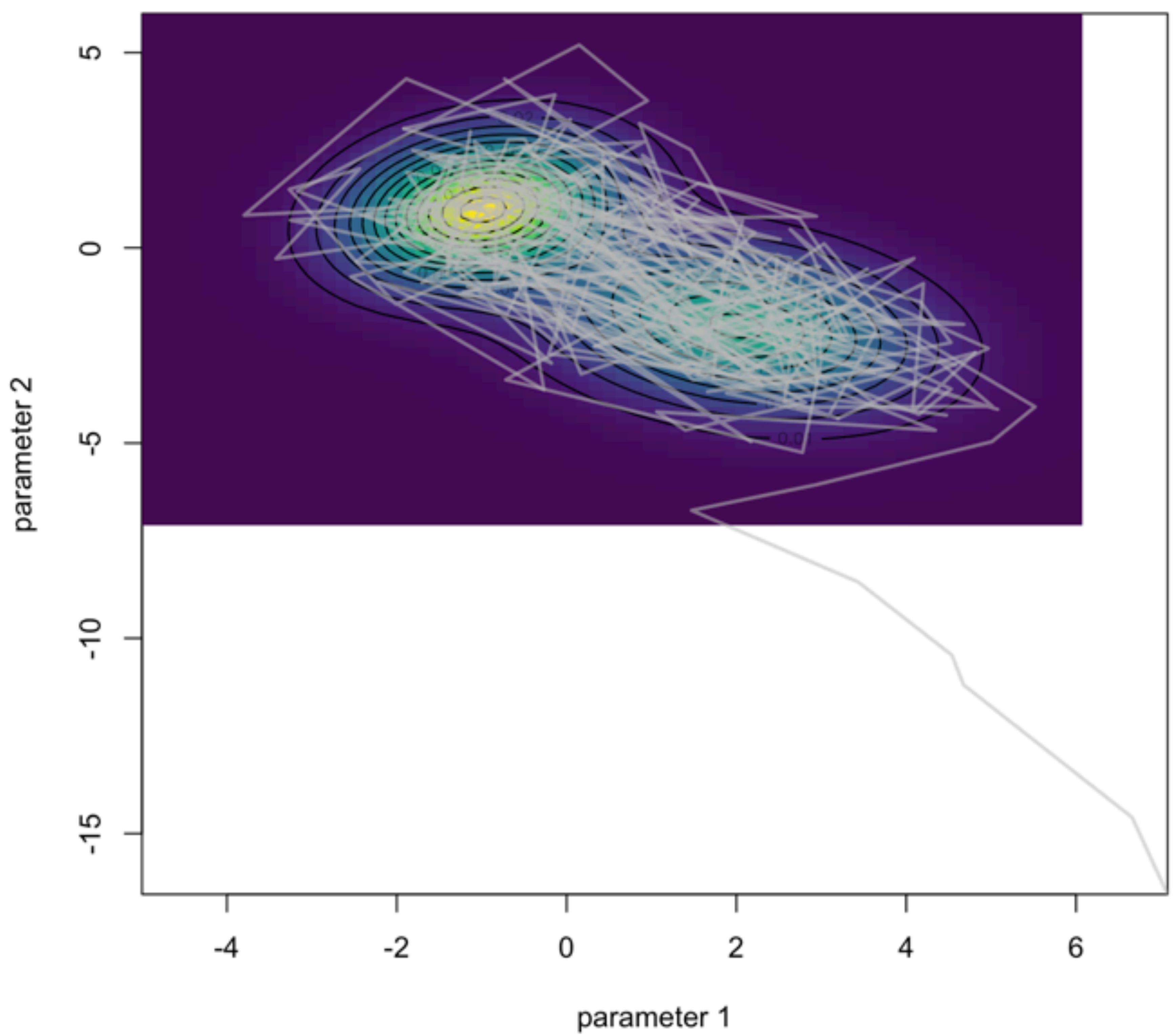


0.02
0.01
0.03
0.05
0.07
0.04
5
0
-5
-10
-15
-4
-2
0
2
4
6
parameter 1
parameter 2

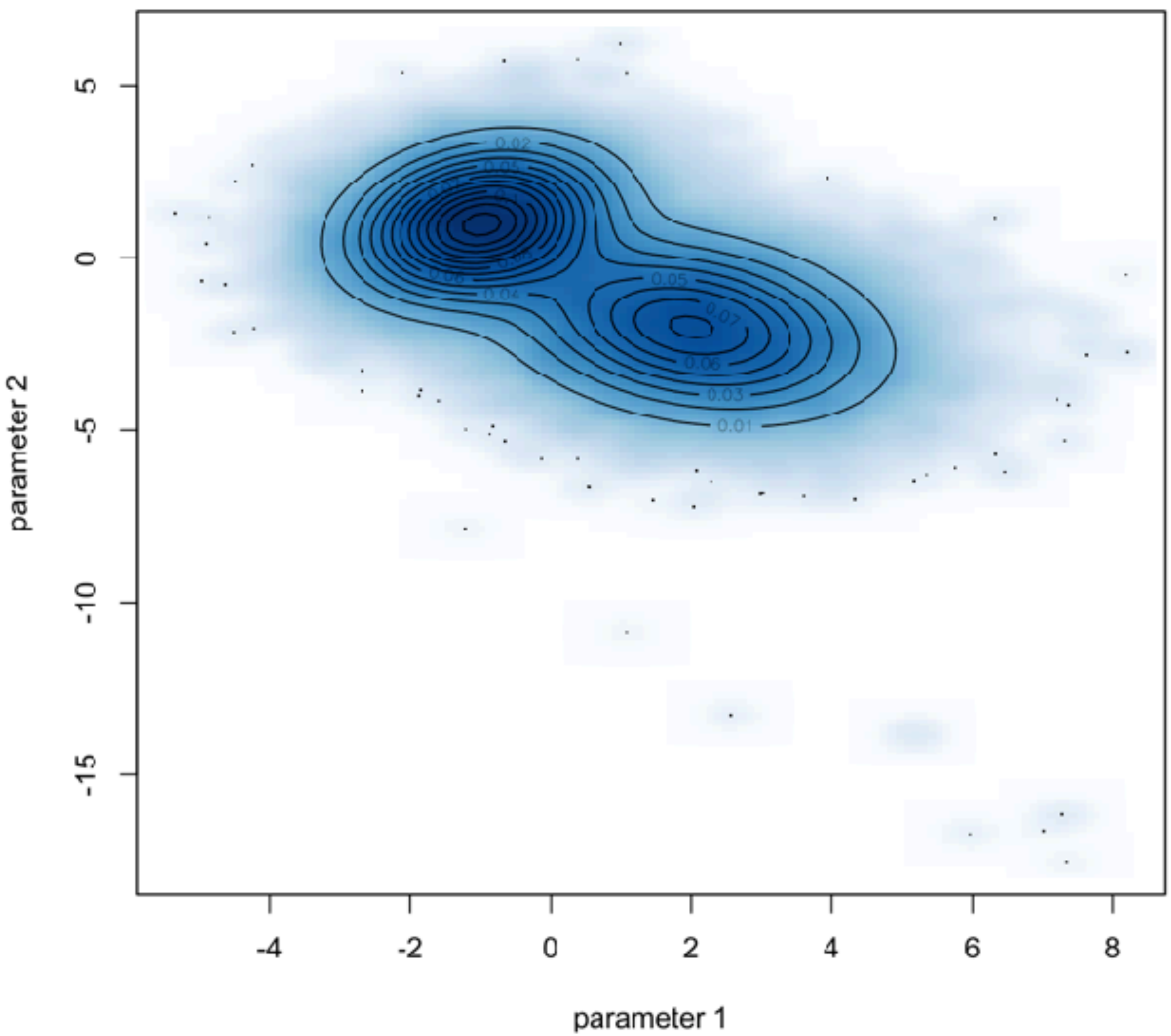
Sample path



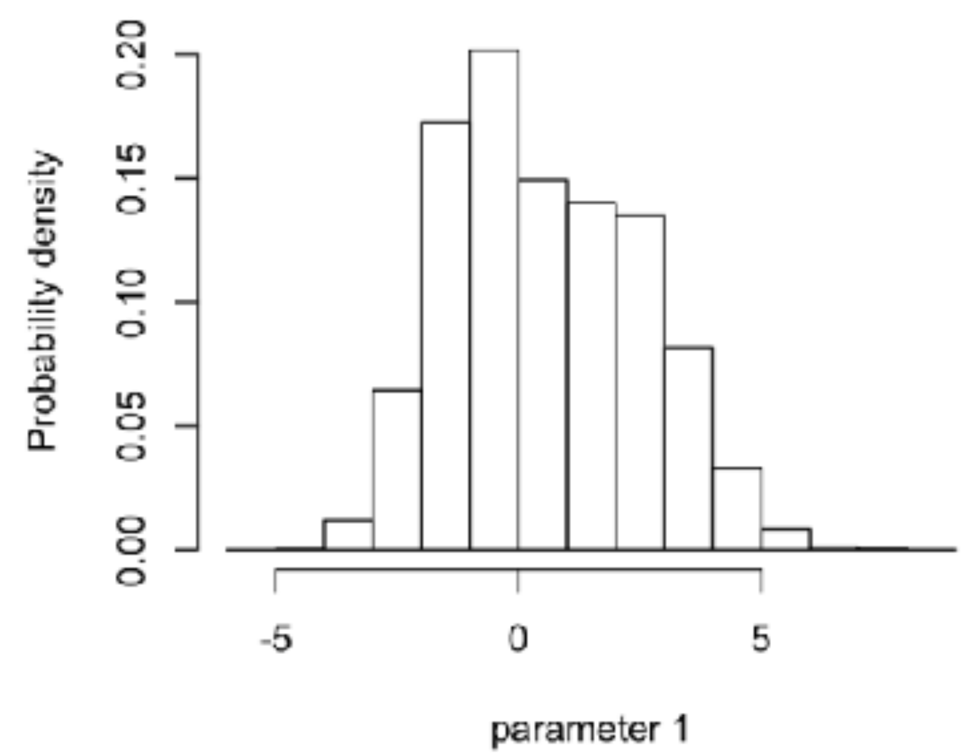
Sample path



Sampled density



Can also get marginals:



Example: Metropolis Algorithm

- Idea is to 'walk' randomly through parameter space, spending more time in places that are higher probability—that way, the overall distribution draws more from higher probability spots

- Setup—we need

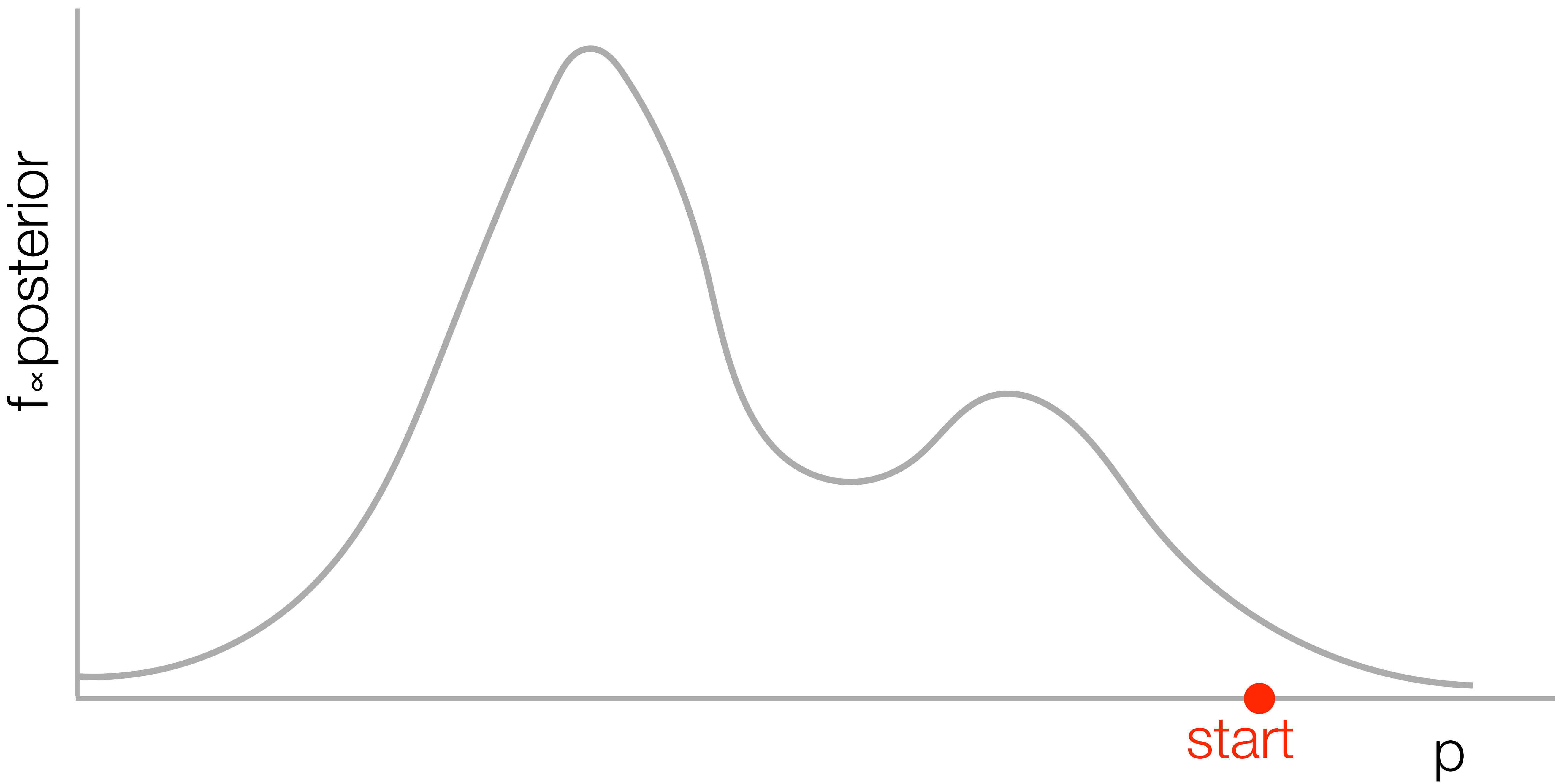
  - A function $f(p)$ proportional to the distribution we want to sample, in our case $f(p) = P(z|p) \cdot P(p)$

  - A proposal distribution (how we choose the next point from the current one) - more on this in a minute

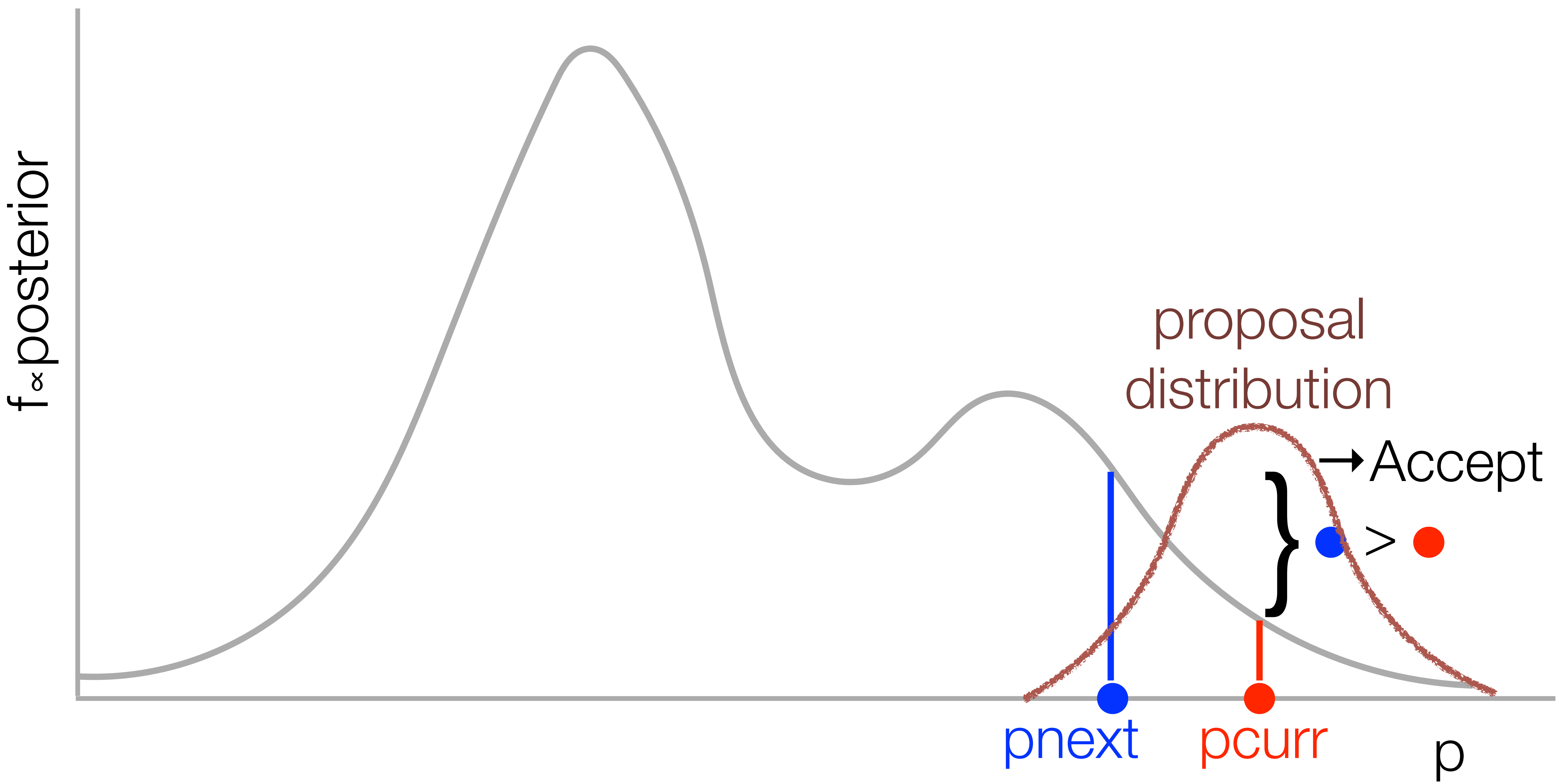
Metropolis Algorithm

- Start at some point in parameter space
- For each iteration
    - Propose a new random point p_{next} based on the current point p_{curr} (using the proposal distribution)
    - Calculate the **acceptance ratio**, $\alpha = f(p_{next})/f(p_{curr})$
        - If $\alpha \geq 1$, the new point is as good or better—accept
        - If $\alpha < 1$, accept with probability α

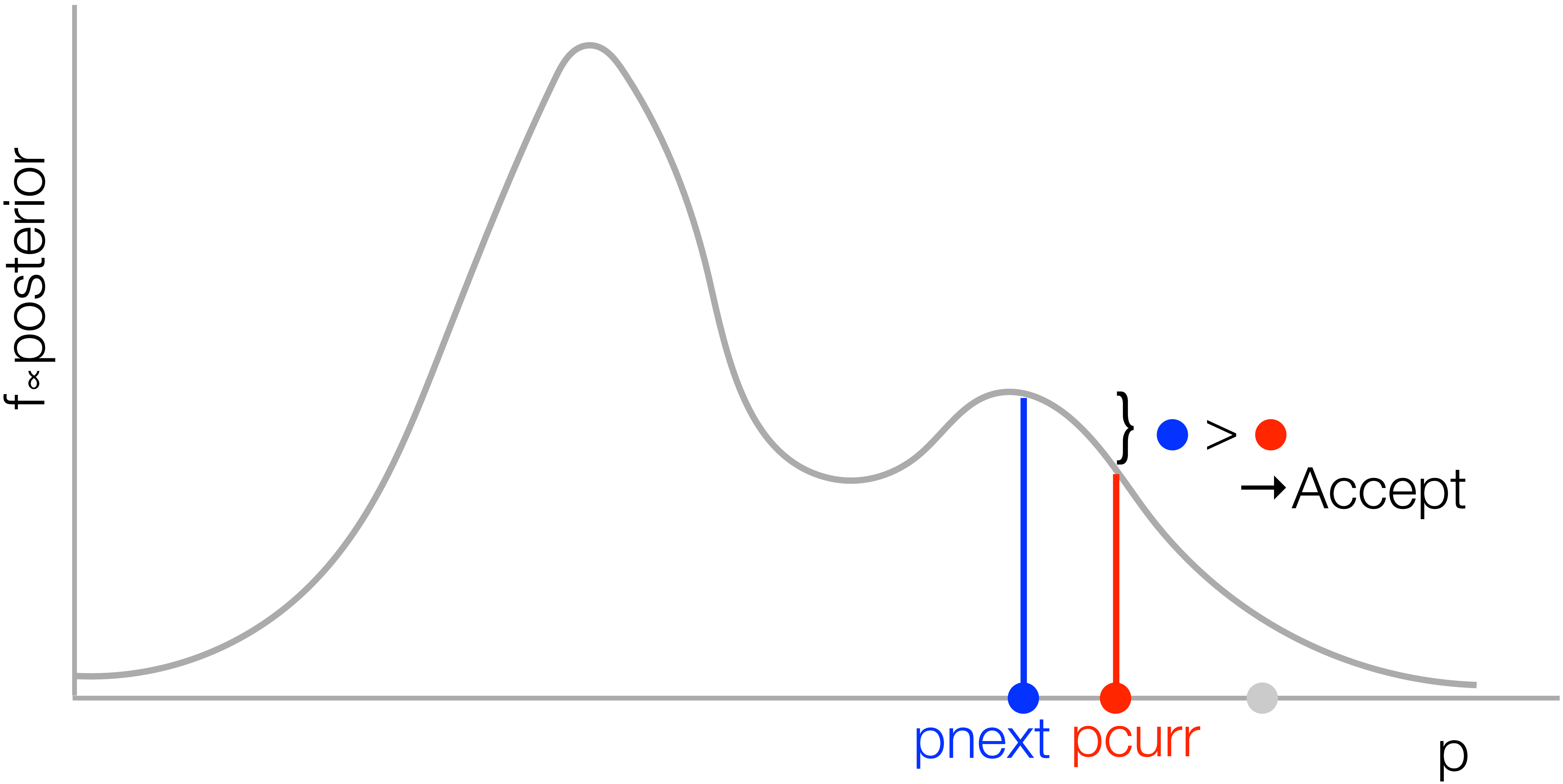
What does the metropolis algorithm do?



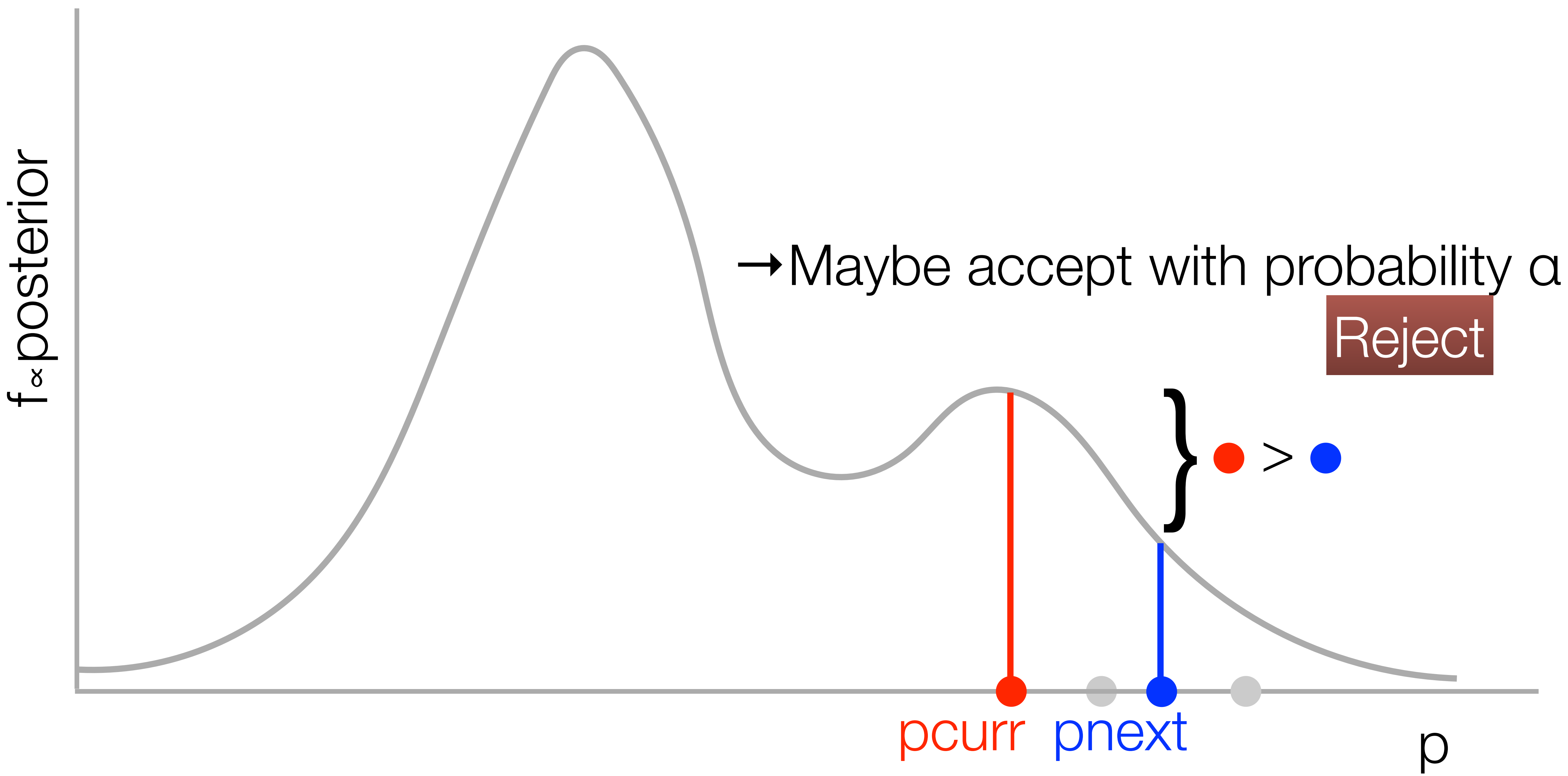
What does the metropolis algorithm do?



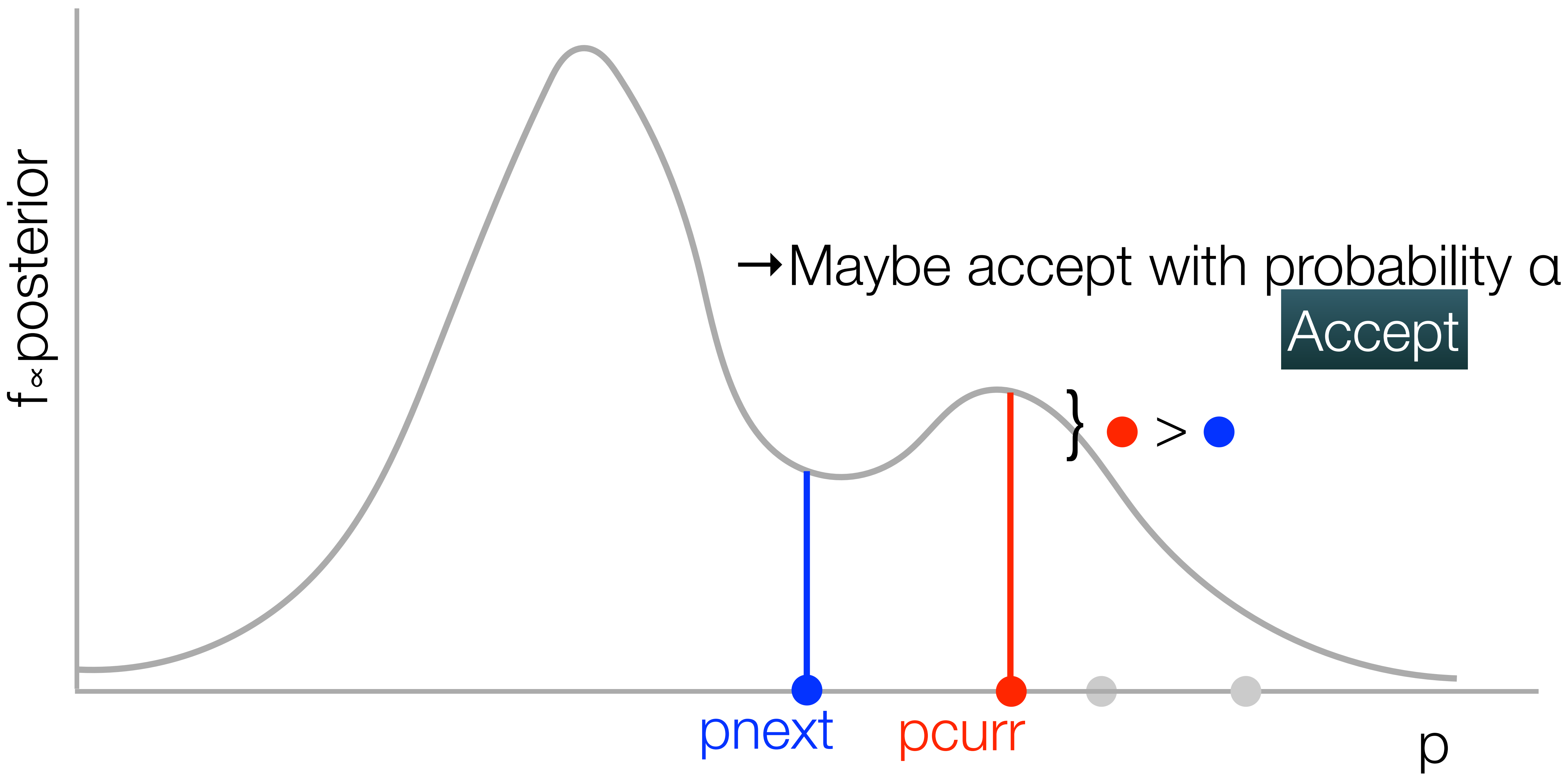
What does the metropolis algorithm do?



What does the metropolis algorithm do?



What does the metropolis algorithm do?



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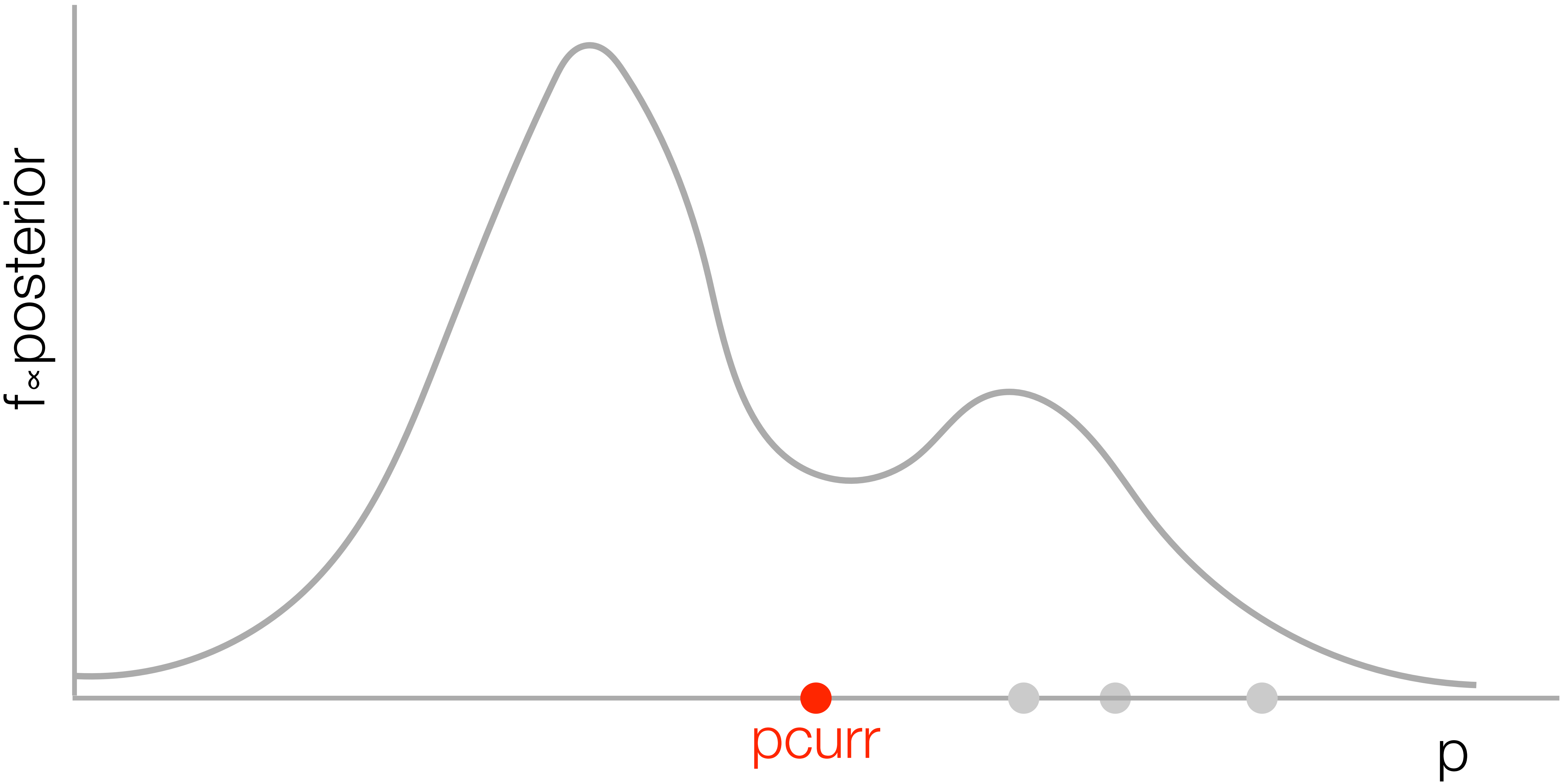
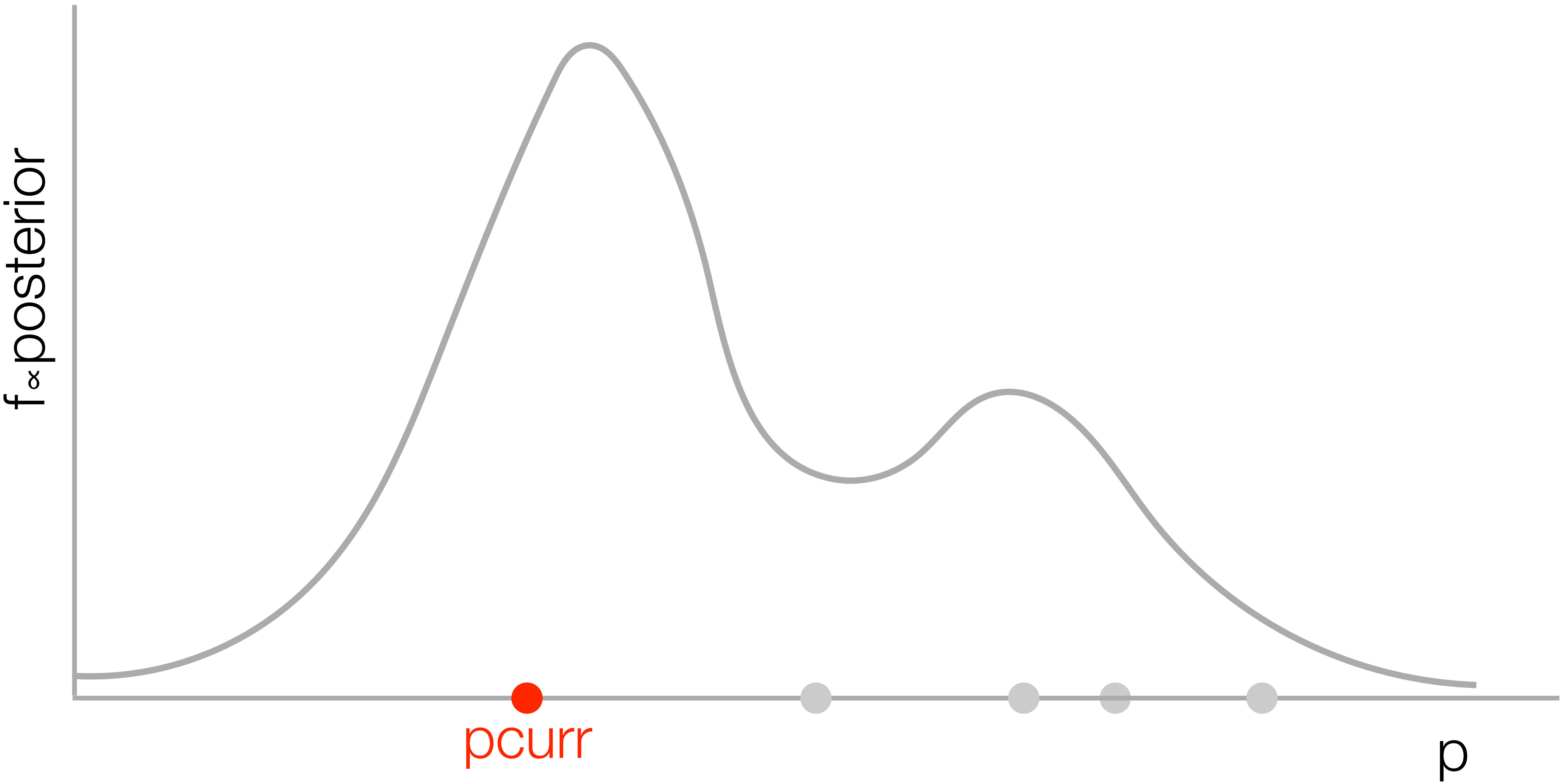


What does the metropolis algorithm do?



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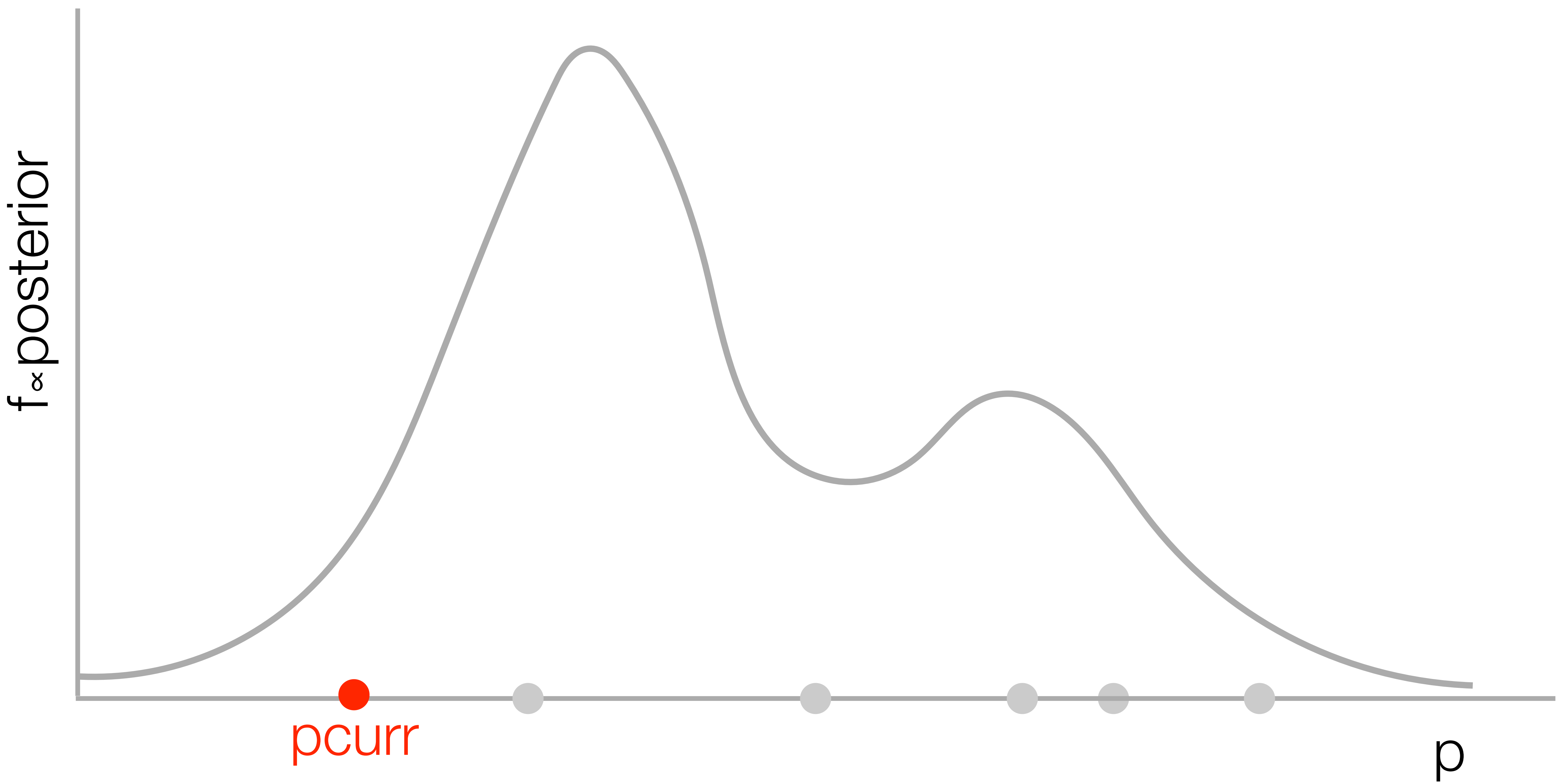
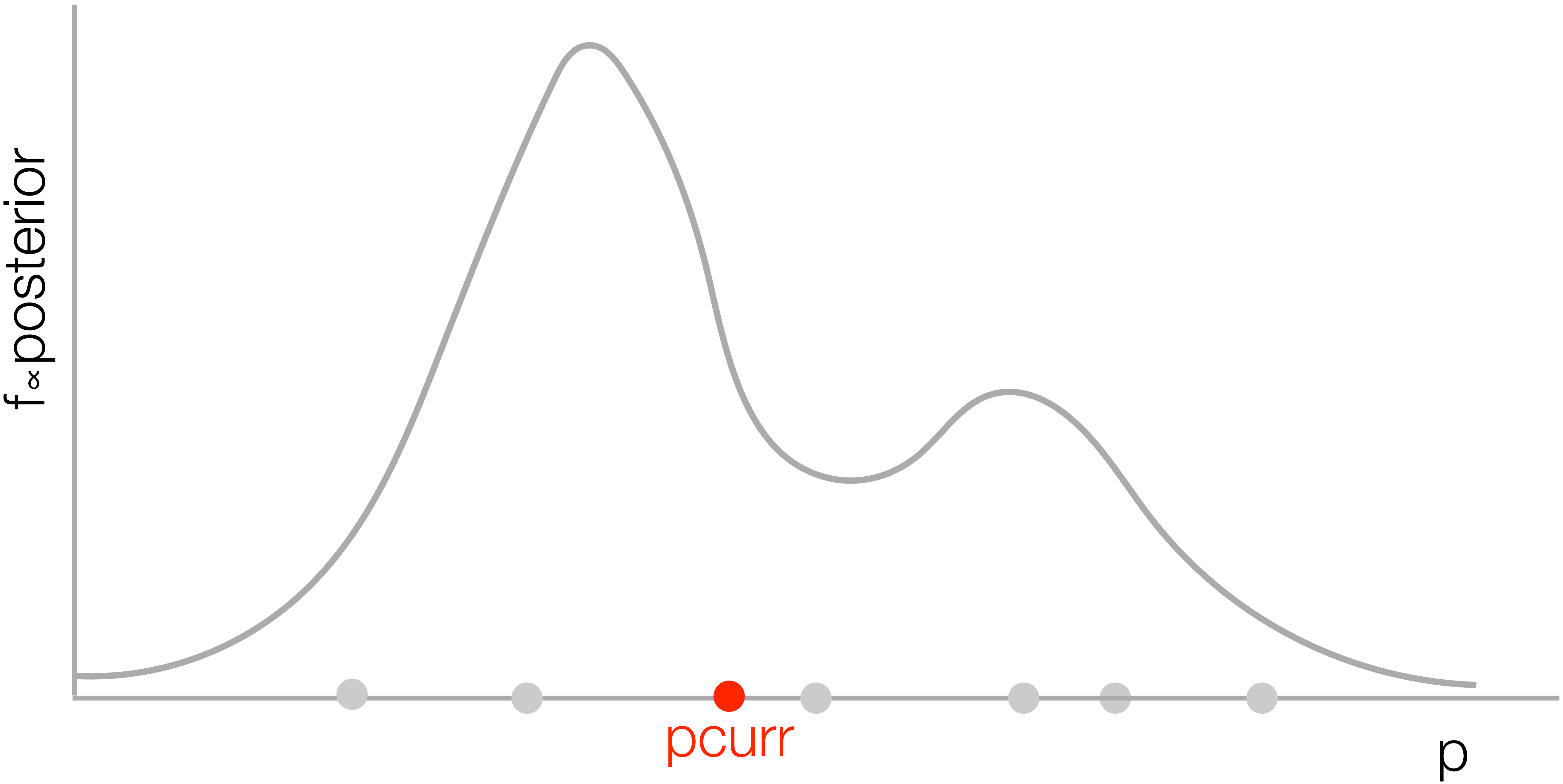
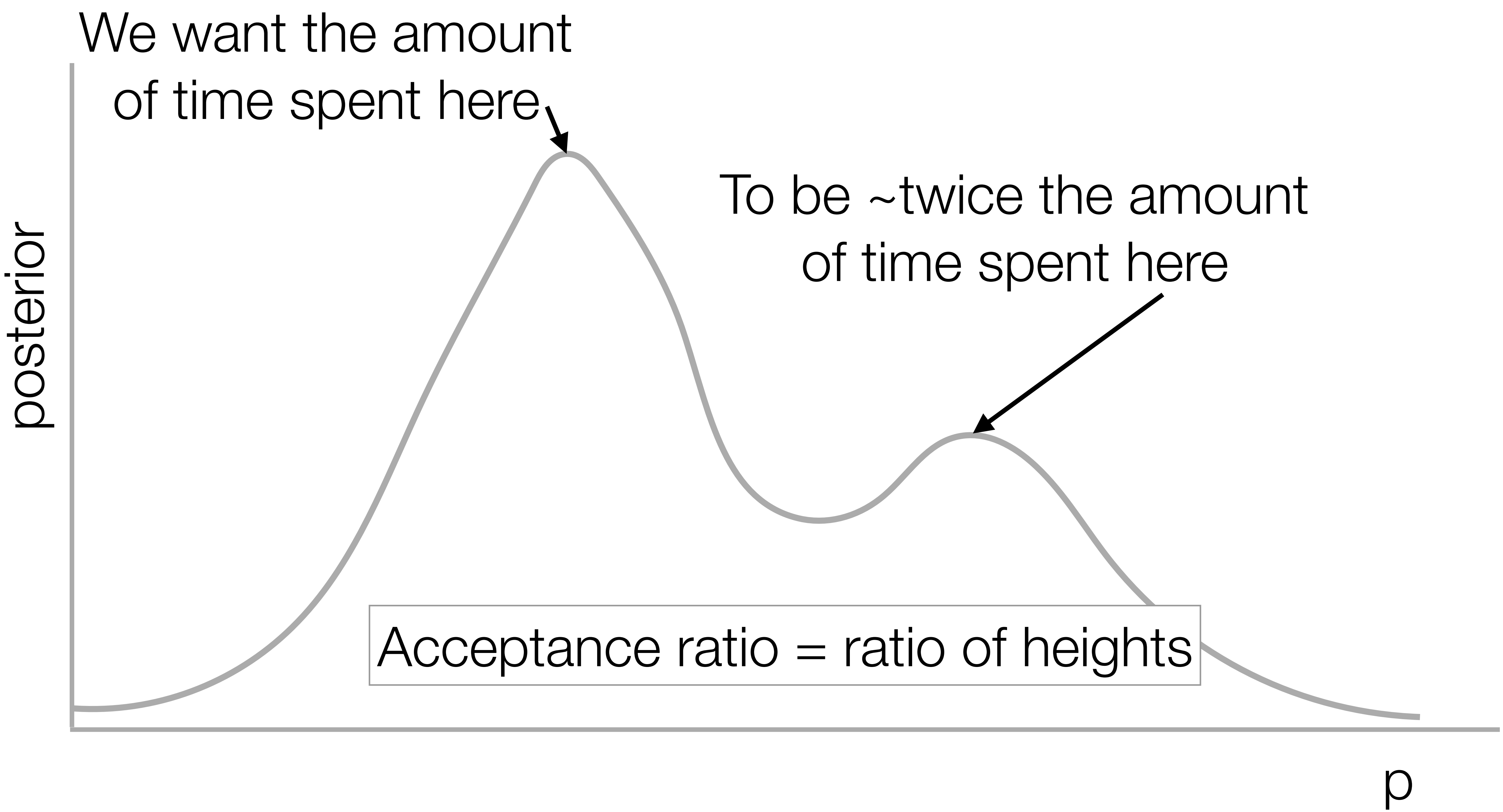


What does the metropolis algorithm do?



Why does this recover the posterior distribution? Key is the acceptance ratio α



Acceptance ratio = ratio of heights

Why does this recover the posterior distribution?

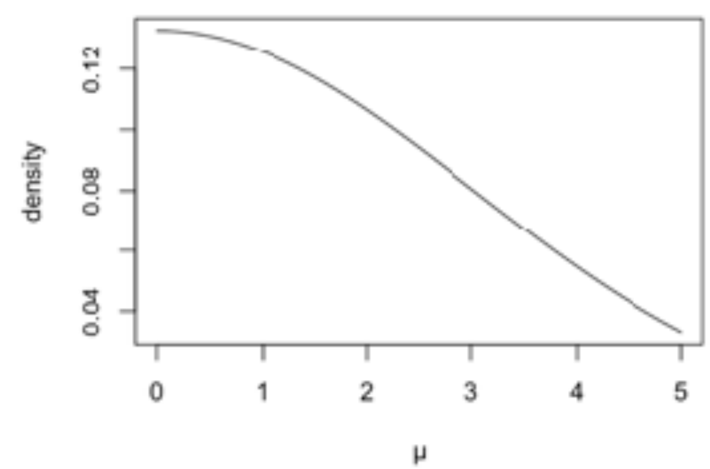
- The acceptance ratio $\alpha = f(p_{next})/f(p_{curr})$
- Note it is equal to $P(p_{next}|z)/P(p_{curr}|z)$ since the denominators cancel
- Suppose we're at the peak
    - If $f(p_{curr}) = 2\ f(p_{next})$, then $\alpha = 1/2$, i.e. we accept with 1/2 probability
- Overall, will mean the number of samples we take from a region will be proportional to the height of the distribution

Proposal Distribution

- A distribution that lets us choose our next point randomly from our current one
- For Metropolis algorithm, must be symmetric
- Common to choose a normal distribution centered on current point
- Width (SD) of normal = proposal width
  - Choice of proposal width can strongly affect how the Markov chain behaves, how well it converges, mixes, etc.

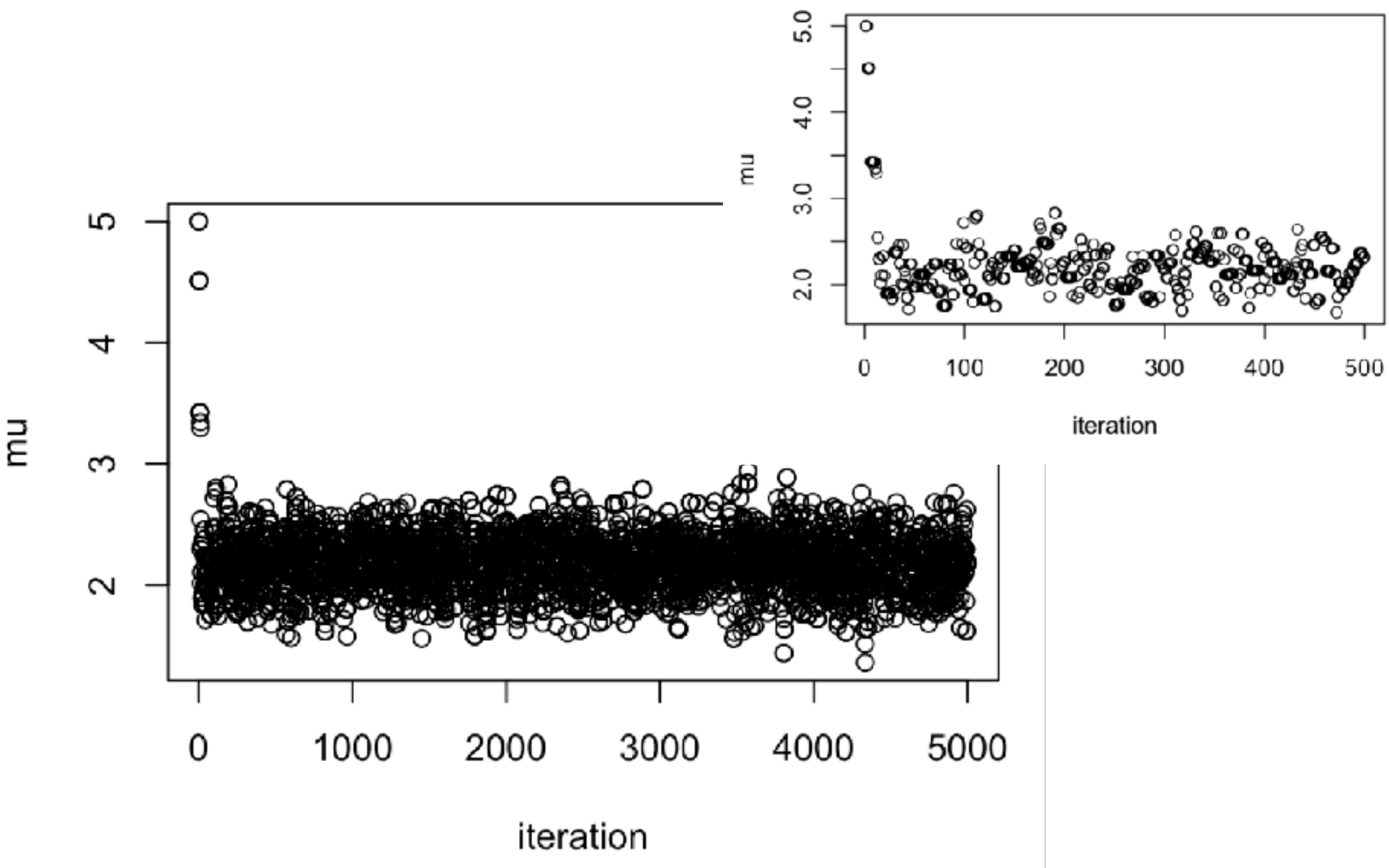
Example

- Model: normal distribution $\mathcal{N}(\mu, \sigma)$
  - Suppose σ is known, μ to be estimated
  - Likelihood: $P(z_i \mid \mu, 1) = f(z_i \mid \mu, 1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(z-\mu)^2}{2}}$ $\quad P(z \mid \mu) = \prod_{i=1}^{n} f(z_i \mid \mu, 1)$
- Prior: $\mu \sim \mathcal{N}(0, 3)$

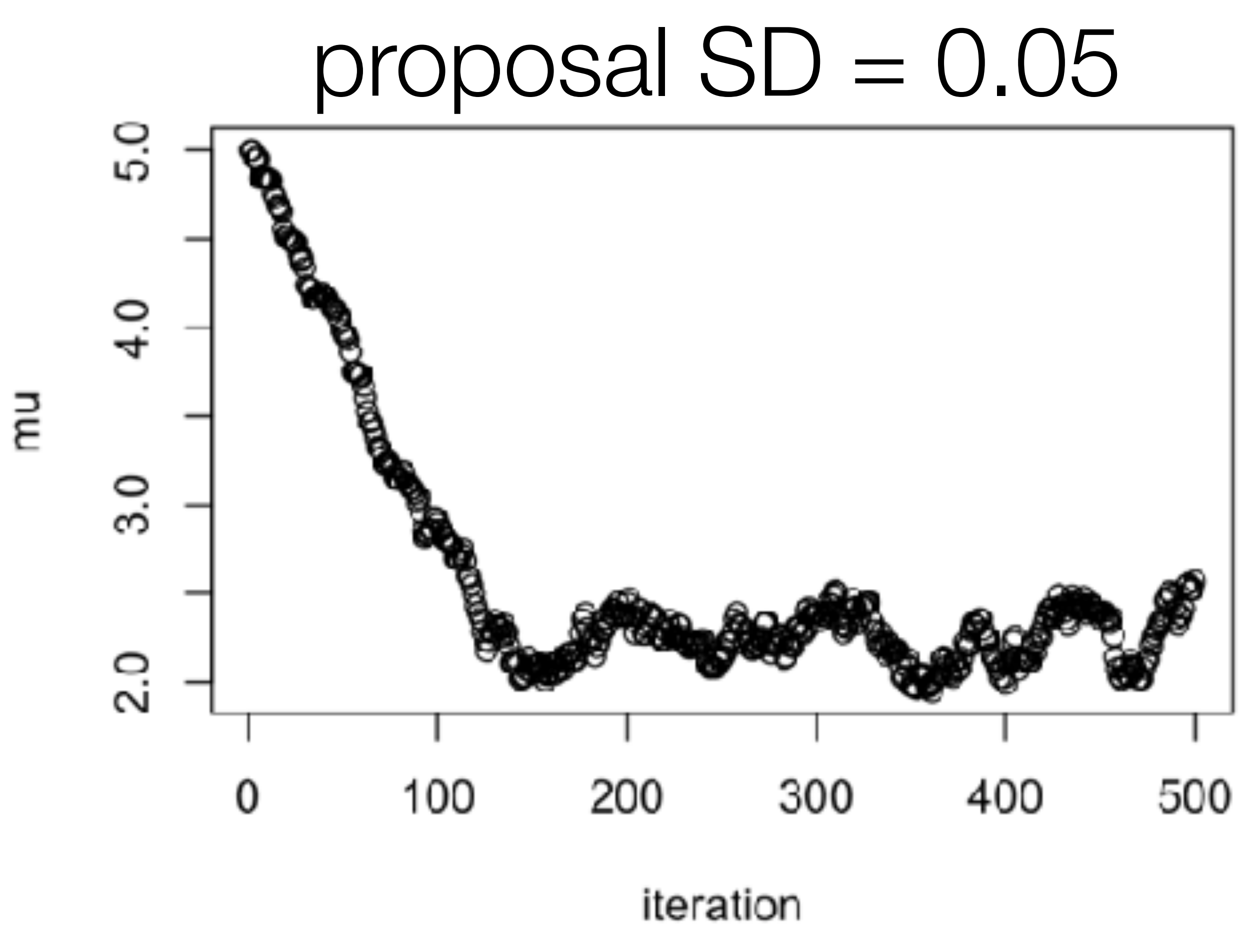


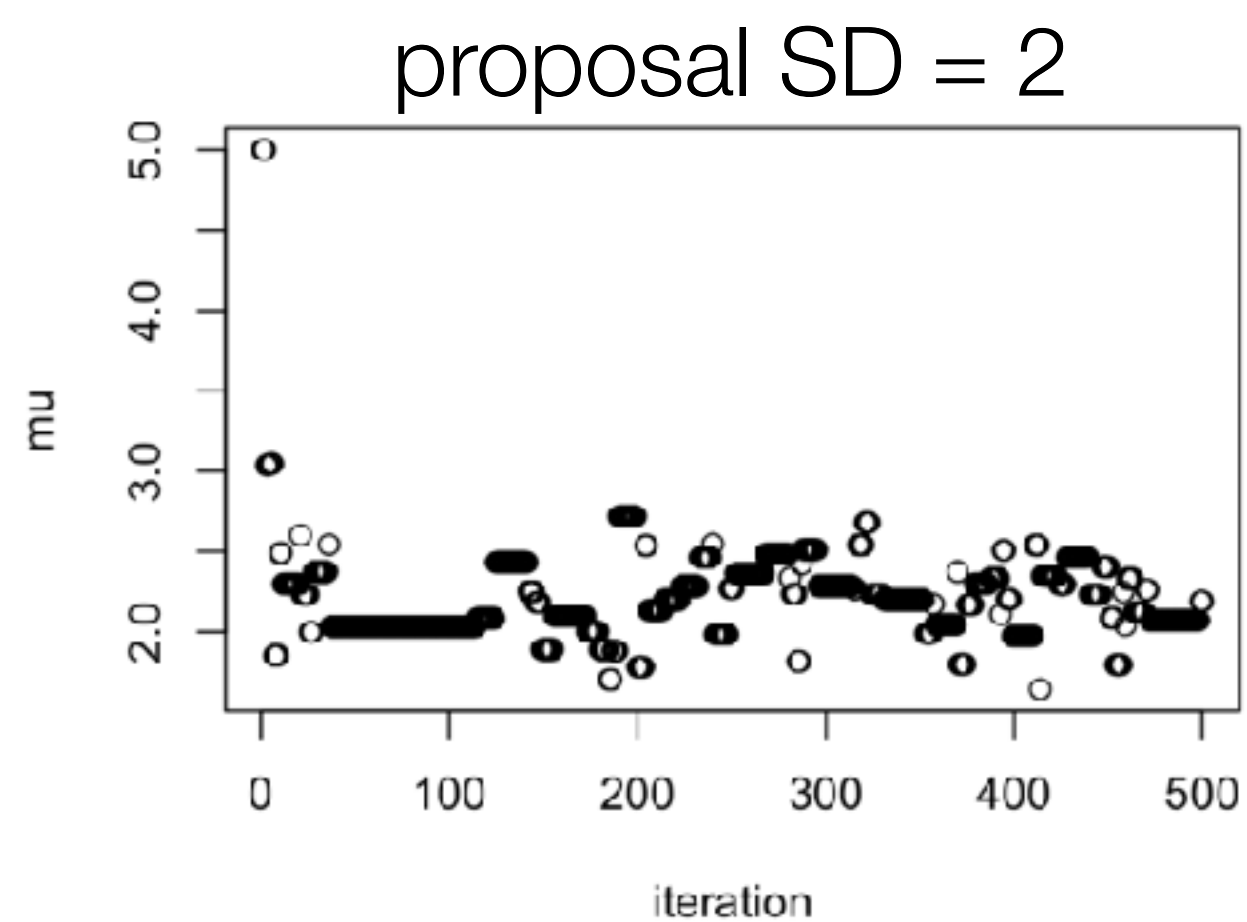
- Suppose we have 20 data points

Example - proposal width: SD = 0.5

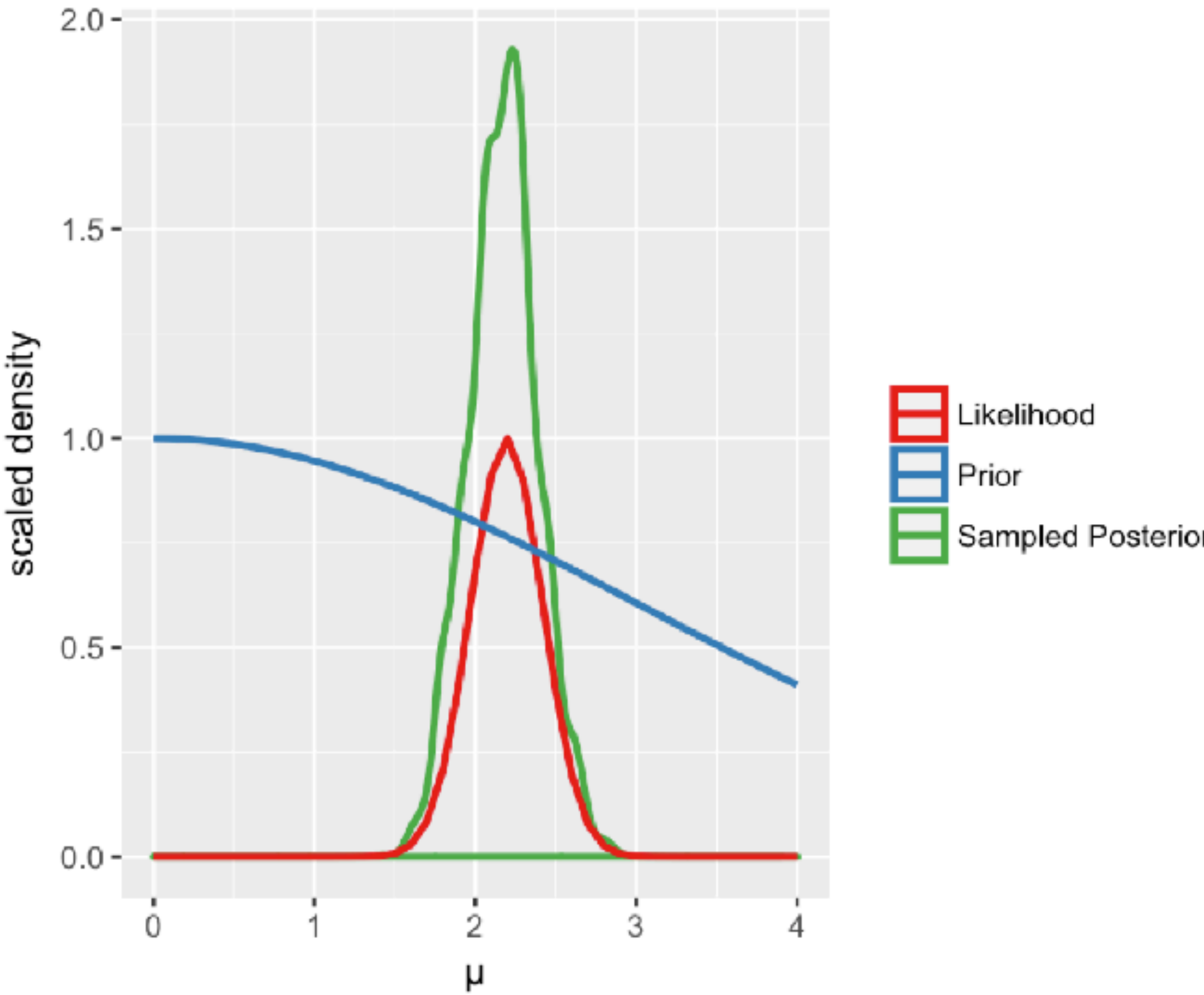


Goldilocks problem:
What happens if we change the proposal width?





Example: prior, likelihood, and posterior (all scaled)

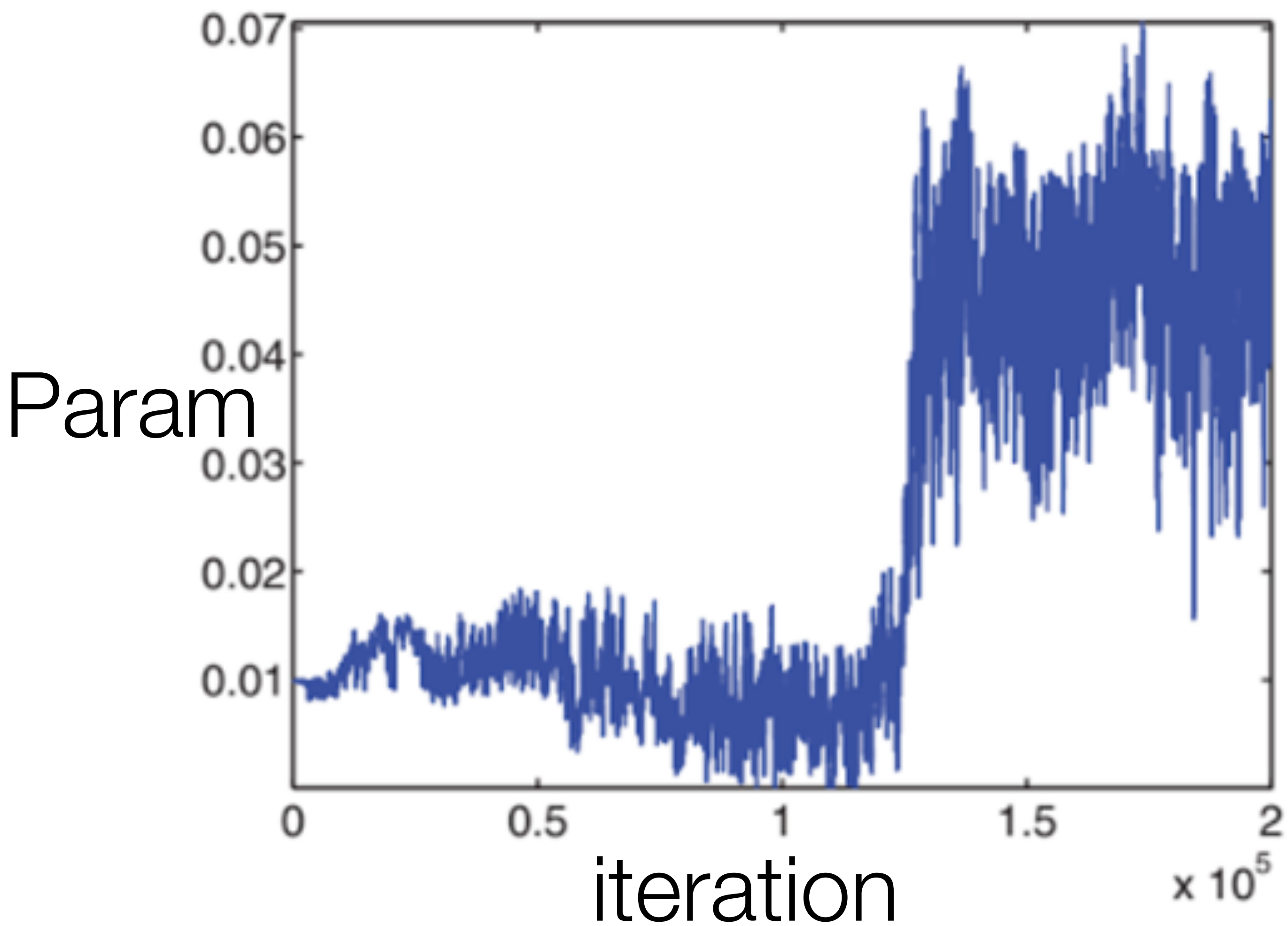


Assessing convergence

- MCMC methods will let us sample the posterior once they've converged to their equilibrium distribution
- How to know once we've reached equilibrium?
  - Visual evaluation of **burn-in**
  - Autocorrelation of elements in chain *k* iterations apart
- Also approaches to use in combination with/instead of burn-in: start with MAP estimation, multiple chains, etc.

Assessing convergence

- Often done visually
- Although, this can be misleading:



Chain shifts after 130,000 iterations due to a local min in sum of squares (Example from R. Smith, *Uncertainty Quantification*)

Metropolis & Metropolis-Hastings Caveats

- Assessing convergence—how long is burn-in?
  - What about when you have unidentifiability or multiple minima?
- Correlated samples
- How to choose a proposal width? (~size of next jump)

Wide range of methods

- Metropolis–Hastings
- Gibbs sampling
- Variations of the above: prior optimization, multi-start, adaptive methods, delayed rejection
  - DRAM (Delayed Rejection Adaptive Metropolis-Hastings)
- Many more!

Examples

American Journal of Epidemiology

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Advance Access publication:
June 9, 2017

Practice of Epidemiology

Application of an Individual-Based Transmission Hazard Model for Estimation of Influenza Vaccine Effectiveness in a Household Cohort

Joshua G. Petrie*, Marisa C. Eisenberg, Sophia Ng, Ryan E. Malosh, Kyu Han Lee, Suzanne E. Ohmit, and Arnold S. Monto

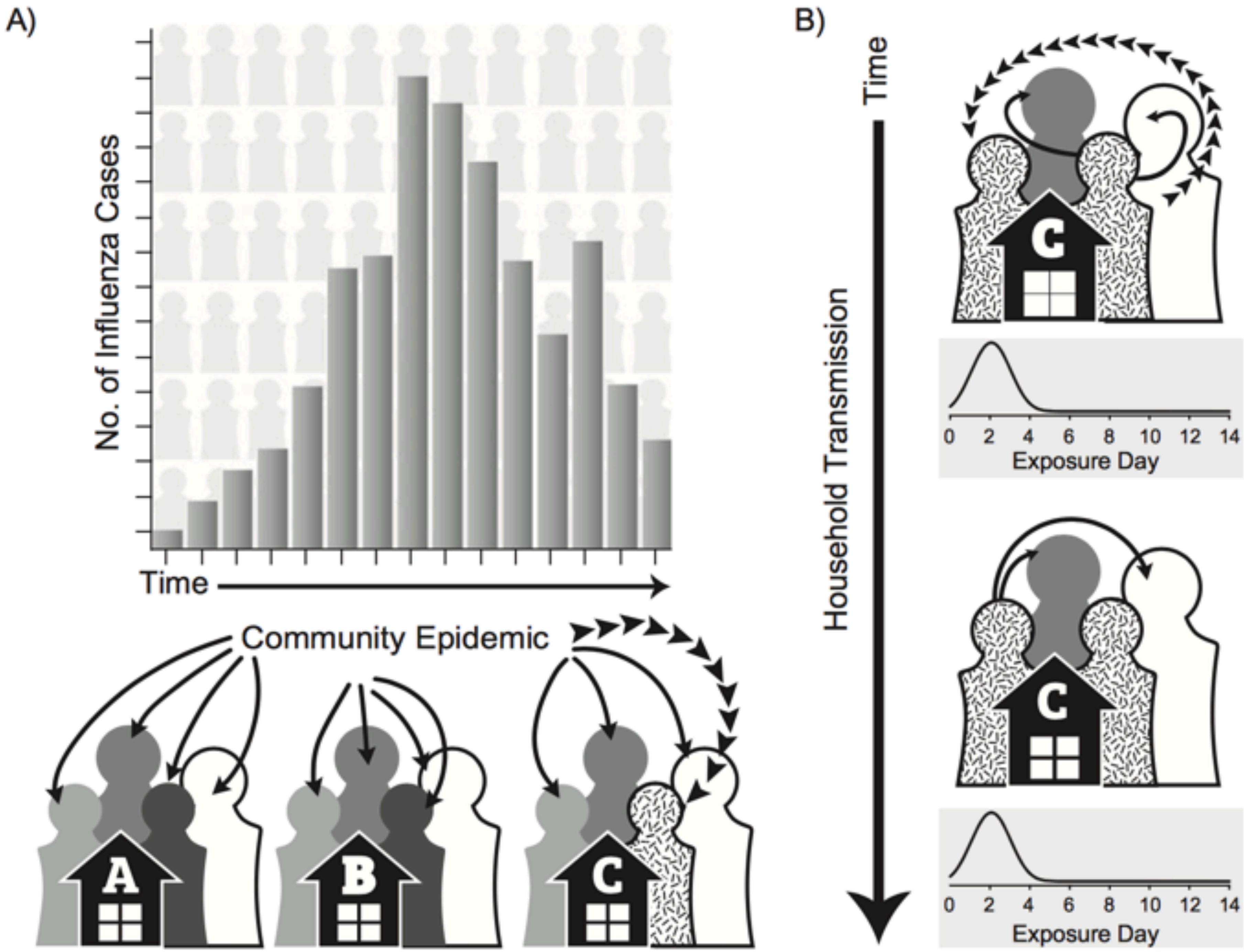

A)
No. of Influenza Cases
Time
Community Epidemic
A
B
C
B)
Time
Household Transmission
C
0 2 4 6 8 10 12 14
Exposure Day
C
0 2 4 6 8 10 12 14
Exposure Day

Table 2. Observed and Individual-Based Transmission Hazard Model–Predicted Influenza A(H3N2) Infections According to Infection Source, Age, Presence of High-Risk Health Condition, and Influenza Vaccination Status, Household Influenza Vaccine Effectiveness Study, Ann Arbor, Michigan, 2010–2011

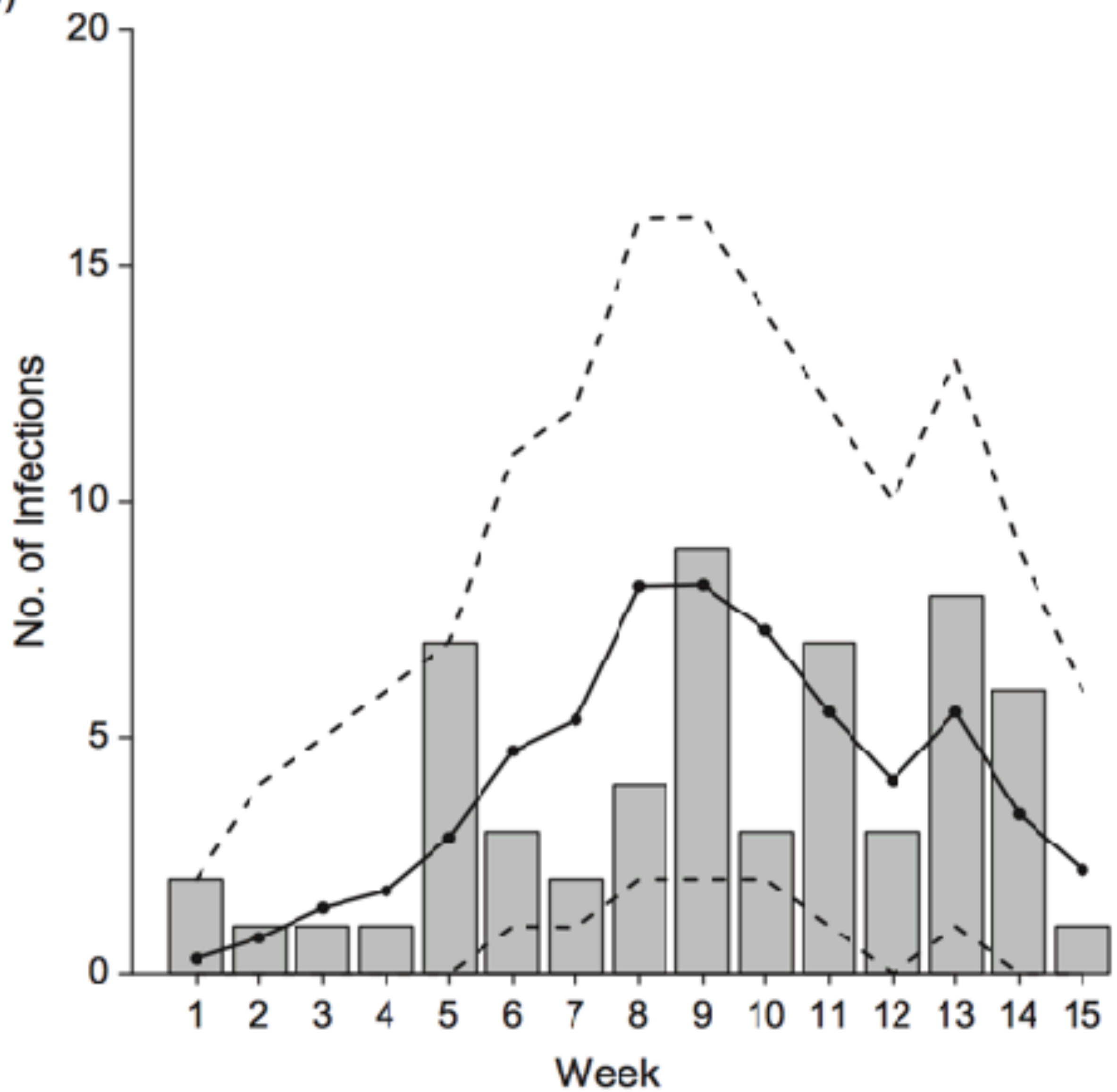
Characteristic	Observed Data			TH Model Predictions				P Value[a]
	No. of Cases ($n = 58$)	Total No. Exposed ($n = 1,441$)	% Positive	Median No. of Cases	95% CrI	% Positive	95% CrI	
Community-acquired	41	1,441	2.8	43	31, 55	3.0	2.2, 3.8	0.70
Household-acquired	17	111	15.3	18	9, 30	13.2	6.6, 20.5	
Secondary	N/O	N/O		15	7, 24			
Tertiary	N/O	N/O		3	0, 9			
Quaternary	N/O	N/O		0	0, 0			
Age category, years								0.80
<9	32	468	6.8	36	22, 50	7.7	4.7, 10.7	
9–17	8	371	2.2	8	3, 14	2.2	0.8, 3.8	
≥18	18	602	3.0	18	9, 27	3.0	1.5, 4.5	
Documented high-risk health condition								0.49
Any	6	162	3.7	5	1, 11	3.1	0.6, 6.8	
None	52	1,279	4.1	56	38, 76	4.4	3.0, 5.9	
Documented influenza vaccination[b]								0.45
Yes	33	864	3.8	32	19, 48	3.7	2.2, 5.6	
No	25	577	4.3	29	16, 44	5.0	2.8, 7.6	
Overall model predictions				62	42, 82	4.3	2.9, 5.7	

Abbreviations: CrI, credible interval; N/O, not observed; TH, transmission hazard.

[a] Simulation-based χ^2 test.

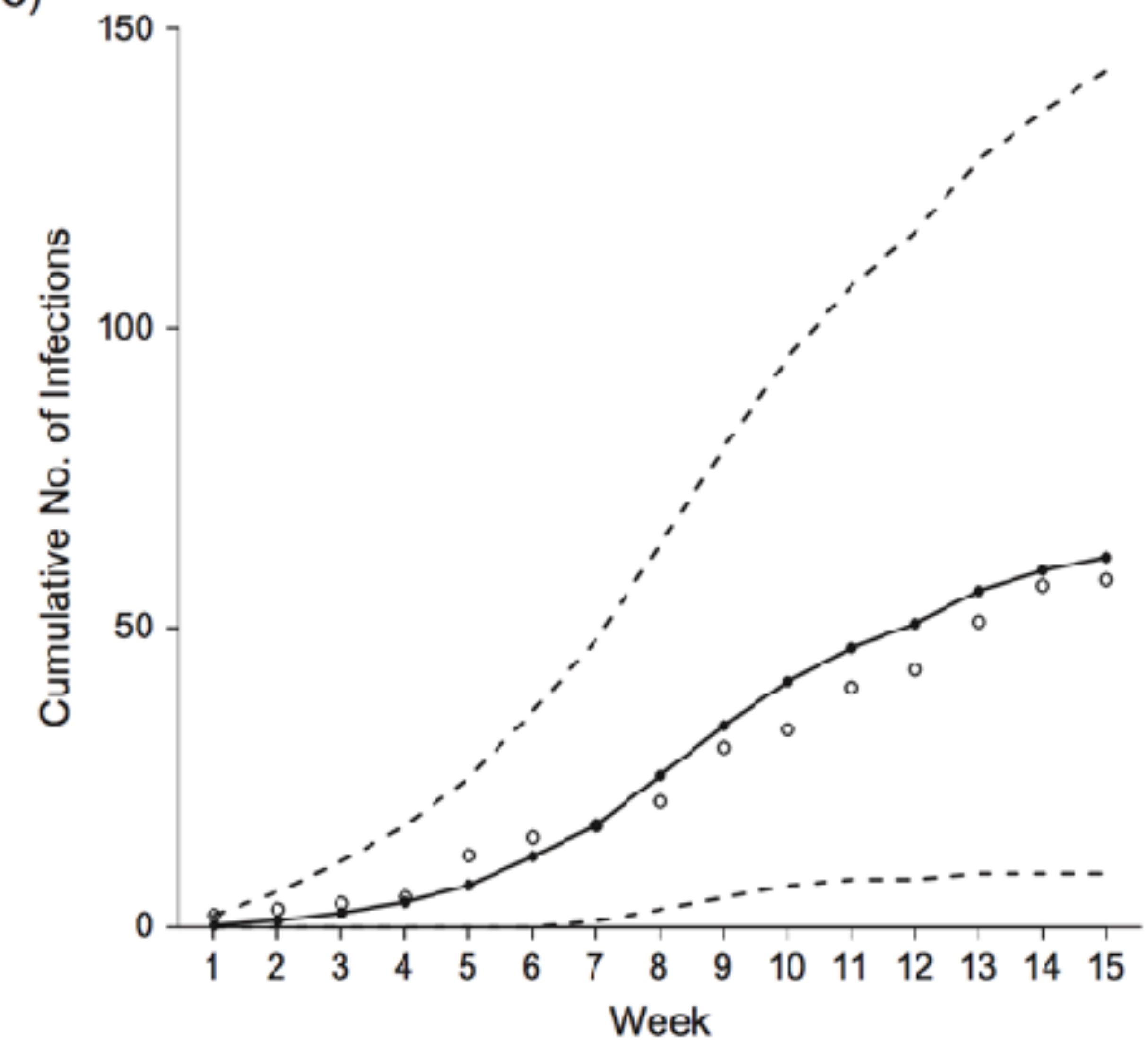
[b] At least 1 dose of 2010–2011 influenza vaccine documented in the electronic medical record or state registry; vaccination must have occurred ≥14 days prior to illness onset for influenza A(H3N2) infected subjects.

B)

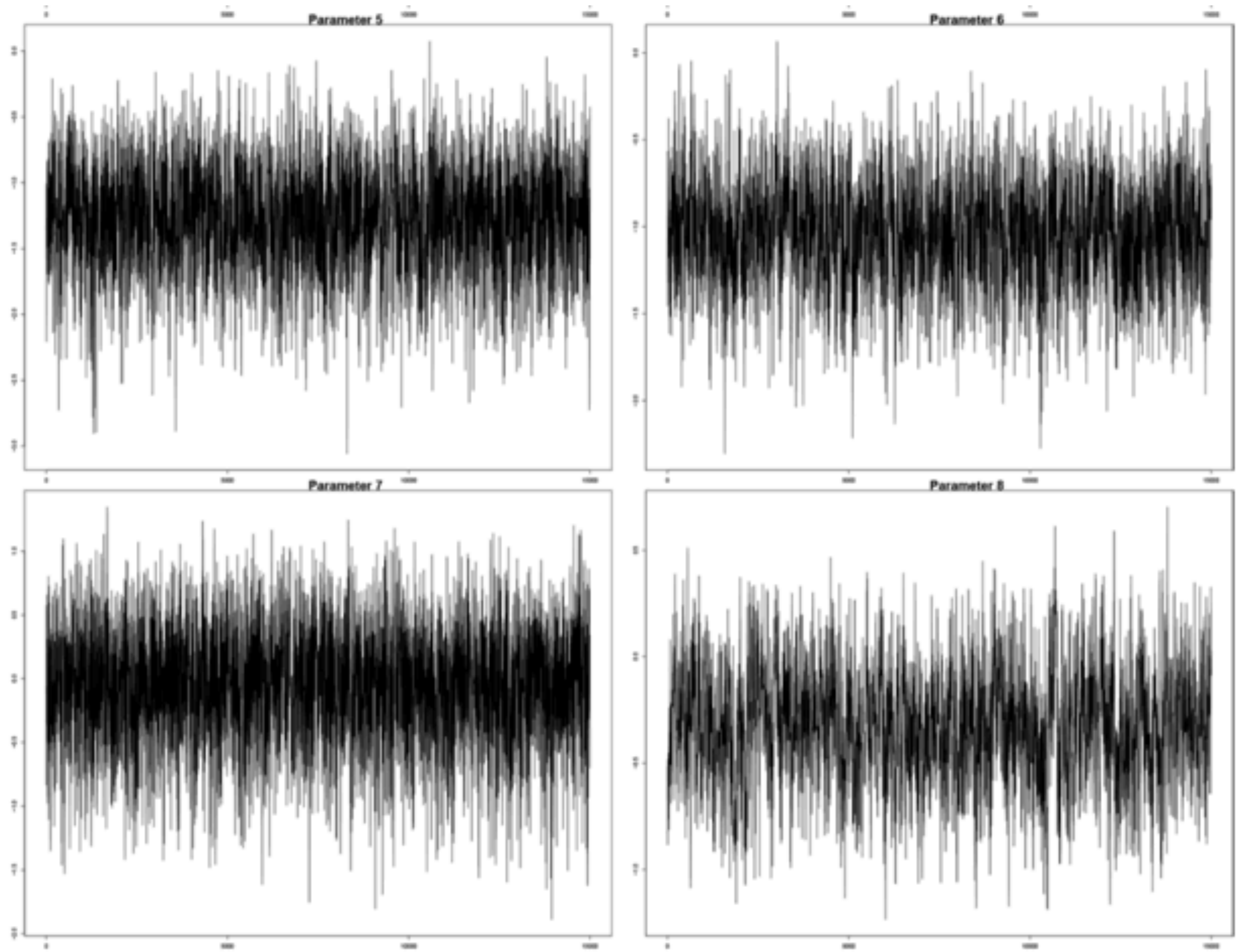


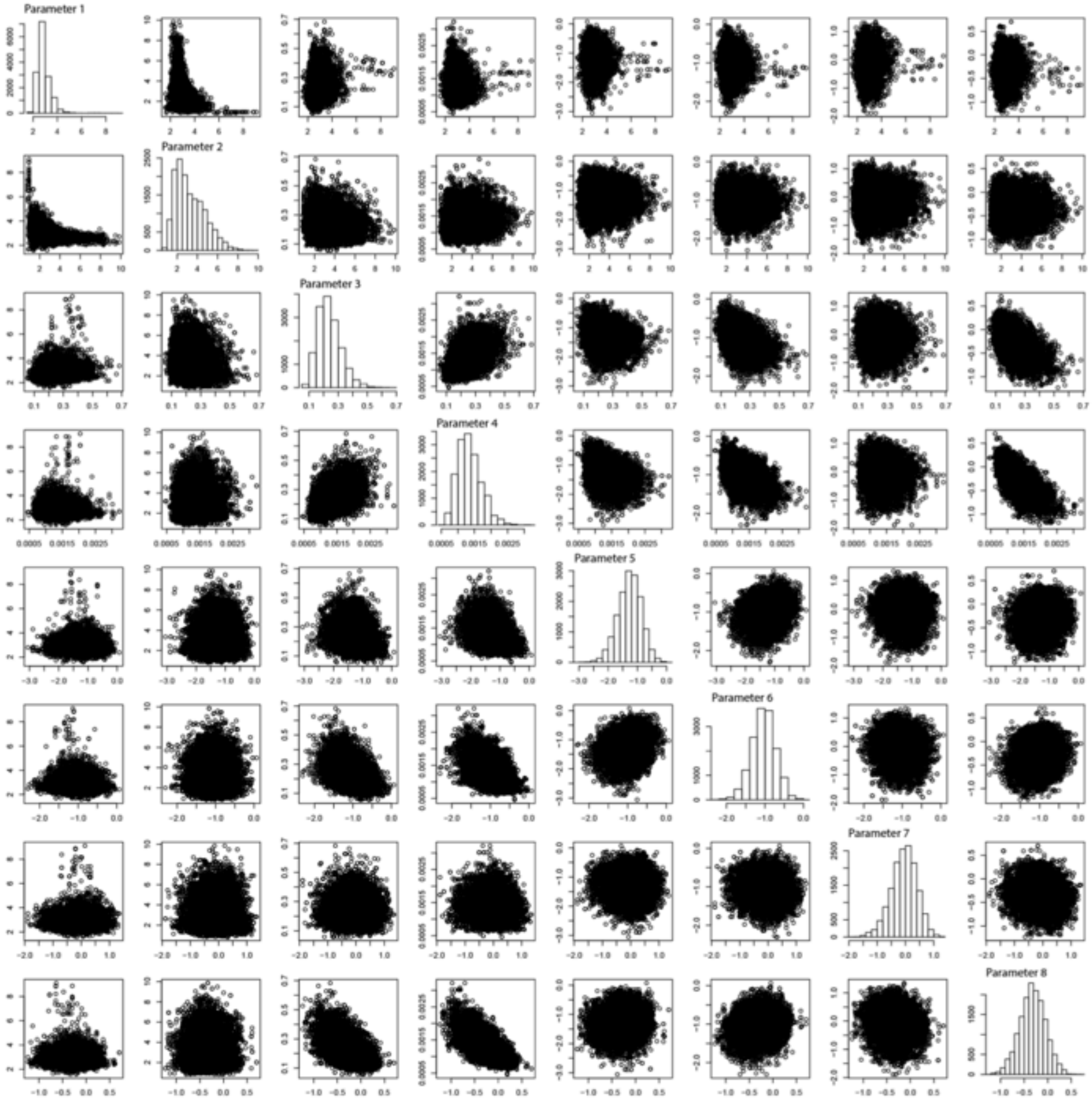
20
15
10
5
0
No. of Infections
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
Week

C)



150
100
50
0
Cumulative No. of Infections
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
Week


Parameter 5
Parameter 6
Parameter 7
Parameter 8

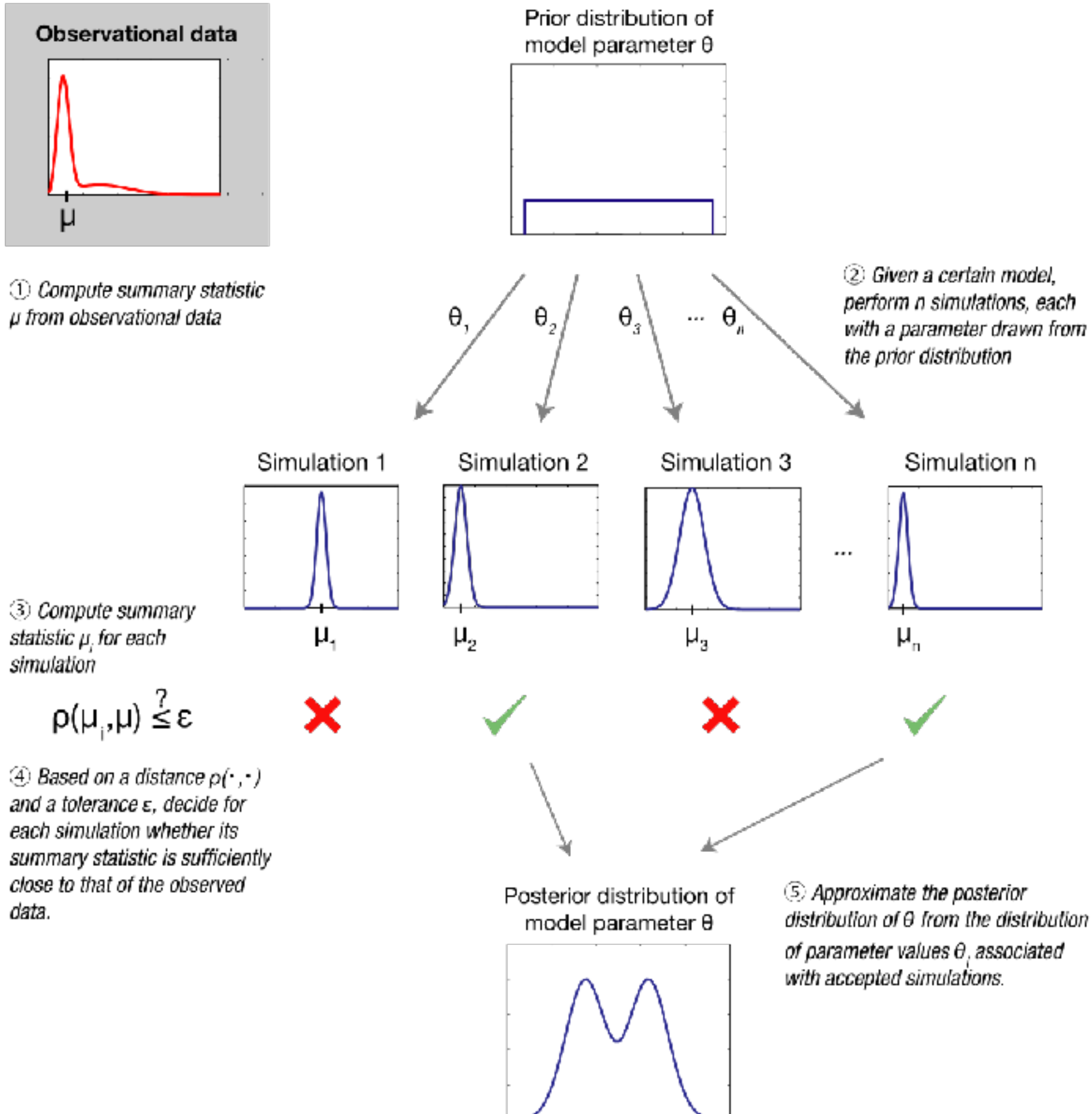

Parameter 1
Parameter 2
Parameter 3
Parameter 4
Parameter 5
Parameter 6
Parameter 7
Parameter 8

Sample Importance Resampling and Approximate Bayesian Computation

- MCMC can be slow—another approach to getting a rough sample of parameter space that matches the data is Sample Importance Resampling
  - Can be used with the true likelihood
  - Or with an approximating function (approximate Bayesian computation)
    - E.g. may take a threshold based on distance between the model and observed data

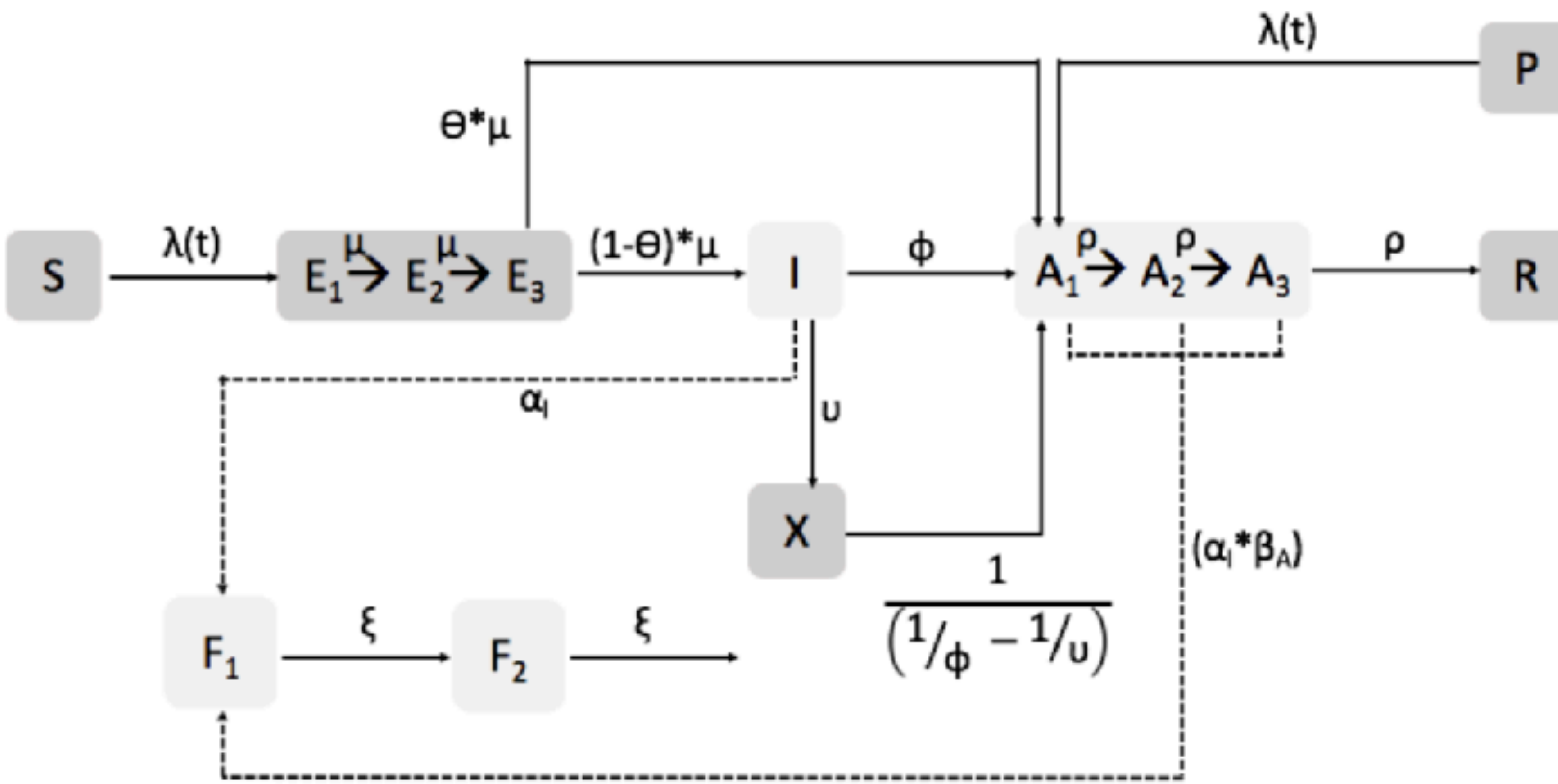
Basic idea

- Draw a sample of parameters from your prior (either drawing at random or with LHS/sobol/etc. sampling)
- Run the model for each sample
- Calculate the likelihood value (or approximation of it) for each sample
- Weight the samples based on the likelihood
- Resample to get the final set of samples

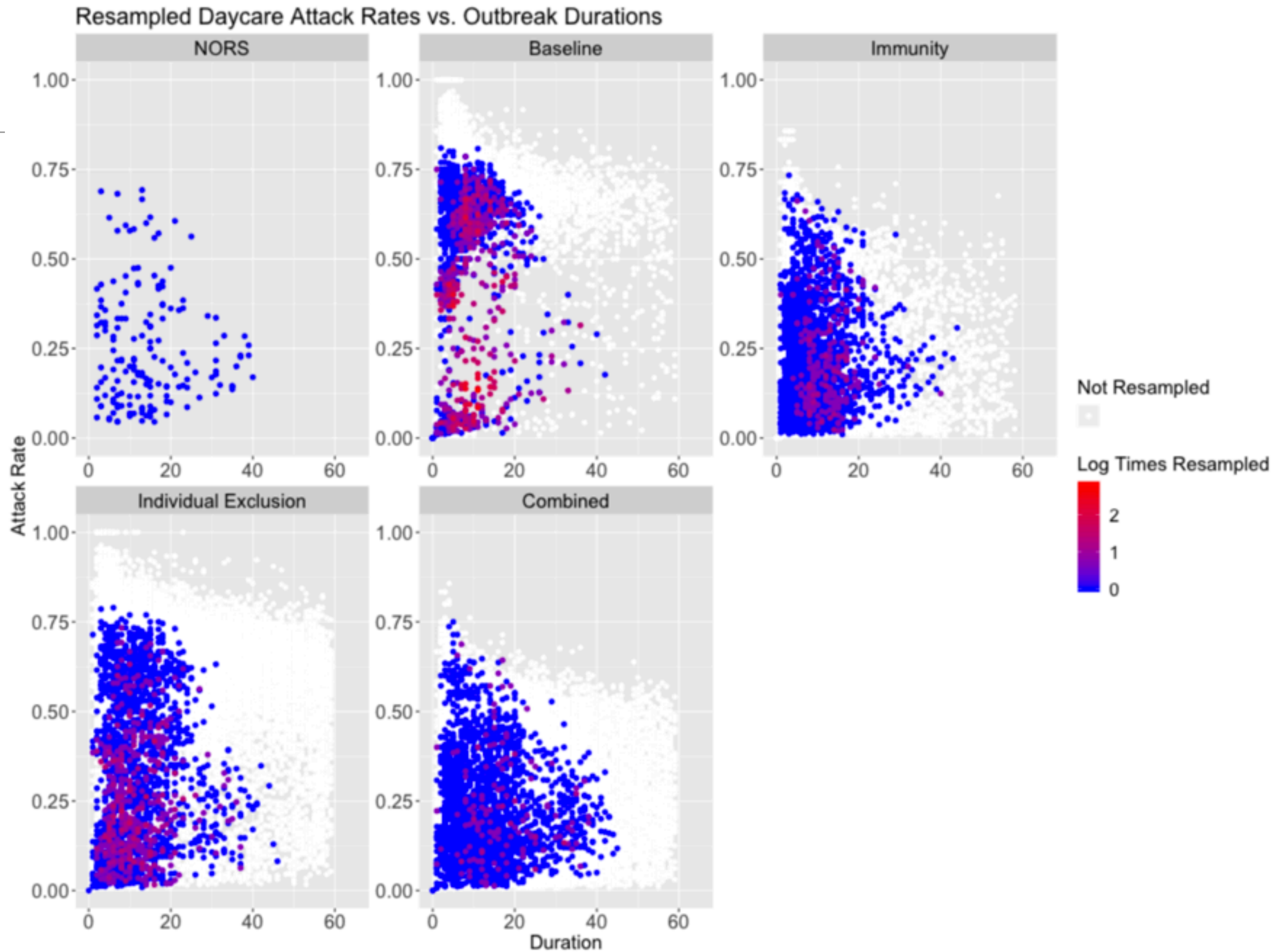


https://en.wikipedia.org/wiki/Approximate_Bayesian_computation

Example: Norovirus model



Havumaki et al. 2020



Resampled Daycare Attack Rates vs. Outbreak Durations
NORS
Baseline
Immunity
Individual Exclusion
Combined
Attack Rate
Duration
0.00
0.25
0.50
0.75
1.00
0
20
40
60
Not Resampled
Log Times Resampled
2
1
0

Readings

- Menzies NA, Soeteman DI, Pandya A, Kim JJ. Bayesian methods for calibrating health policy models: a tutorial. PharmacoEconomics. 2017 Jun 1;35(6):613-24.