Using MCMC for inference using Hamiltonian Monte Carlo with Stan

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random@yorku.ca

Send me an email message and I'll add your name to a Piazza Course with useful links.

- Working with uncertainty
  - Frequentist vs. Bayesian inference
- Evolution of MCMC
  - MH, Gibbs, Hamiltonian MC
- Using Stan for HMC
  - Non-linear mixed model
  - Simple ODE model

Sally Clark

- Young lawyer, gives birth to first son in September 1996
- son dies, apparently of SIDS, at 10 weeks
- second son born a year later
- dies, apparently of SIDS, at 8 weeks
- only evidence of trauma consistent with resuscitation attempts
- charged with two counts of murder

Sir Roy Meadow

- distinguished pediatrician
- as expert witness testifies:
  - probability of one SIDS death: $\frac{1}{8{,}500}$
  - probability of two: $\left(\frac{1}{8{,}500}\right)^2 = \frac{1}{72{,}250{,}000}$
  - 'if she's innocent, the chances of this happening are 1 in 72 million'
- jury convicts Sally Clark of murder in November 1999
- first appeal lost in October 2000
- second appeal succeeds and Sally Clark is released in January 2003
- she dies in 2007 at the age of 42

H_0: Sally is innocent

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Y: 2 children die for no apparent cause

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Criticism: 1) assumes independence

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Correct p-value is larger - maybe $\frac{1}{10{,}000}$!

BUT:

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So we really want $P(y^+ | H_0)$?

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- Must be close!?
- Is $P(y^+ | H_0)$ a good proxy for $P(H_0 | y)$?

BUT:

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Don't we really want $P(H_0 | Y)$?

- Must be close!?
- Is $P(Y^+ | H_0)$ a good proxy for $P(H_0 | Y)$?

Does it establish guilt beyond a reasonable doubt?

BUT:

So we really want $P(Y^+ | H_0)$?

Don't we really want $P(H_0 | Y)$?

- Must be close!?
- Is $P(Y^+ | H_0)$ a good proxy for $P(H_0 | Y)$?

Let's find out:

$$P(H_0 | Y) = \frac{P(H_0, Y)}{P(Y)} = \frac{P(Y | H_0) P(H_0)}{P(Y)}$$

Bayesian tree:

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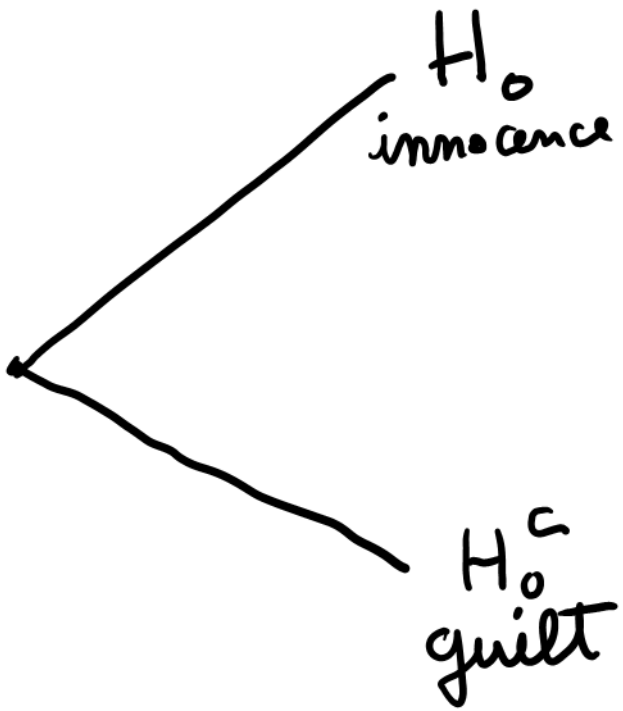

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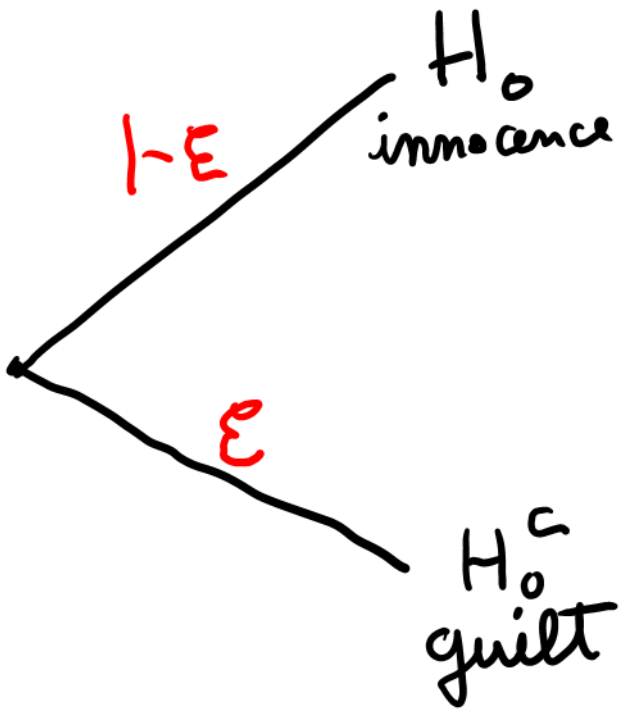
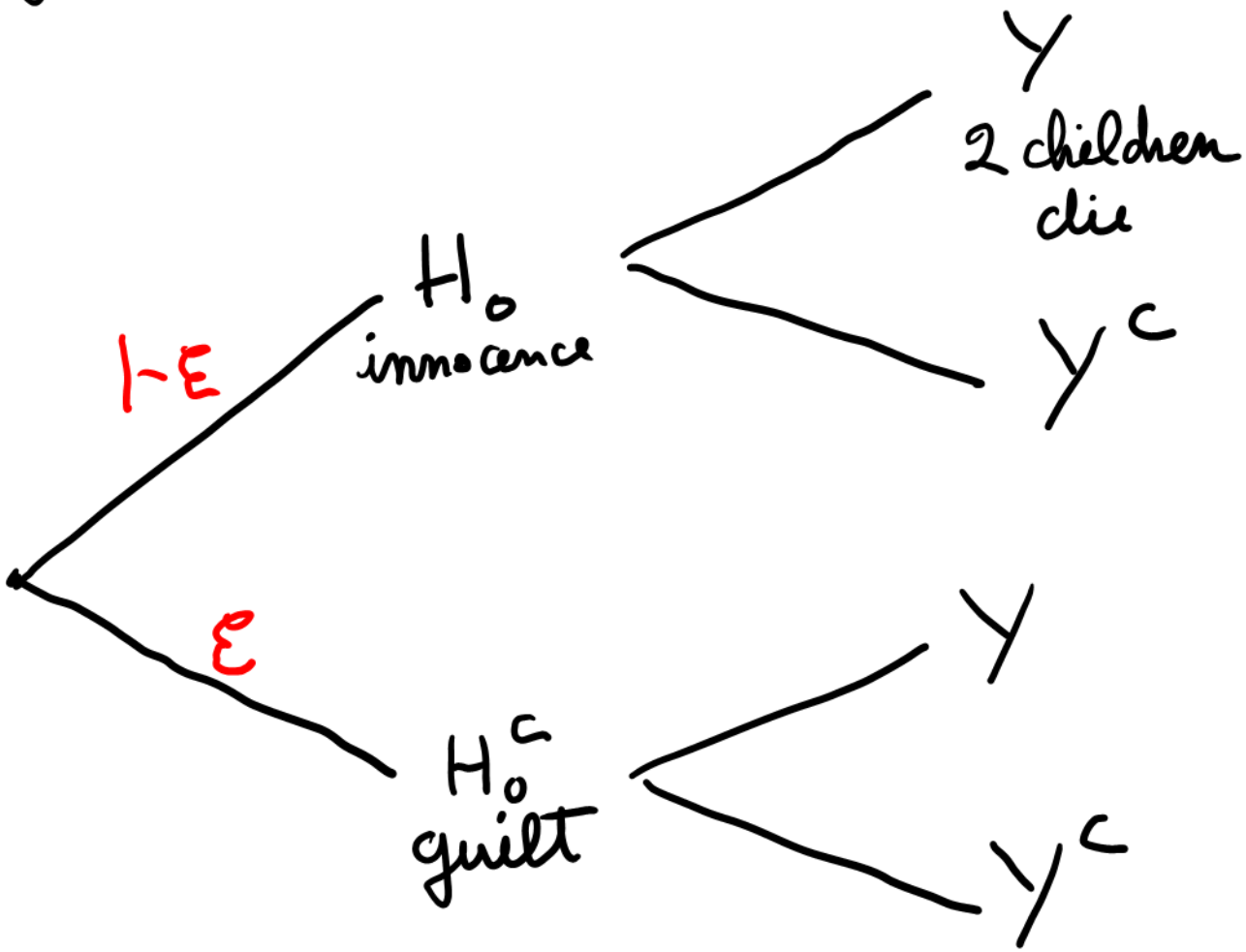


E = very small number

Bayesian tree:



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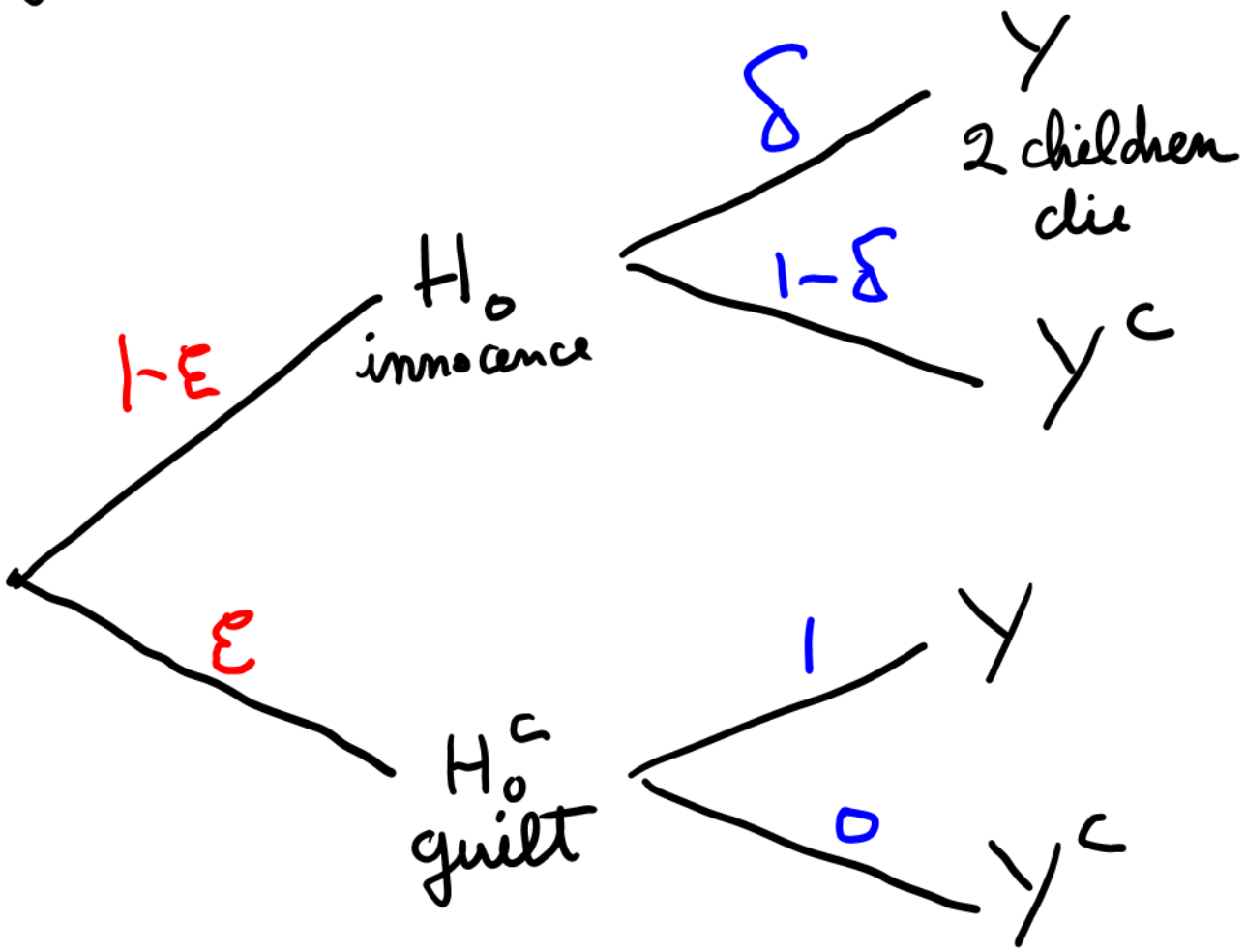
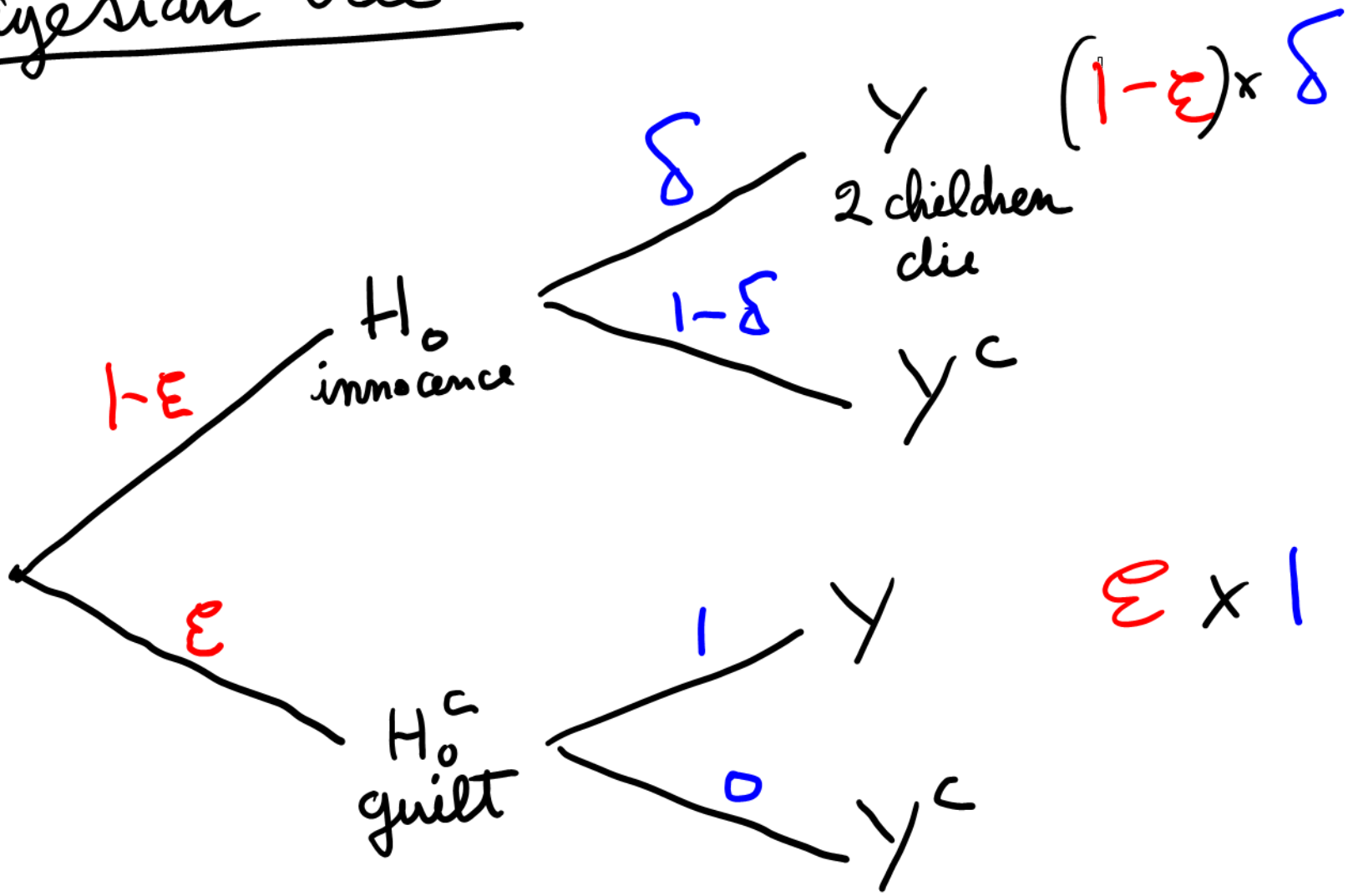


δ = very small number

Bayesian tree:



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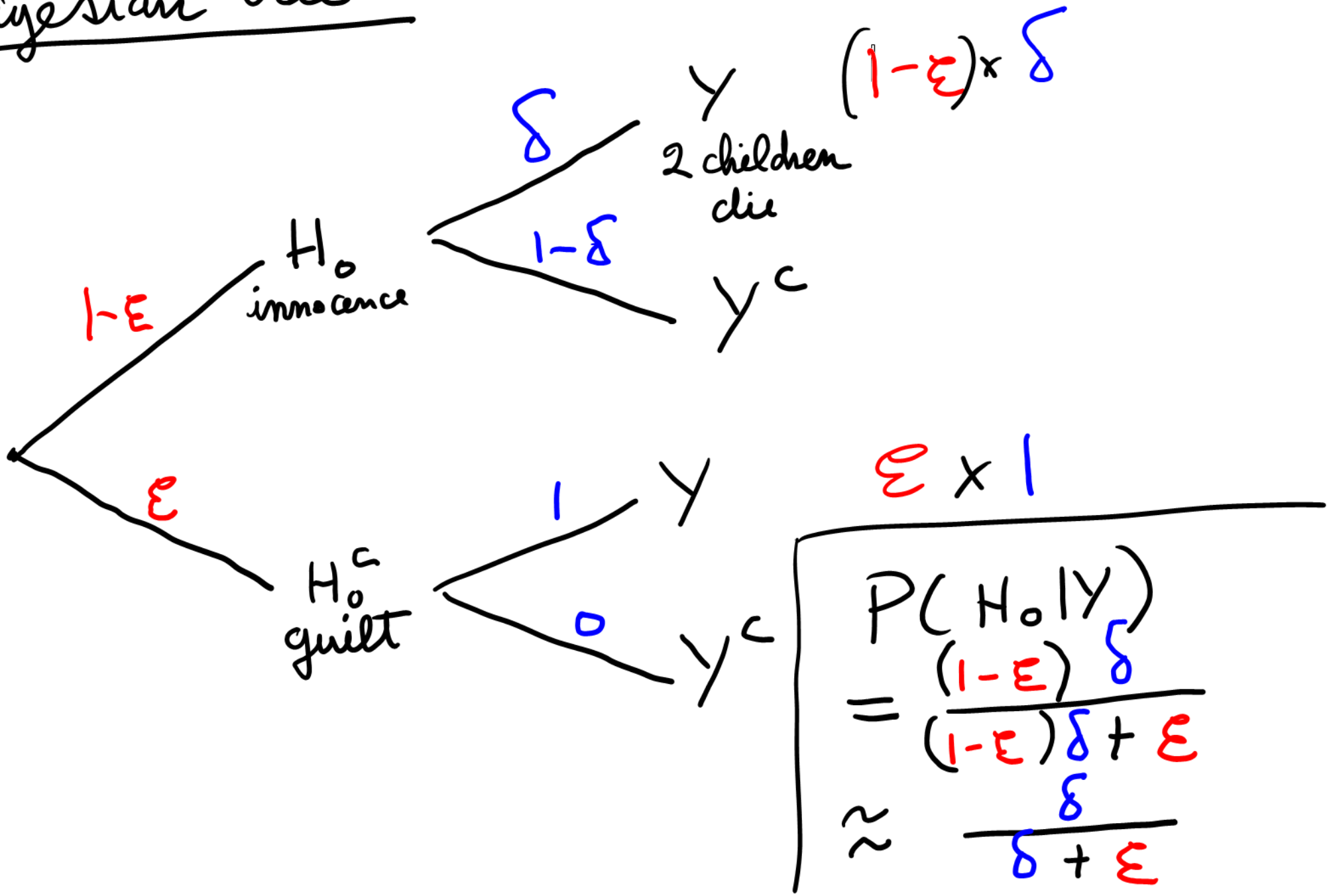

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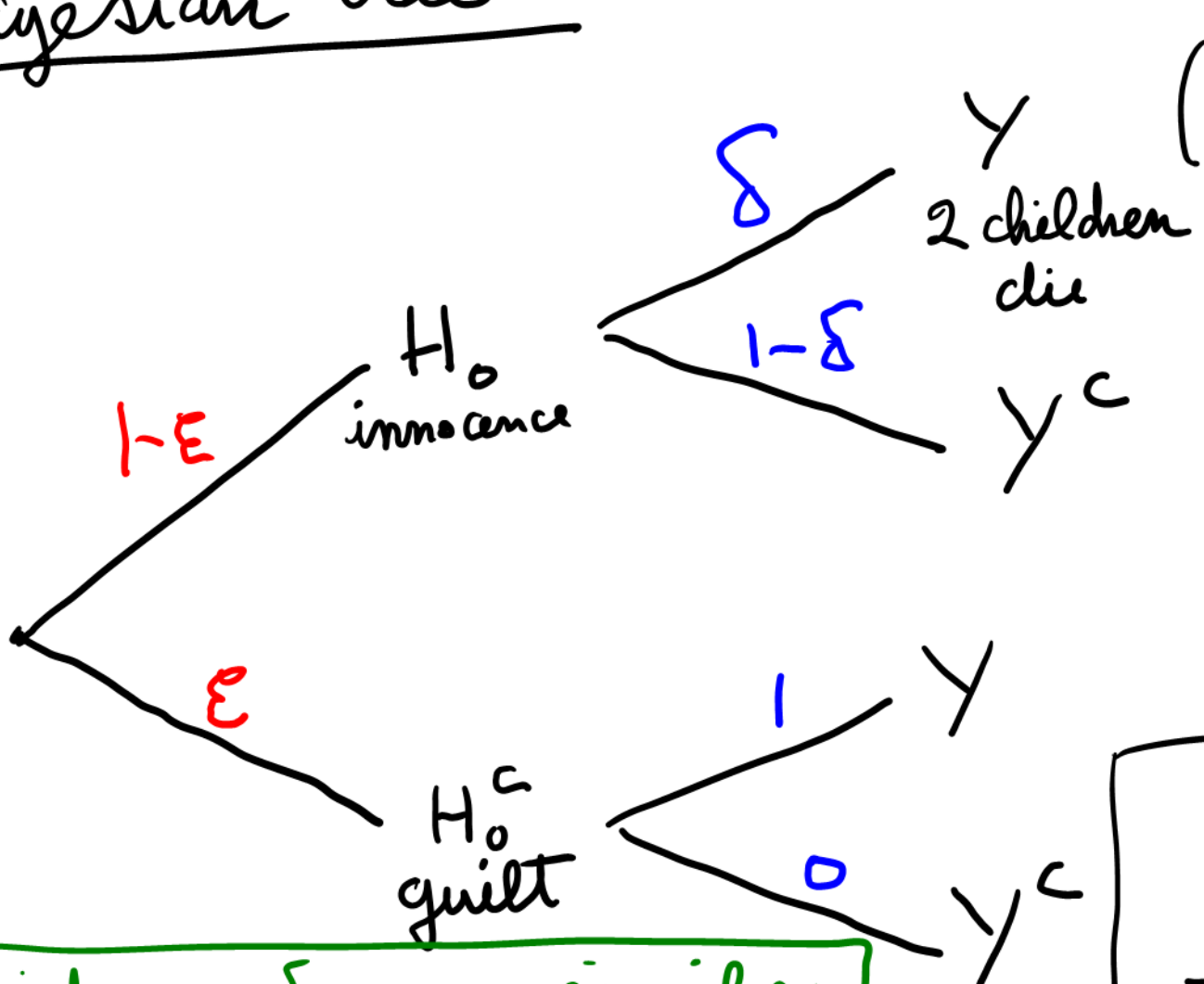


$(1-\varepsilon) \times \delta$

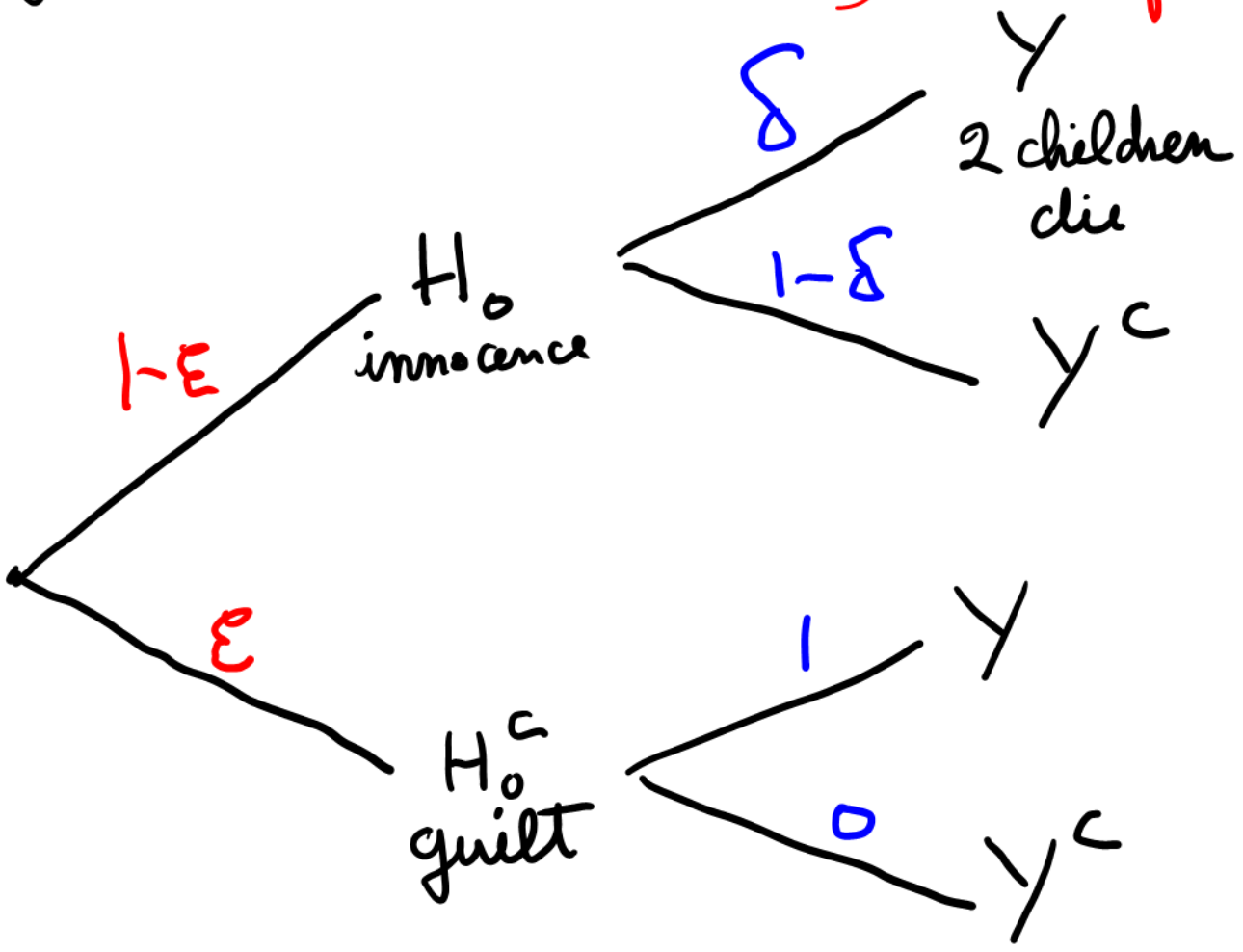
$\varepsilon \times 1$

$$P(H_0|Y) = \frac{(1-\varepsilon)\,\delta}{(1-\varepsilon)\,\delta + \varepsilon} \approx \frac{\delta}{\delta + \varepsilon}$$

So if ε & δ are similar then $P(H_0|Y) \approx \frac{1}{2}$

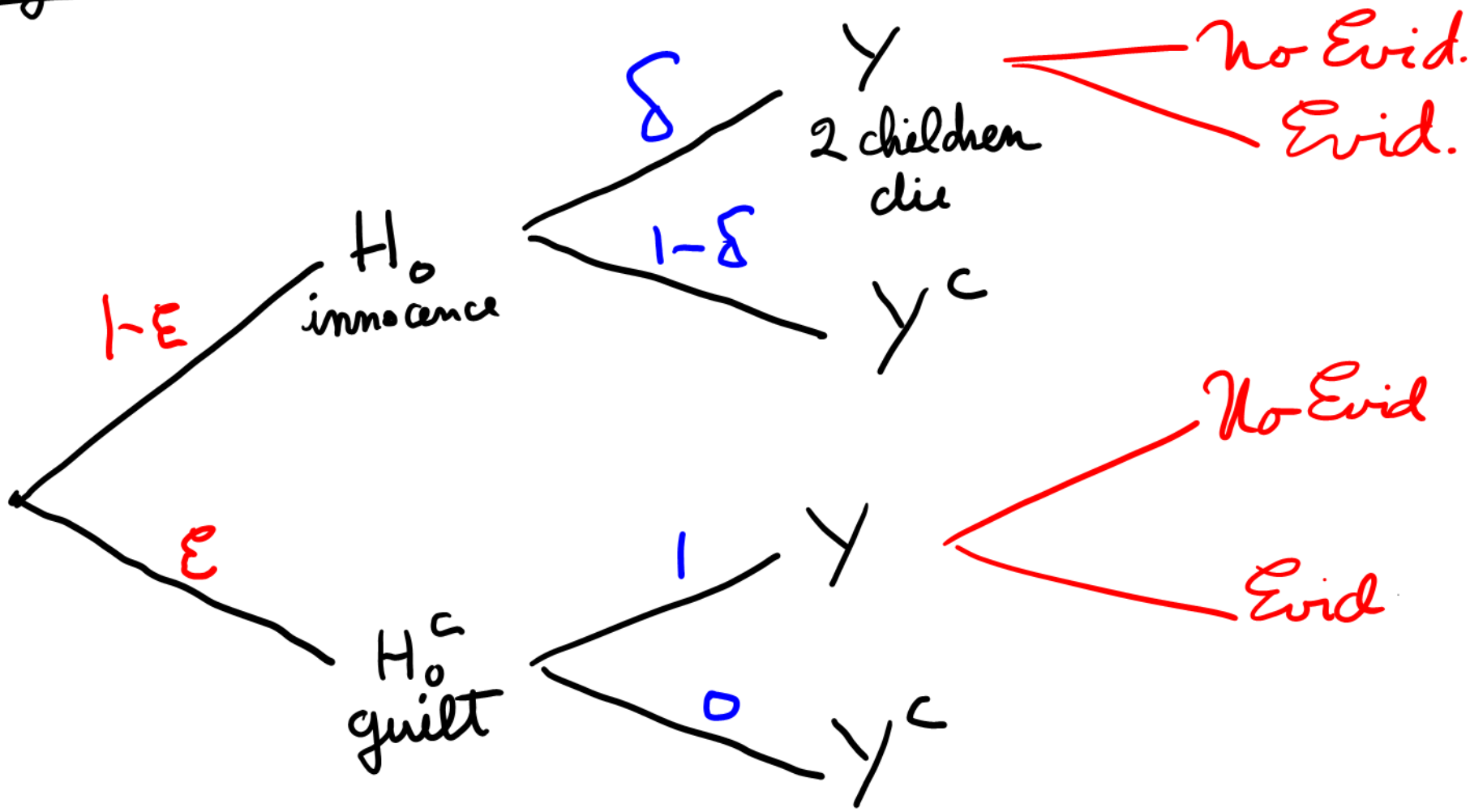
Bayesian tree:

But this ignores lack of evidence



If it's a crime, it's a "perfect" crime - and, presumably, only a small proportion of crimes are perfect crimes.

Bayesian tree:



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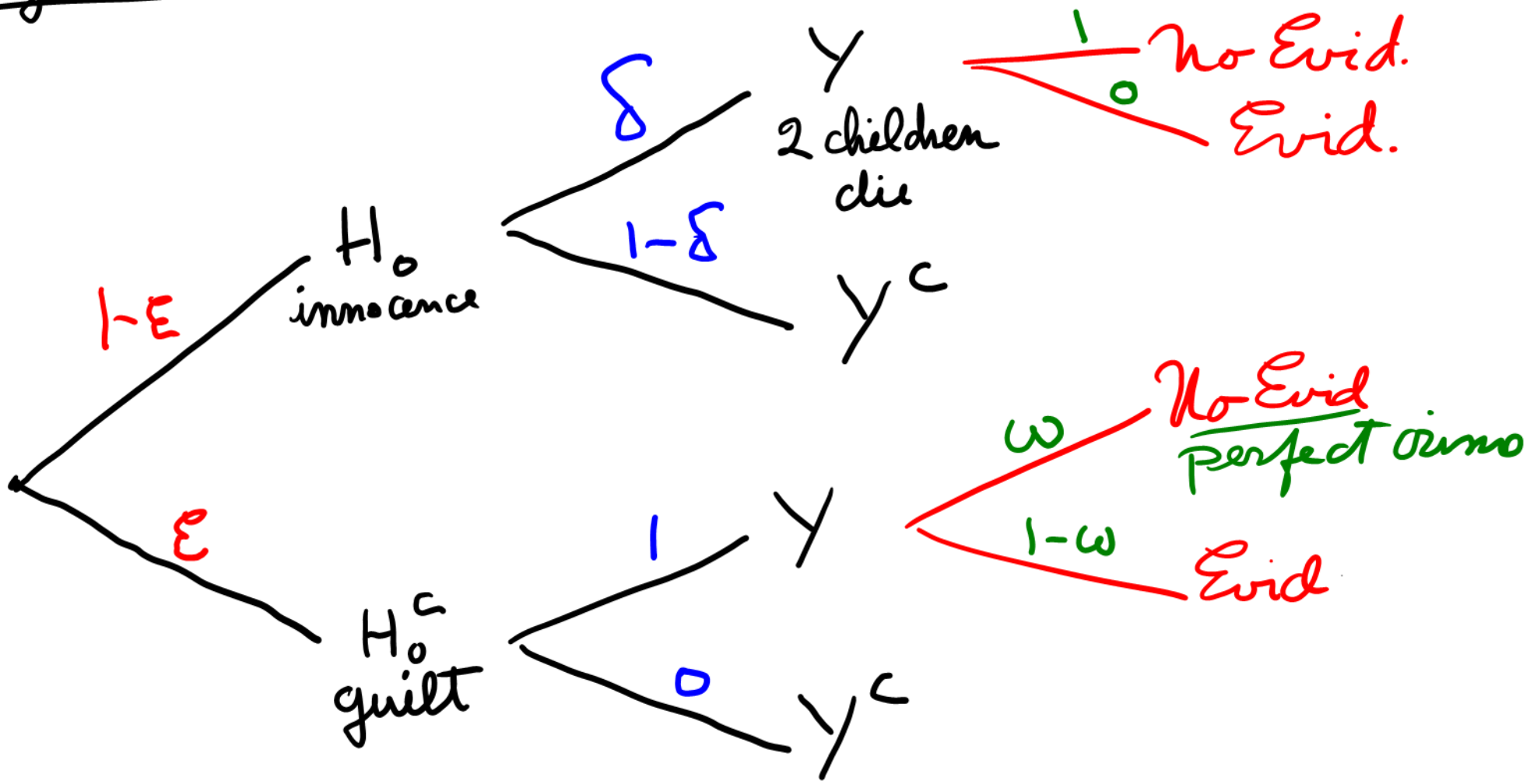

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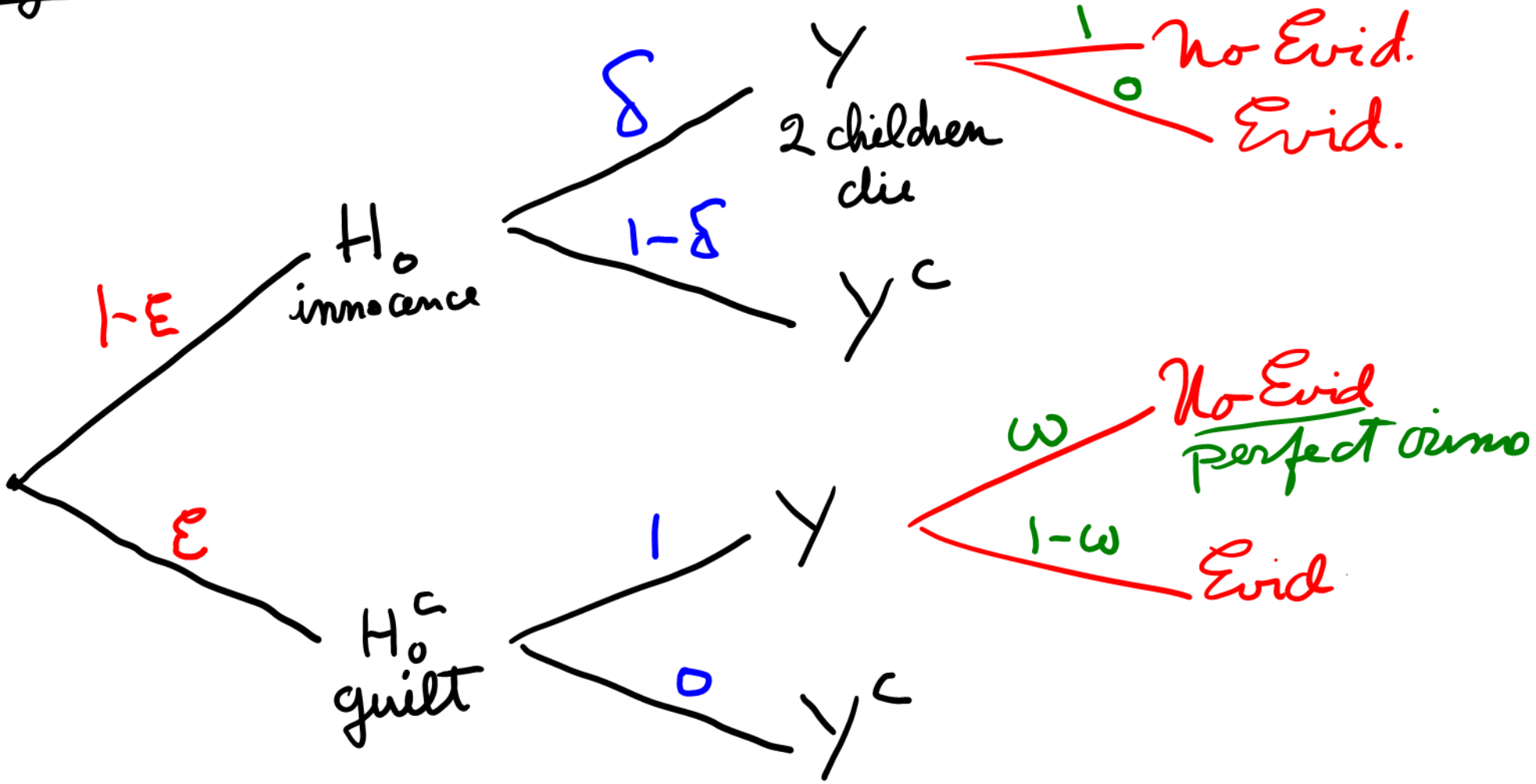

$$Pr(H_0 \mid Y \& No\ Evid) \approx \frac{\delta}{\delta + \varepsilon\omega} \approx \text{close to } 1\ !!$$

Sally Clark was innocent beyond a reasonable doubt.

$P(y^+ | H_0)$

was a very poor proxy for

$P(H_0 | y)$

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- But many (most?) scientists only know about $P(Y^+ | H_0)$.
- Many have been trained to be adamantly opposed to using "subjective" Bayesian methods instead of "objective" Frequentist methods.

— Using the p-value as a proxy for $P(H_0 | Y)$ has come to be known as the "Prosecutor's Fallacy"

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- But many (most?) scientists testifying don't know of other ways

— Using the p-value as a proxy for $P(H_0 | Y)$ has come to be known as the "Prosecutor's Fallacy"

So, how did we get to this? Why are we using p-values if they are so bad?

Dilemma

Dilemma

Θ : unknown state of nature

Dilemma

θ : unknown state of nature

Y : what's observed

Dilemma

Θ : unknown state of nature

Y : what's observed

What does Y say about Θ?

Dilemma

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Model: $p(Y|\Theta)$

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From this we can get p-values, confidence intervals, size-α tests.

Dilemma

Θ : unknown state of nature

Y : what's observed

What does Y say about Θ?

Model: $p(Y \mid \Theta)$

From this we can get p-values, confidence intervals, size-α tests.

But not $p(\Theta \mid Y)$ (posterior)

For that we need to start with $p(\Theta)$ (prior)

To get what you really want, you need to pay a price many are reluctant to pay.

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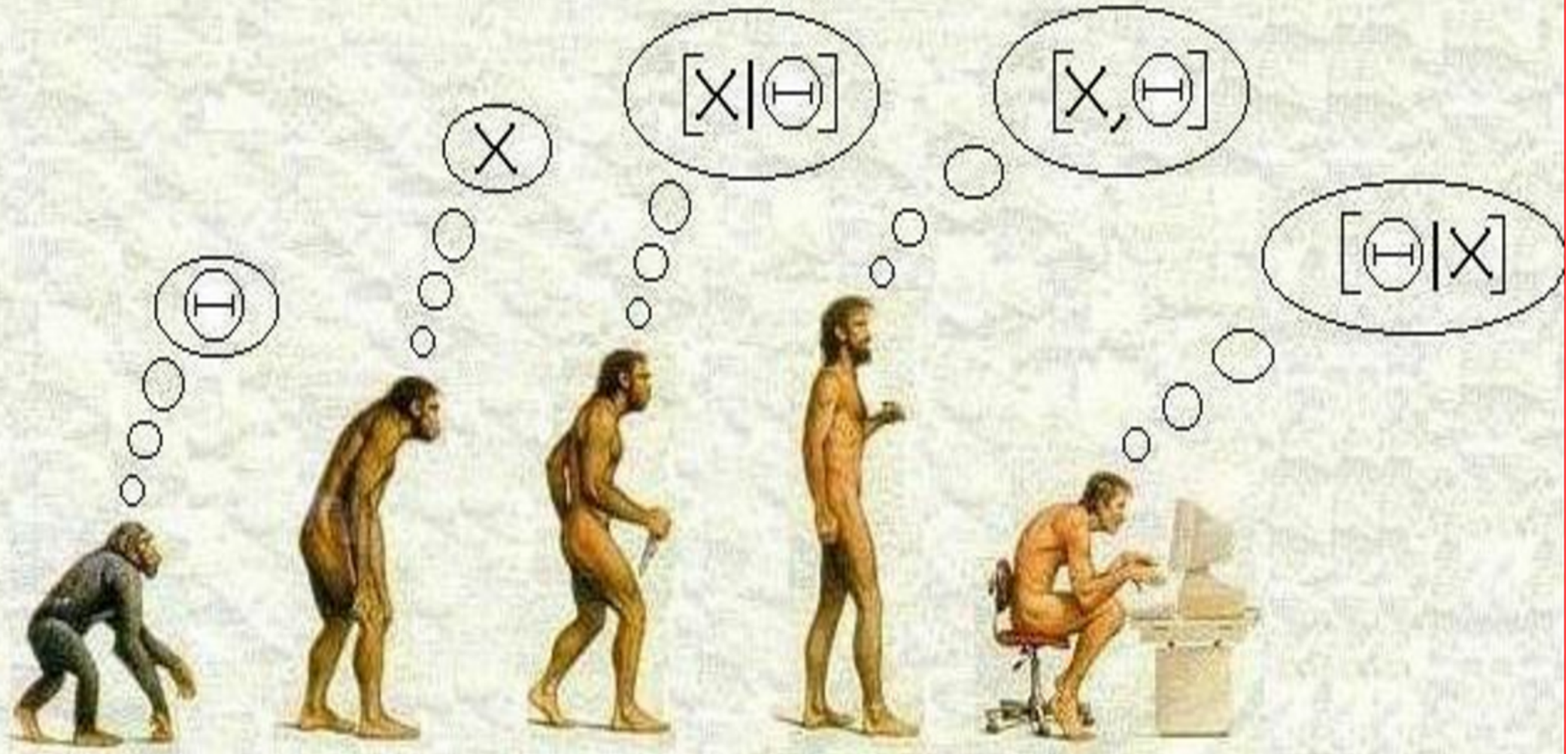
A historical perspective

(YET ANOTHER) HISTORY OF LIFE AS WE KNOW IT...



HOMO APRIORIUS

HOMO PRAGMATICUS

HOMO FREQUENTISTUS

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HOMO BAYESIANIS

(YET ANOTHER) HISTORY OF LIFE AS WE KNOW IT...

Cicero

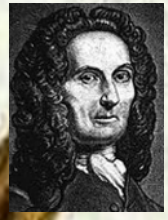
HOMO APRIORIUS | HOMO PRAGMATICUS | HOMO FREQUENTISTUS | HOMO SAPIENS | HOMO BAYESIANIS

(YET ANOTHER) HISTORY OF LIFE AS WE KNOW IT...

Cicero

early 1700s

de Moivre



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Pascal $P(\theta|x)$ using uniform $p(\theta)$

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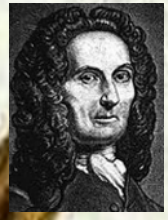

late 1700s
1800s

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$[X|\Theta]$

$[X,\Theta]$

$[\Theta|X]$

early 1700s
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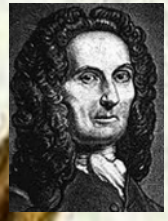

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Controversial

Uniform of $P \in (0,1)$
not same as
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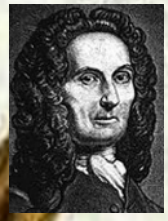

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Controversial

Uniform of $p \in (0,1)$ not same as Uniform of odds $\omega \in (0,\infty)$ – which is not even a probability

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Pascal
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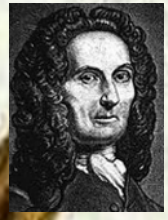

late 1700s
1800s

1920
Fisher – p-values
Neyman – decision theory
Pearson – hypothesis testing

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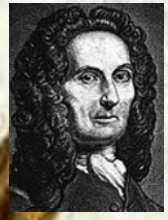

late 1700s 1800s

1920
Fisher
Neyman
Pearson

1940-60
Fisher - fiducial
Fraser - structural

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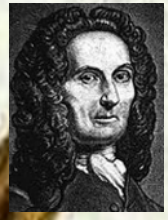

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MCMC
1950s+

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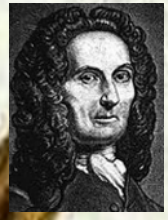

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MCMC
1950s+

HMC
1990s+

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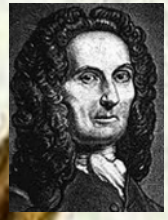

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Bayesian Renaissance

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Philosophical Basic problem

Philosophical

Basic problem

Given a model $P(x|\theta)$

Philosophical Basic problem

Given a model $P(X|\theta)$

To get $P(\theta|X)$

you need to be willing

to specify $P(\theta)$

Philosophical Basic problem

Given a model $P(x|\theta)$

To get $P(\theta|x)$

you need to be willing

to specify $P(\theta)$

Then $P(x,\theta) = P(x|\theta)P(\theta)$

and $P(\theta|x) = \frac{P(x,\theta)}{P(x)}$

Philosophical Basic problem

Given a model $P(X|\theta)$ (Model)

To get $P(\theta|X)$

you need to be willing

to specify $P(\theta)$ (Prior)

Then $P(X,\theta) = P(X|\theta)P(\theta)$

and $P(\theta|X) = \frac{P(X,\theta)}{P(X)}$ (Posterior)

Philosophical Basic problem

Given a model $P(x|\theta)$ (model)

To get $P(\theta|x)$

you need to be willing

to specify $P(\theta)$ (prior)

Then $P(x,\theta) = P(x|\theta)P(\theta)$

and $P(\theta|x) = \frac{P(x,\theta)}{P(x)}$ (posterior)

- You need a prior to get a posterior.
- Can we justify a particular prior?

Frequentists only use $P(x|\theta)$
and don't need $P(\theta)$

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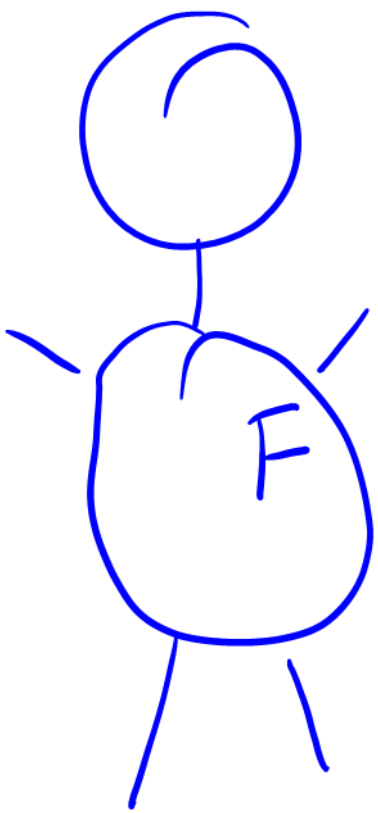
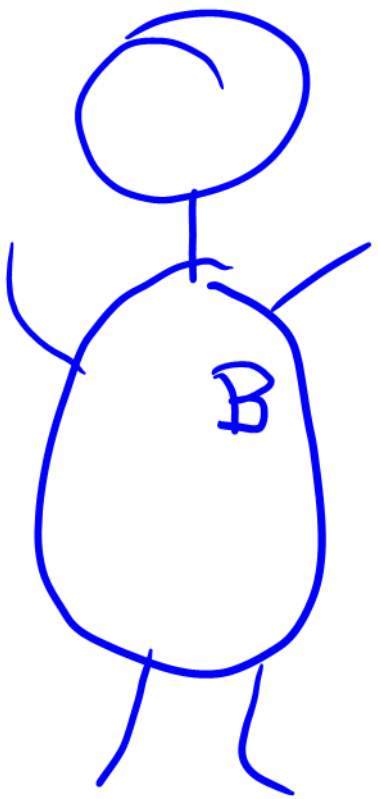
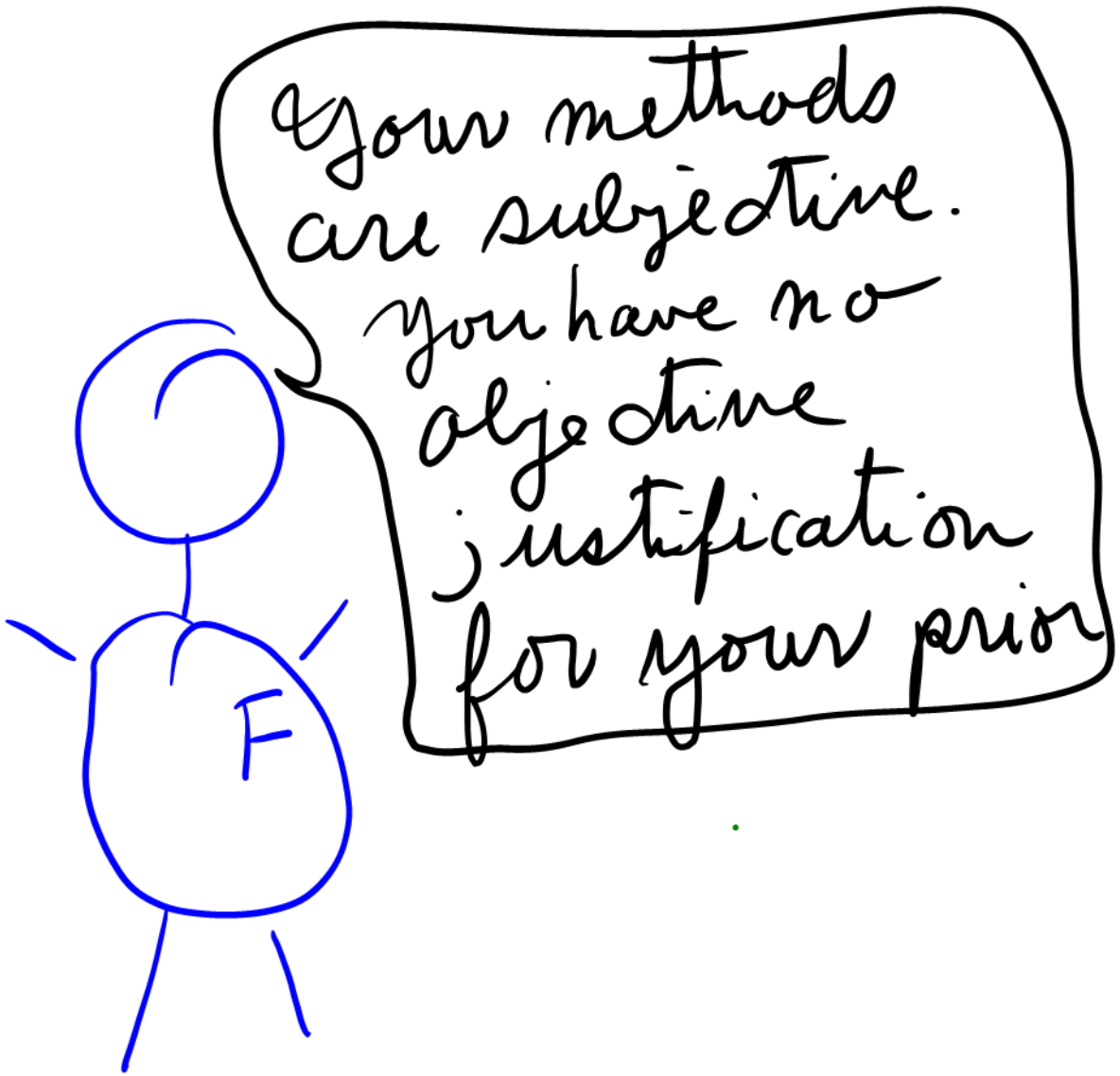
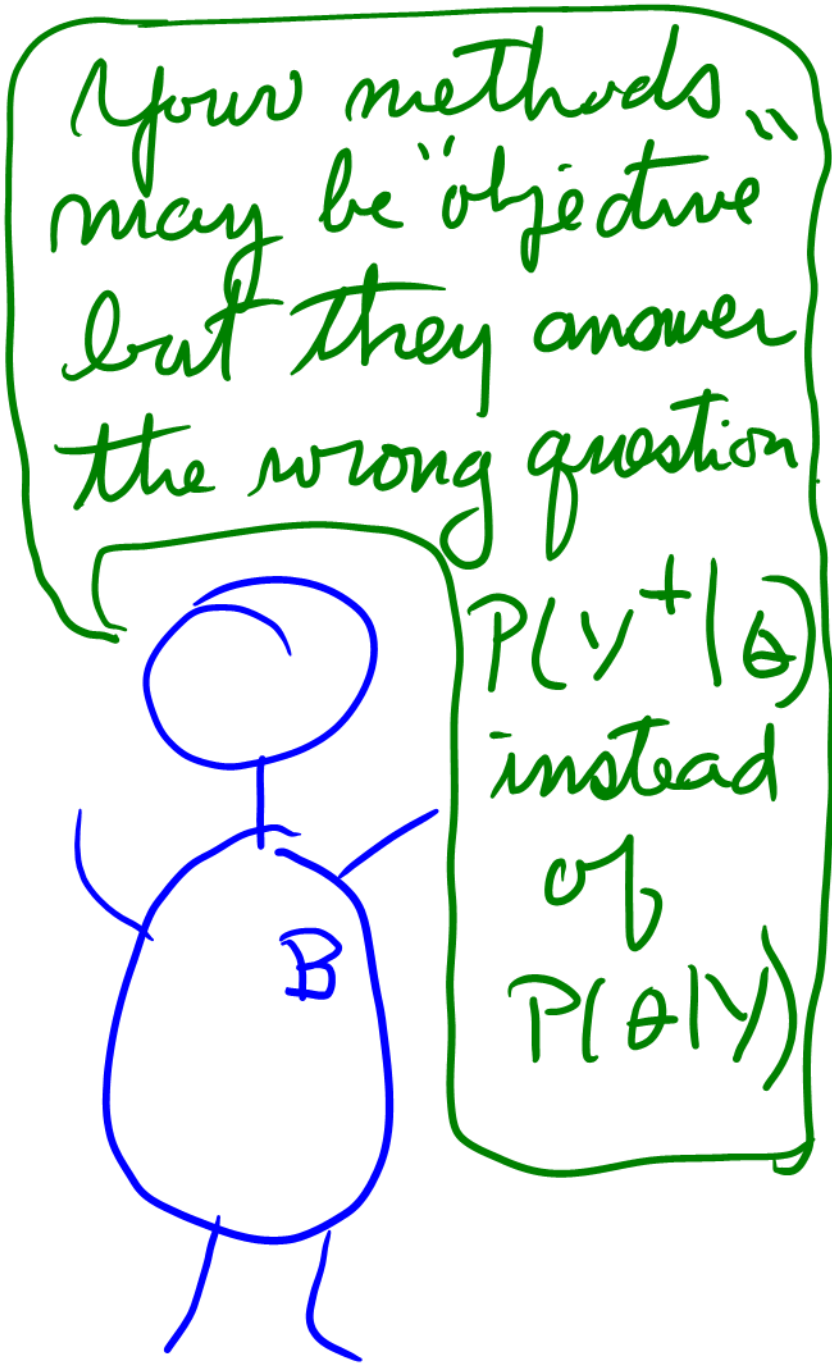
and don't need $P(\theta)$





Frequentists only use $P(x|\theta)$ and don't need $P(\theta)$





Frequentists only use $P(x|\theta)$ and don't need $P(\theta)$

Your methods are subjective. You have no objective justification for your prior

Your methods may be "objective" but they answer the wrong question

$P(y^+|\theta)$ instead of $P(\theta|y)$

Practical problem:

$$p(x, \theta) = p(x|\theta)\, p(\theta)$$

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$$p(\theta|x) = \frac{p(x, \theta)}{p(x)}$$

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$$p(x) = \int p(x, \theta)\, d\theta$$

Practical problem:

$$p(x, \theta) = p(x|\theta)\, p(\theta)$$

$$p(\theta|x) = \frac{p(x, \theta)}{p(x)}$$

$$p(x) = \int p(x, \theta)\, d\theta$$

If θ has high dimension this becomes easily impossible.

Practical problem:

$$p(x, \theta) = p(x|\theta)\, p(\theta)$$

$$p(\theta|x) = \frac{p(x, \theta)}{p(x)}$$

MCMC (mid 20th C.) comes to the rescue:
It's possible to sample from $p(\theta|x)$ knowing only $p(x, \theta)$

Posteriors without priors?

Fisher - Fiducial inference

Fraser - Structural inference

Objective Bayesian inference

Baking the Bayesian omelette without breaking the Bayesian egg.

Emerging practice:

Using weakly informative priors.

Posteriors without priors?

Fisher - Fiducial inference
Fraser - Structural inference
Objective Bayesian inference

→ The reason why thinking of a 95% CI for a linear regression parameter as a 95% "probability" interval is harmless.

Baking the Bayesian omelette without breaking the Bayesian egg.

Emerging practice:
Using weakly informative priors.

Posteriors without priors?

Fisher - Fiducial inference
Fraser - Structural inference
Objective Bayesian inference

Baking the Bayesian omelette without breaking the Bayesian egg.

Emerging practice:
Using weakly informative priors.

→ The reason why thinking of a 95% CI for a linear regression parameter as a 95% "probability interval" is harmless.

But don't take it for granted
Remember Sally Clark

Improper vs proper priors

Posteriors.

Problems

HxC

Markov Chain Monte Carlo

We use $p(\theta, x) = p(x|\theta)\, p(\theta)$

Markov Chain Monte Carlo

We use $p(\theta, x) = p(x|\theta)\, p(\theta)$

joint — model × prior

Samples from $P(\theta|X)$ using only $p(\theta, x)$

i.e. no need to find elusive $P(x)$

Markov Chain Monte Carlo

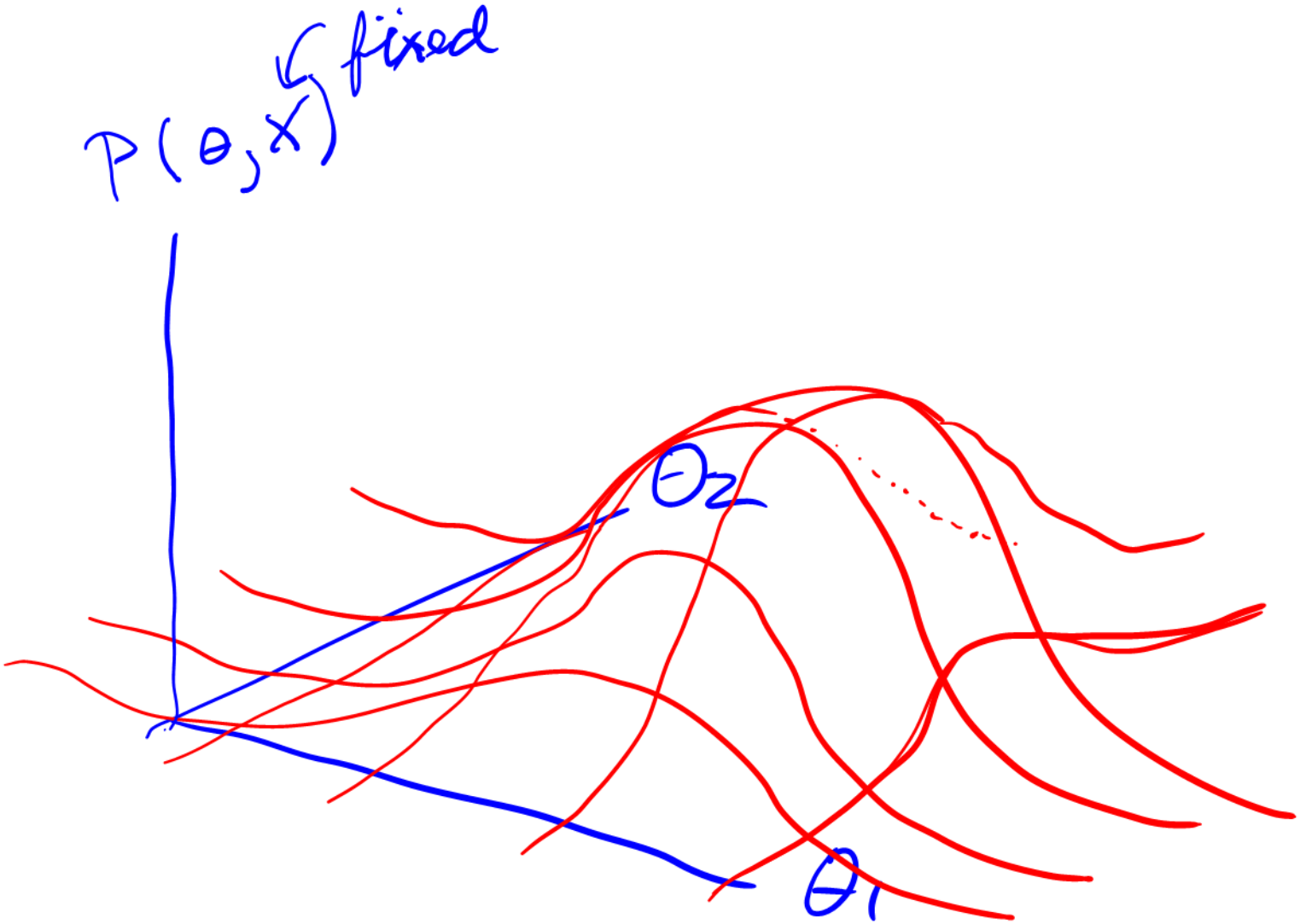
We use $p(\theta, x) = p(x|\theta)\, p(\theta)$

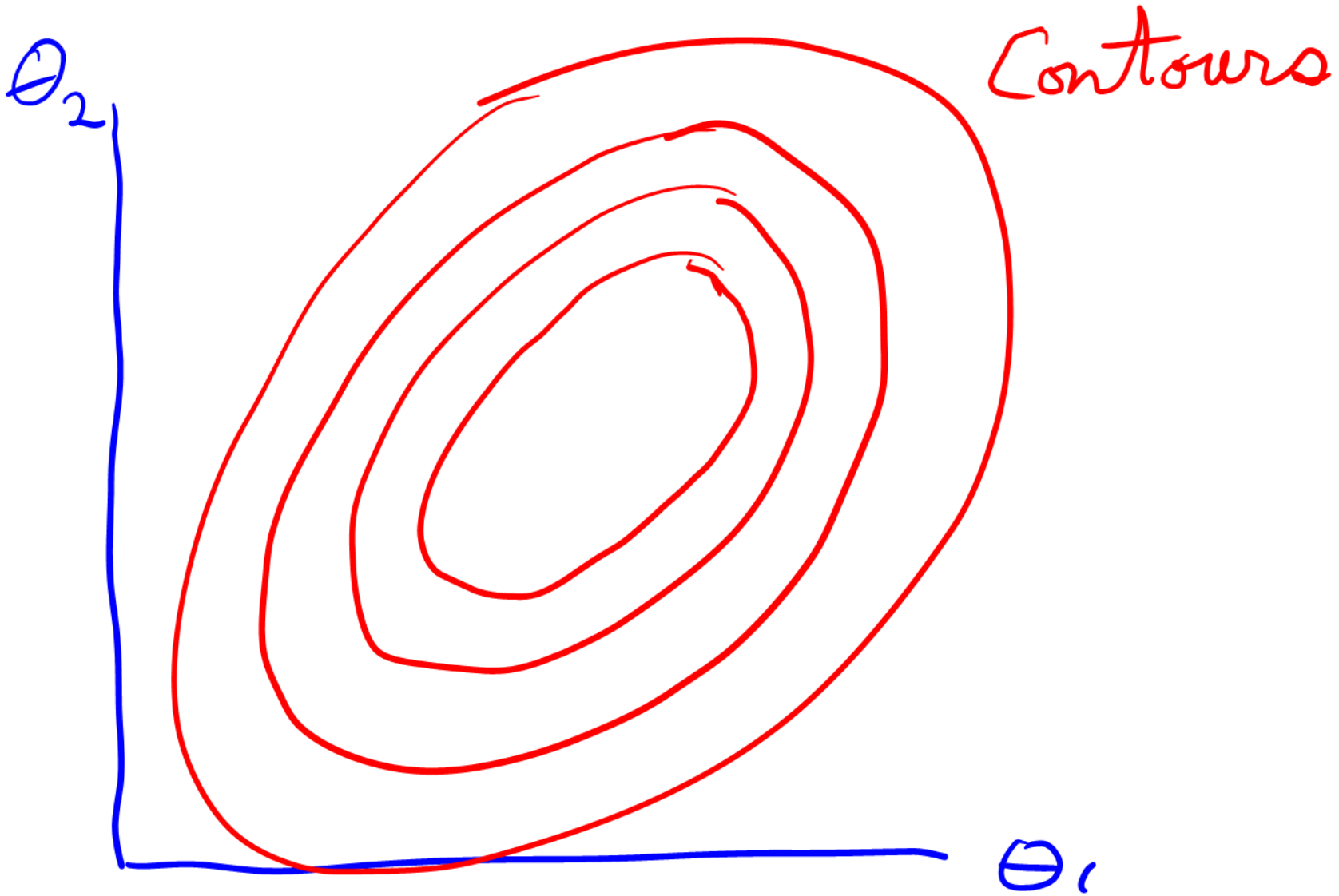
joint — model × prior

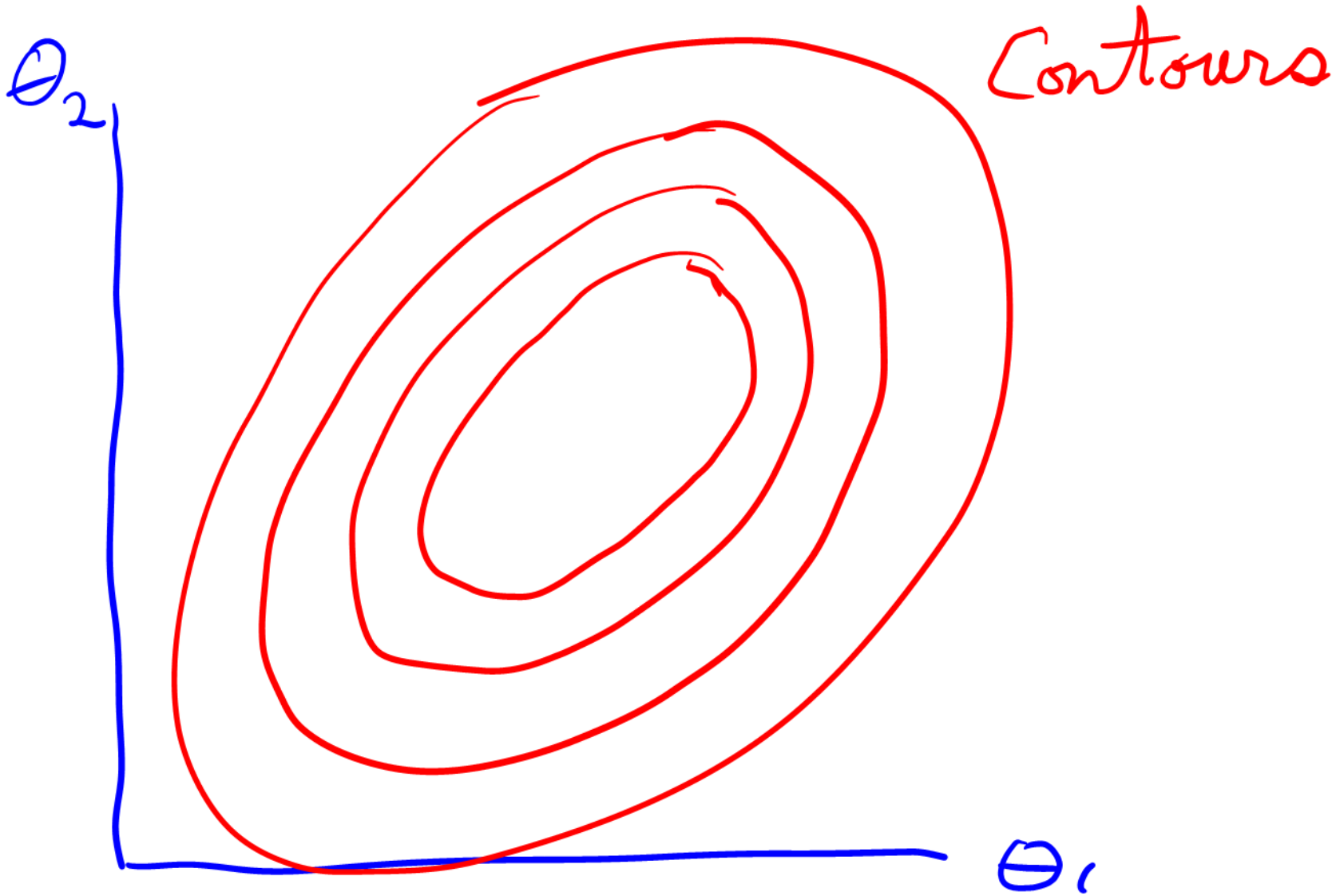
Samples from $P(\theta|x)$ using only $p(\theta, x)$

i.e. no need to find elusive $P(x)$

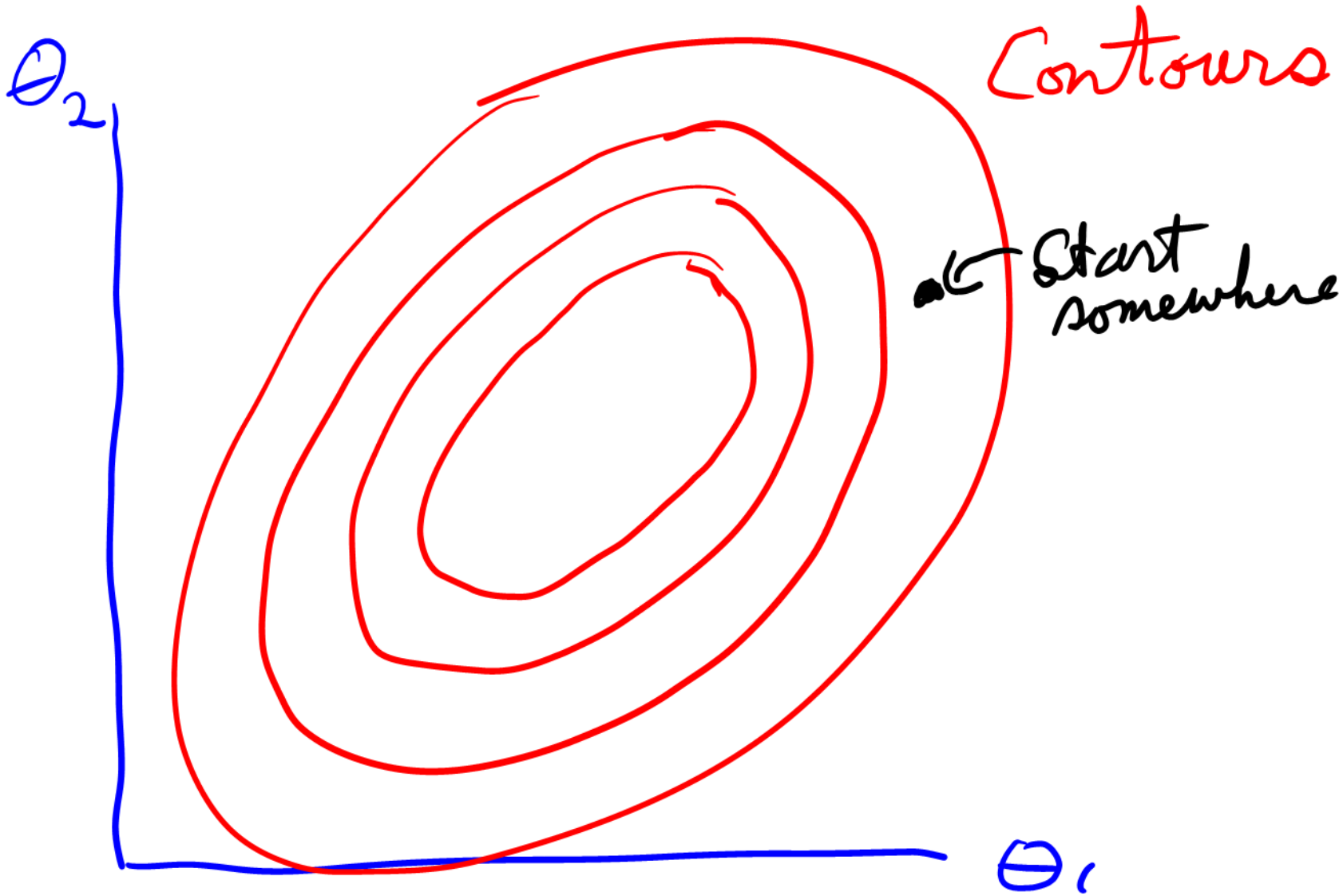
With x fixed, think of $P(\theta, x)$ as defining a mountain over θ space


p(θ, x)
fixed
θ2
θ1

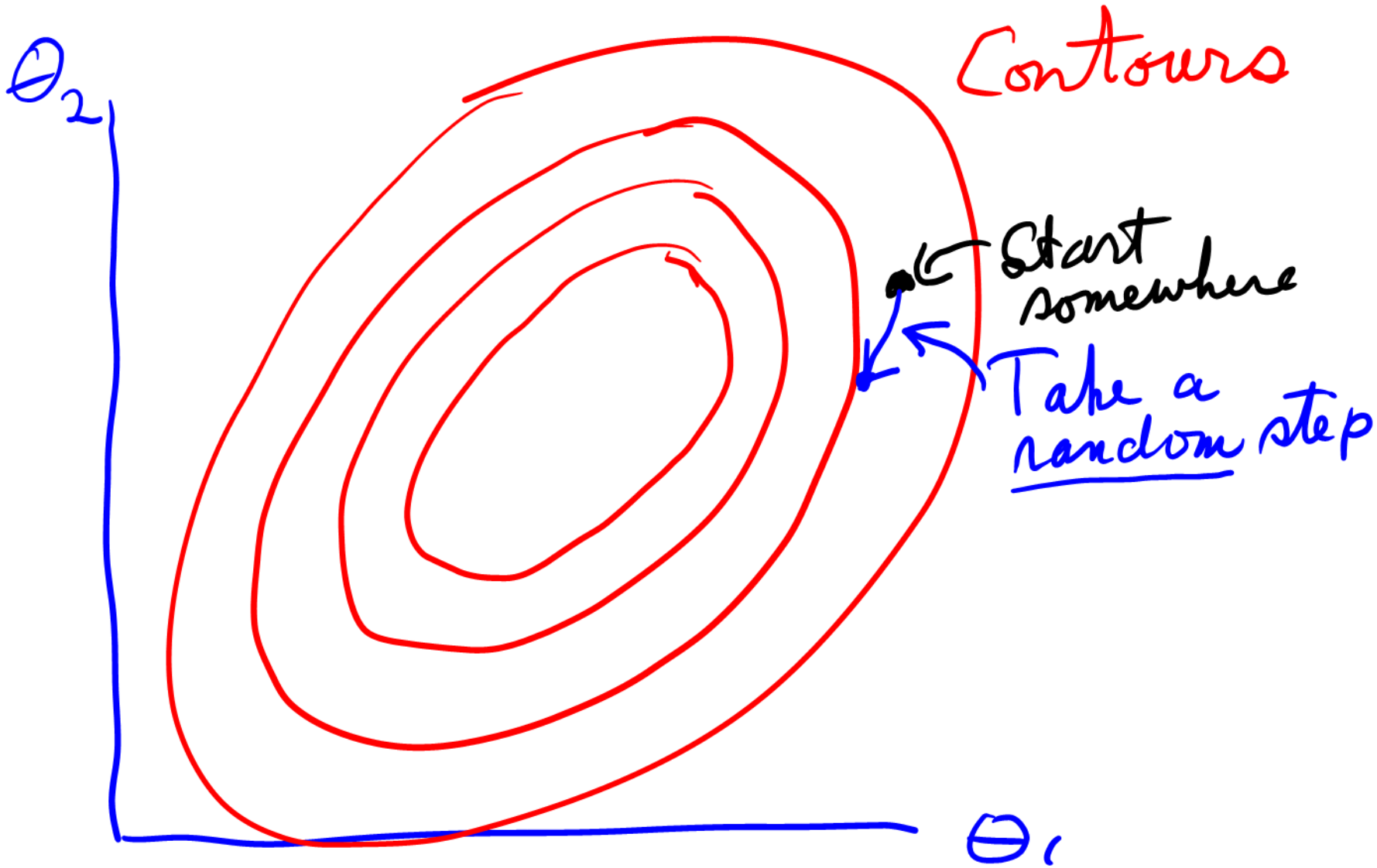

θ_2
Contours
θ_1



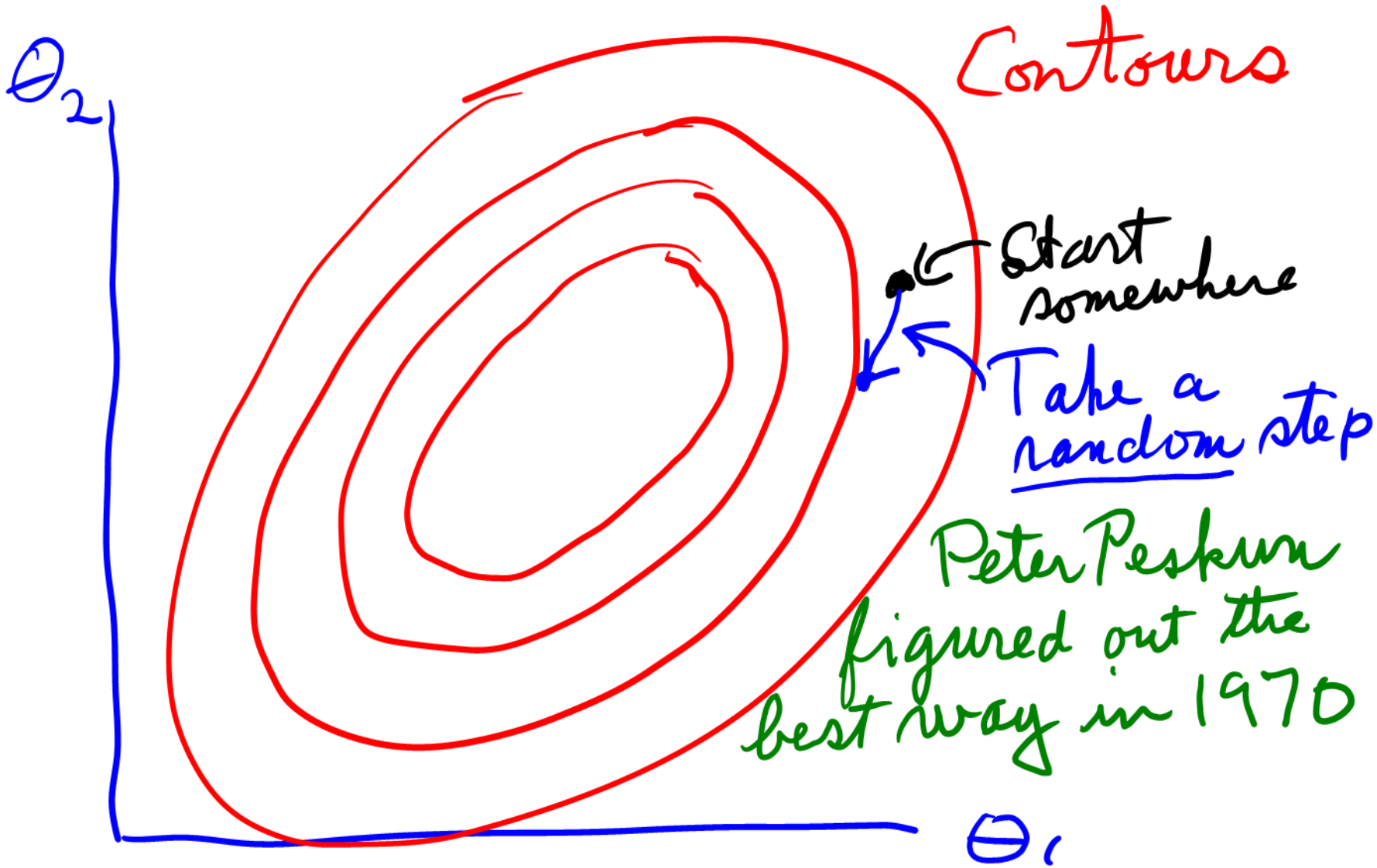
Metropolis-Hastings algorithm



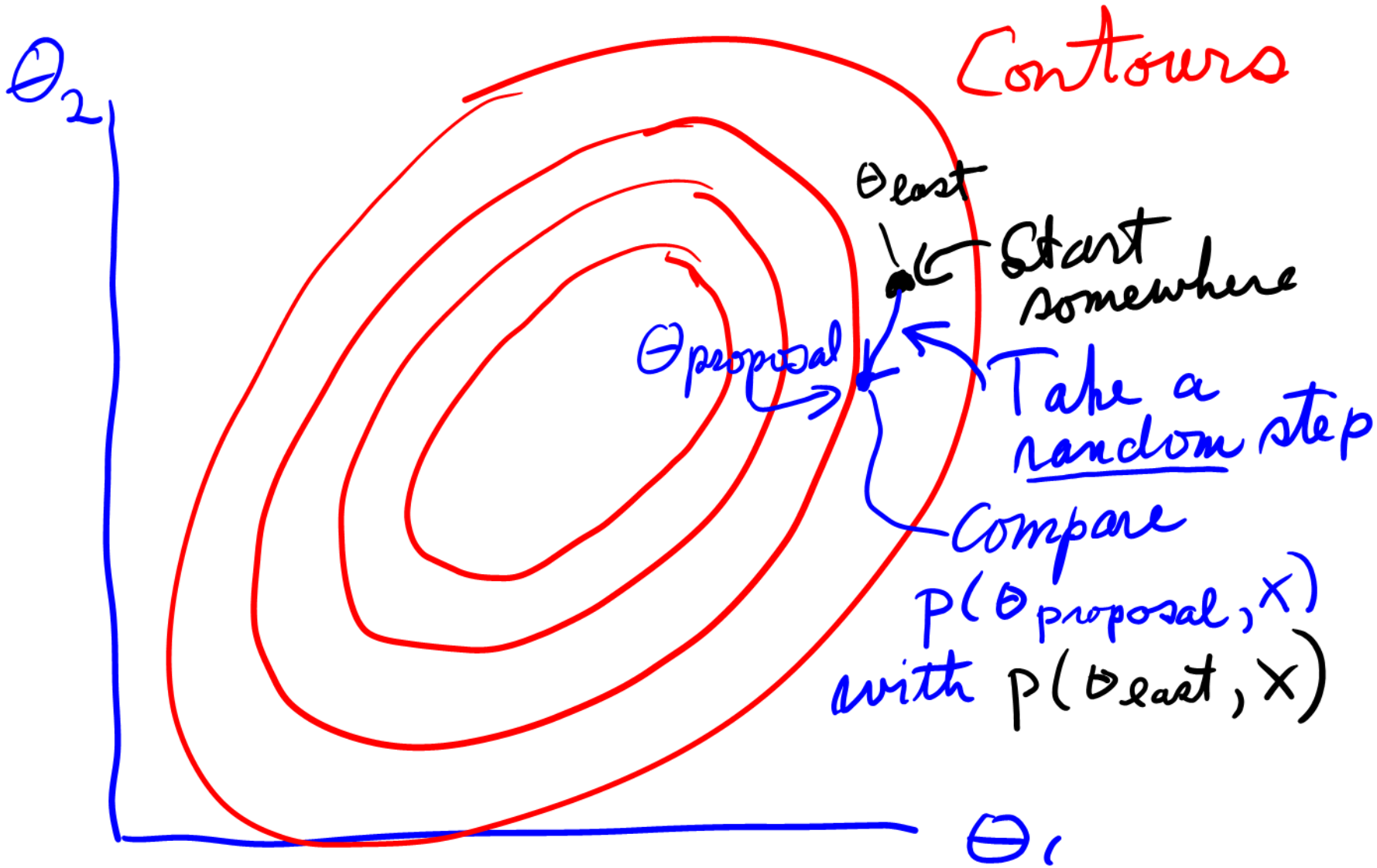
Metropolis-Hastings algorithm



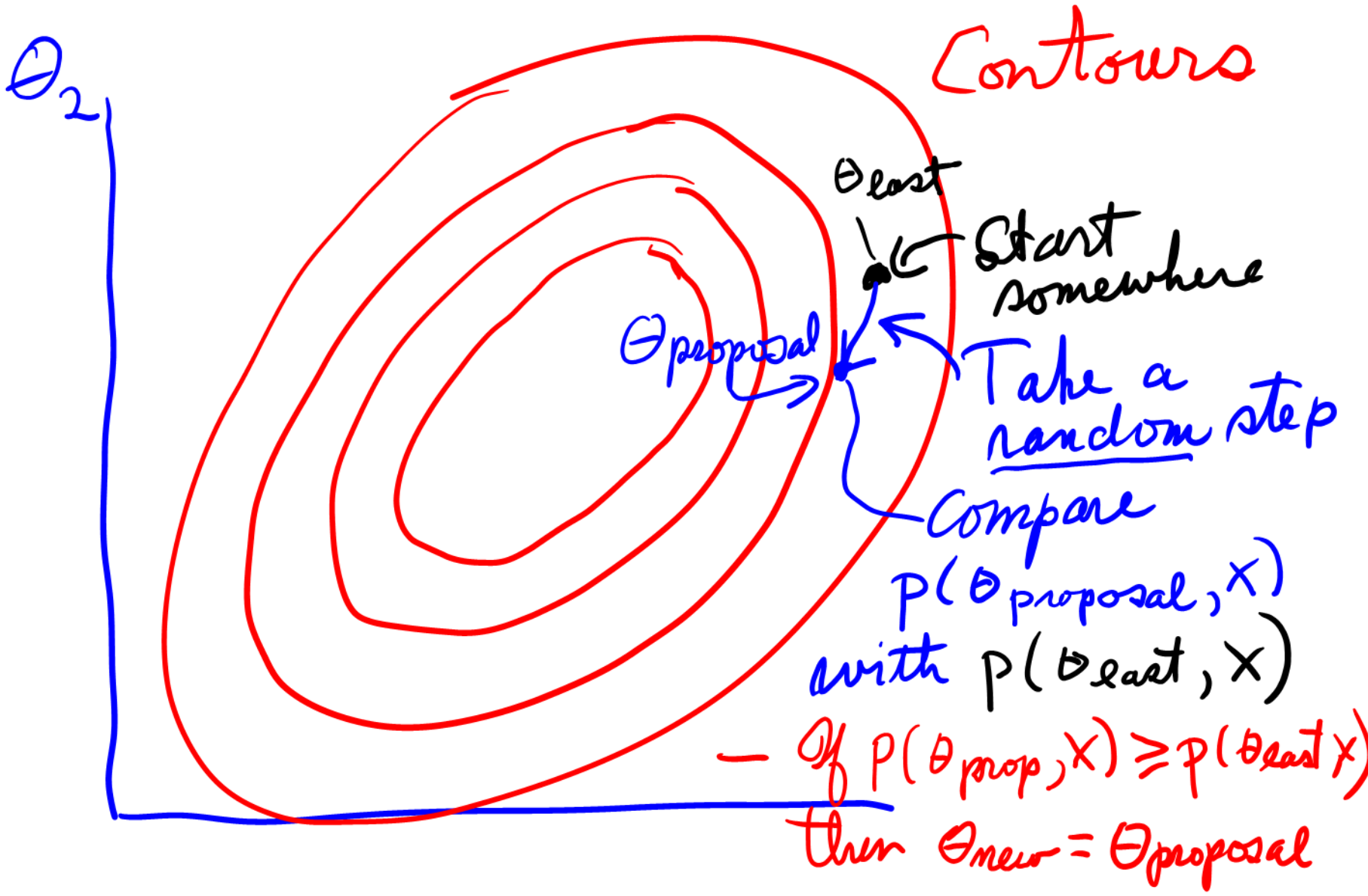
Metropolis-Hastings algorithm

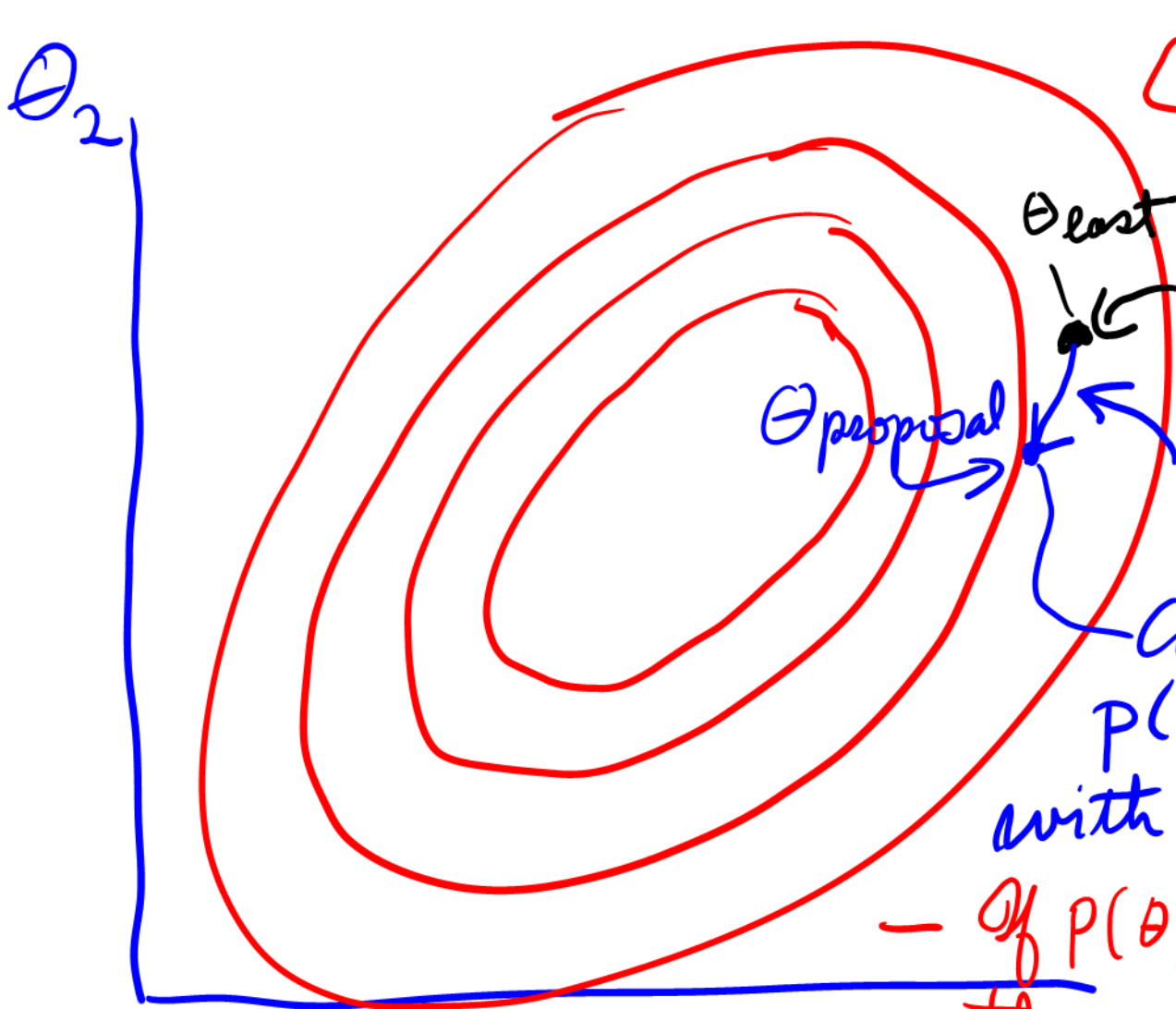


Metropolis-Hastings algorithm



Metropolis-Hastings algorithm


Contours
θ_2
θ_{last}
Start somewhere
$\theta_{proposal}$
Take a random step
Compare
$p(\theta_{proposal}, X)$
with $p(\theta_{last}, X)$
– If $p(\theta_{prop}, X) \geq p(\theta_{last} X)$
then $\theta_{new} = \theta_{proposal}$


θ_2
Contours
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Start somewhere
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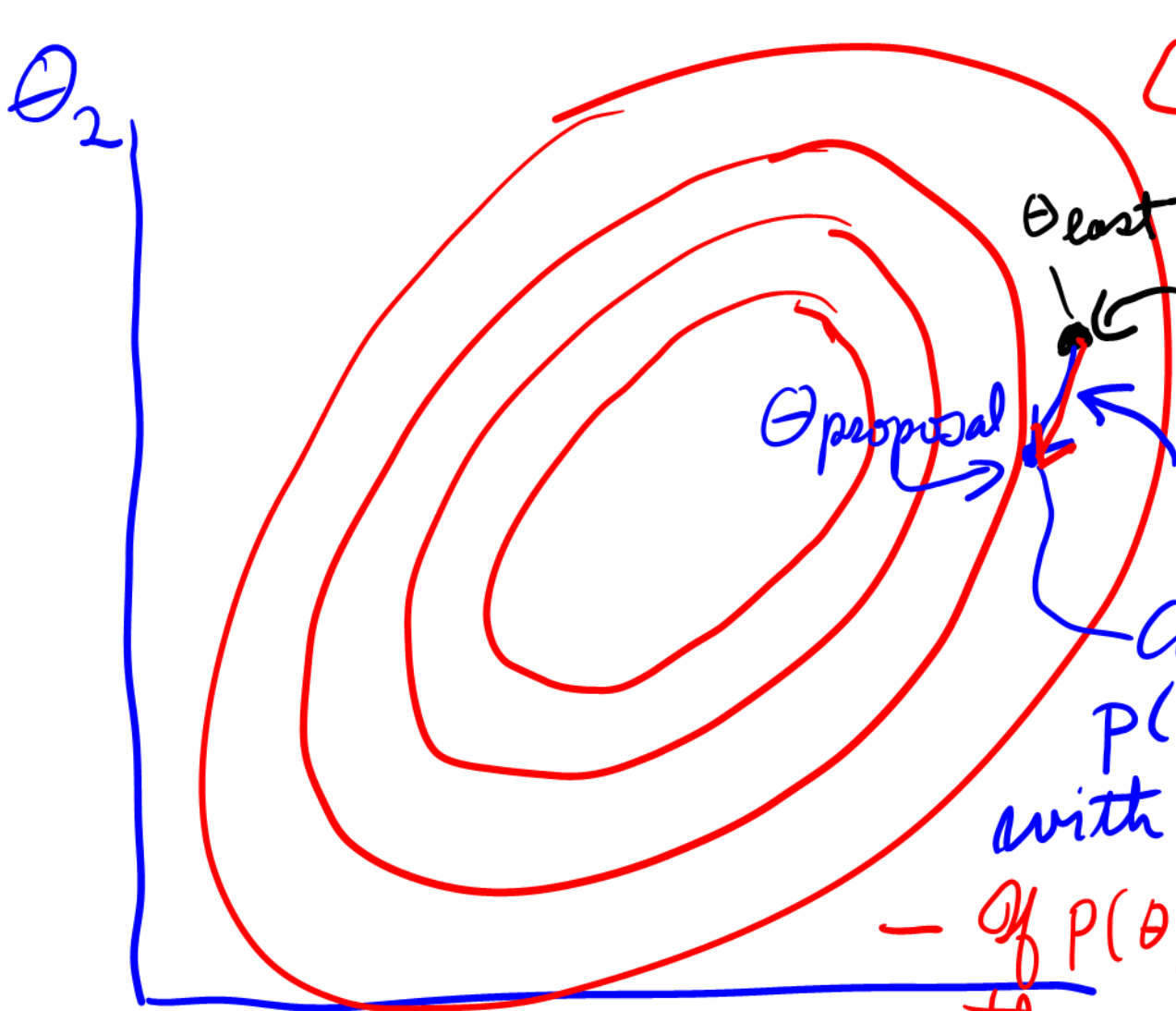
Take a random step
Compare
$p(\theta_{proposal}, X)$
with $p(\theta_{last}, X)$
– If $p(\theta_{prop}, X) \geq p(\theta_{last} X)$
Then $\theta_{new} = \theta_{proposal}$
– Otherwise, i.e if you have moved down in probability, ~~set~~ $\theta_{new} = \theta_{proposal}$ with prob $\frac{p(\theta_{prop}, X)}{p(\theta_{last}, X)}$
else $\theta_{new} = \theta_{last}$


θ_2
Contours
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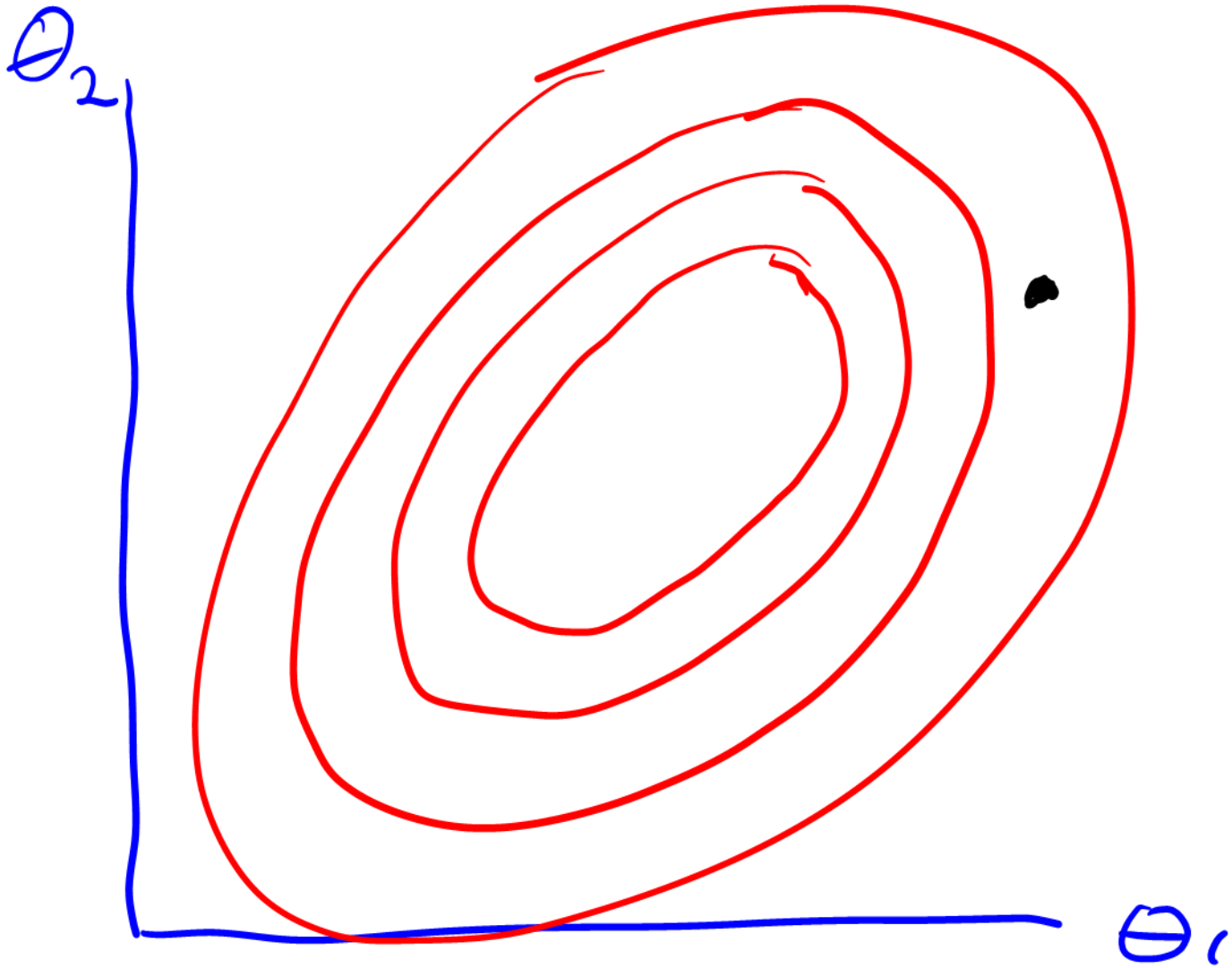
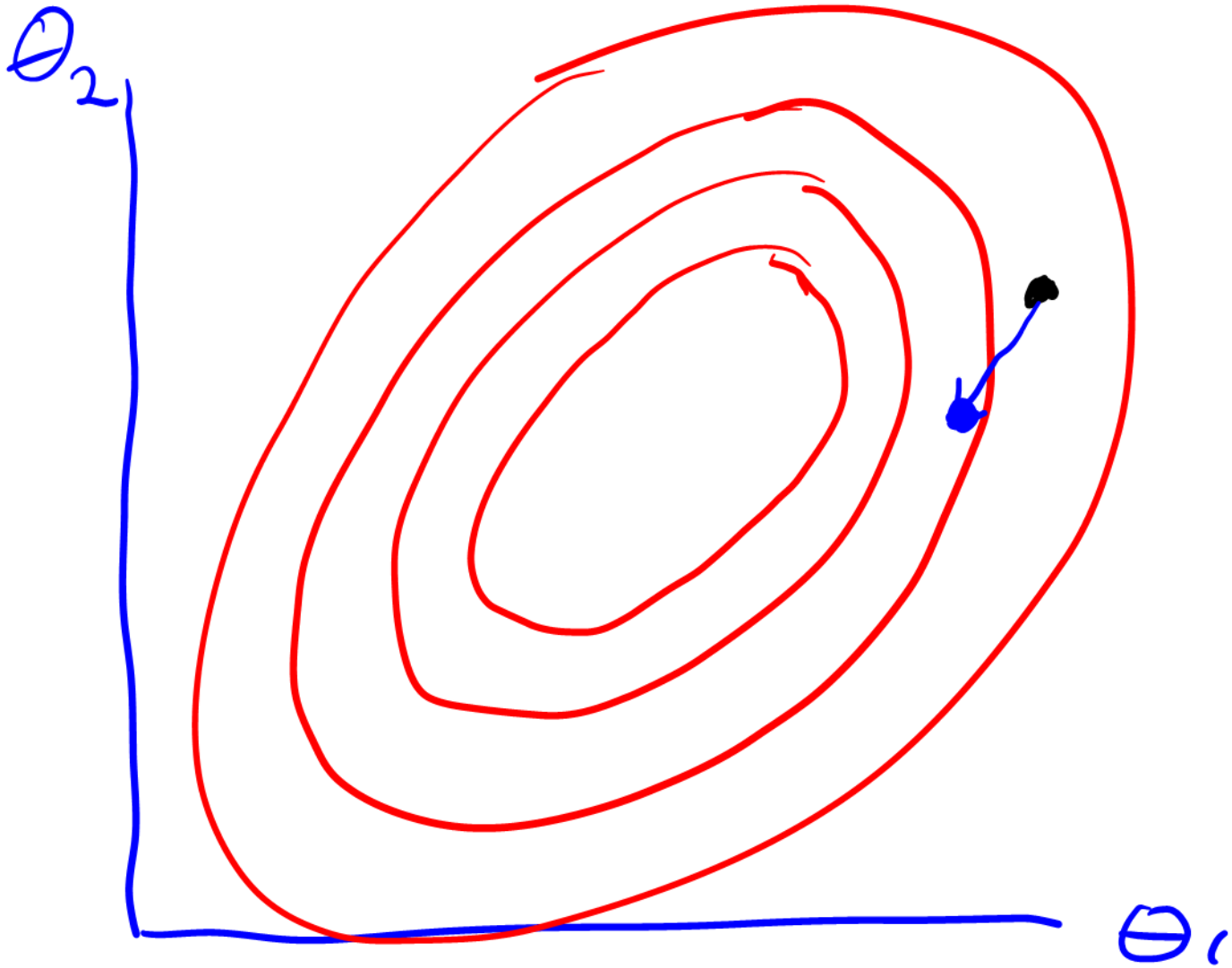
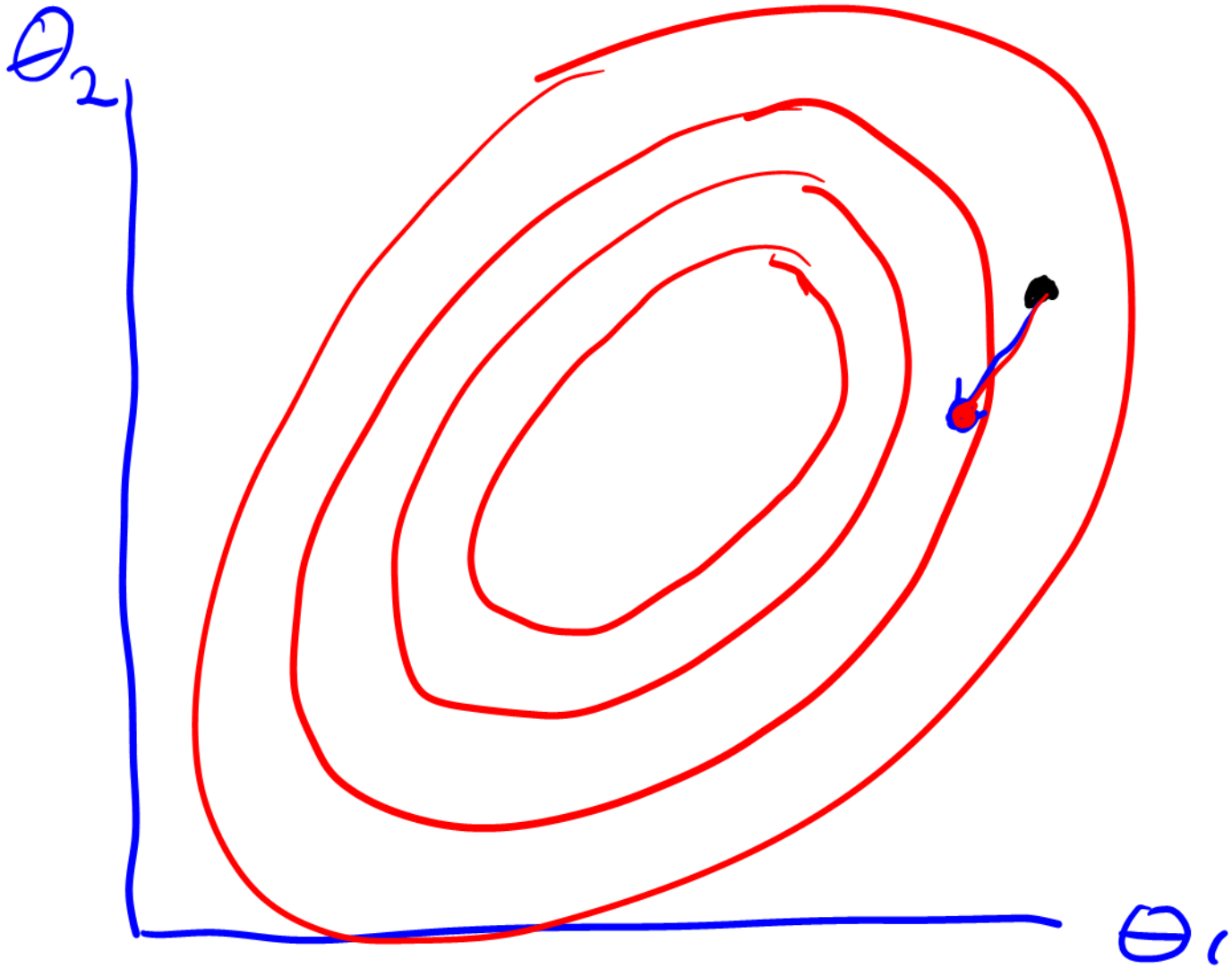
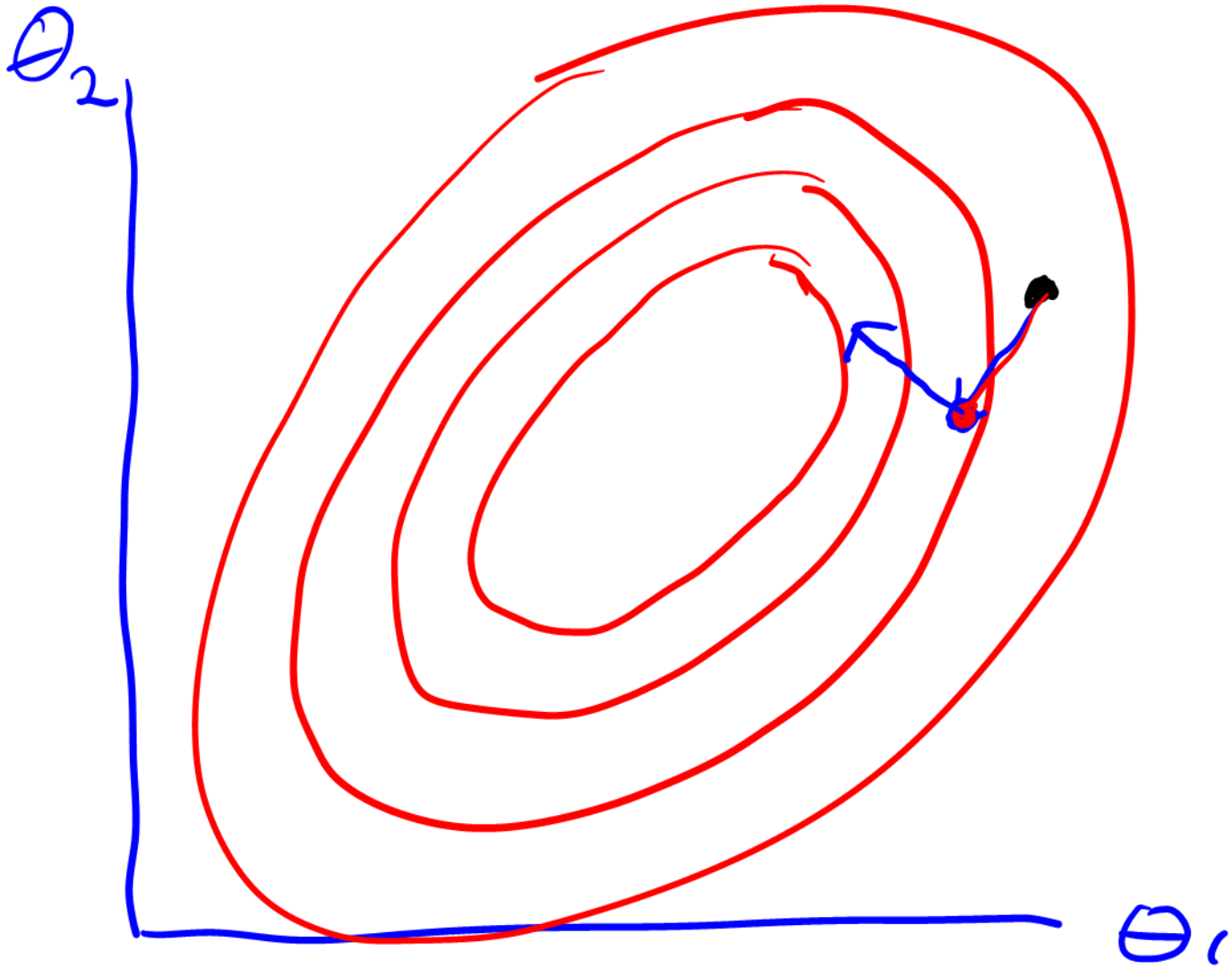
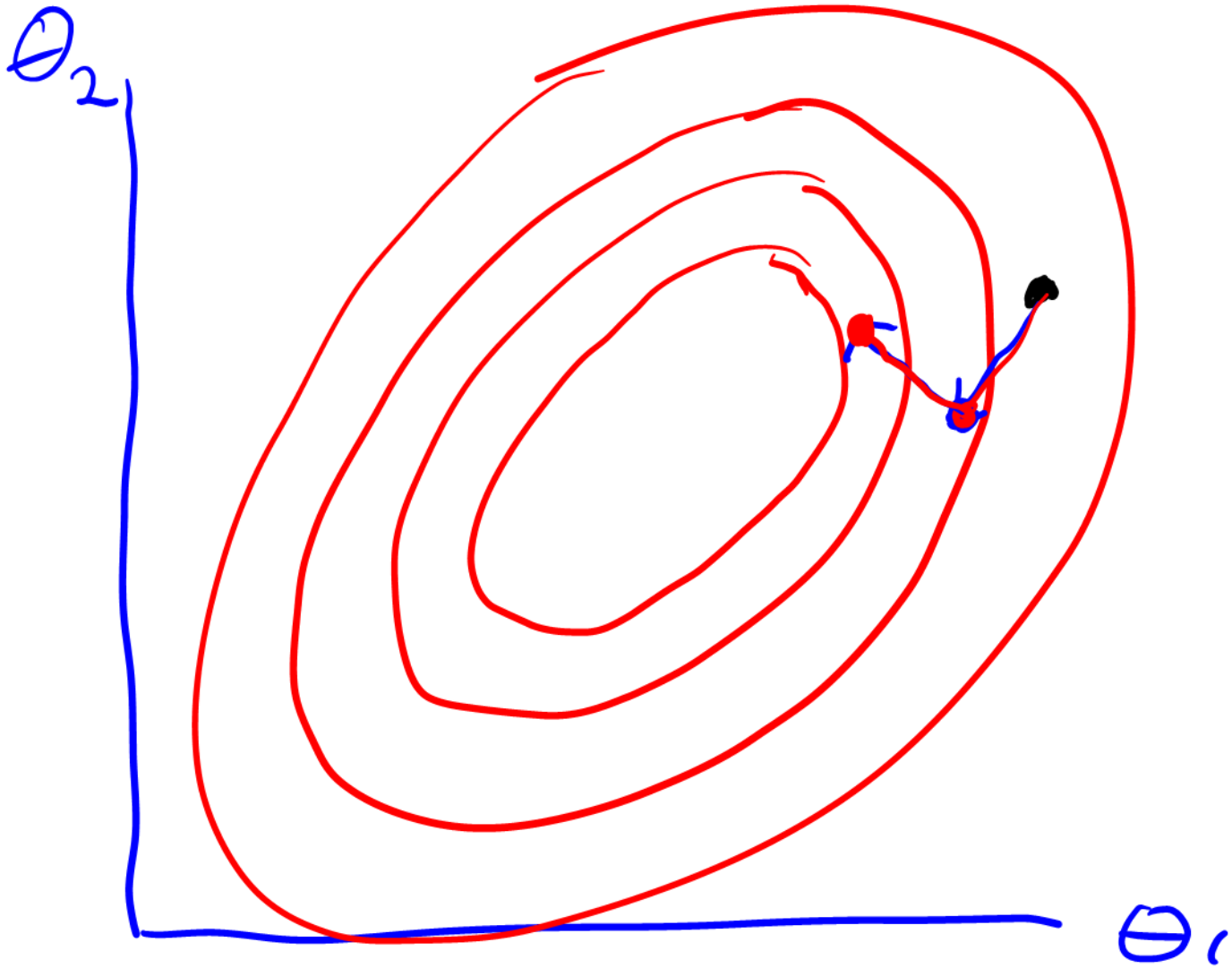
Start somewhere
$\theta_{proposal}$
Take a random step
Compare
$p(\theta_{proposal}, X)$
with $p(\theta_{last}, X)$
– If $p(\theta_{prop}, X) \geq p(\theta_{last} X)$
Then $\theta_{new} = \theta_{proposal}$
– Otherwise, i.e if you have moved down in probability, ~~but~~ $\theta_{new} = \theta_{proposal}$ with prob $\frac{p(\theta_{prop}, X)}{p(\theta_{last}, X)}$
else $\theta_{new} = \theta_{last}$

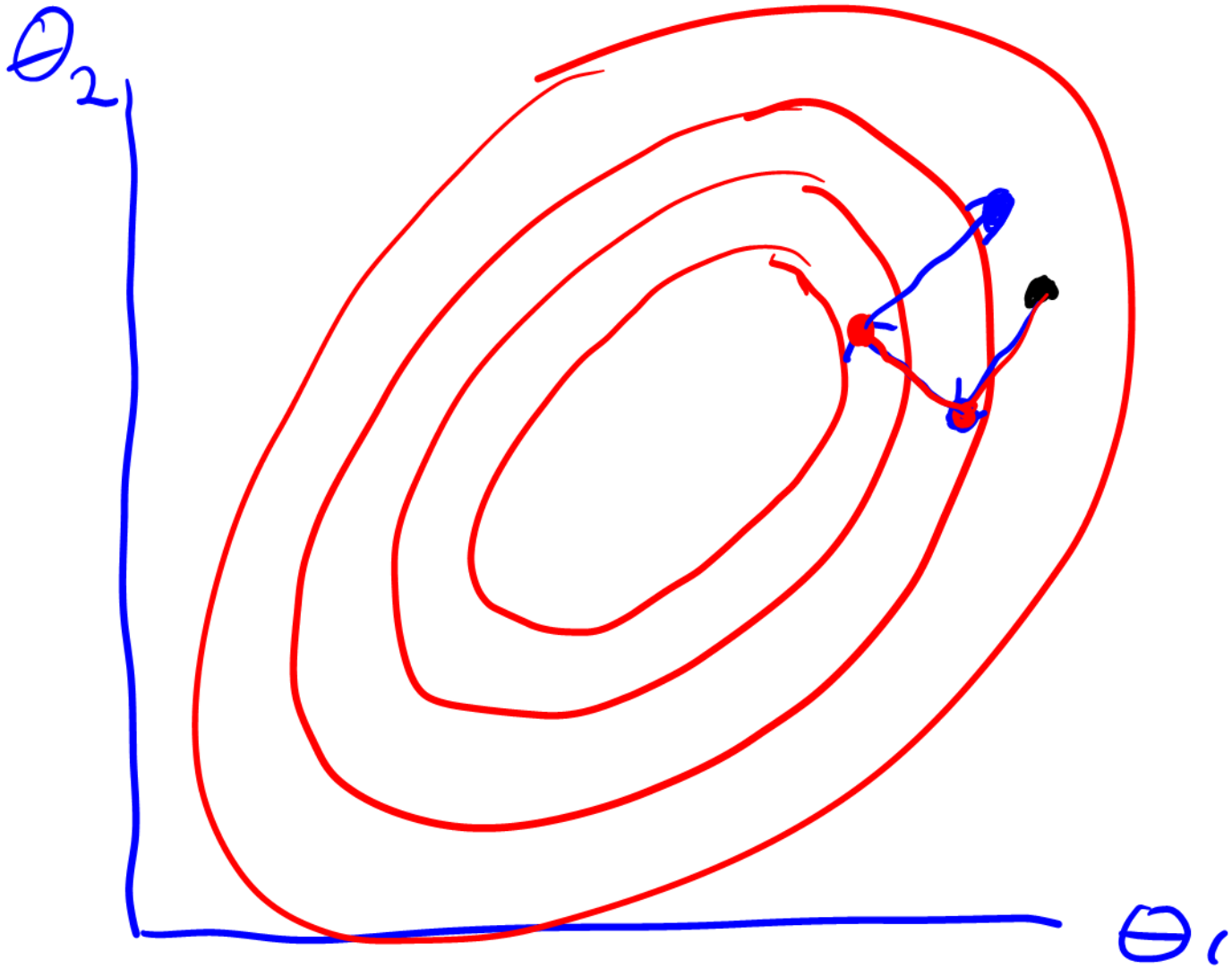

θ_2
θ_1

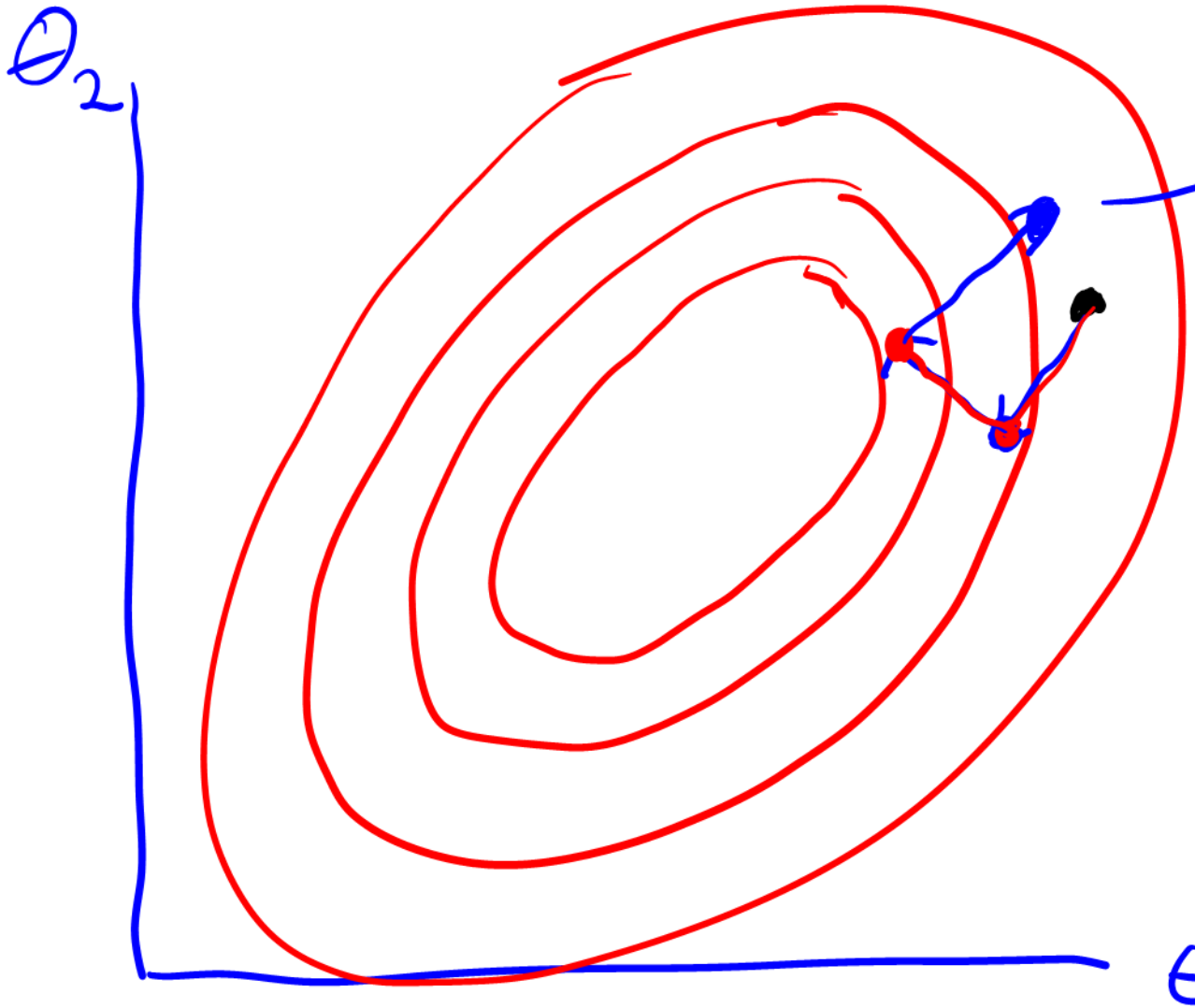

θ_2
θ_1


θ_2
θ_1


θ_2
θ_1


θ_2
θ_1

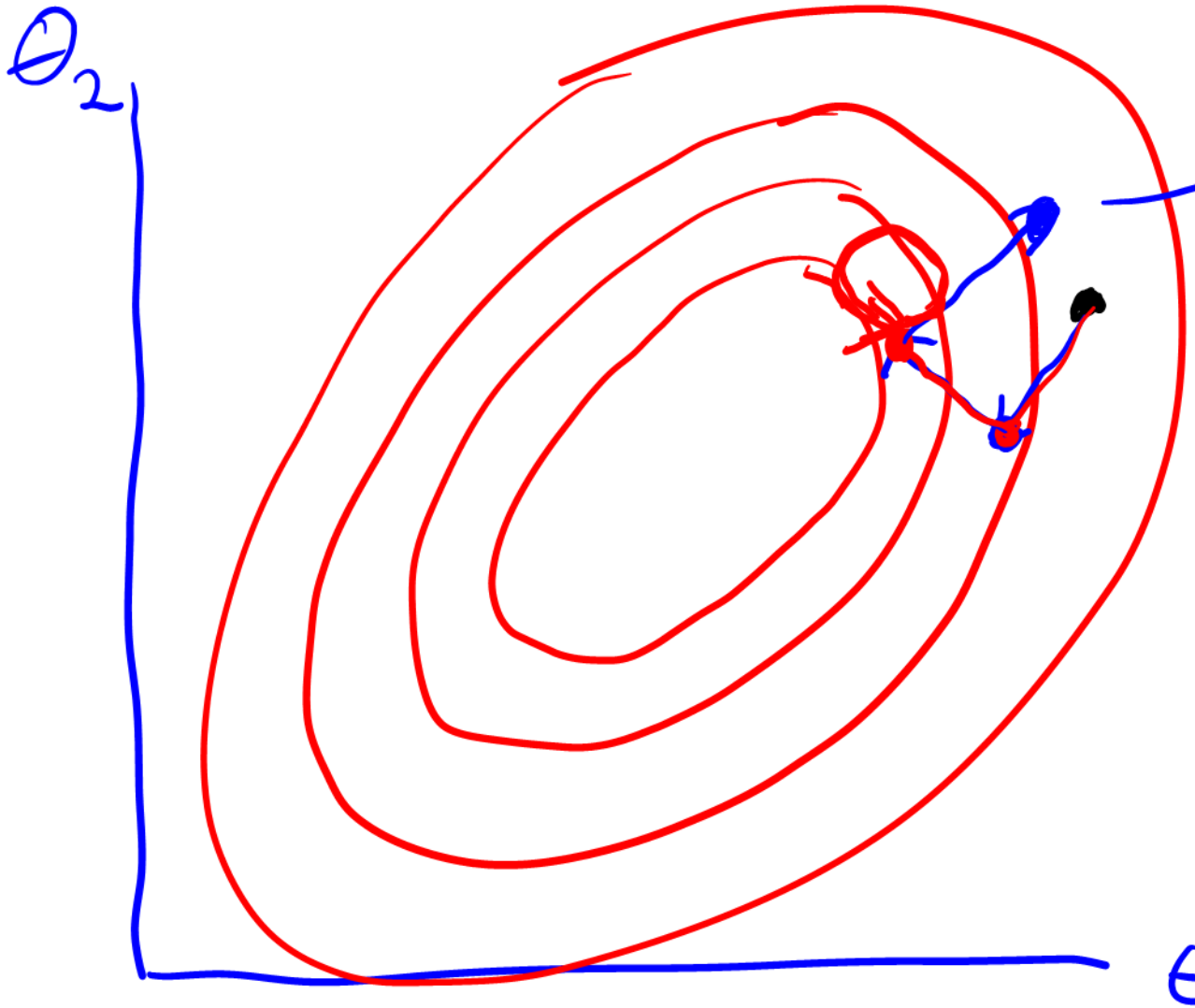

θ_2
θ_1



Toss a biased coin with

$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

If Heads move, if Tails stay



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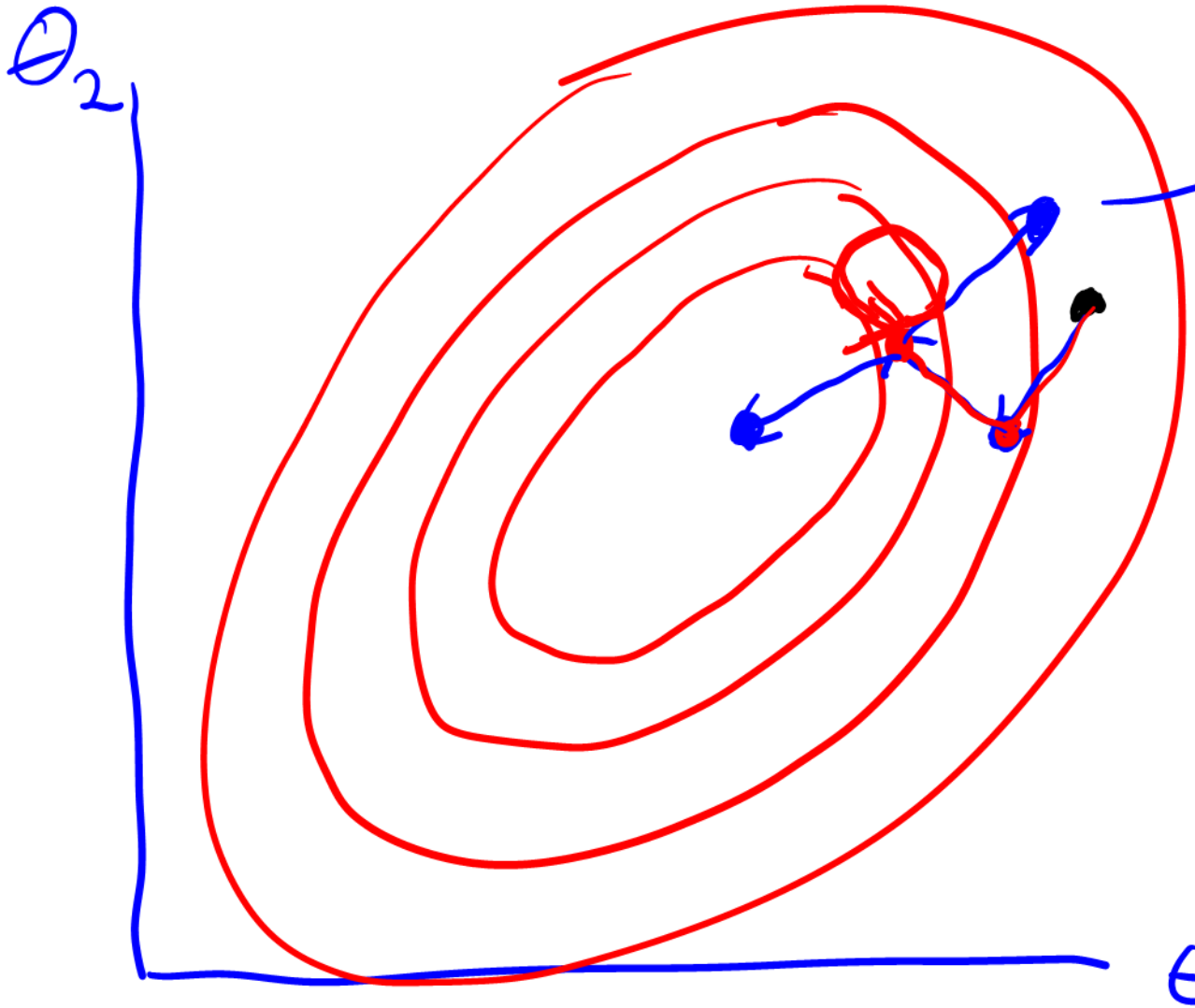
$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

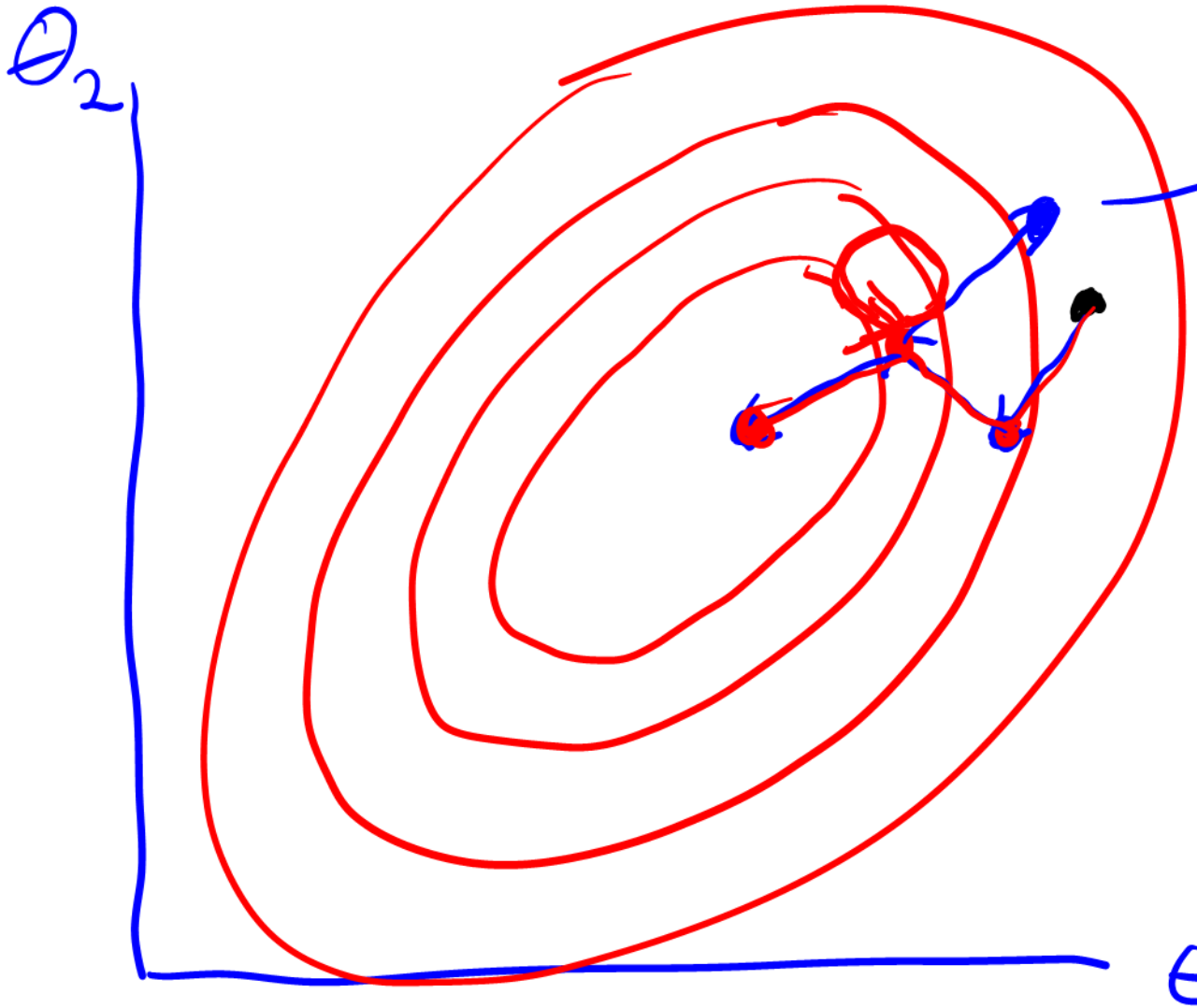
If Heads move, if Tails stay



Toss a biased coin with

$P(H) = \frac{P(\cdot)}{P(\cdot)}$

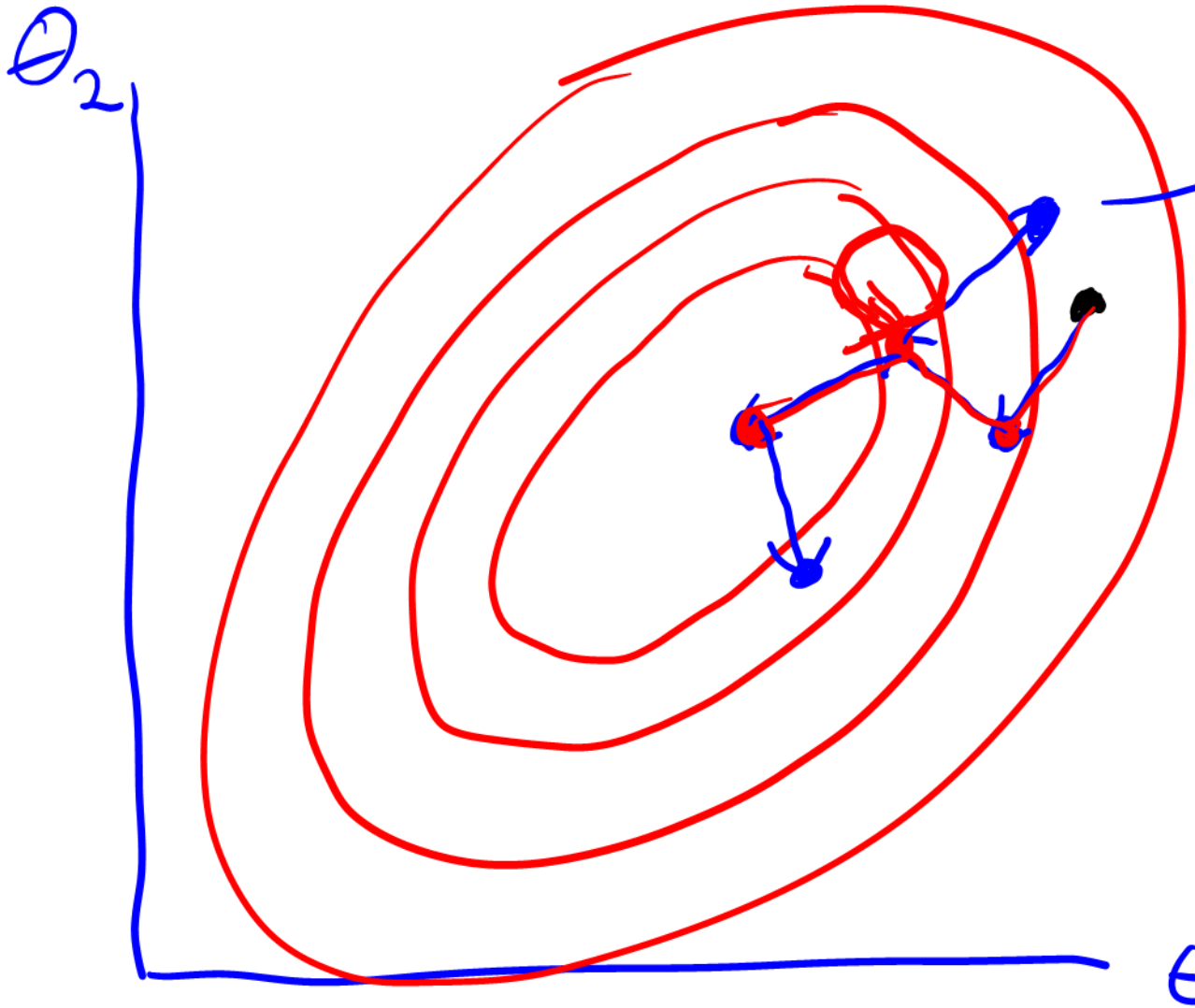
If Heads move, if Tails stay



toss a biased coin with

$p(H) = \frac{p(\cdot)}{p(\cdot)}$

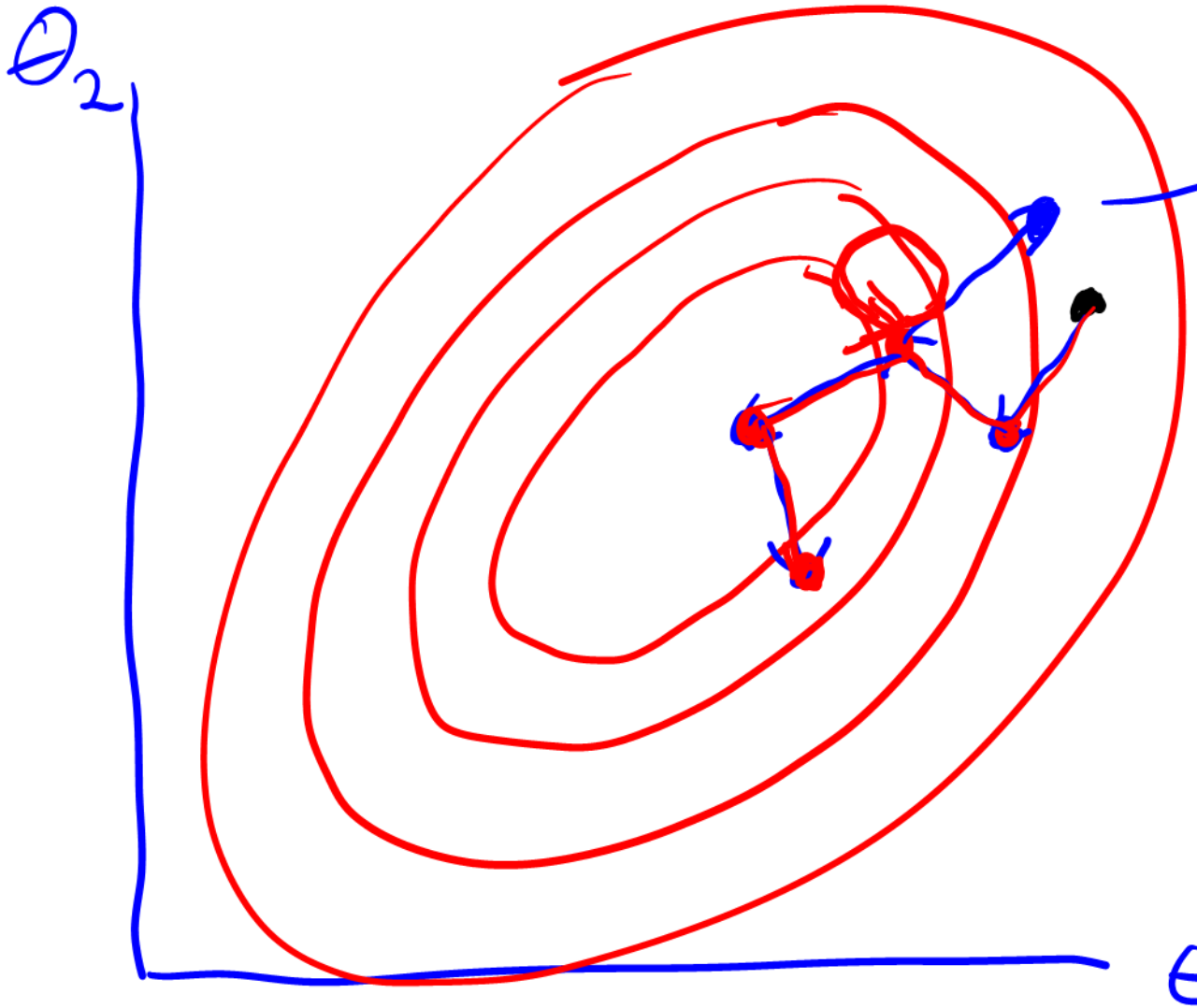
If Heads move, if Tails stay



Toss a biased coin with

$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

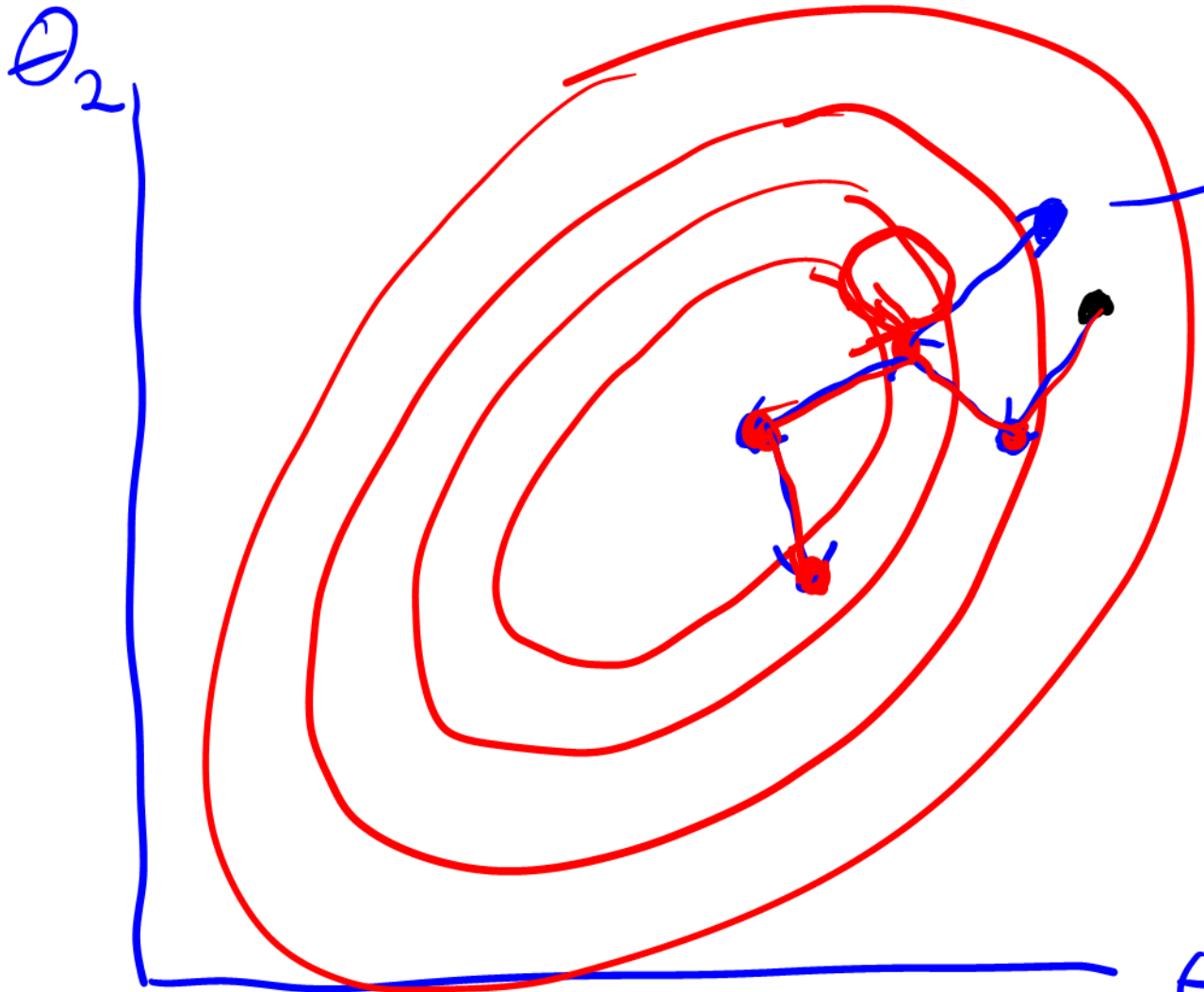
If Heads move θ_1, if Tails stay



Toss a biased coin with

$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

If Heads move, if Tails stay

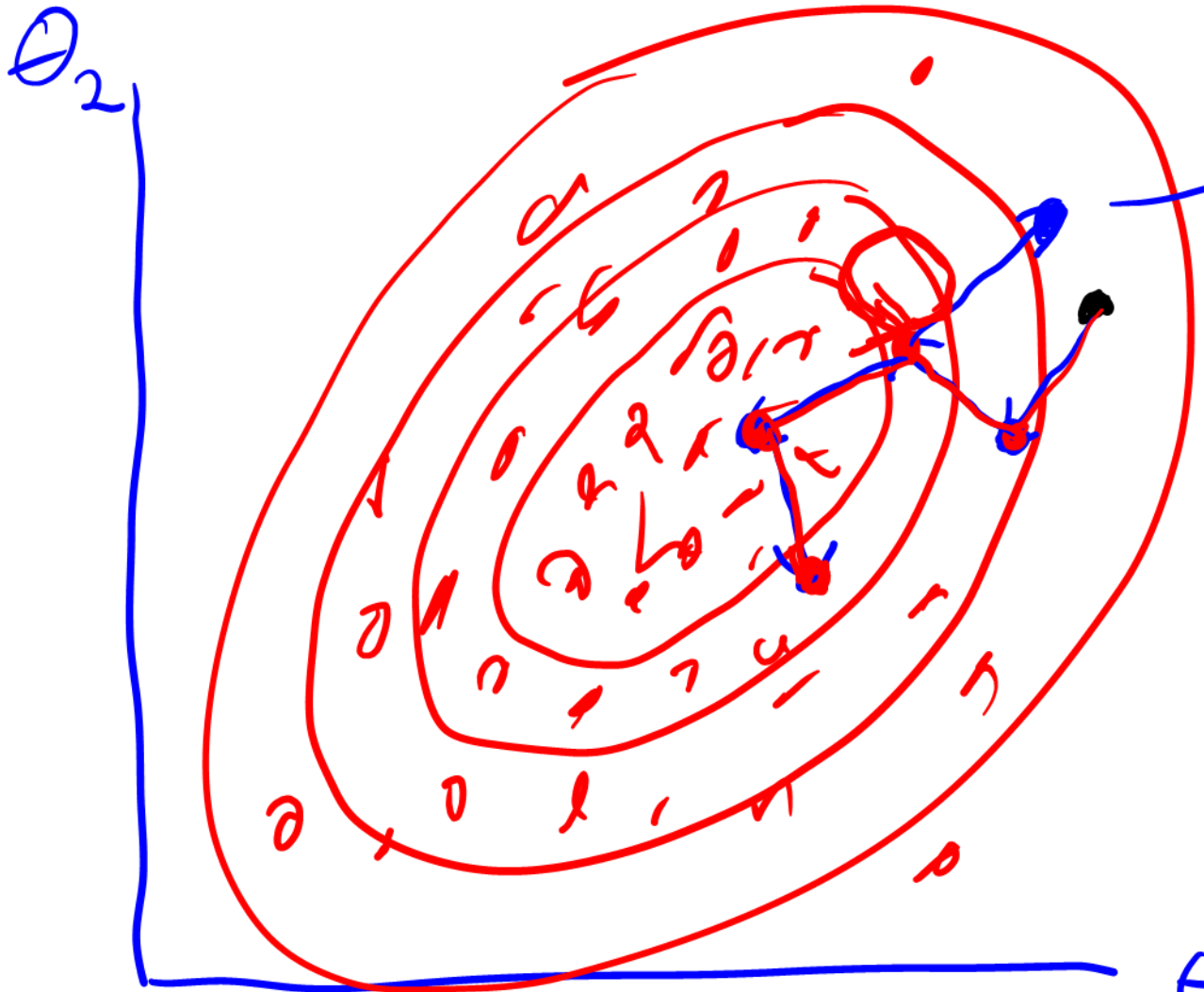


Toss a biased coin with

$$p(H) = \frac{p(\theta_1)}{p(\theta_1) + p(\theta_2)}$$

If Heads move, if Tails stay

Keep doing this for a very long time

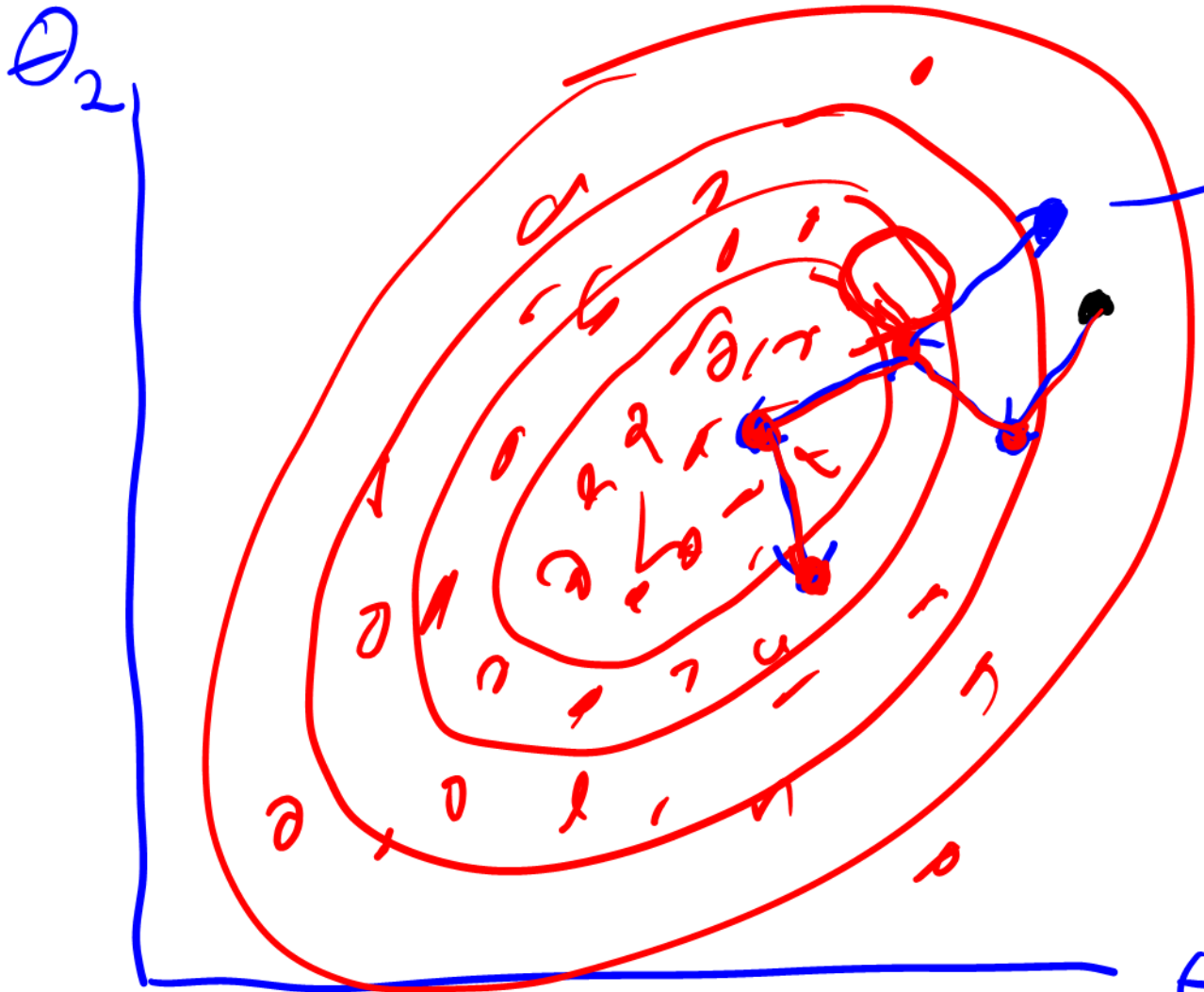


Toss a biased coin with

$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

If Heads move if Tails stay

Keep doing this for a very long time



Toss a biased coin with

$$p(H) = \frac{p(\cdot)}{p(\cdot)}$$

If Heads move
If Tails stay

Generates a sample from $P(\theta|X)$

That's the XX-H algorithm

That's the XX-H algorithm

Can be very slow in high dimensions with non-elliptical contours, e.g.

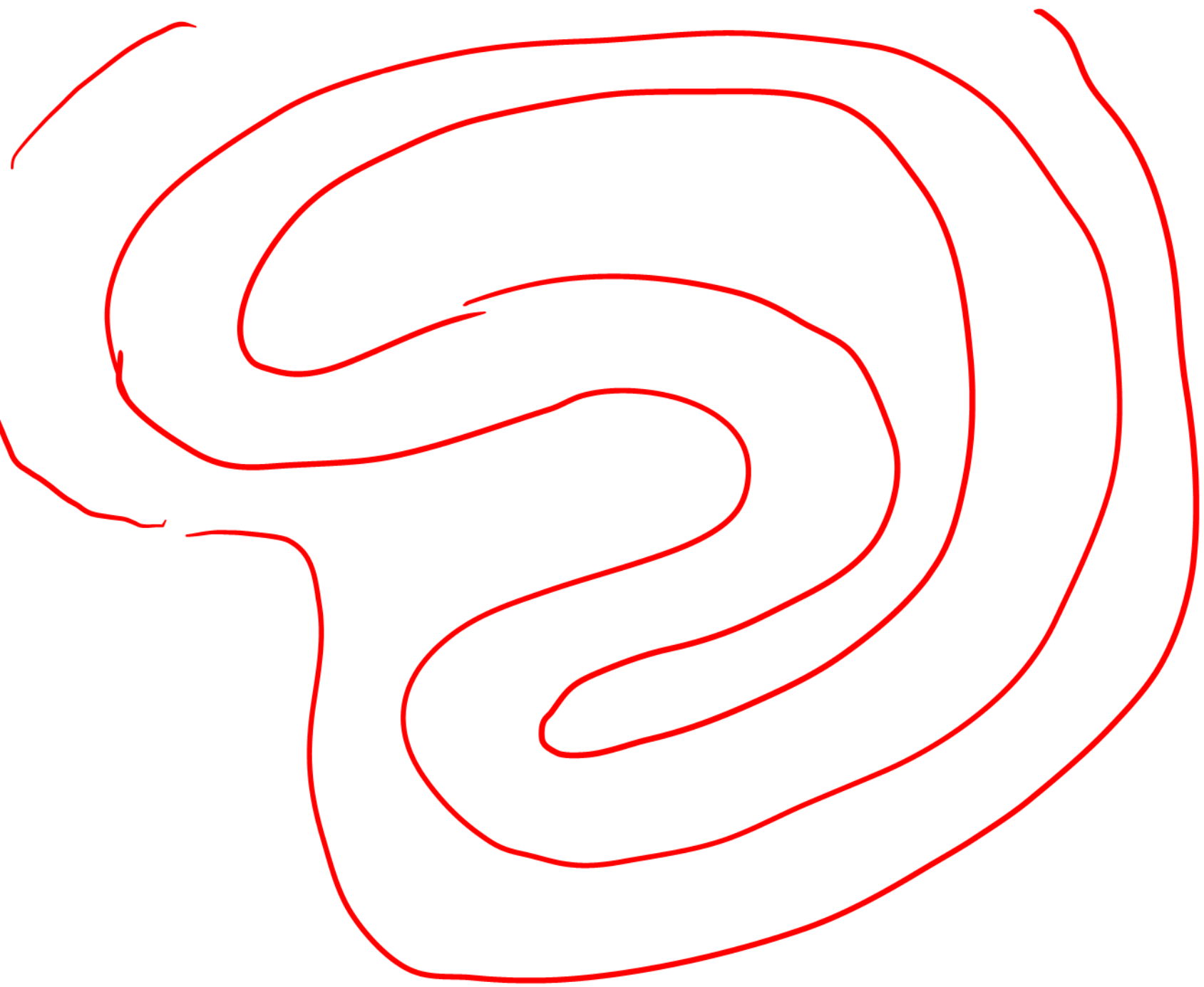
Can get stuck in corners for a long time!

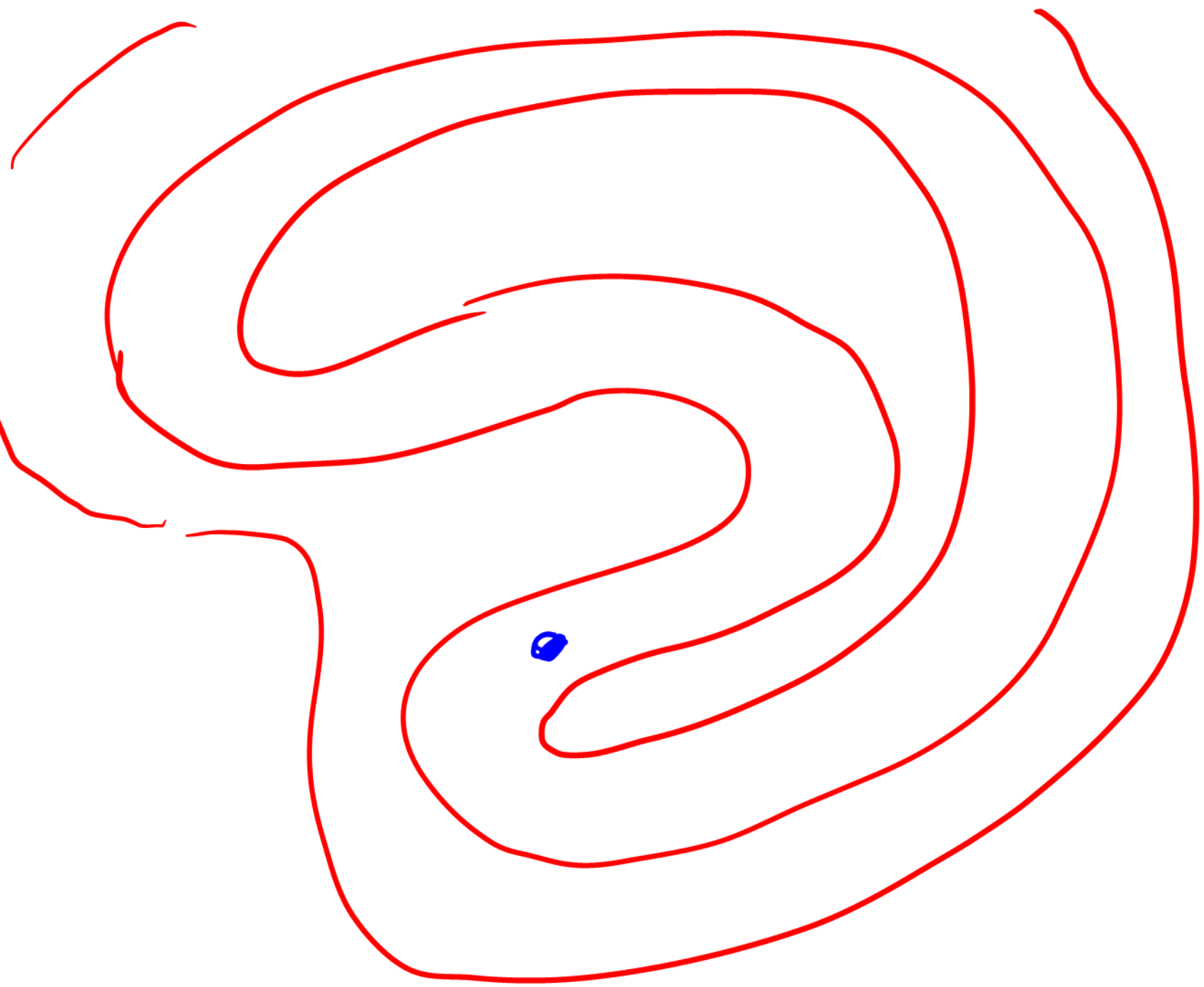
Hamiltonian Monte Carlo

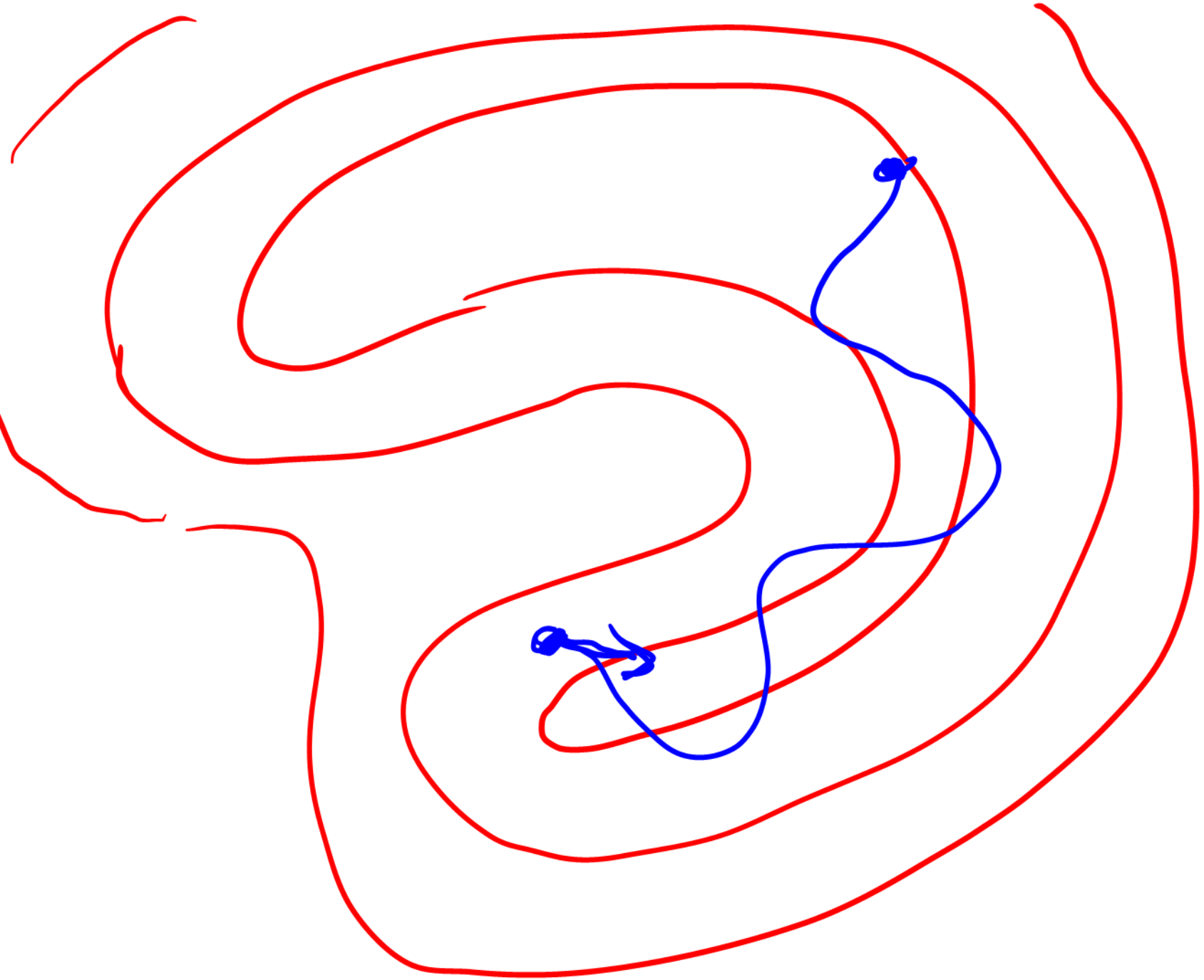
- Turn the mountain into a bowl by using $-\log p(\theta, x)$
- Instead of random steps, go for a ride on a frictionless skateboard with swivel wheels - starting with a random push.

$-\log p(\theta, x)$

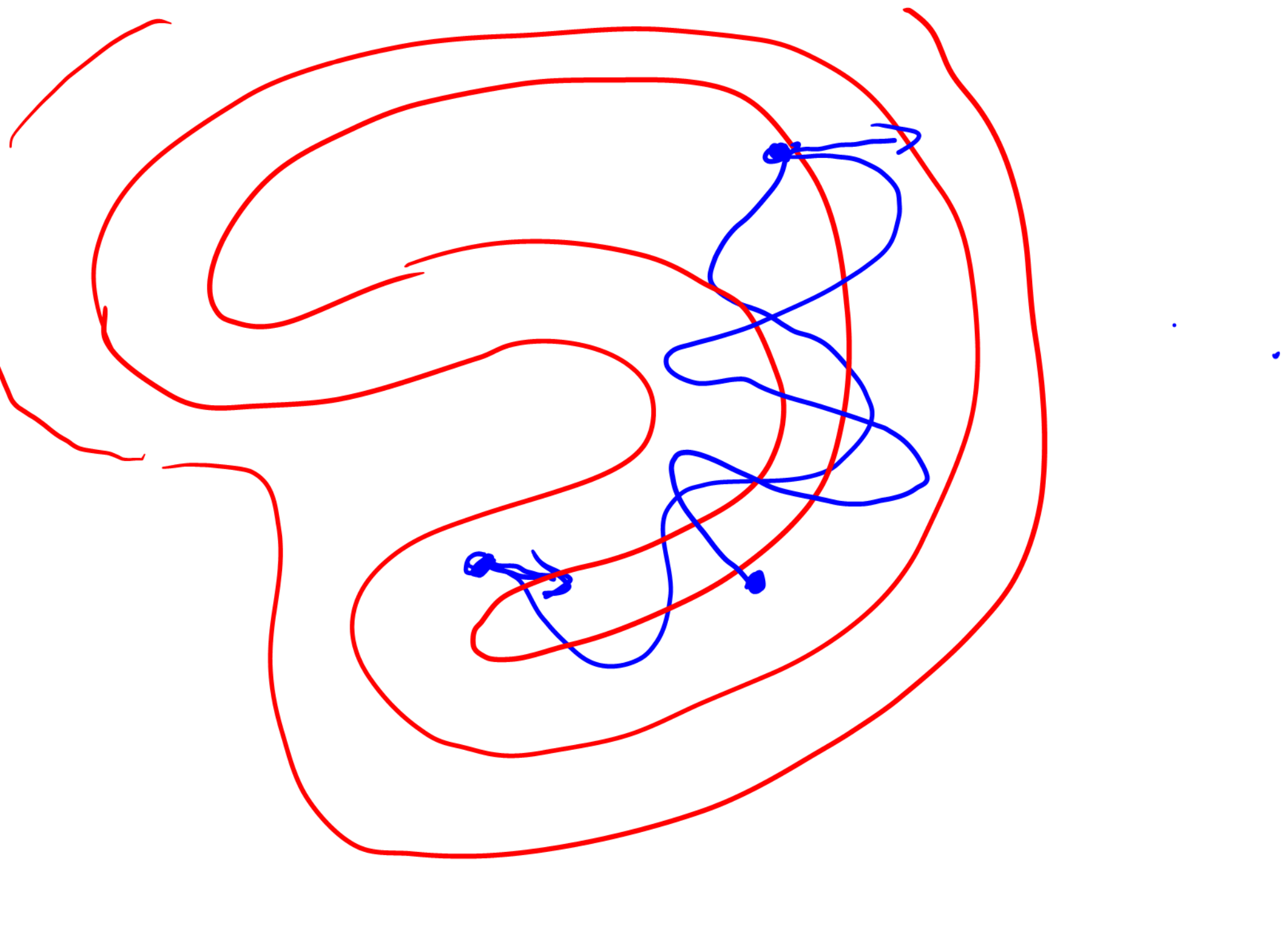
θ

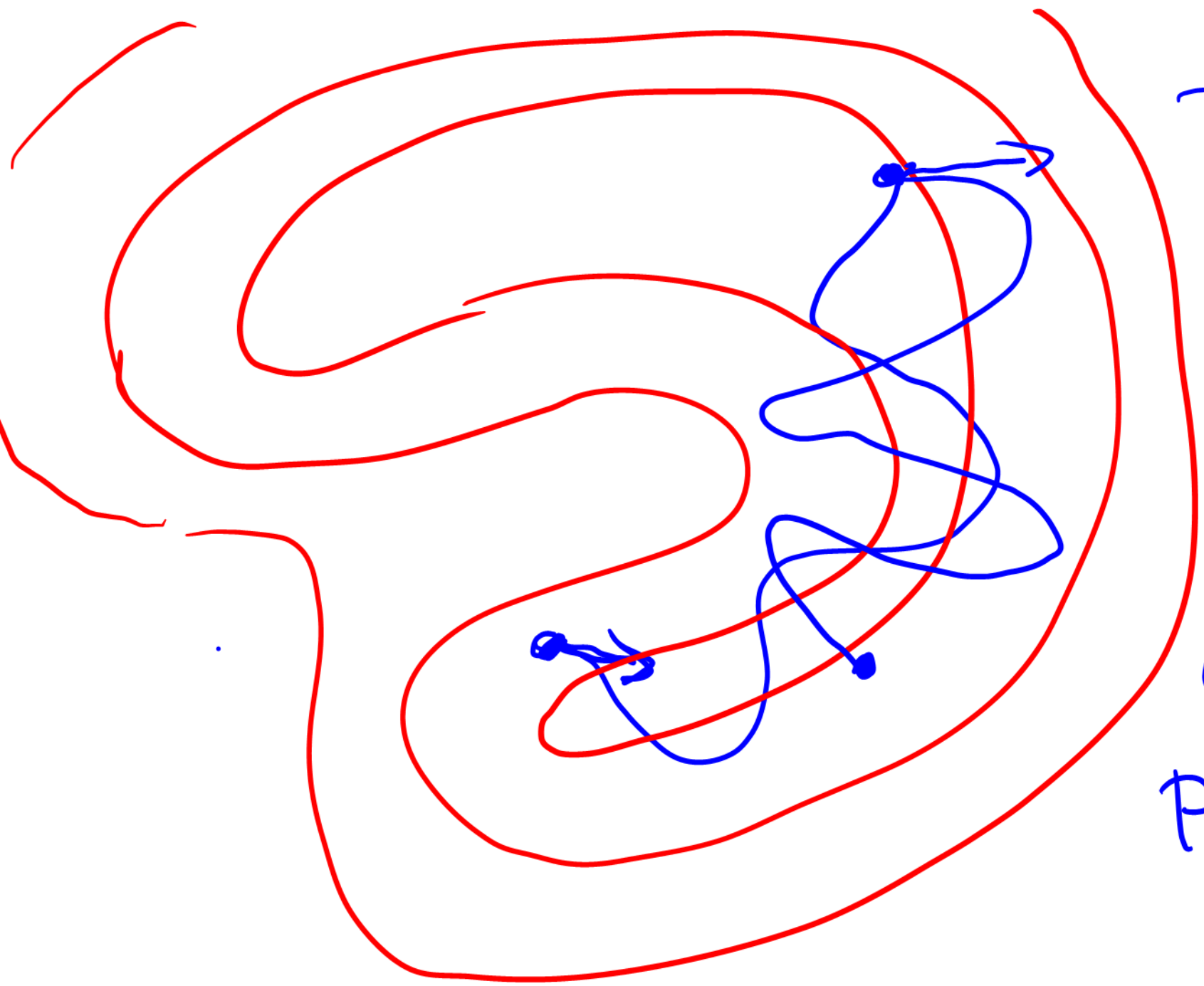




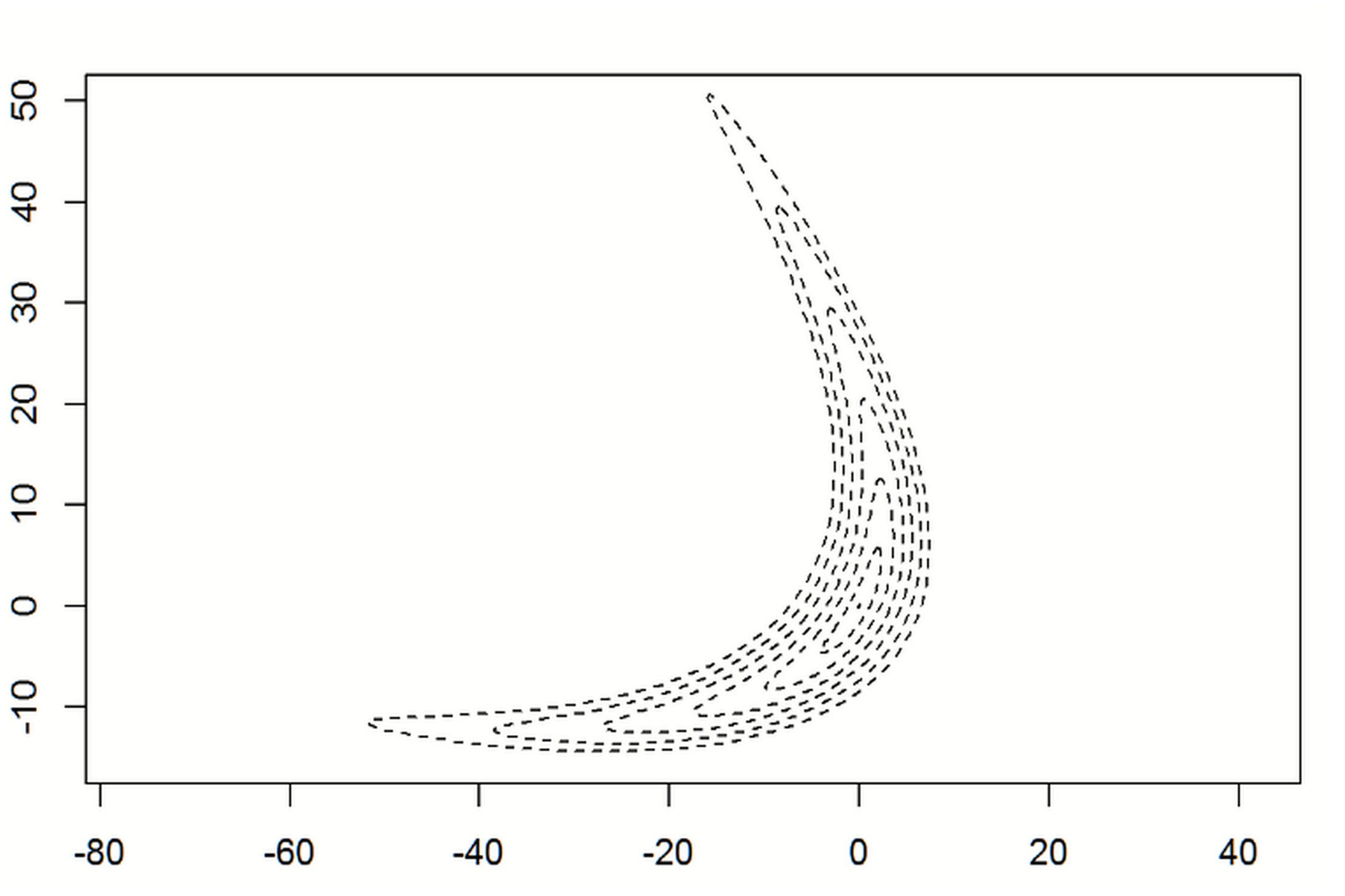


Stop after a set time.





This can do a much better job of covering $p(\theta|x)$.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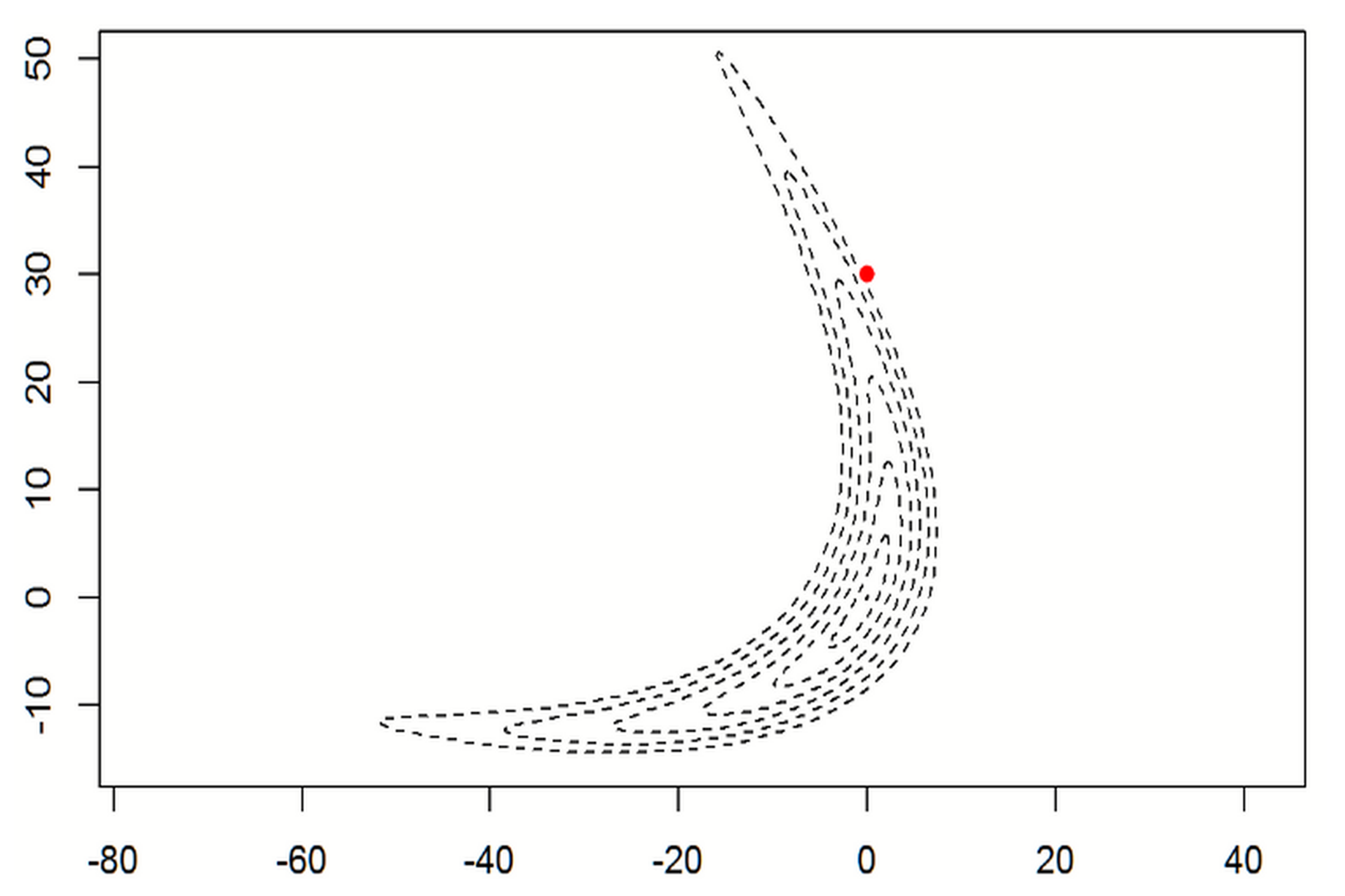
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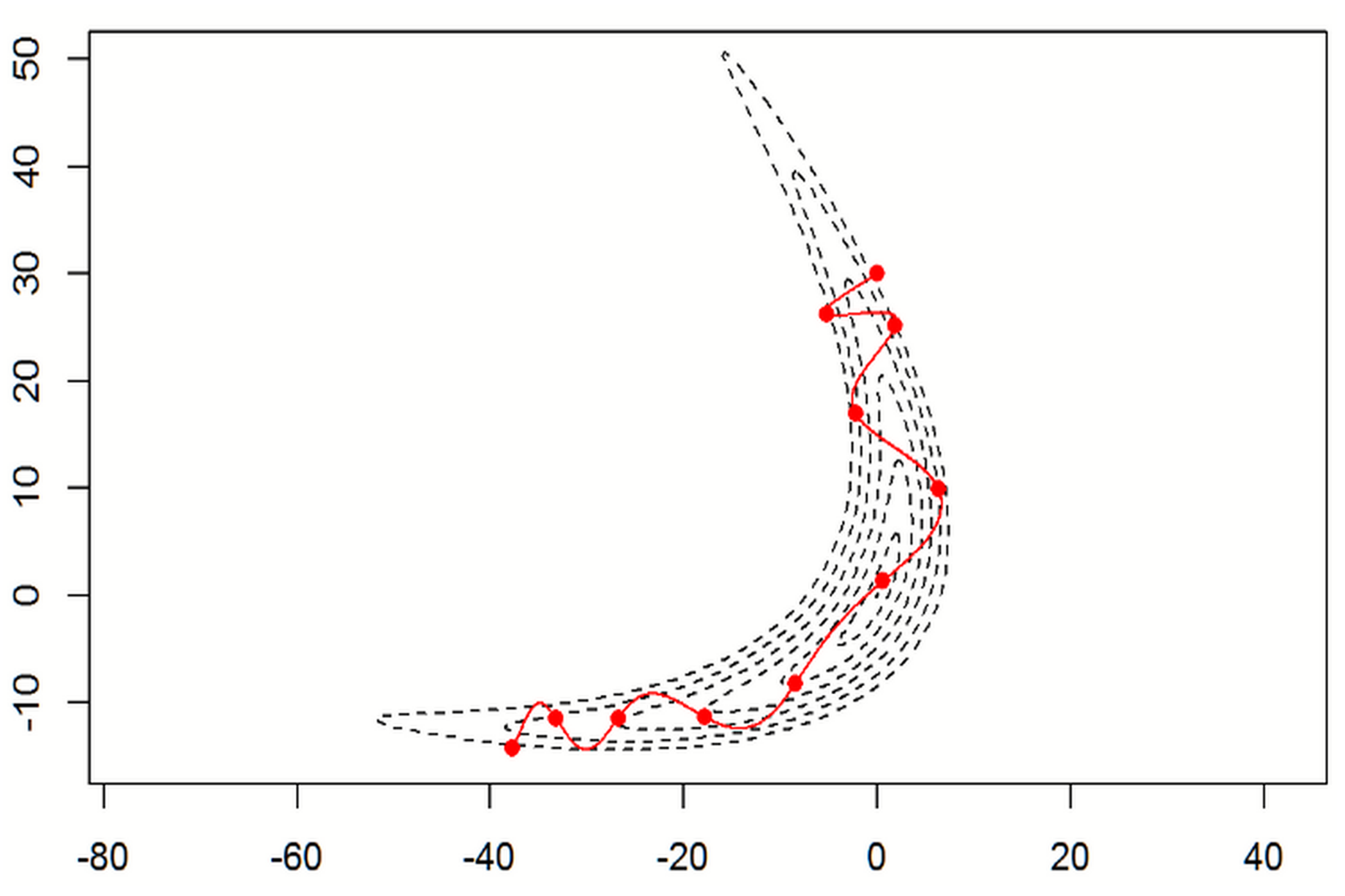
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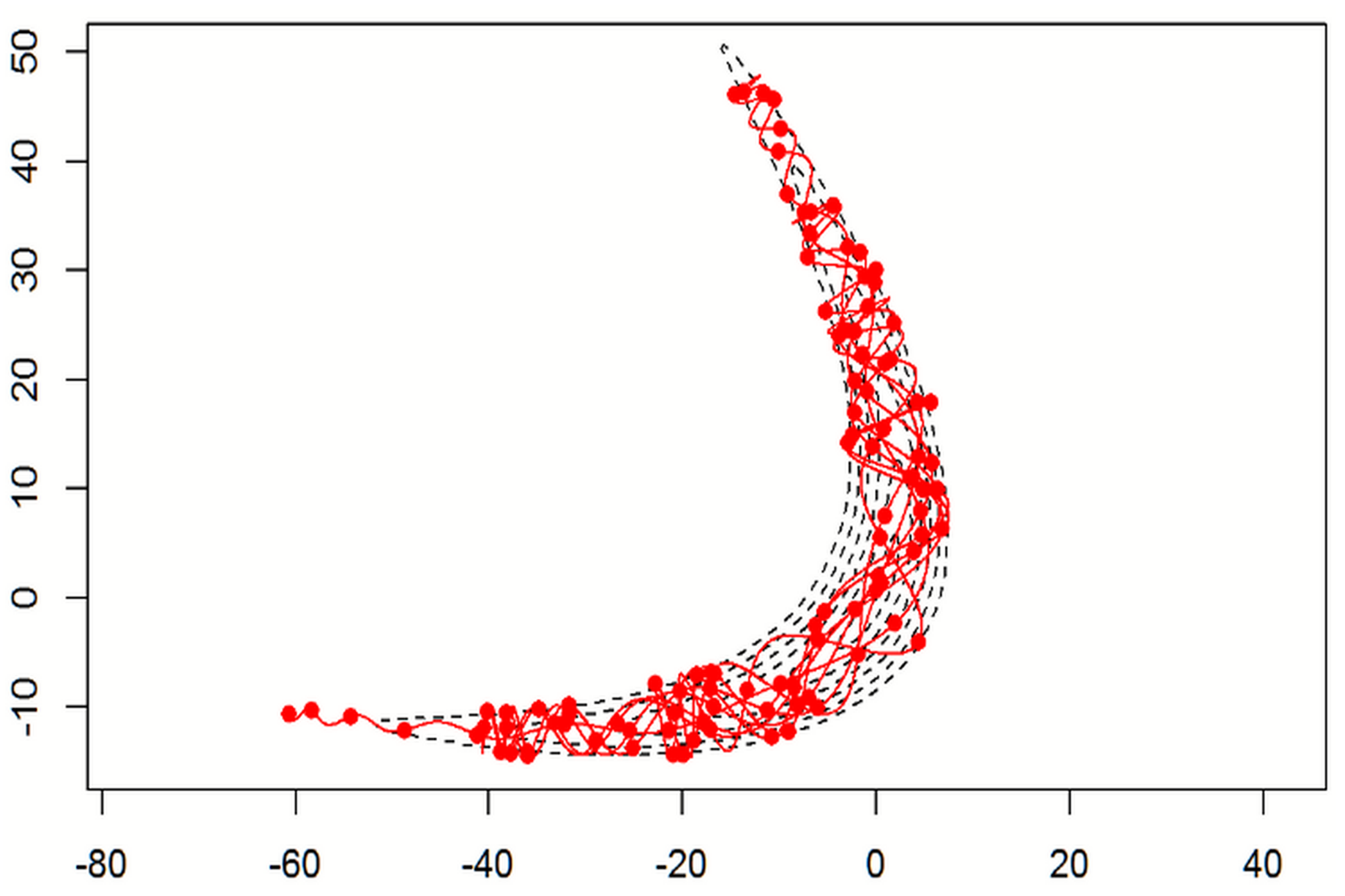
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L : # of leaps (leapfrog) steps

ε : size of each step

$L\varepsilon$: "distance" travelled in θ-space

If too small - too much like random walk

If L too large - too much computing time

If ε too large - bad numerical approximation to continuous path and too high likelihood of rejecting proposal.

From Neal (2011)

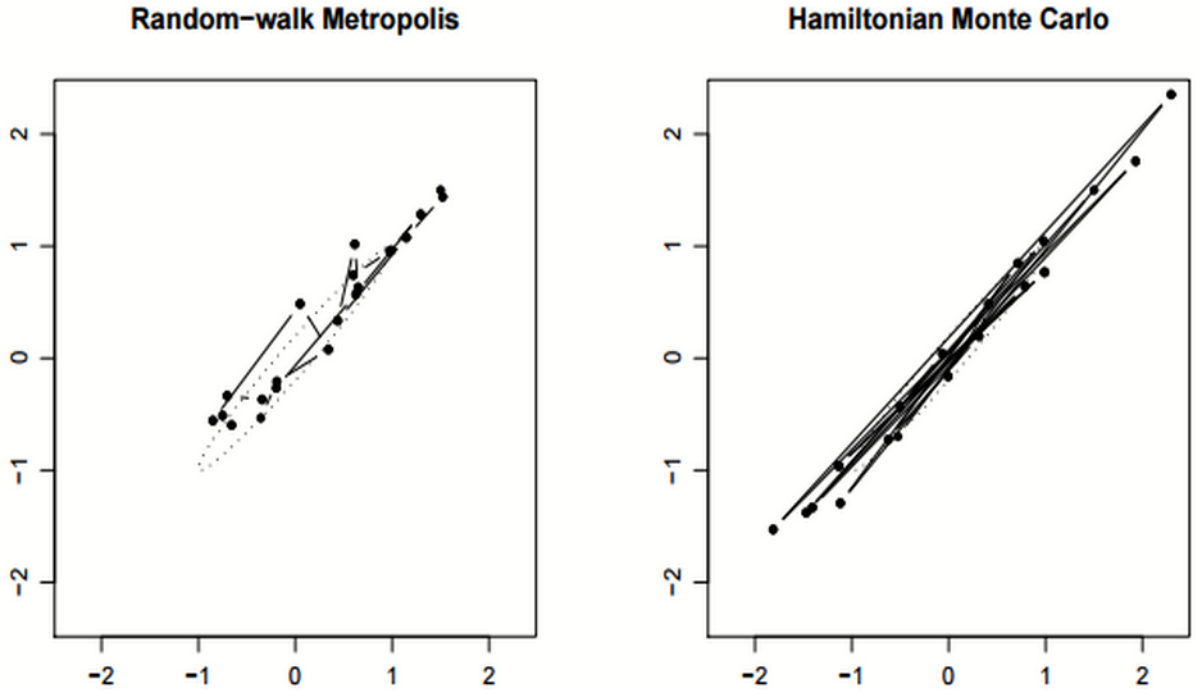

Figure 4: Twenty iterations of the random-walk Metropolis method (with 20 updates per iteration) and of the Hamiltonian Monte Carlo method (with 20 leapfrog steps per trajectory) for a 2D Gaussian distribution with marginal standard deviations of one and correlation 0.98. Only the two position coordinates are plotted, with ellipses drawn one standard deviation away from the mean.

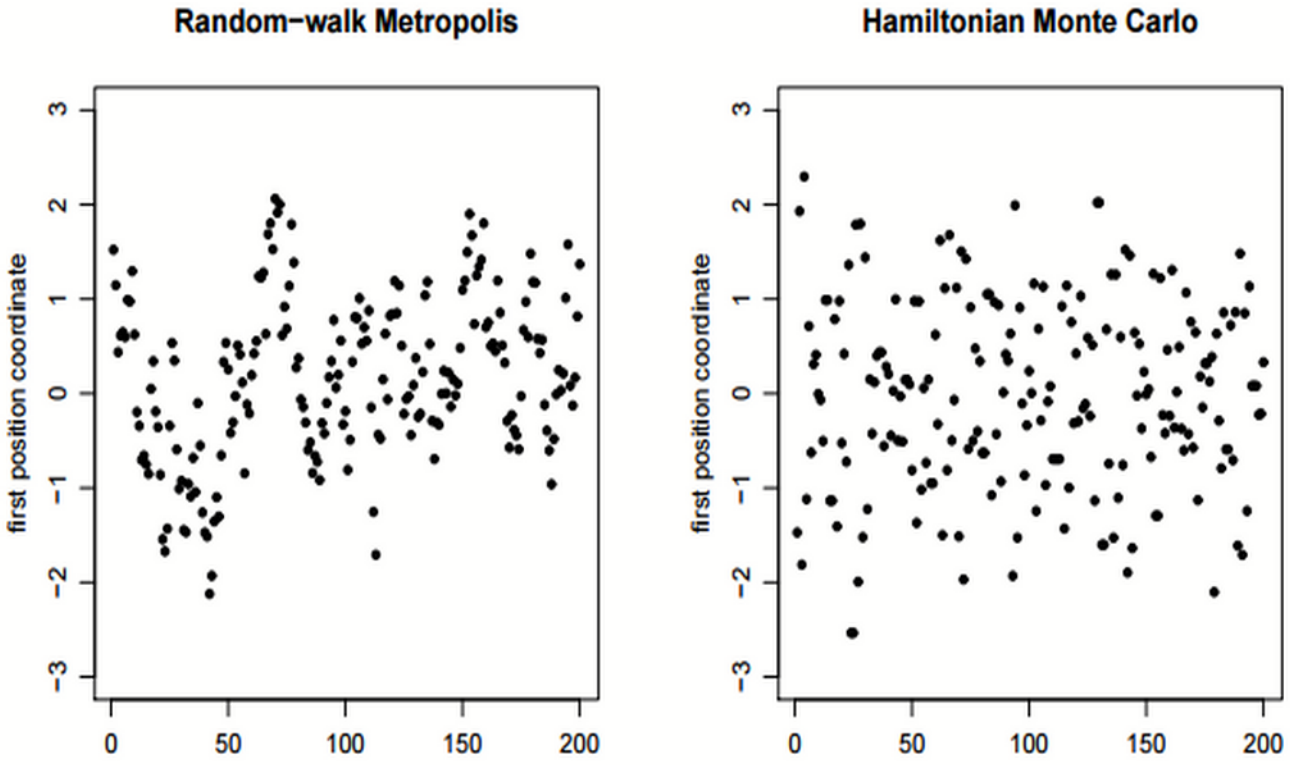

Figure 5: Two hundred iterations, starting with the twenty iterations shown above, with only the first position coordinate plotted.

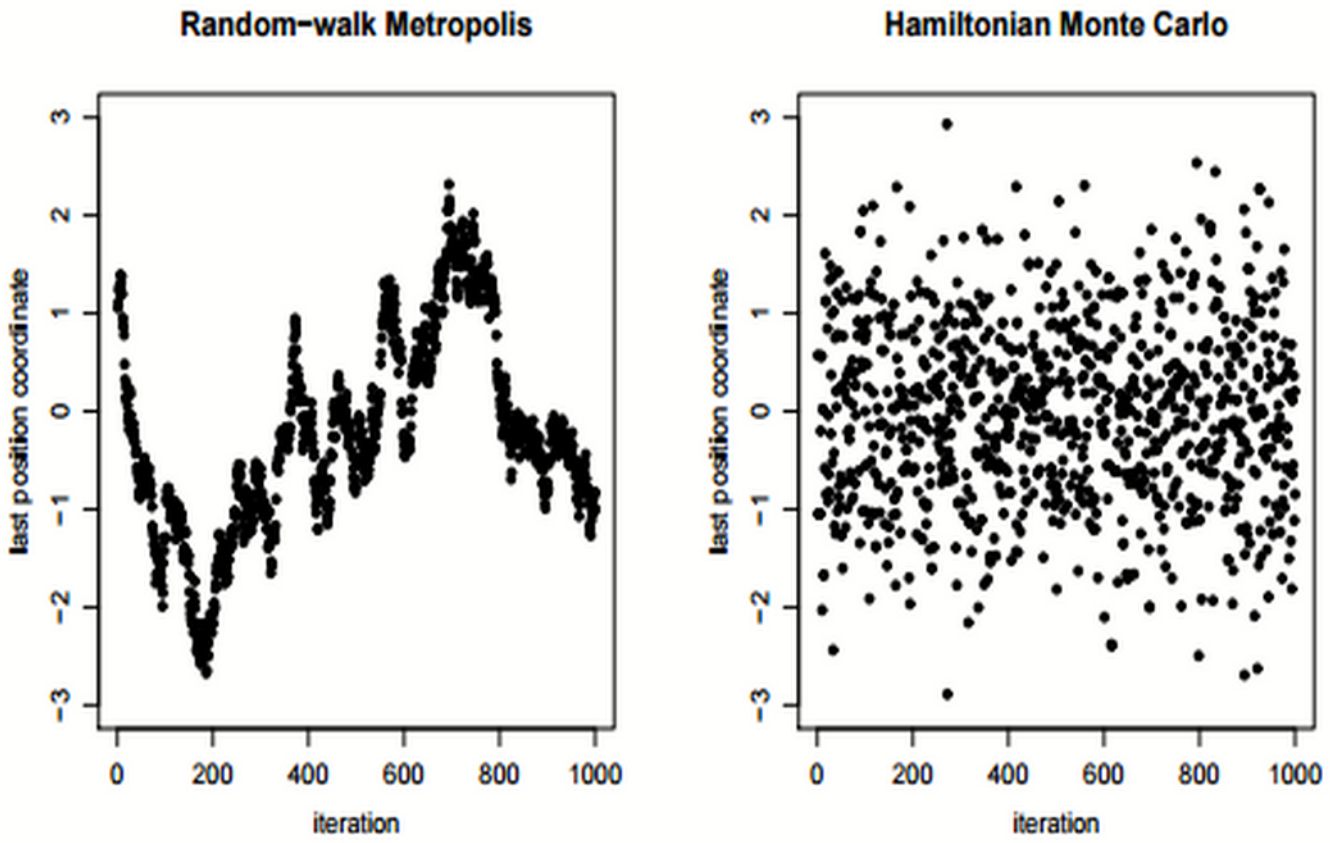

Figure 6: Values for the variable with largest standard deviation for the 100-dimensional example, from a random-walk Metropolis run and an HMC run with $L = 150$. To match computation time, 150 updates were counted as one iteration for random-walk Metropolis.

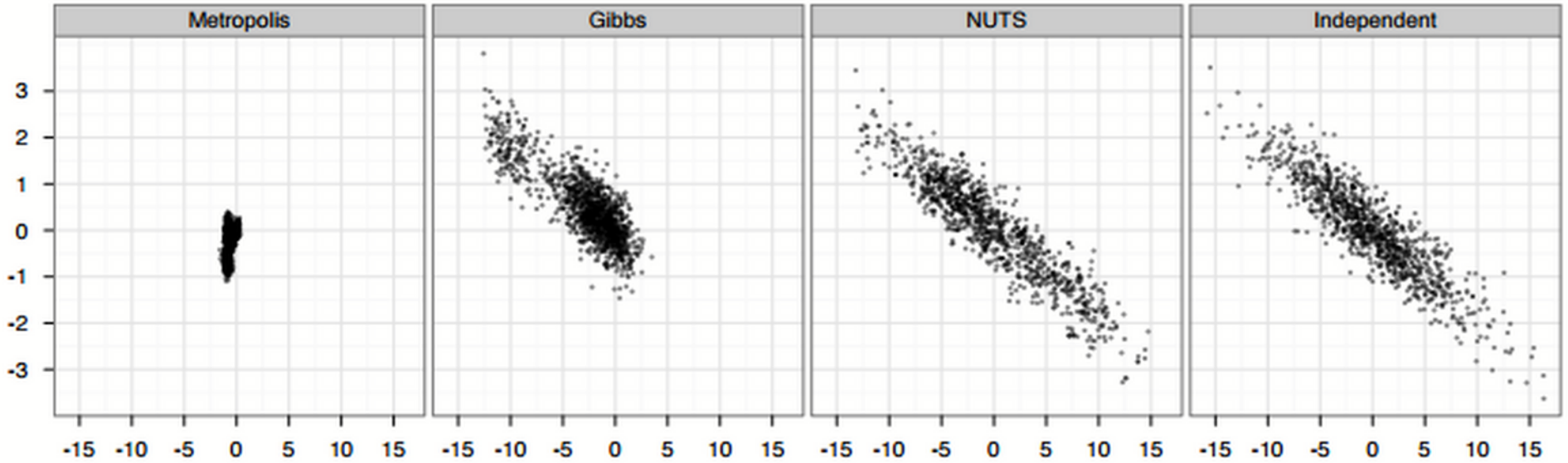

Figure 7: Samples generated by random-walk Metropolis, Gibbs sampling, and NUTS. The plots compare 1,000 independent draws from a highly correlated 250-dimensional distribution (right) with 1,000,000 samples (thinned to 1,000 samples for display) generated by random-walk Metropolis (left), 1,000,000 samples (thinned to 1,000 samples for display) generated by Gibbs sampling (second from left), and 1,000 samples generated by NUTS (second from right). Only the first two dimensions are shown here.

from Hoffman & Gelman (2014)