Bayesian approaches to parameter estimation

Epid 814 - Marisa Eisenberg

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 $P(p|z)$

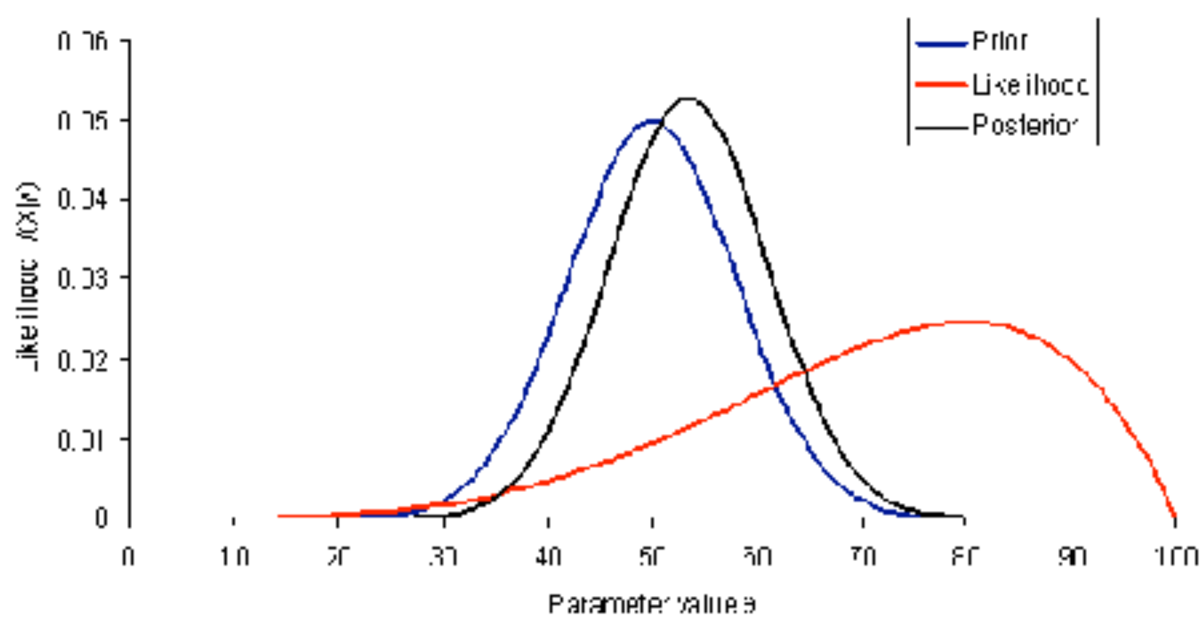
- If we only need a point estimate, MAP gets around needing to estimate $P(z)$

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

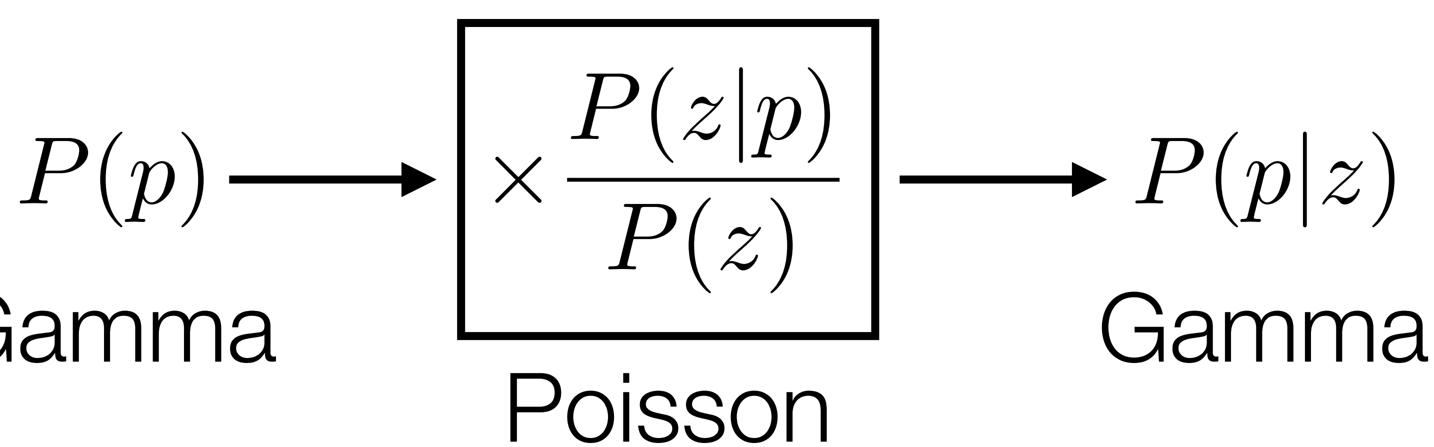


Conjugate Priors

- 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

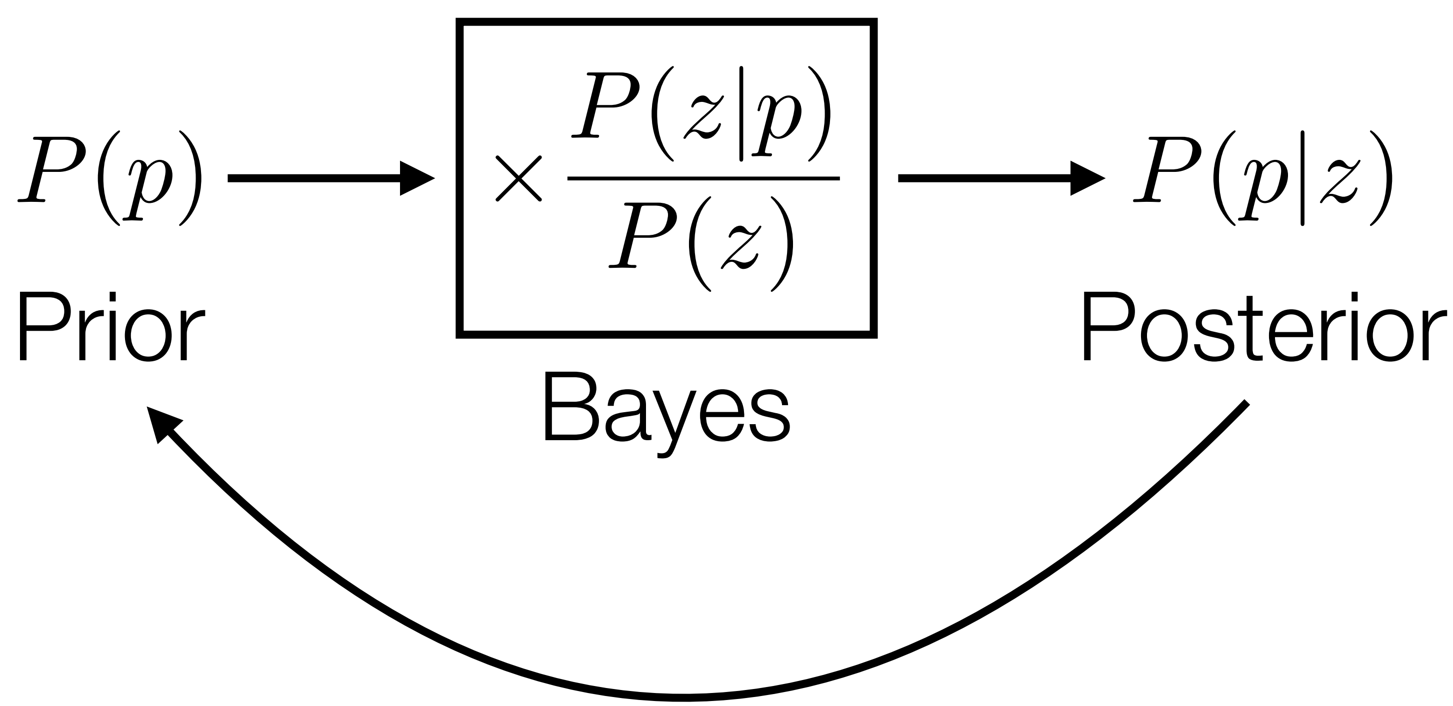
- For example, a gamma distribution is the conjugate prior for a Poisson likelihood.



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

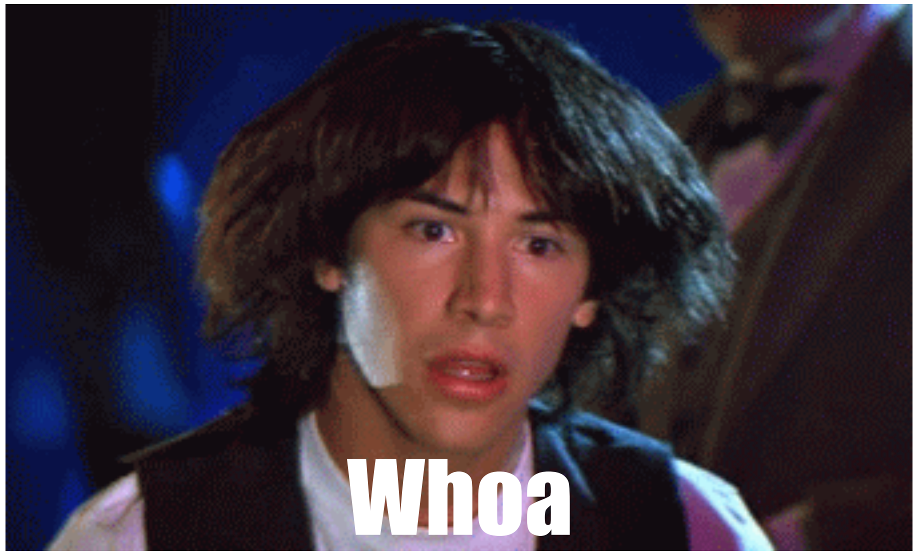
$$P(z|\theta) = \theta^z (1 - \theta)^{1-z}$$

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

- 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
- Sampling-based methods—in particular, **Markov chain Monte Carlo (MCMC)**

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: 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

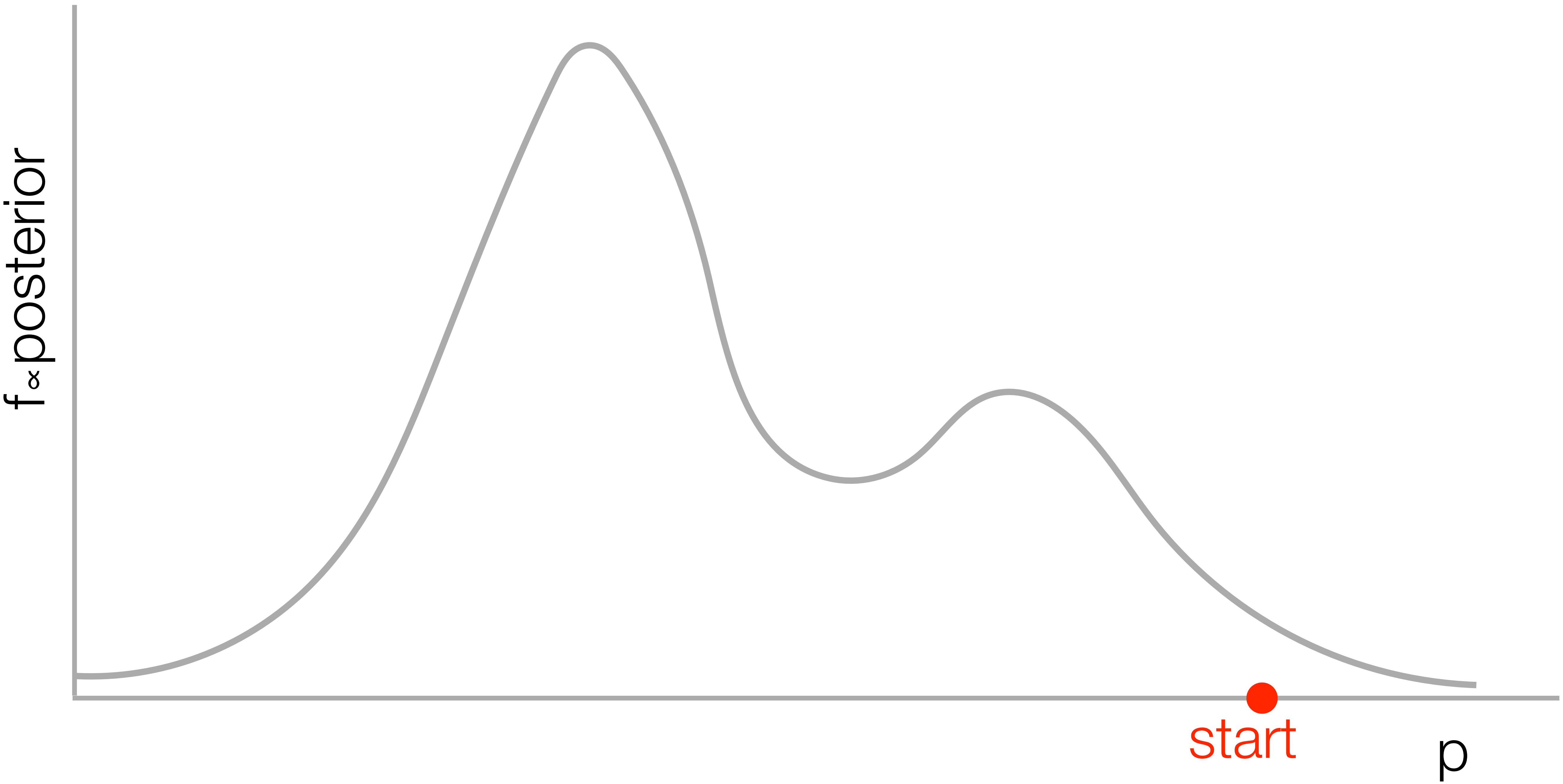
Metropolis Algorithm

- 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

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.

What does the metropolis algorithm do?



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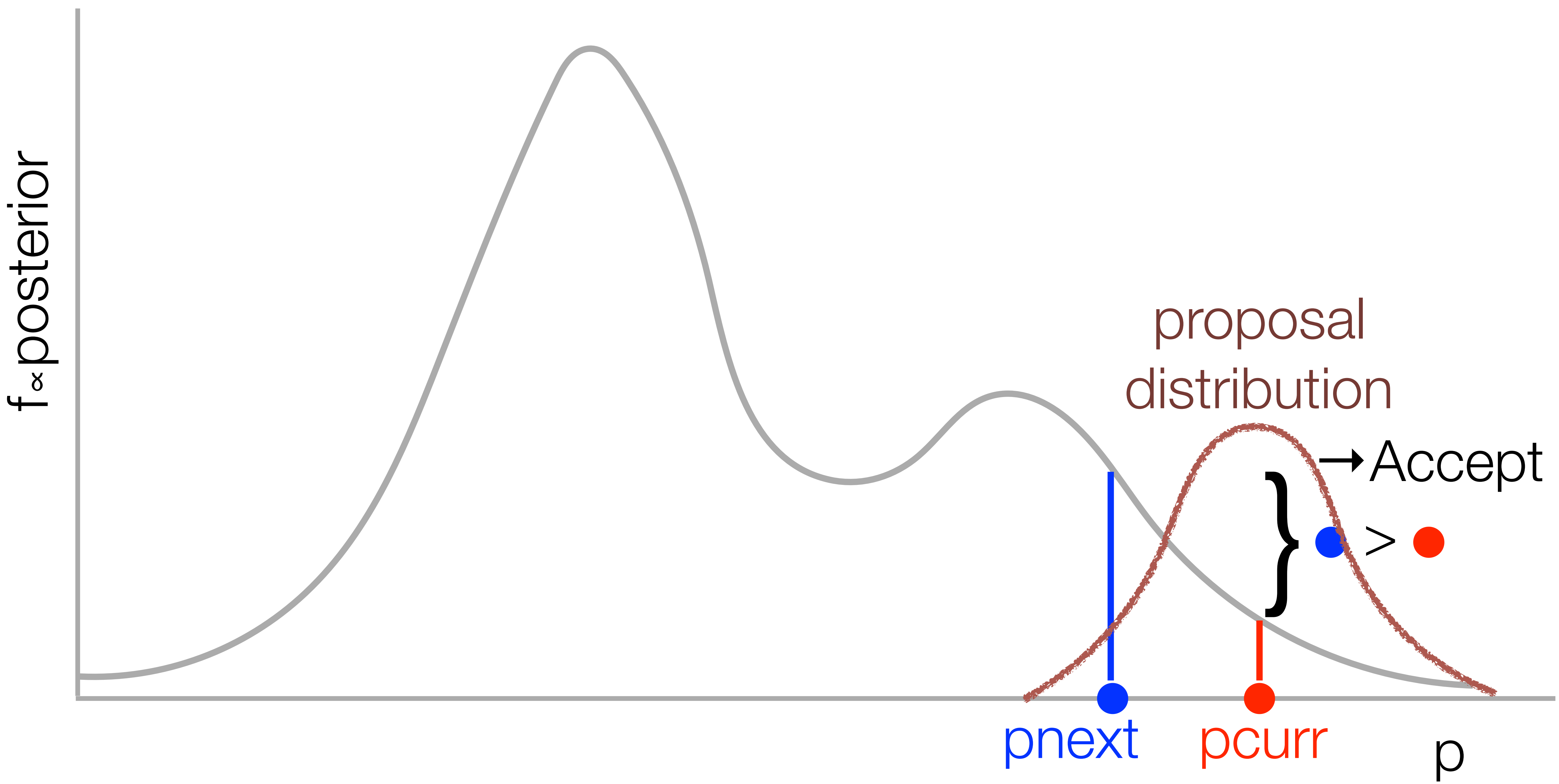

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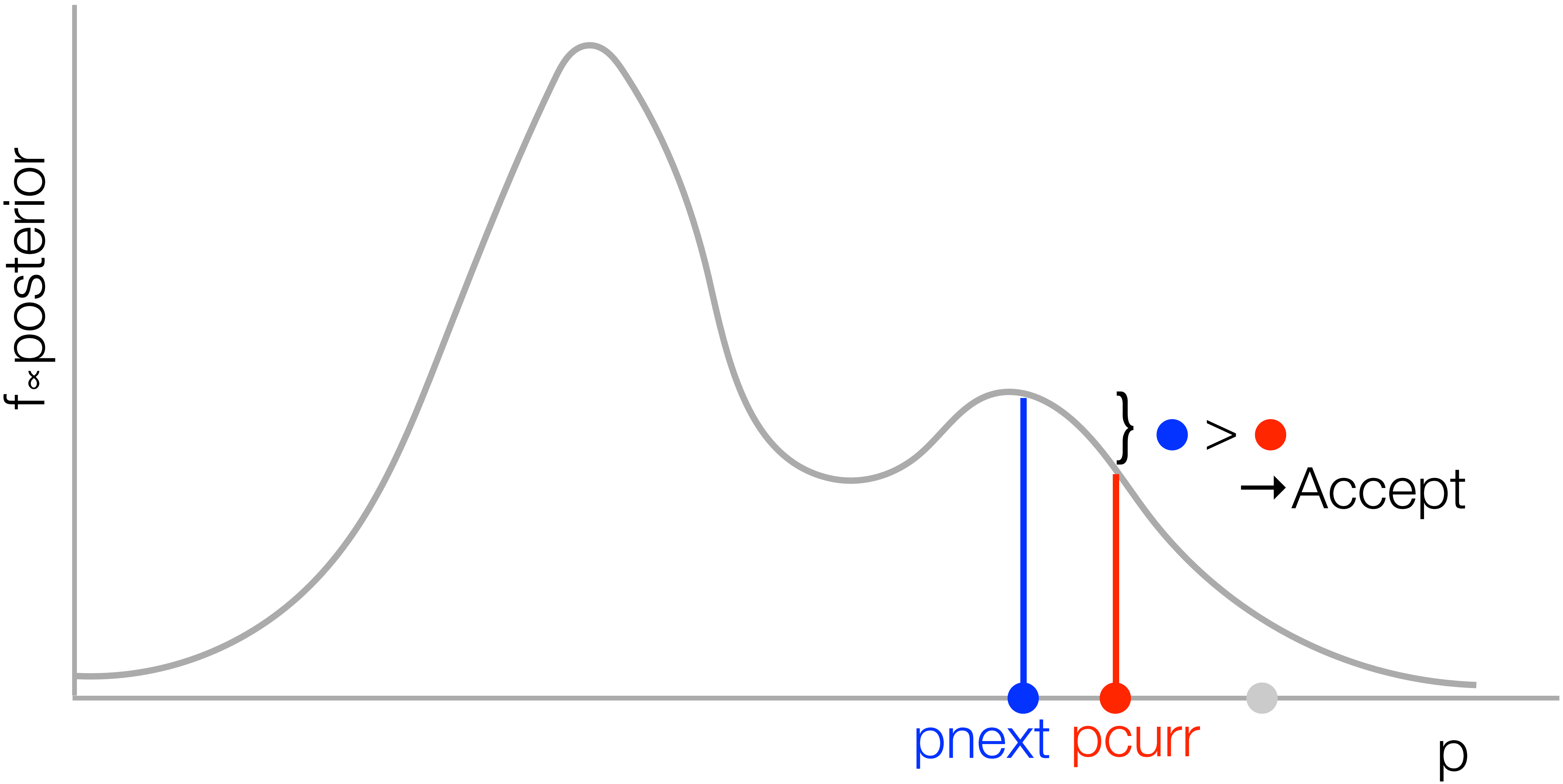

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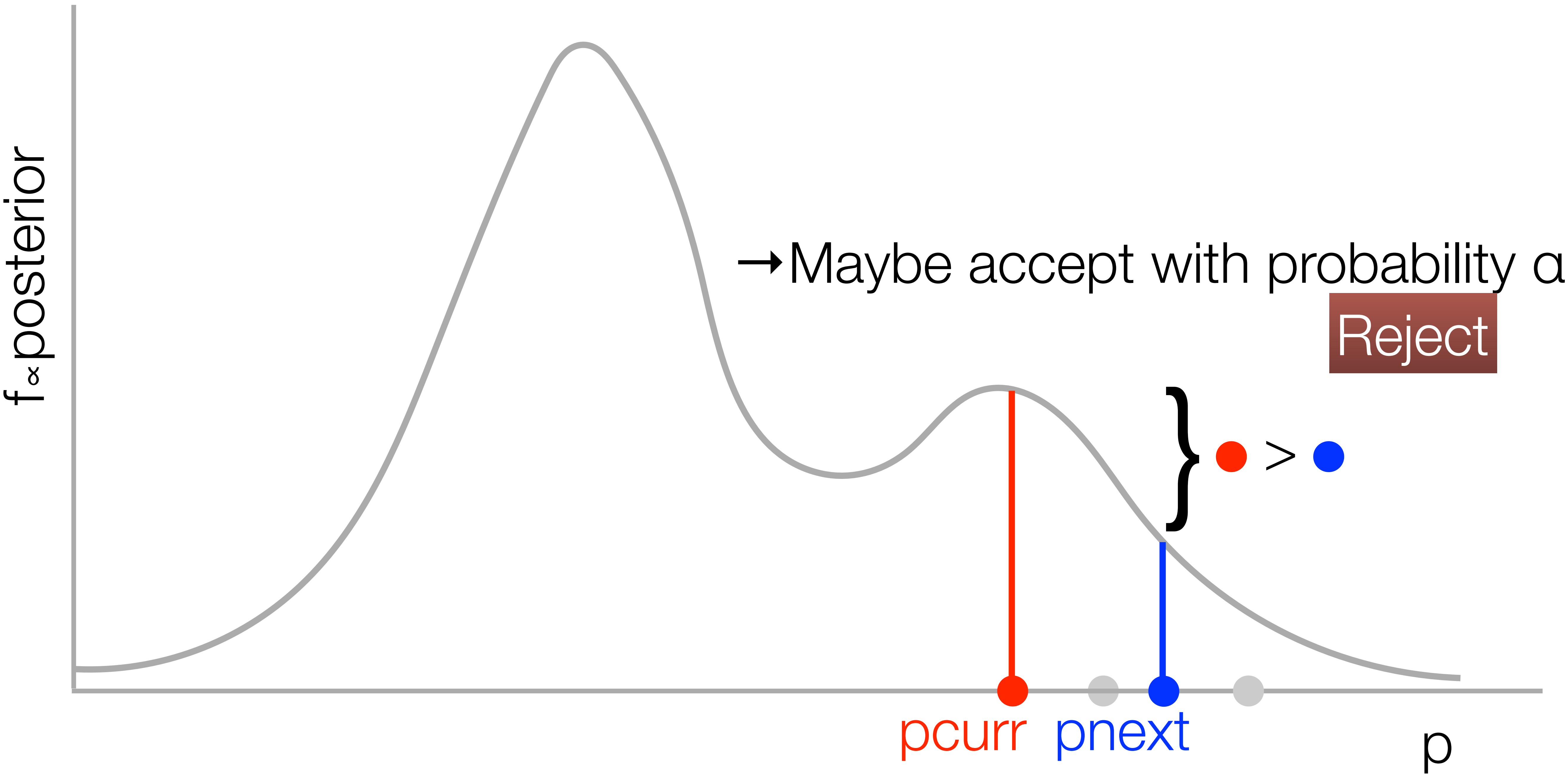

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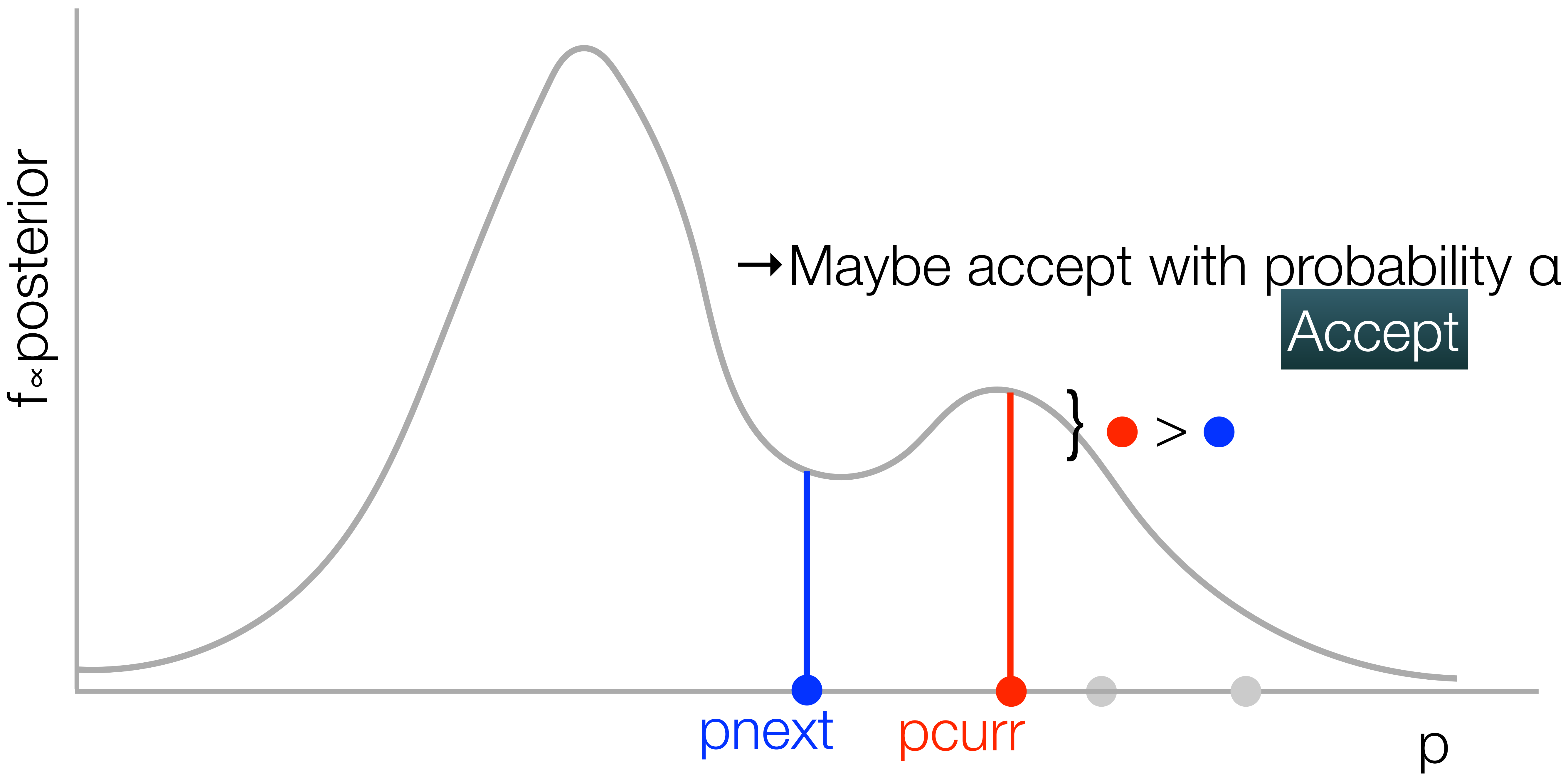
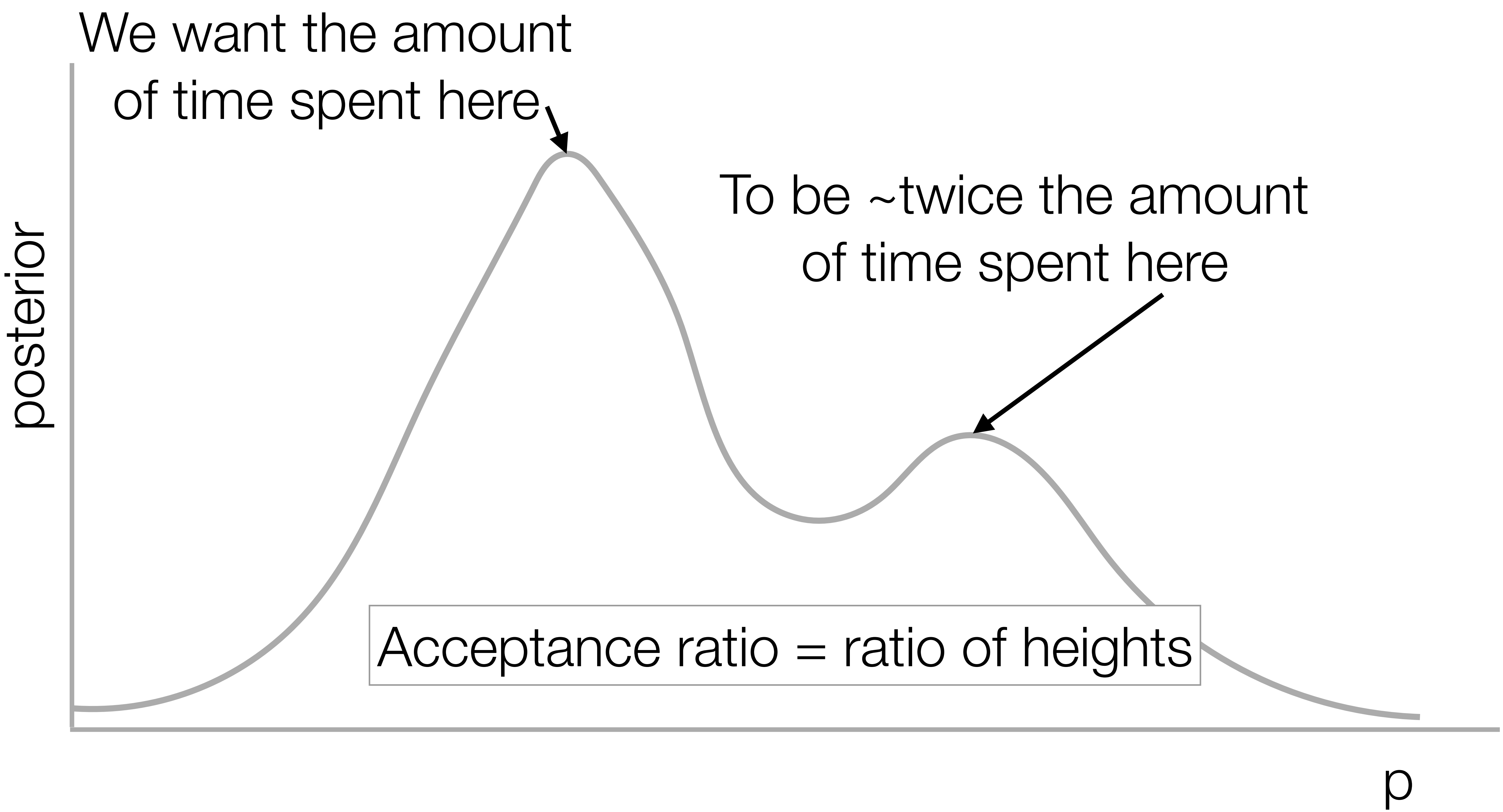


Why does this recover the posterior distribution? Key is the acceptance ratio α

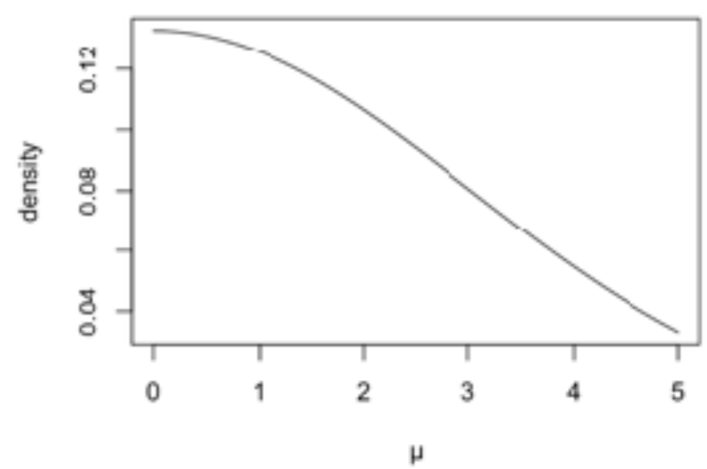


Why does this recover the posterior distribution?

- 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

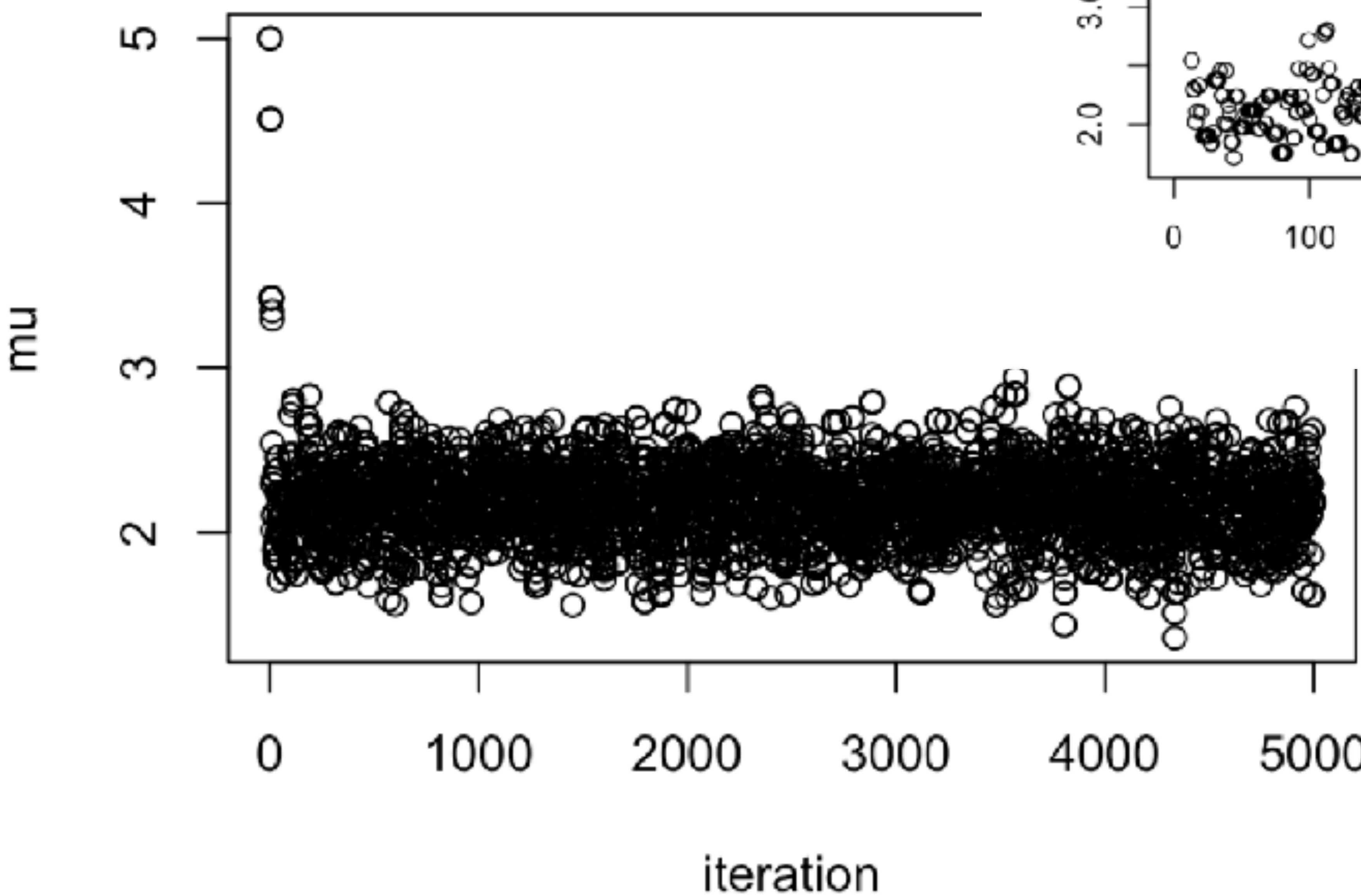
Example

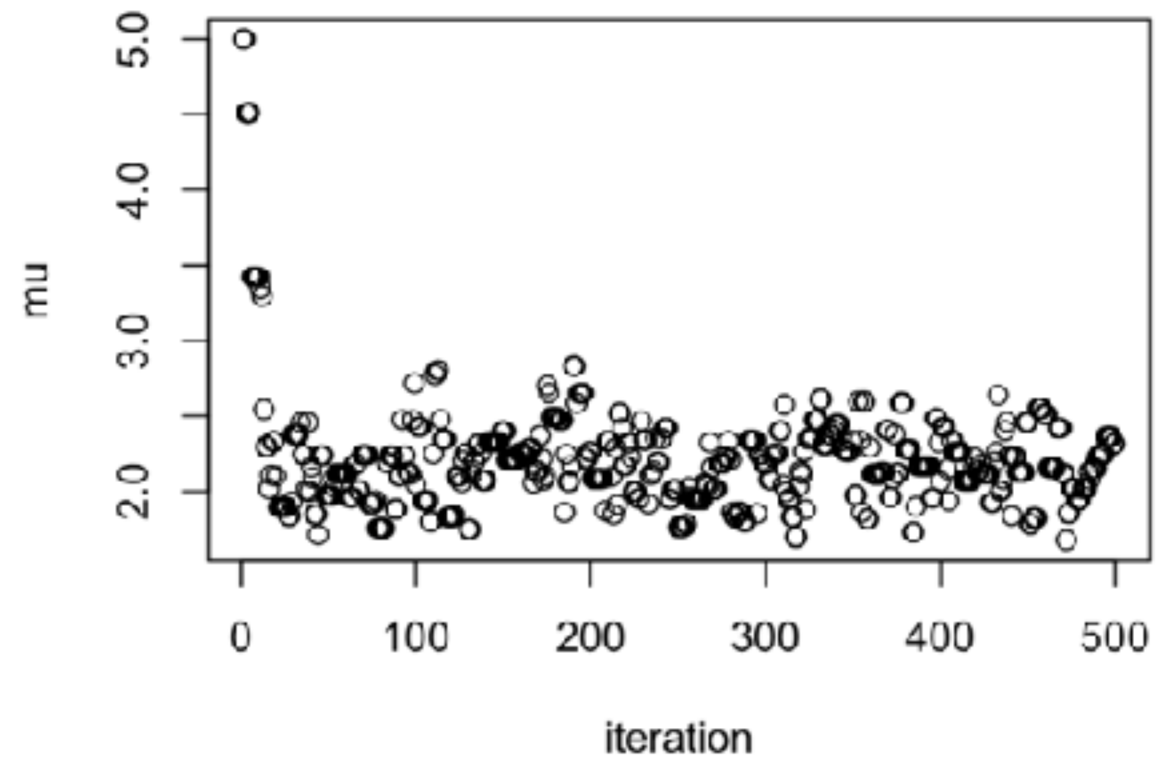
- Model: normal distribution $\mathcal{N}(\mu, \sigma)$
  - Suppose σ is known, μ to be estimated
  - Likelihood: $P(z_i \mid \mu, 1) = f(z_i \mid \mu, 1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(z-\mu)^2}{2}}$ $\quad P(z \mid \mu) = \prod_{i=1}^{n} f(z_i \mid \mu, 1)$
- Prior: $\mu \sim \mathcal{N}(0, 3)$



- Suppose we have 20 data points

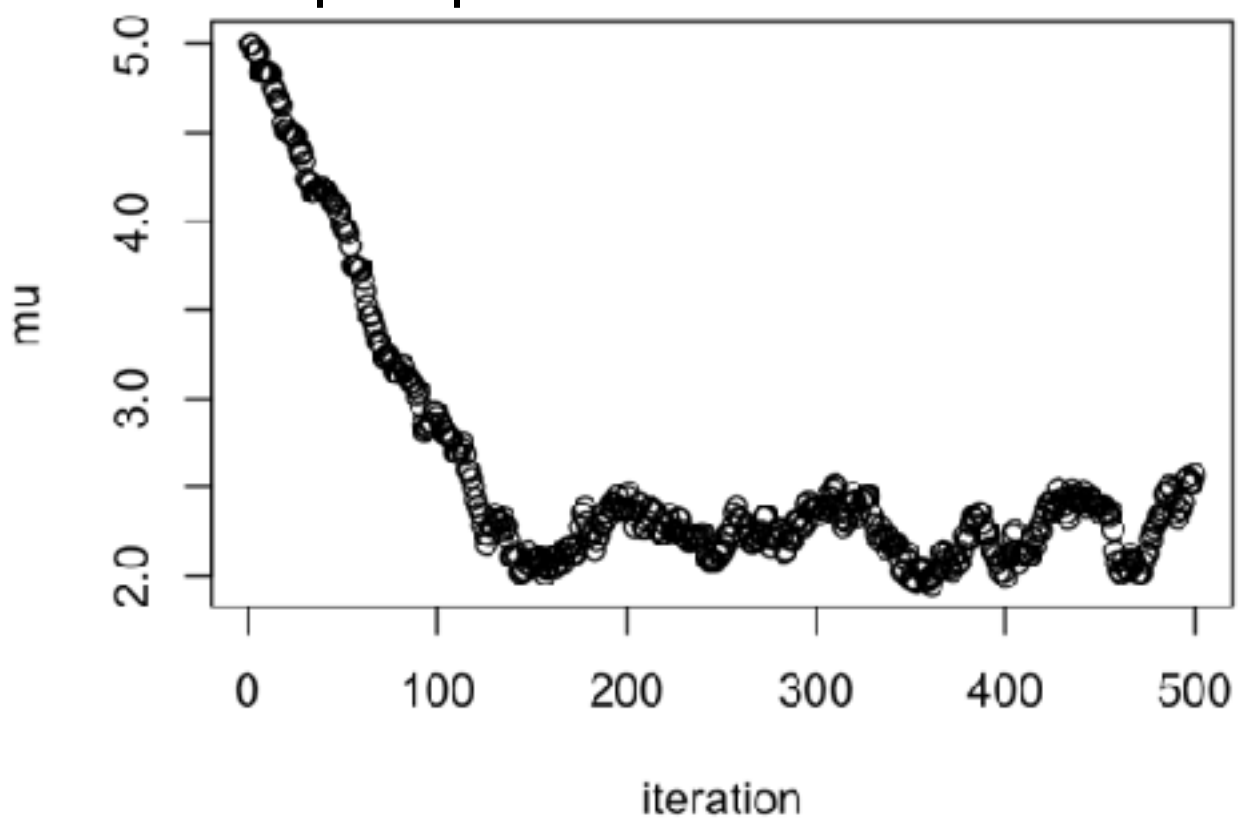
Example - proposal width: SD = 0.5



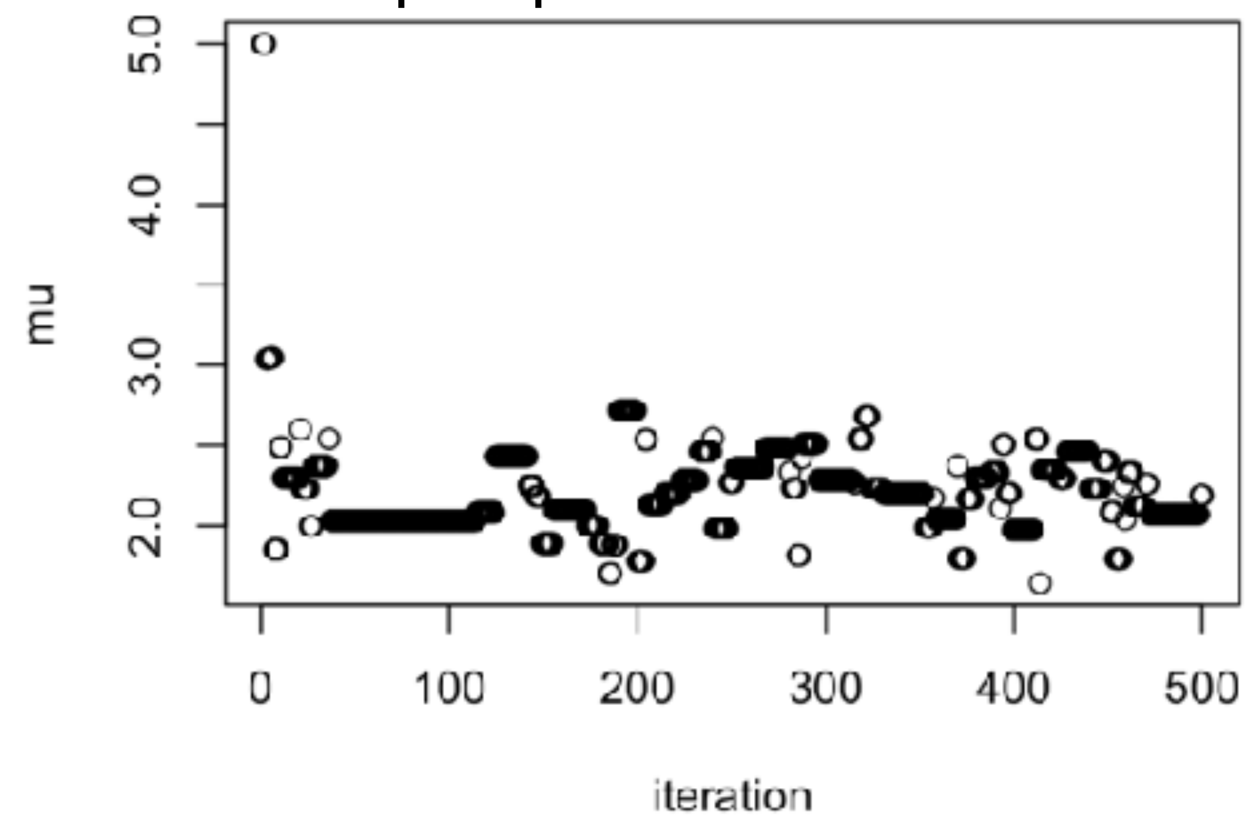


Goldilocks problem:
What happens if we change the proposal width?

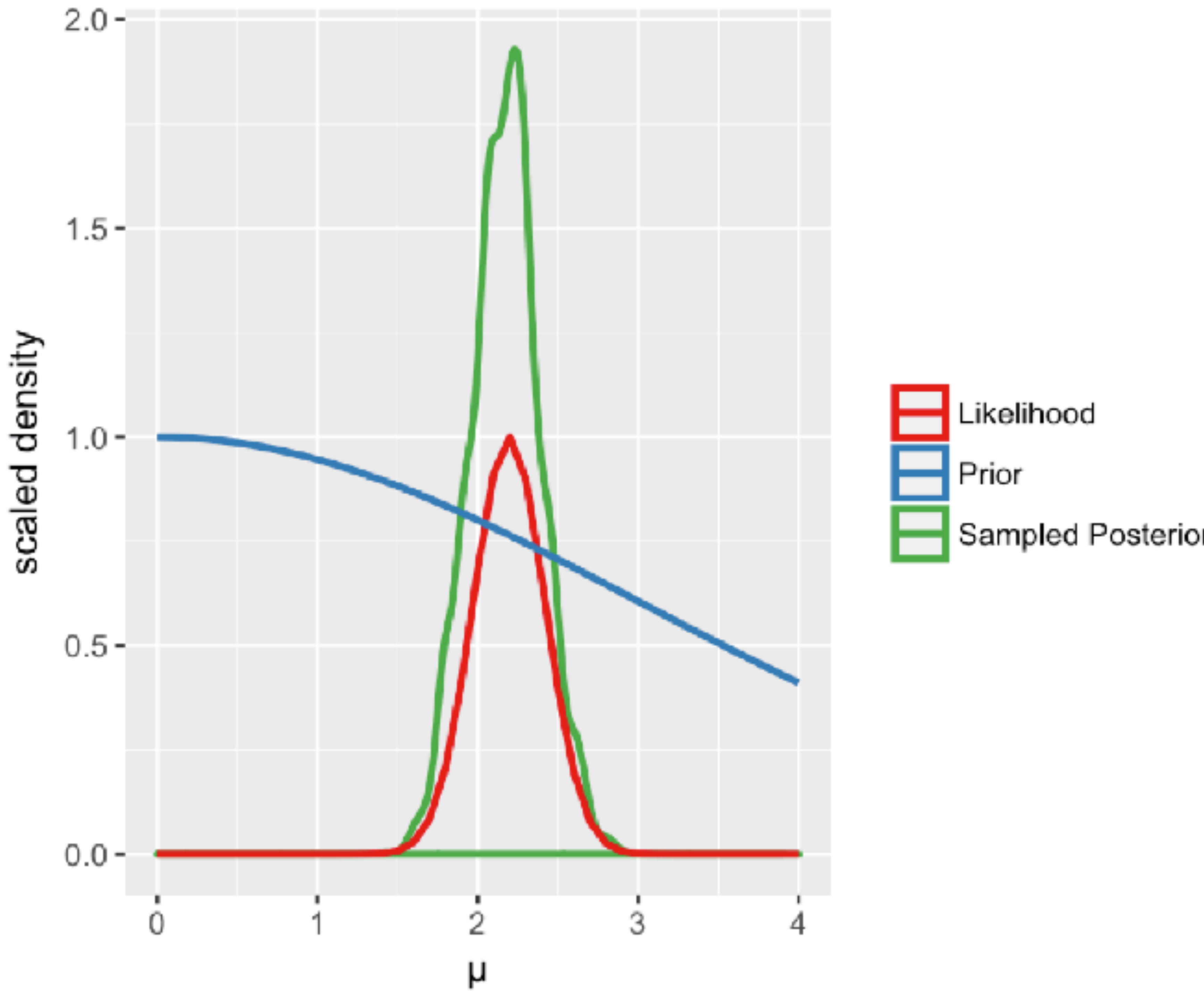
proposal SD = 0.05



proposal SD = 2



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

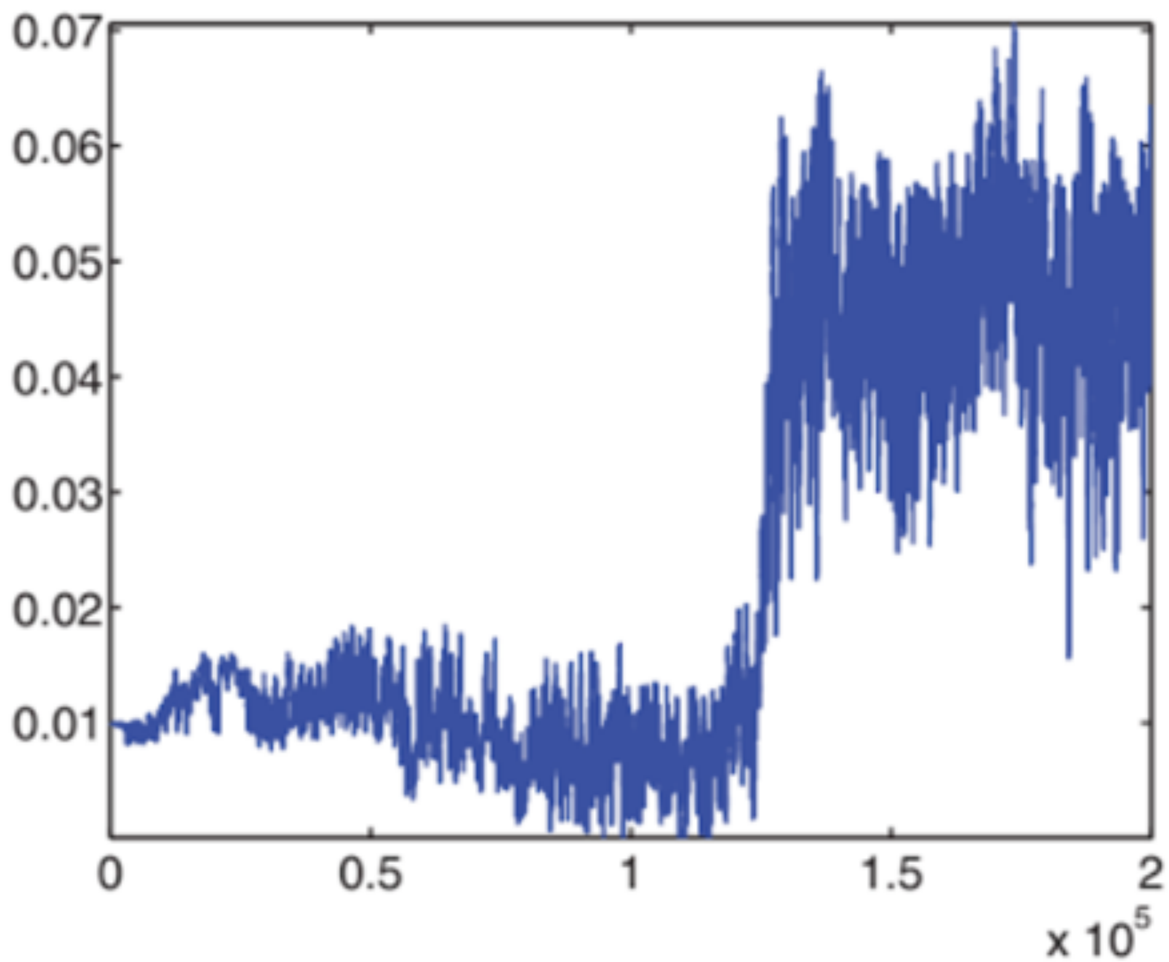


Assessing convergence

- 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**
  - Acceptance ratio
  - Autocorrelation of elements in chain *k* iterations apart
- Careful about MCMC results reported in literature

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?
- Correlated samples
- How to choose a proposal width? (~size of next jump)

Next time

- Code our own Metropolis sampler
- Then, next week:
    - More on priors—uninformed priors (e.g. Jeffreys), identifiability issues
    - Work with sampling packages & more realistic models!