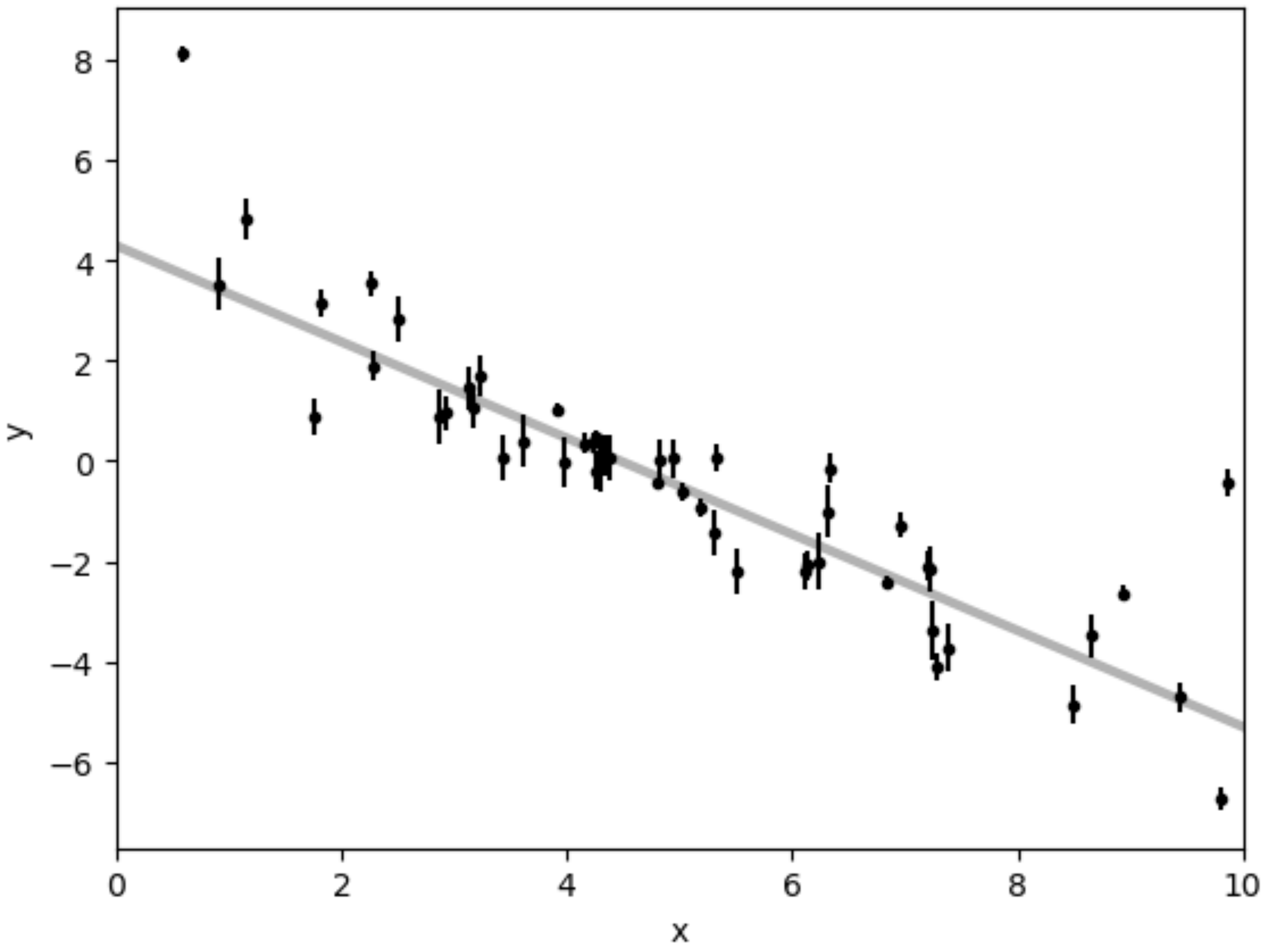
Advanced Sampling Techniques

LSST Discovery Fellowship Program Day 3

Greg Gilbert | LSST Discovery Workshop | 22 May 2025

Fitting a line to data



Modeling choices

Physical
What processes do you include?
What approximations do you make?

Statistical
Are data i.i.d.?
Is there correlated noise?
Do you account for data collection?

Model specification
Parameterization
Priors
Convergence criteria

Sampler
Grid search
Maximum likelihood
Markov Chain Monte Carlo
Nested Sampling

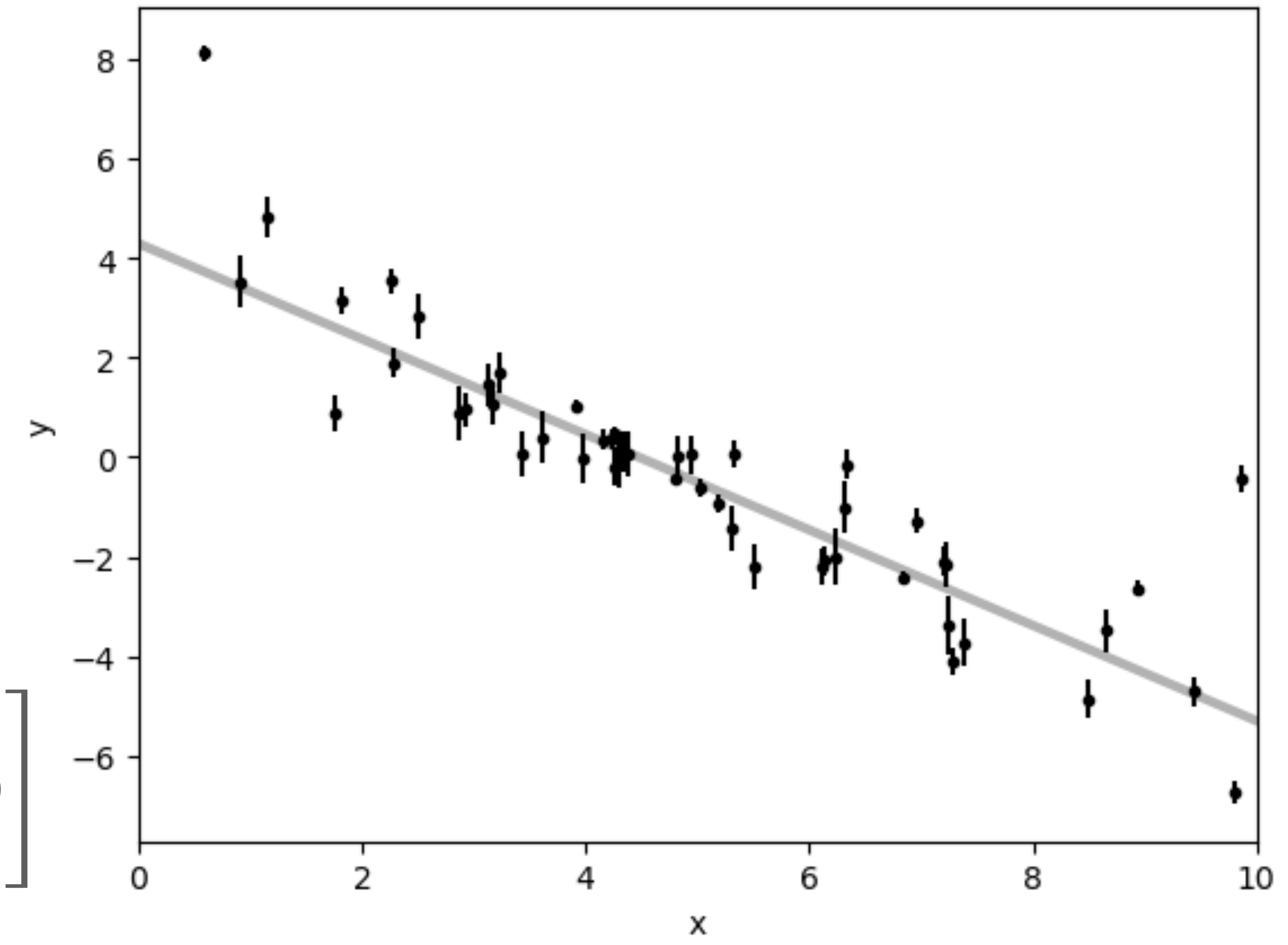
Fitting a line to data

We will build a generative model

$$y_{\text{mod}} = mx + b$$

$$\sigma^2_{\text{tot}} = \sigma^2_{\text{obs}} + s^2$$

$$\ln \mathscr{L}(\theta) = -\frac{1}{2}\sum_i \left[\frac{(y_{\text{obs},i} - y_{\text{mod},i})^2}{\sigma^2_{\text{tot},i}} + \ln(2\pi\sigma^2_{\text{tot},i})\right]$$



We have already made many implicit and explicit assumptions about the data generating process

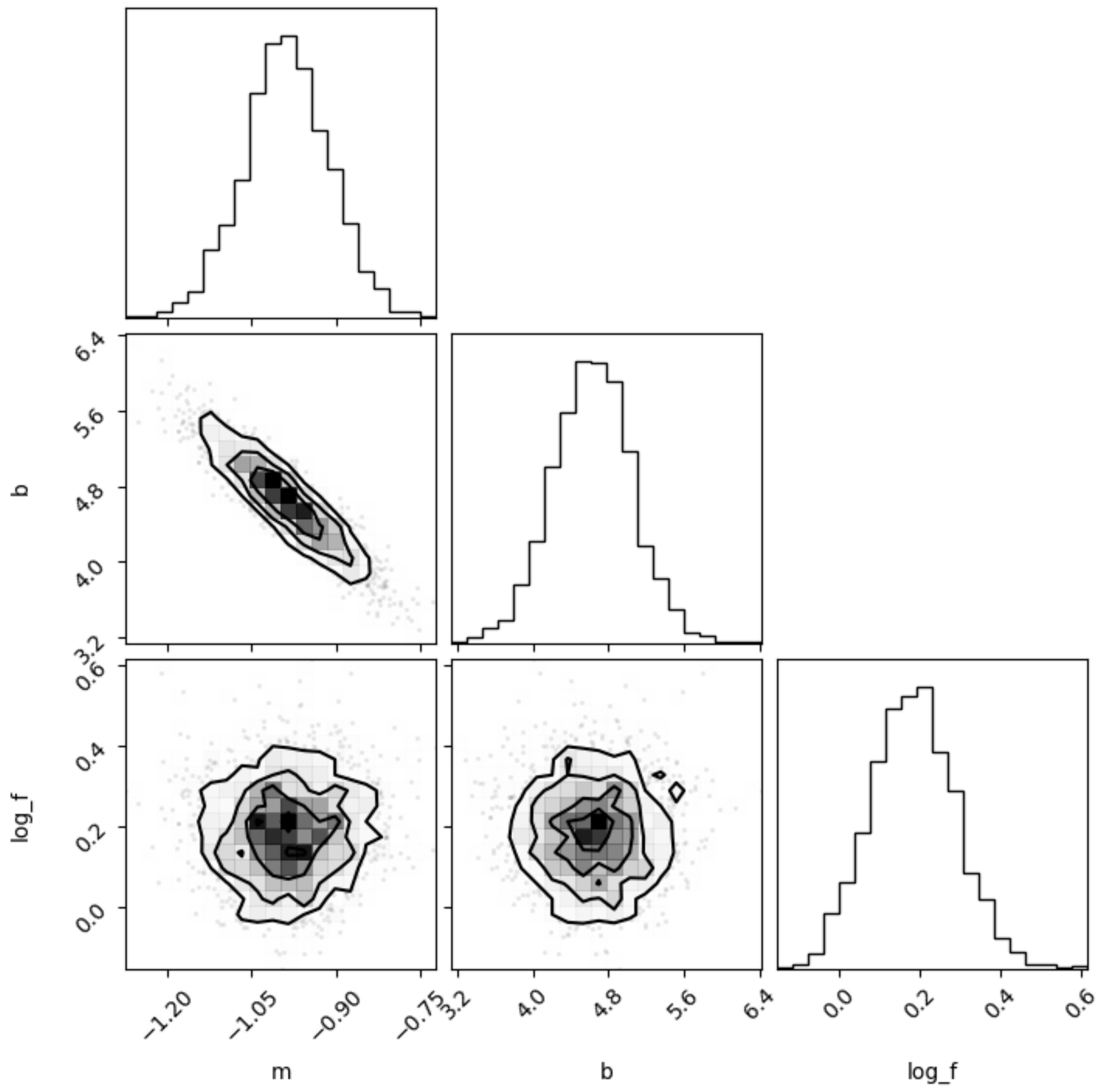
Fitting a line to data

```python
import pymc3 as pm
import pymc3_ext as pmx

with pm.Model() as model:
    m = pm.Uniform("m", lower=-10, upper=10)
    b = pm.Uniform("b", lower=-10, upper=10)
    log_f = pm.Normal("log_f", mu=0, sd=10)

    y_mod = pm.Deterministic("y_mod", m*x + b)
    s_mod = pm.math.sqrt(pm.math.exp(log_f)**2 + y_err**2)


    lnlike = pm.Normal("lnlike", mu=y_mod, sd=s_mod, observed=y_obs)

with model:
    trace = pmx.sample(chains=2, tune=1000, draws=1000, target_accept=0.9, return_inferencedata=True)
```

```
Multiprocess sampling (2 chains in 4 jobs)
NUTS: [log_f, b, m]
```

100.00% [4000/4000 00:00<00:00 Sampling 2 chains, 0 divergences]

Look at those lovely Gaussian posteriors!



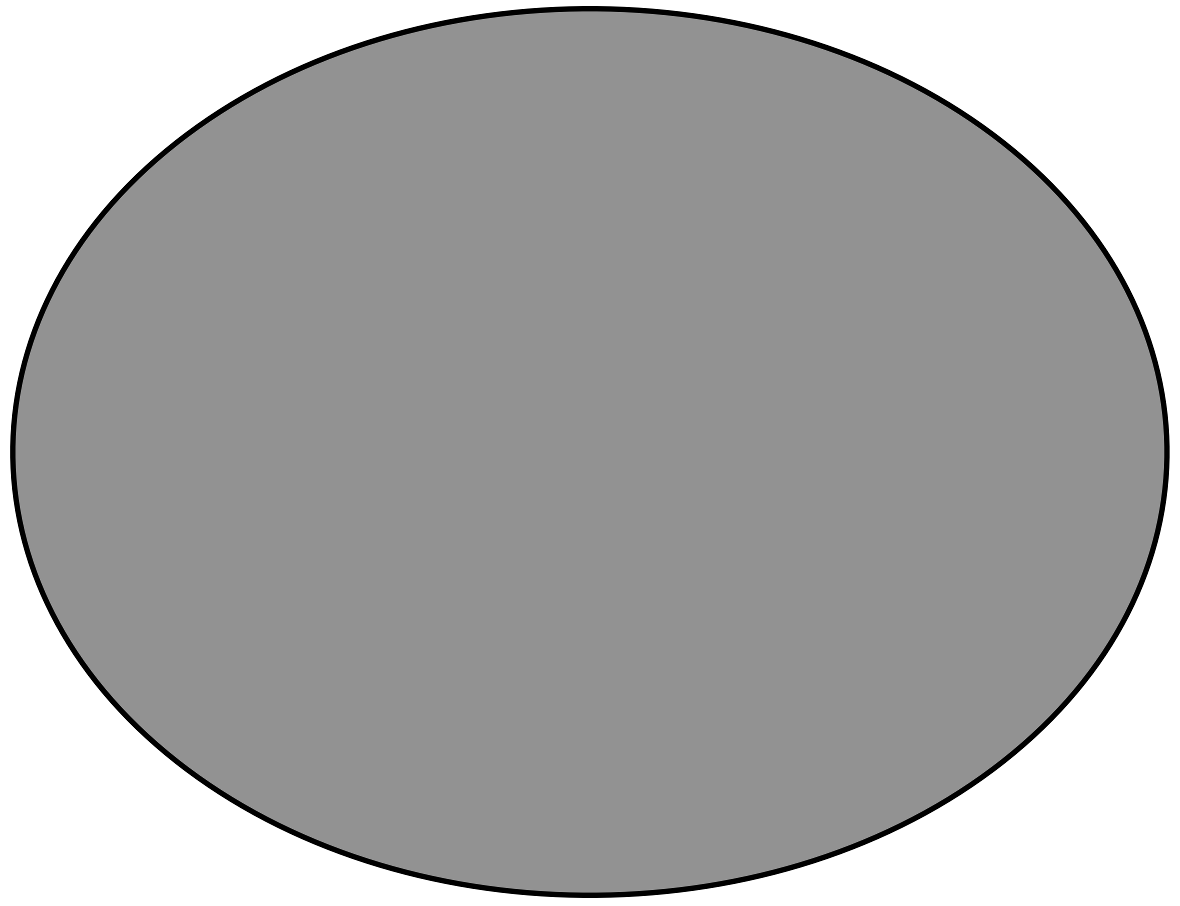
Easy mode: low-dimensional Gaussian

Small parameter covariances

Smooth, homogenous, isotropic posterior topology

Computationally cheap

So simple!



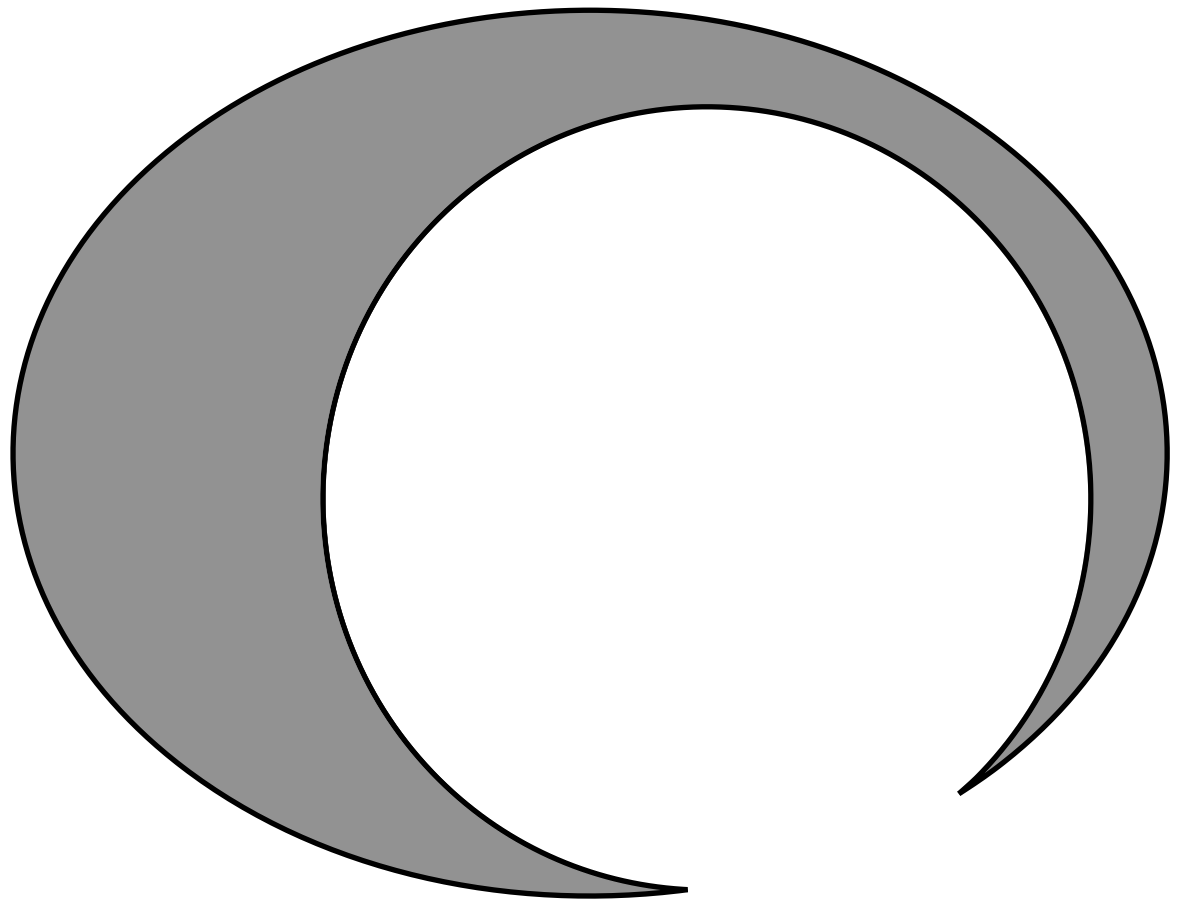
Hard mode: real data

Strong or unknown covariances

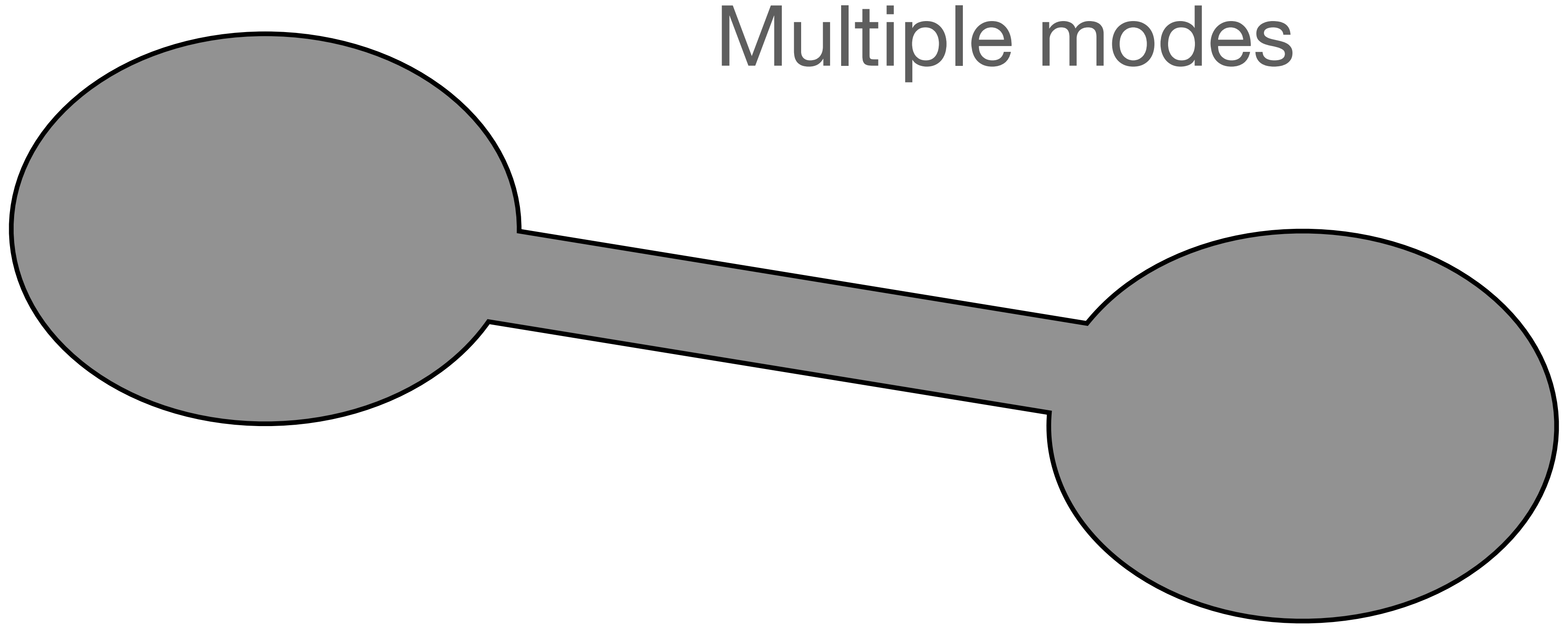
Inhomogeneous (and unknown) posterior topology

Computational cost rapidly scales with number of free parameters

Strong curvature

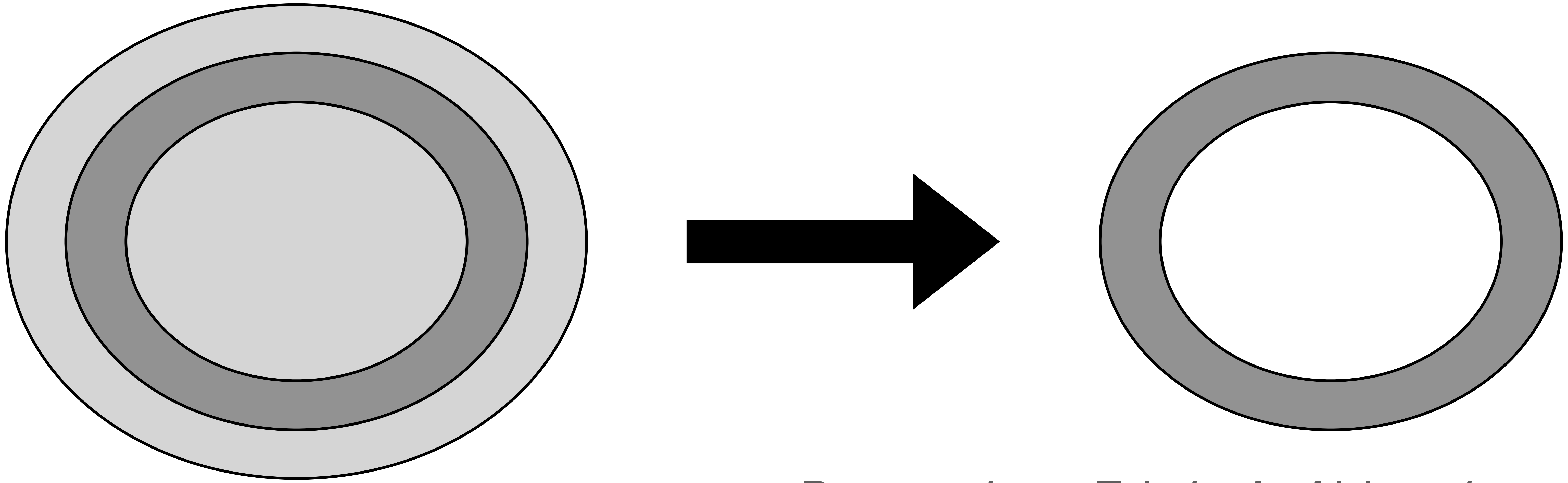


Multiple modes



Sneaky mode: high dimensions

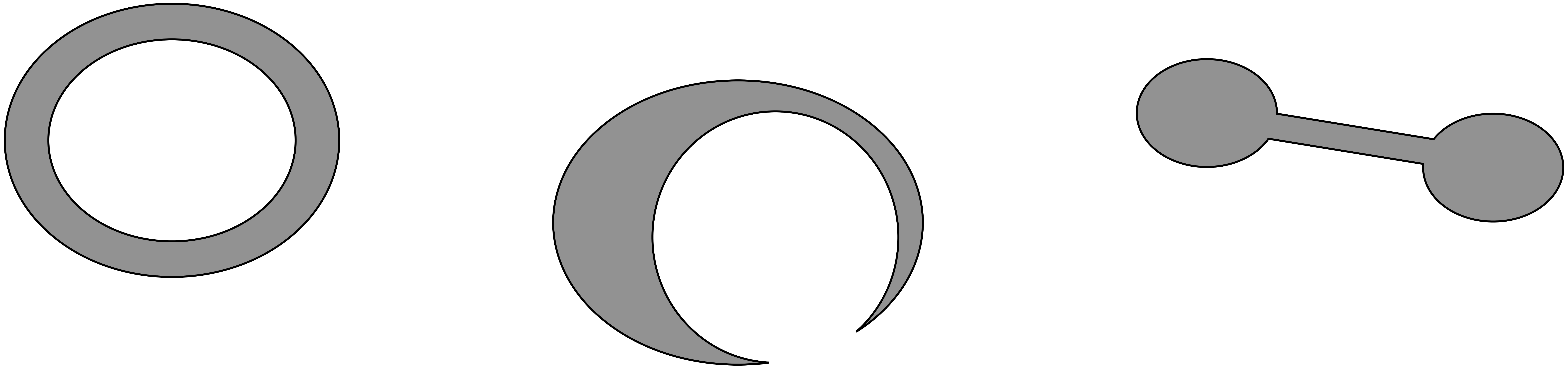
As the number of free parameters increases, the “typical set” is a thin shell, even for low-covariance topologies



Do your best Edwin A. Abbott impression and imagine this is a 10-dimensional Gaussian

Talk about approaching center in every dimension at the same time

Mission: generate samples from complicated posterior topologies



Option 1: Change the sampler

Ensemble Samplers
Hamiltonian Monte Carlo
Nested sampling

Option 2: Change the topology

Re-parameterize
Importance sampling
Umbrella sampling

Bayes Theorem

Likelihood

Prior

$$P(\theta \mid D) = \frac{P(D \mid \theta)\, P(\theta)}{P(D)}$$

Posterior

Evidence

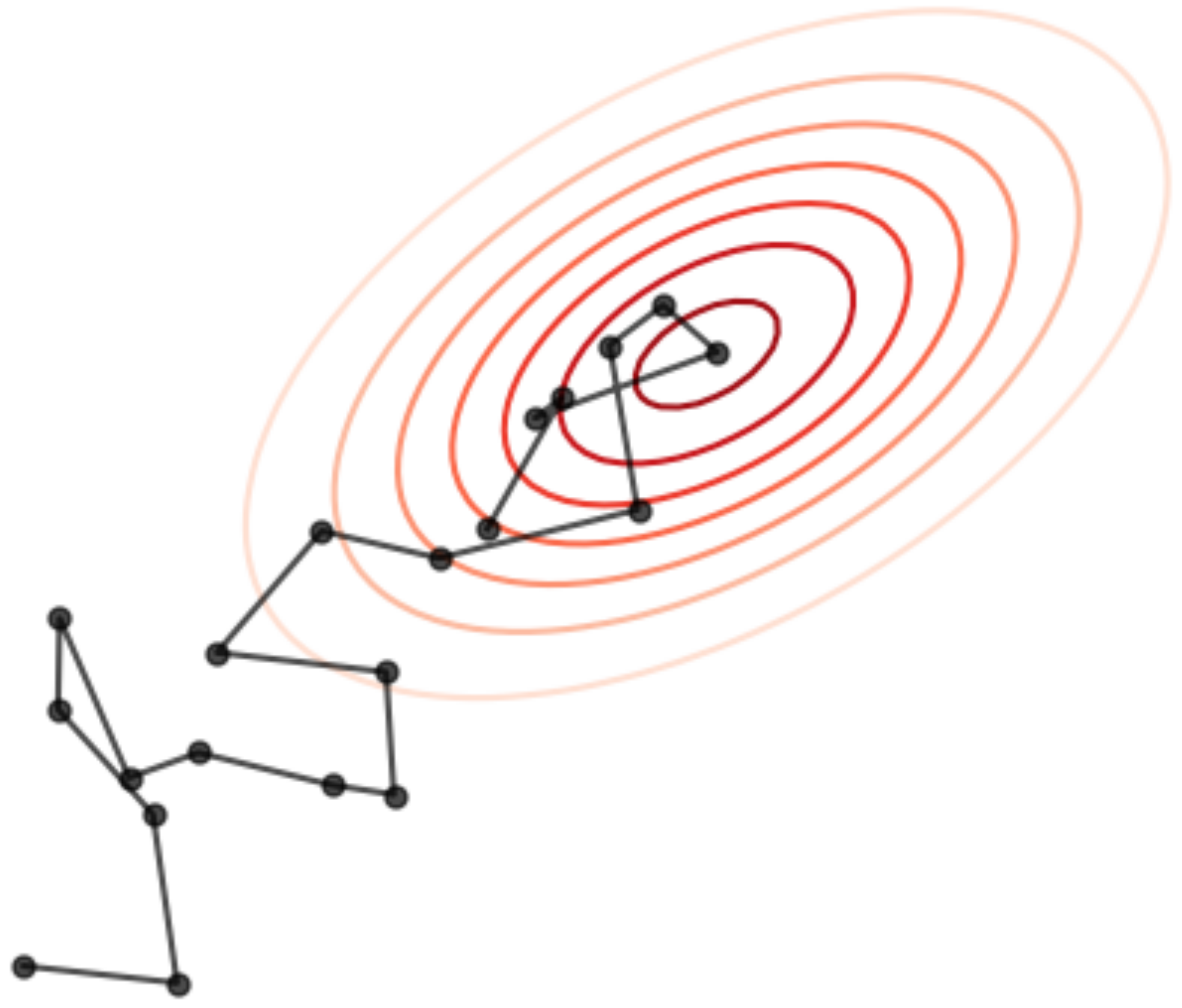
MCMC generates **samples from the posterior**

Random Walk Monte Carlo

1. Choose an initial θ

2. Loop over N iterations
   a. Propose a new θ' from proposal $q(\theta)$
   b. Compute acceptance ratio $\alpha = p(\theta')/p(\theta)$
   c. Generate random number $u \sim U(0,1)$
      - If $u \leq \alpha \rightarrow$ accept, $\theta_{i+1} = \theta'$
      - If $u > \alpha \rightarrow$ reject, $\theta_{i+1} = \theta$

3. Stop when N_{eff} is above desired threshold



MCMC Variations

Method	Description
Metropolis-Hastings	Walkers move according to fixed proposal distribution
Gibbs Sampling	Walkers propose steps one variable at a time
Differential Evolution	Scales steps size according to ensemble of walkers
Affine Invariant	Adapts proposals to geometry of walker ensemble
Parallel Tempering	Runs ensemble of walkers at different “temperatures”
Hamiltonian	Simulates “momentum” for each walker to take long steps through parameter space

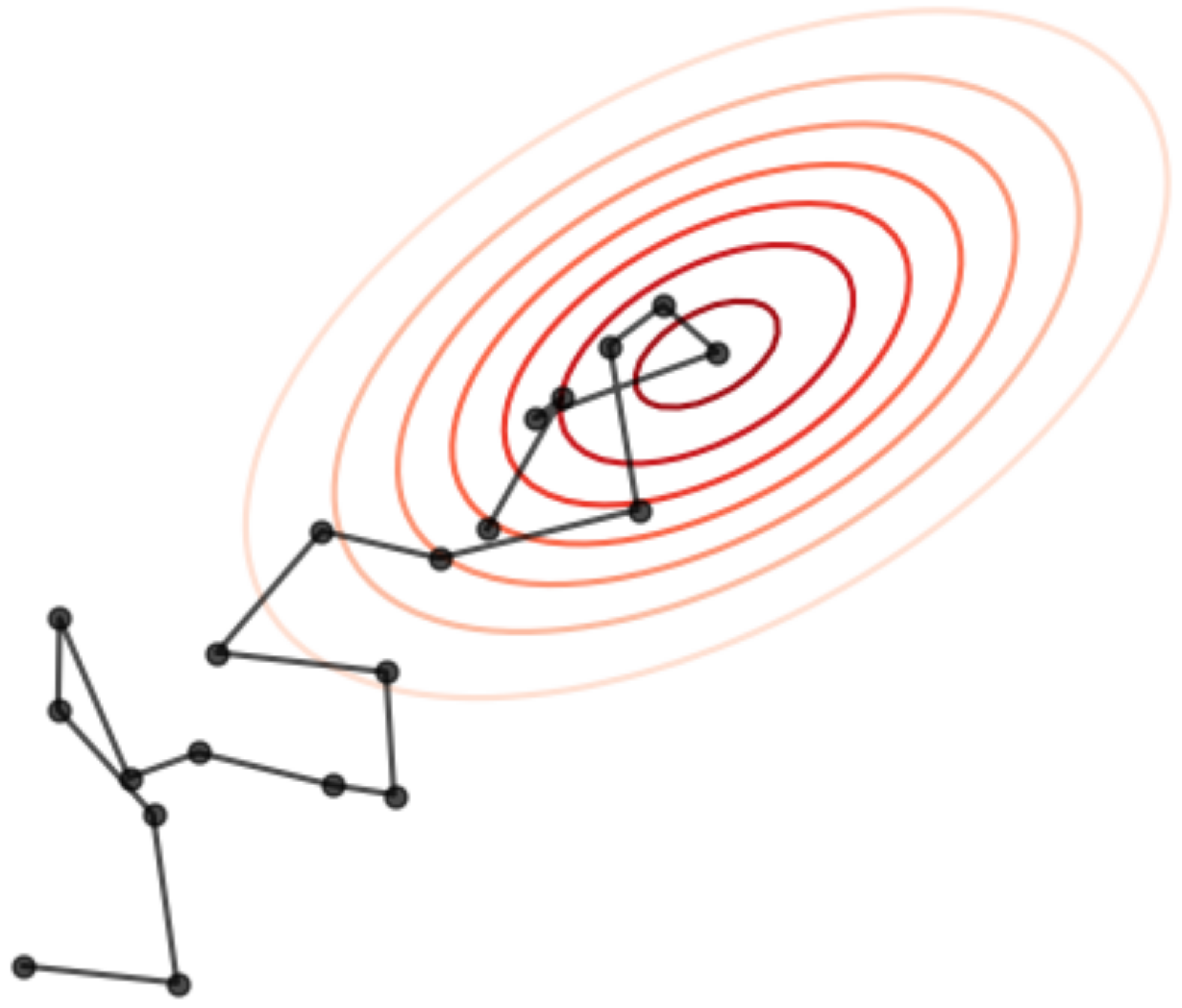
Metropolis-Hastings Monte Carlo

Almost identical to Random Walk Monte Carlo, but algorithm is modified to allow for asymmetric proposal steps

$$\text{Random Walk : } \alpha = \frac{p(\theta')}{p(\theta)}$$

$$\text{Metropolis-Hastings : } \alpha = \frac{p(\theta')}{p(\theta)} \frac{q(\theta \mid \theta')}{q(\theta' \mid \theta)}$$

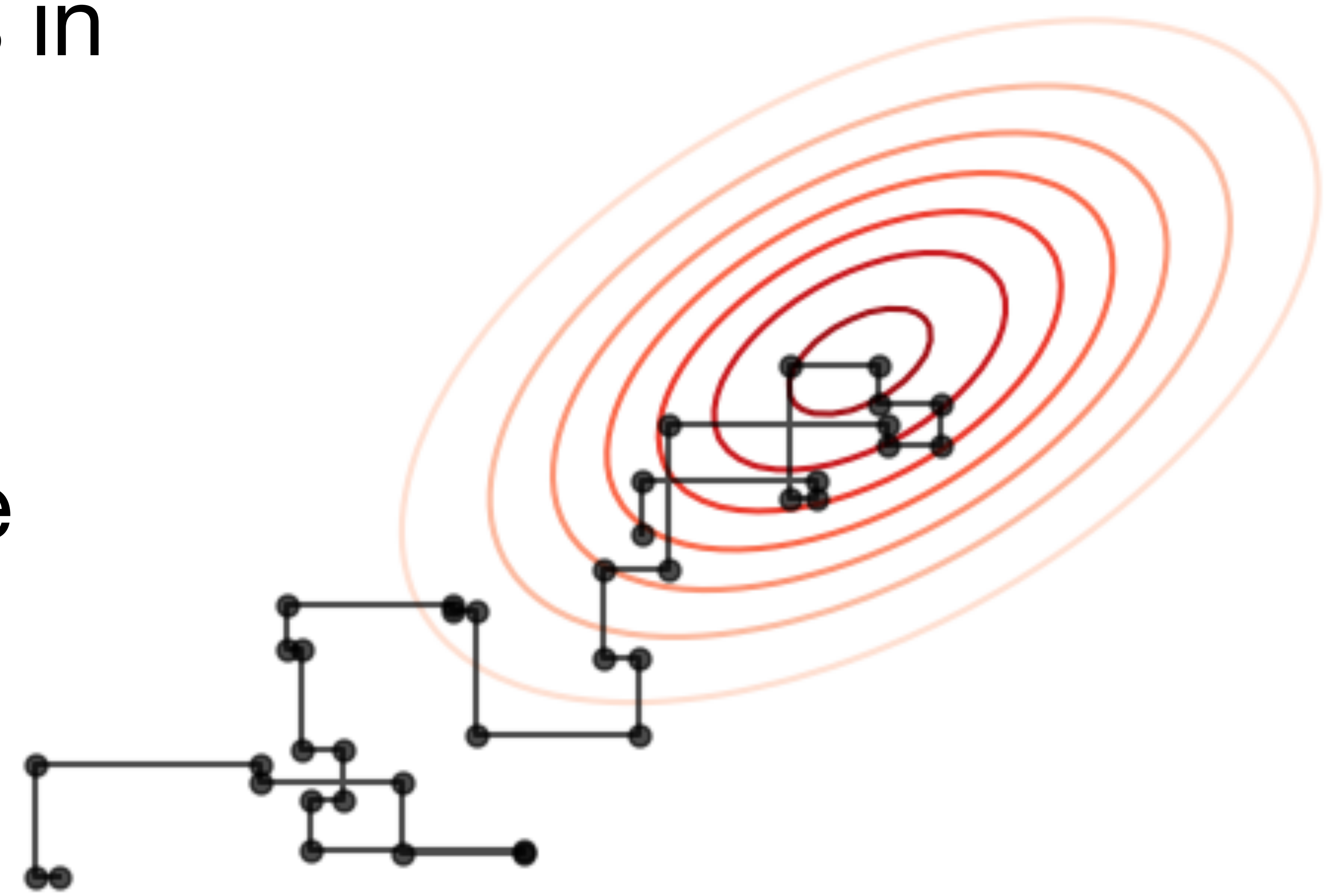
Proposal Distribution



Gibbs Sampling

Very similar to Metropolis-Hastings, but steps in one parameter at a time

This can be beneficial for high-dimensional problems when acceptance fraction would be low by stepping in all parameters at once.



Ensemble Samplers

Differential Evolution

Ter Braak (2004, 2006)

Affine Invariant

Goodman & Weare (2010)

Parallel Tempering

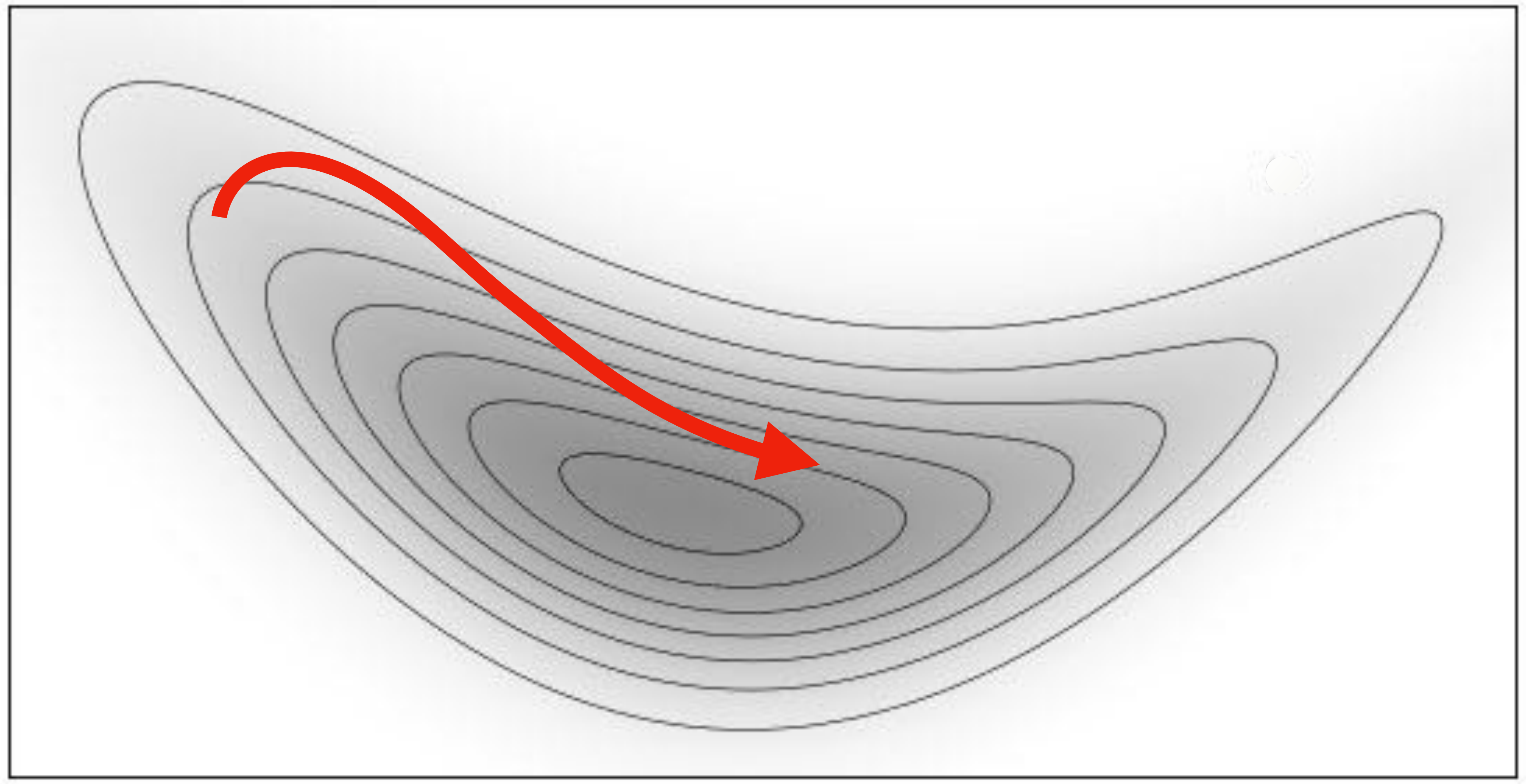
Earl & Deem (2005)

Hamiltonian Monte Carlo

Instead of “walkers” we have “particles” described by both position θ and momentum ν

Particle motion is analogous to rolling a ball around a basin

Higher computational cost per step
Higher acceptance fraction $\alpha \gtrsim 0.9$
Short autocorrelation length $\tau \approx 2$



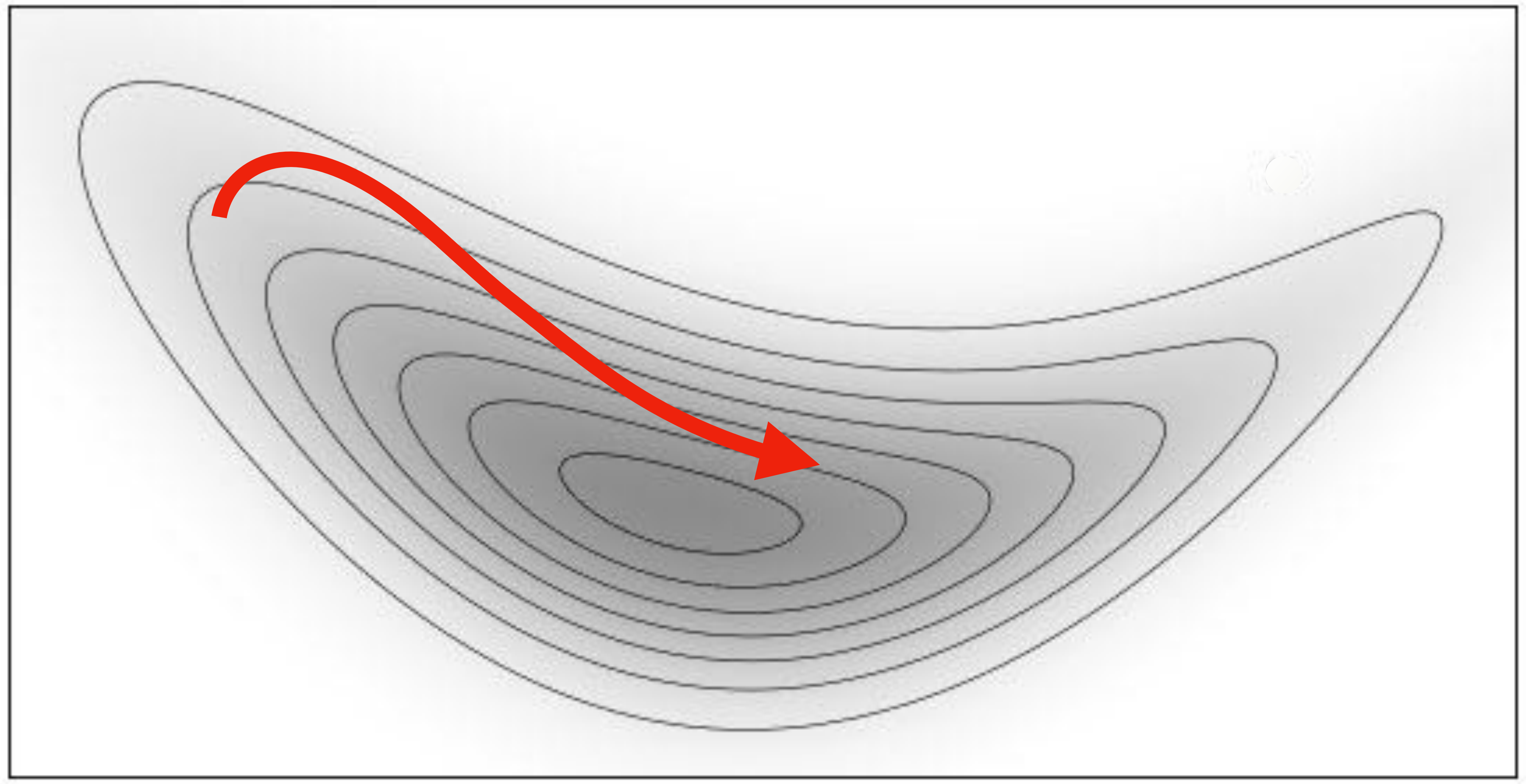
Step size can now be large and traces the curvature of the posterior topology

Hamiltonian Monte Carlo

1. Define a Hamiltonian system
   $H = U(\theta) + K(\nu)$

2. For each step…
   a. Give momentum a ‘kick’
   b. Integrate particle trajectory
   c. Almost always accept proposal

3. Stop at predetermined N
   Is this still true?



$$\boxed{U(\theta) \propto -\log[p(\theta \,|\, D)]}$$

Bayes Theorem

Likelihood

Prior

$$P(\theta \mid D) = \frac{P(D \mid \theta)\, P(\theta)}{P(D)}$$

Posterior

Evidence

Nested sampling generates **samples from the prior***

*subject to constraint $L > \lambda$, with the goal of calculating Z

MCMC vs Nested Sampling

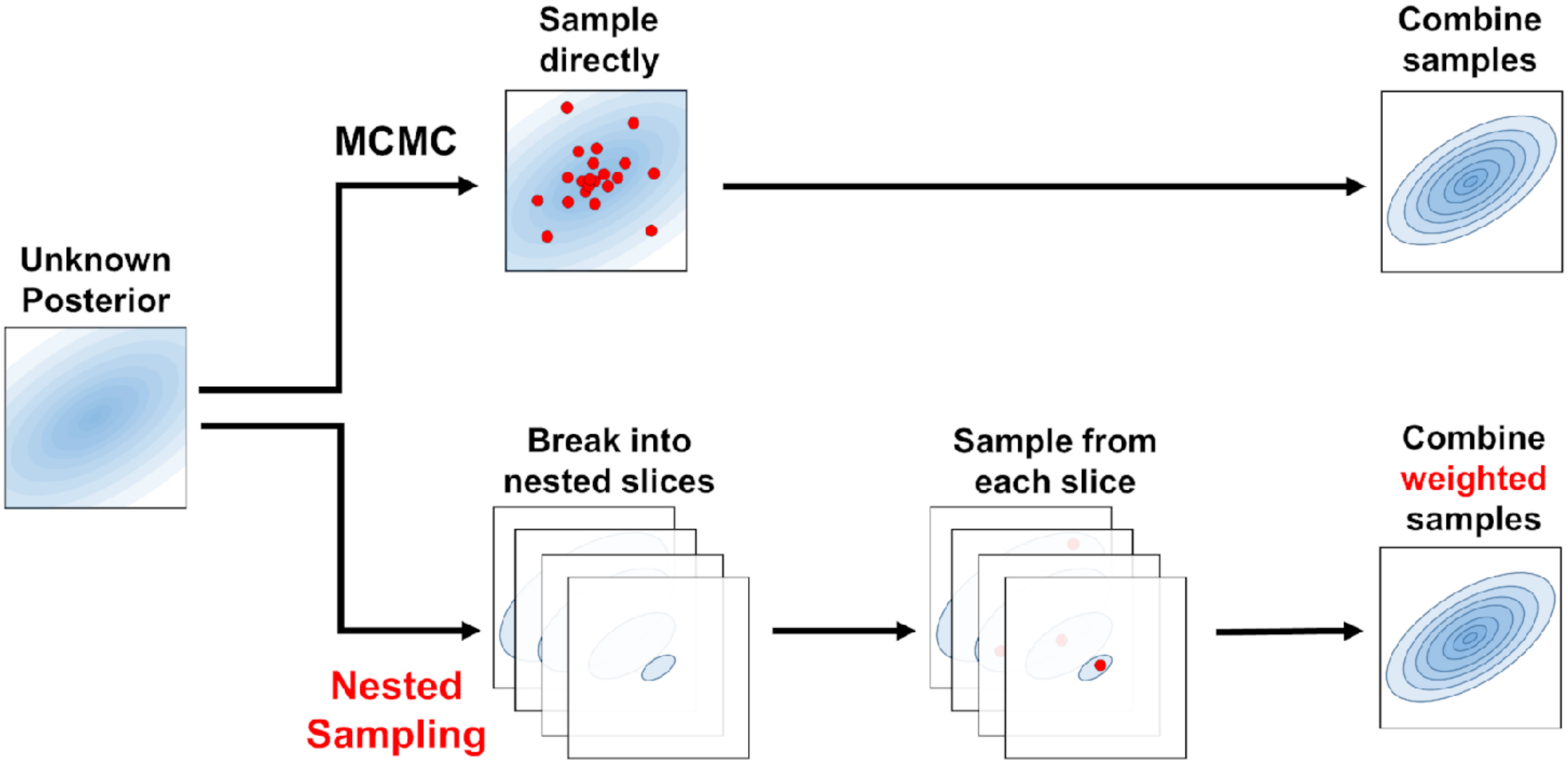


Image Credit: Speagle 2020

Nested Sampling

// Initialize live points.

Draw K "live" points$\{\boldsymbol{\Theta}_1, \ldots, \boldsymbol{\Theta}_K\}$ from the prior $\pi(\boldsymbol{\Theta})$.

// Main sampling loop.

while stopping criterion not met **do**

  Compute the minimum likelihood $\mathcal{L}^{\min}$ among thecurrent set of live points.

  Add the kth live point $\boldsymbol{\Theta}_k$ associated with $\mathcal{L}^{\min}$to a list of "dead" points.

  Sample a new point $\boldsymbol{\Theta}'$ from the prior subject to the constraint$\mathcal{L}(\boldsymbol{\Theta}') \geq \mathcal{L}^{\min}$.

  Replace $\boldsymbol{\Theta}_k$ with $\boldsymbol{\Theta}'$.

  // Check whether to stop.

  Evaluate stopping criterion.

end

// Add final live points.

while $K > 0$ **do**

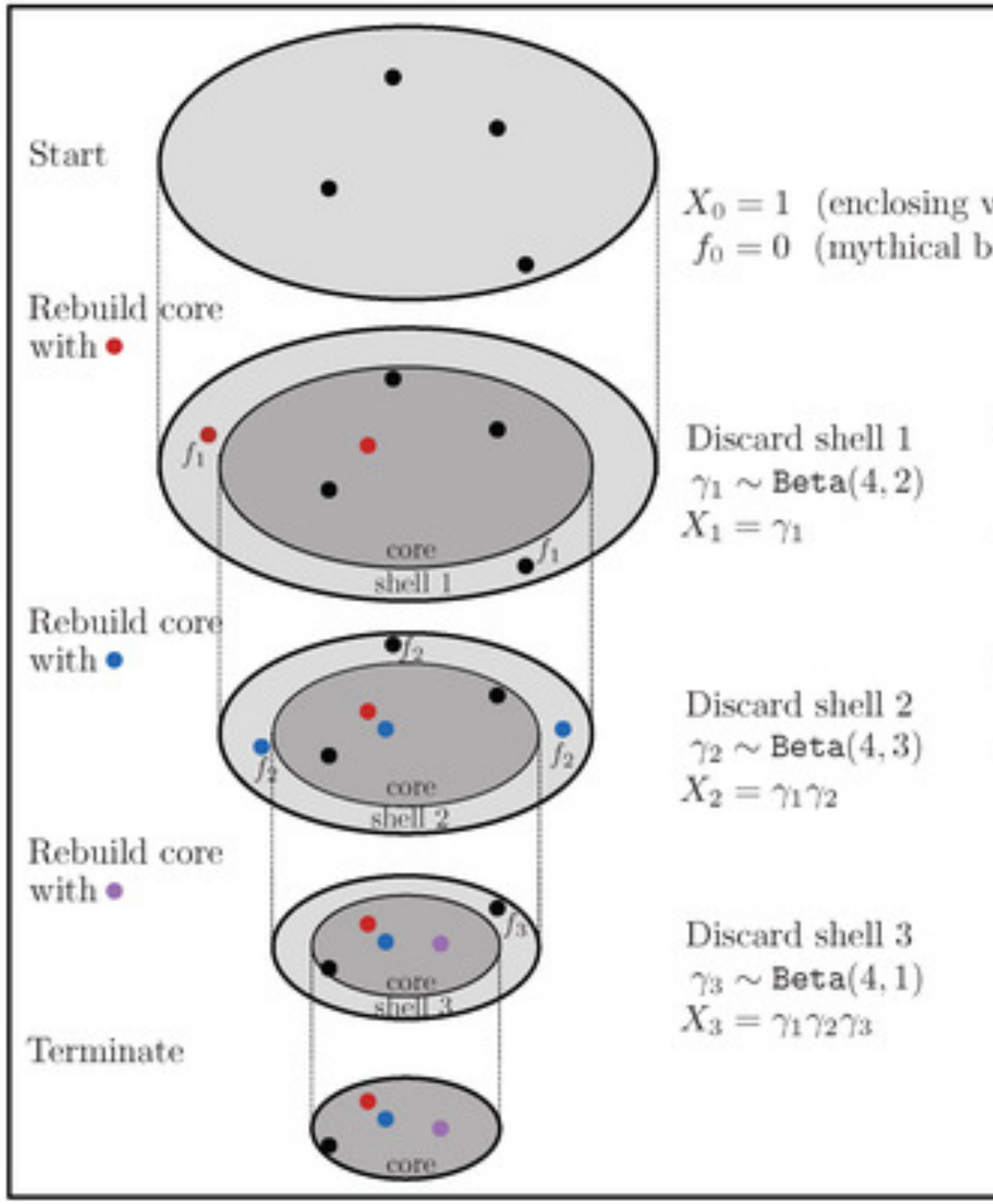
  Compute the minimum likelihood $\mathcal{L}^{\min}$ among thecurrent set of live points.

  Add the kth live point $\boldsymbol{\Theta}_k$ associated with $\mathcal{L}^{\min}$to a list of "dead" points.

  Remove $\boldsymbol{\Theta}_k$ from the set of live points.

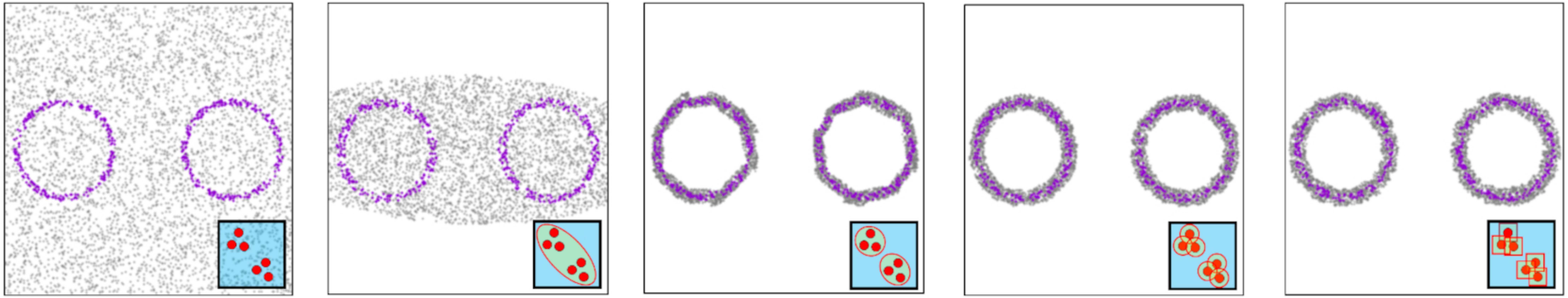
  Set $K = K - 1$.

end



Nested Sampling

Bounding Distributions



Unit Cube
(no bound)

Single
Ellipsoid

Multiple
Ellipsoids

Overlapping
Balls

Overlapping
Cubes

Nested Sampling

Here’s where I show the math going from prior volume to evidence to posterior