

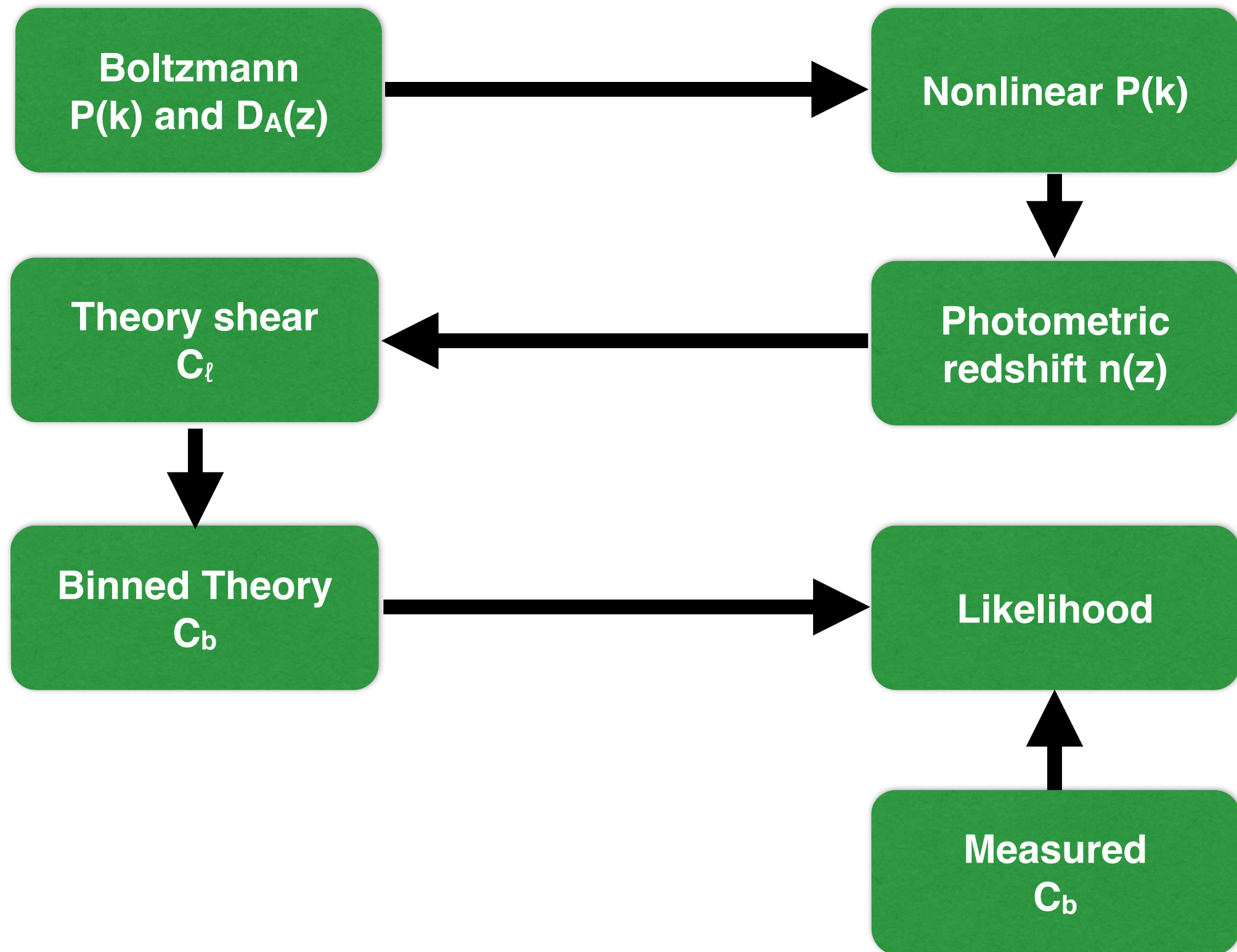
# Observations to Models

## Lecture 3

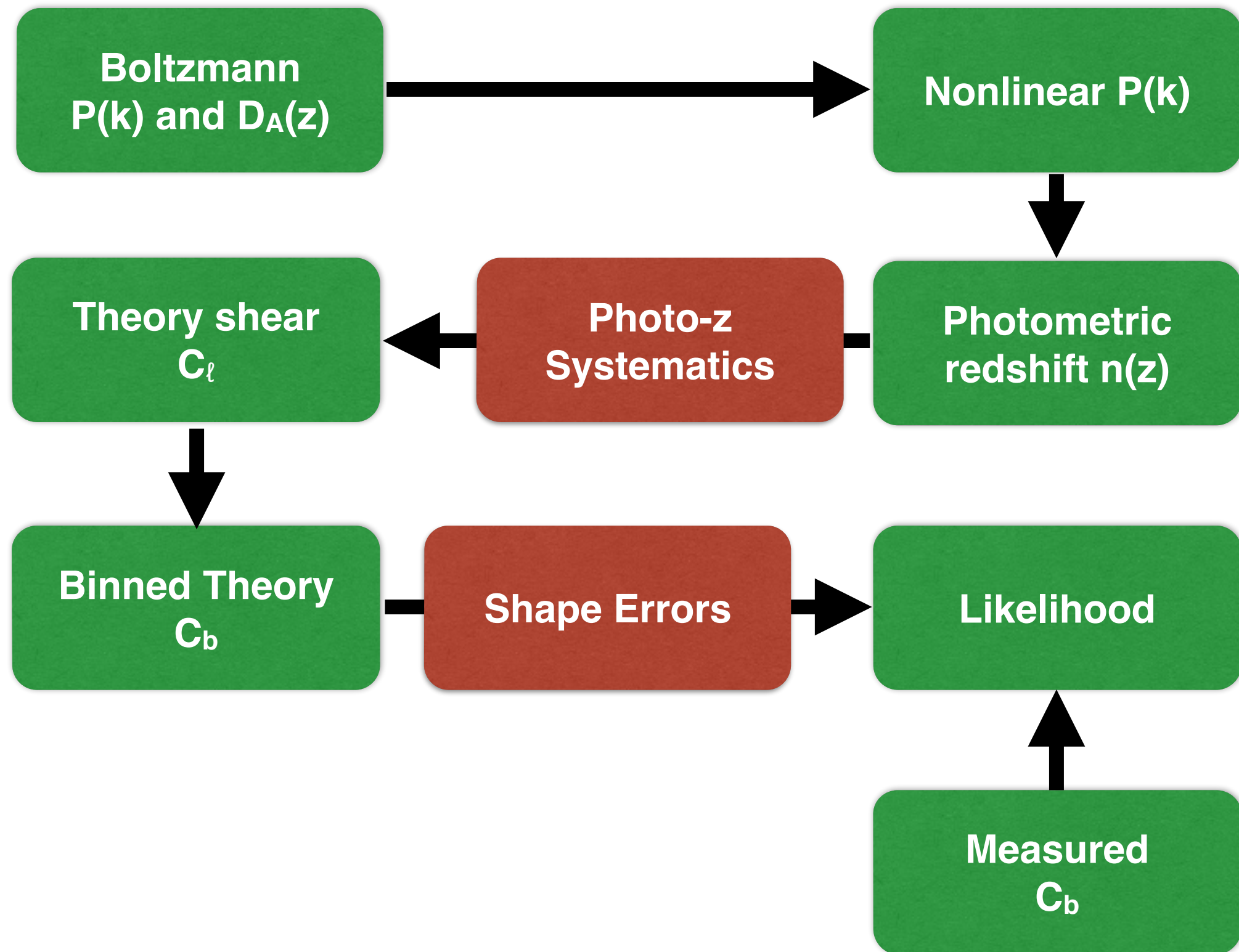
Exploring likelihood spaces  
with CosmoSIS

Joe Zuntz  
University of Manchester

# Defining Likelihood Pipelines



# Defining Likelihood Pipelines



# Modular Likelihood Pipelines

- Each box is an independent piece of code (*module*)
- With well-defined inputs and outputs
- This lets you replace, compare, insert, and combine code more easily

# CosmoSIS

- CosmoSIS is a parameter estimation framework
- Connect inference methods to cosmology likelihoods

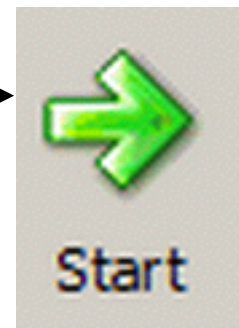
<https://bitbucket.org/joezuntz/cosmosis>

# Setting up CosmoSIS on teaching machines

- Open VirtualBox



- Click "start"



- Password cosmosis

- Click Terminal



> su

- use password **cosmosis**

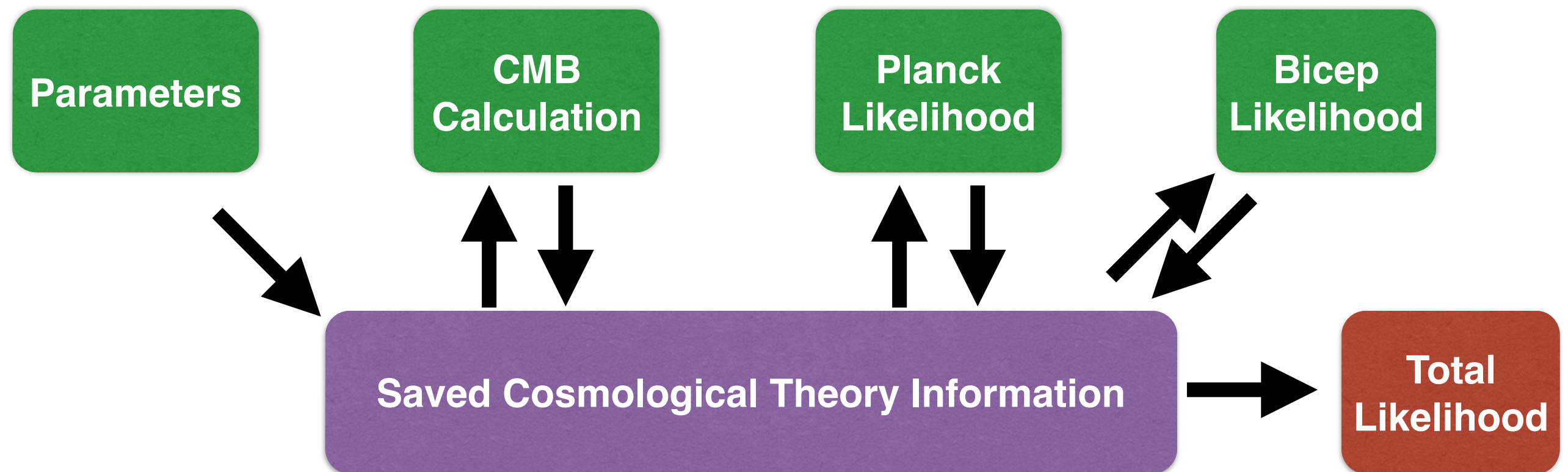
> cd /opt/cosmosis

> source config/setup-cosmosis

# Pipeline Example

```
> cosmosis demos/demo2.ini
```

```
> postprocess -o plots -p demo2 demos/demo2.ini
```



<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo2>

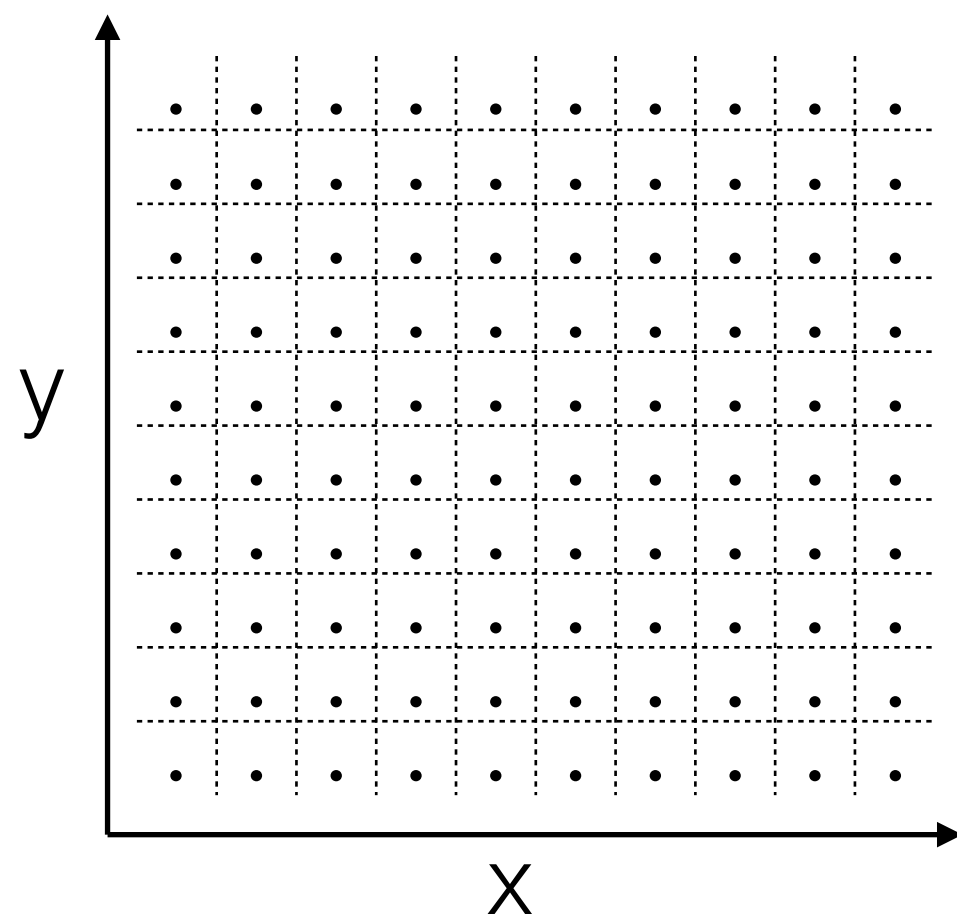
# Basic Inference Methods

- You've made a posterior function from a likelihood function and a prior
  - Now what?
- Explore the parameter space and build constraints on parameters
  - Remember: “the answer” is a probability distribution



# Basic Inference: Grids

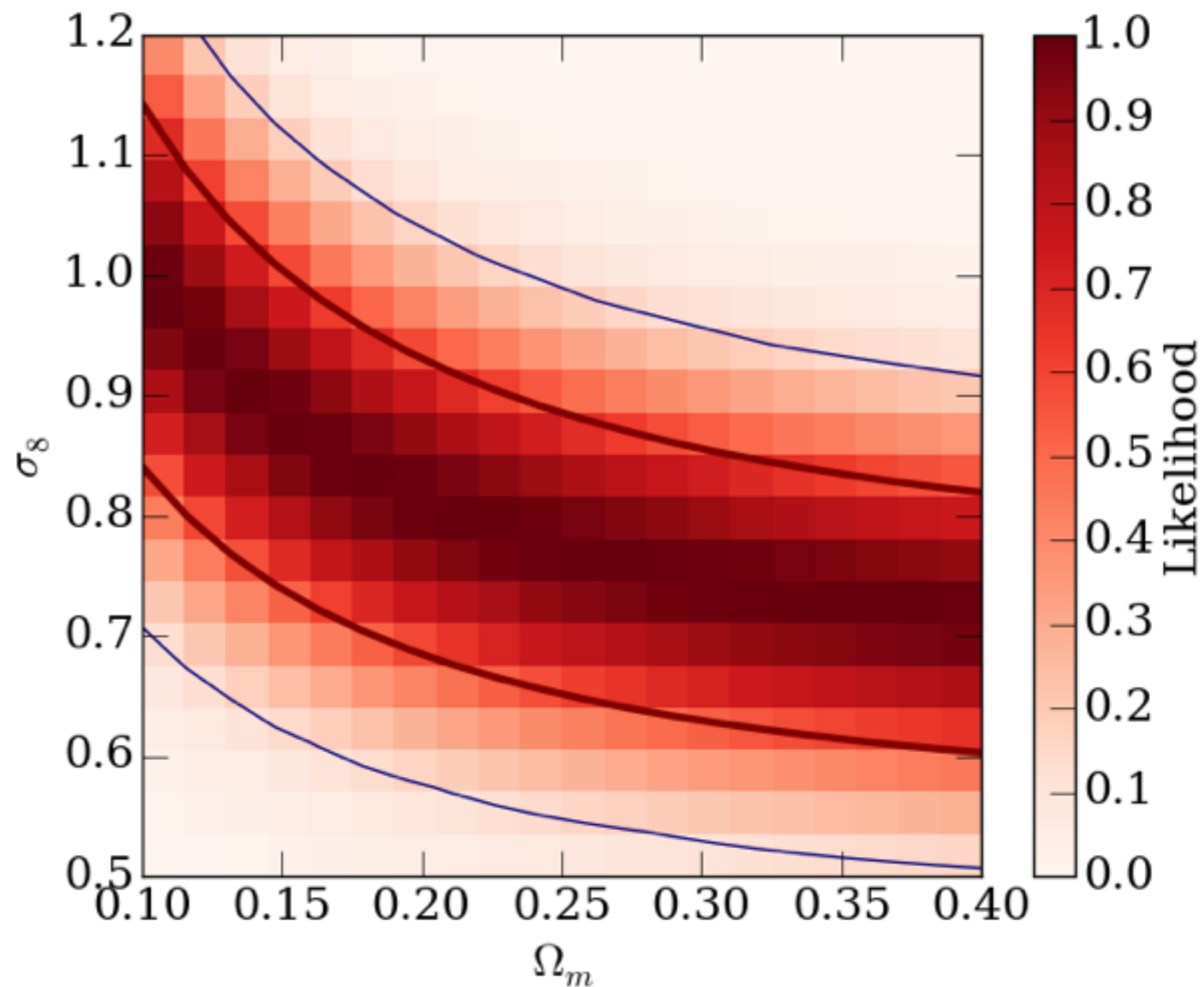
- Low number of parameters  
⇒ can try grid of all possible  
parameter combinations
- Number of posterior evaluations  
= (grid points per param)<sup>(number params)</sup>
- Approximate PDF integrals as sums



# Basic Inference: Grids

- Get constraints on lower dimensions by summing along axes

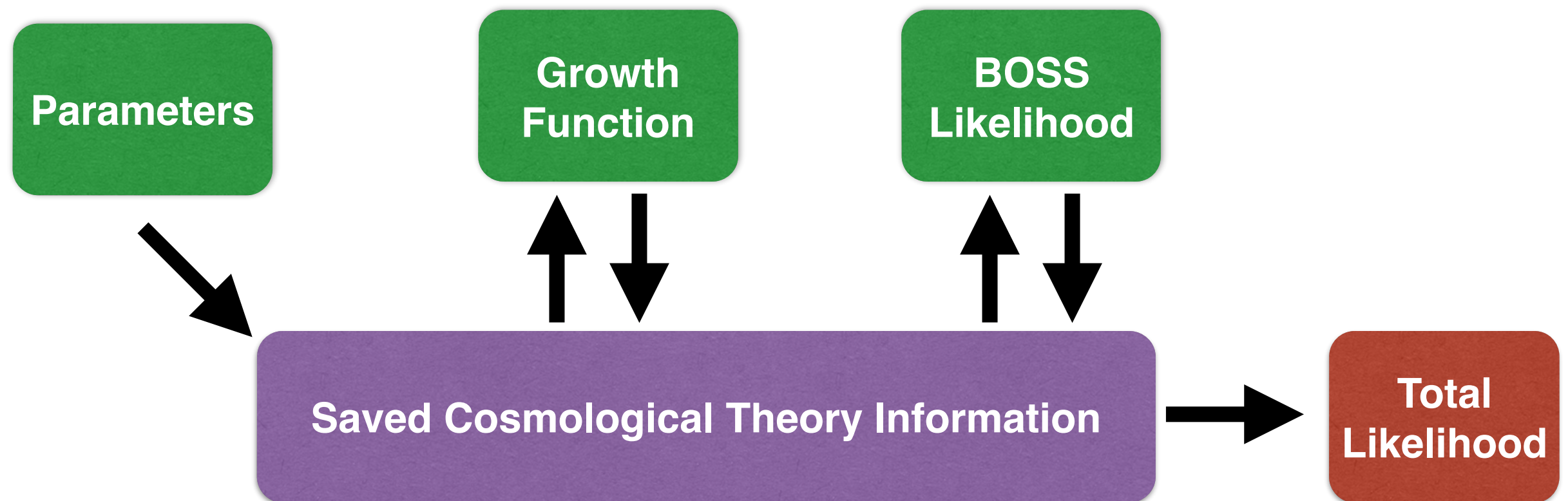
$$\begin{aligned} P(X) &= \int P(XY) dy \\ &\approx \sum_i \delta Y_i P(X, Y_i) \\ &\propto \sum_i \delta P(X, Y_i) \end{aligned}$$



# Grid Example

```
> cosmosis demos/demo7.ini
```

```
> postprocess -o plots -p demo7 demos/demo7.ini
```

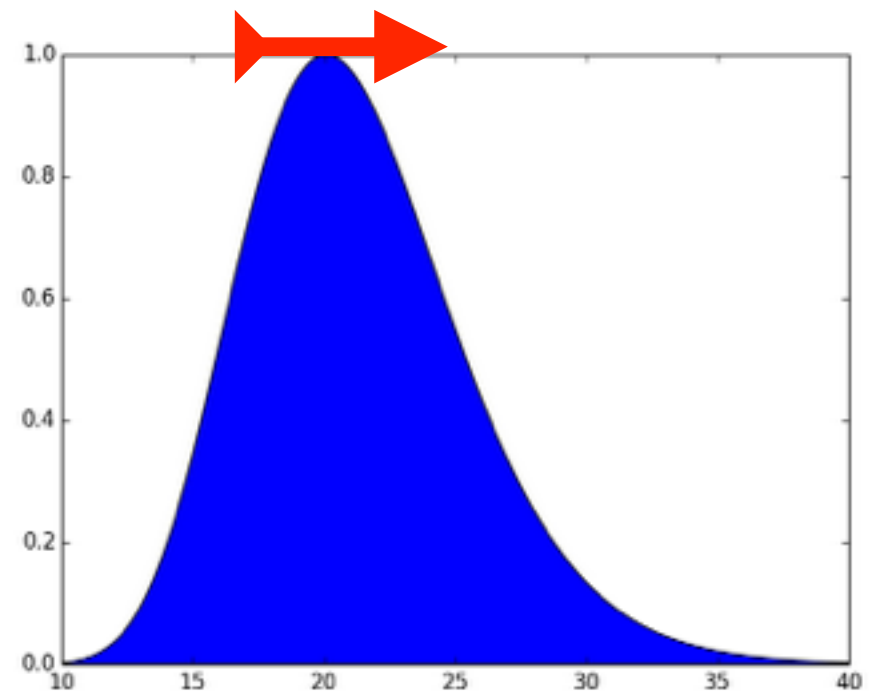


<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo7>

# Basic Inference:

## Maximum Likelihood/Posterior

- The modal value of a distribution can be of interest, especially for near-symmetric distributions
- Find mode by solving  $\text{gradient}=0$
- Maximum-likelihood (ML)  
Maximum a Posteriori (MAP)



# Basic Inference:

## Maximum Likelihood/Posterior

- In 1D cases solve:

$$\frac{dP}{dx} = 0 \quad \text{or} \quad \frac{d \log P}{dx} = 0$$

- Multi-dimensional case:

$$\underline{\nabla} P = 0 \quad \text{or} \quad \underline{\nabla} \log P = 0$$

# Basic Inference:

## Maximum Likelihood/Posterior

- Around the peak of a likelihood the curvature is related to distribution width
- Usually easiest to do with logs, for example for a Gaussian:

$$\left. \frac{d^2 \log P}{dx^2} \right|_{x=\mu} = -\frac{1}{\sigma^2}$$

# ML Exercise

- Find the maximum likelihood of our LMC cepheid likelihood, assuming fixed  $\sigma_i$ :

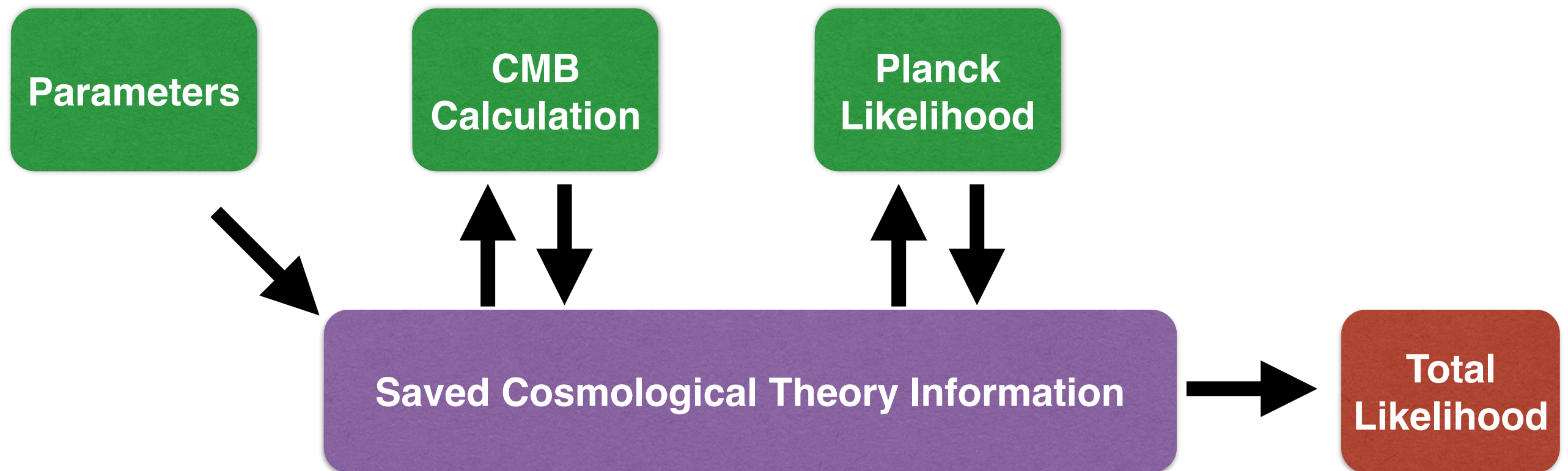
$$P(V_i^{\text{obs}} | \mathbf{p}) \propto \frac{1}{\sigma_{\text{int}}^2 + \sigma_i^2} \exp -0.5 \left( \frac{(V_i^{\text{obs}} - (\alpha + \beta \log_{10} P_i))^2}{\sigma_{\text{int}}^2 + \sigma_i^2} \right)$$

- Much easier to use  $\log(P)$

# ML Example

```
> cosmosis demos/demo4.ini
```

```
> postprocess -o plots -p demo4 demos/demo4.ini
```



<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo4>



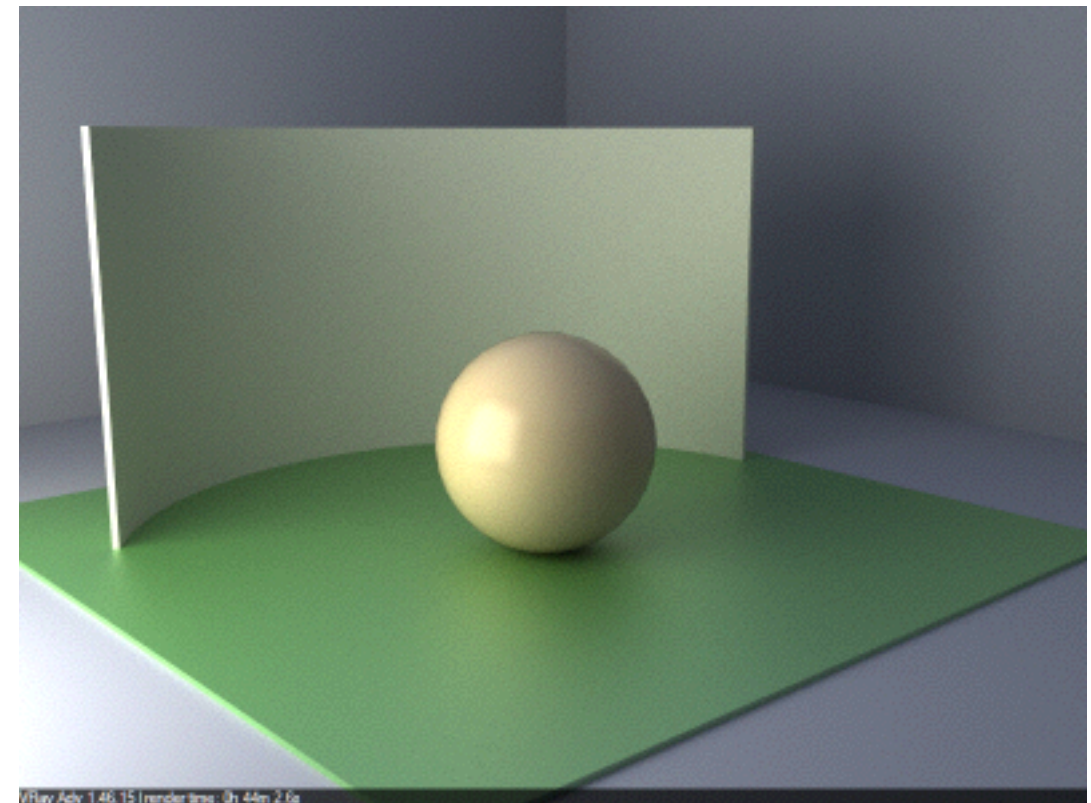
# Basic Inference:

## Maximum Likelihood/Posterior

- In simple cases you can solve these analytically. Otherwise need some kind of optimization
  - Numerical solvers - various algorithms; google scipy.minimize for a nice list
  - Usually easier with gradients e.g. Newton-Raphson
  - See also Expectation-Maximization algorithm

# Monte Carlo Methods

- Collection of methods involving repeated sampling to get numerical results
  - e.g. chance of dealing two pairs in five cards?
- Multi-dimensional integrals, graphics, fluid dynamics, genetics & evolution, AI, finance

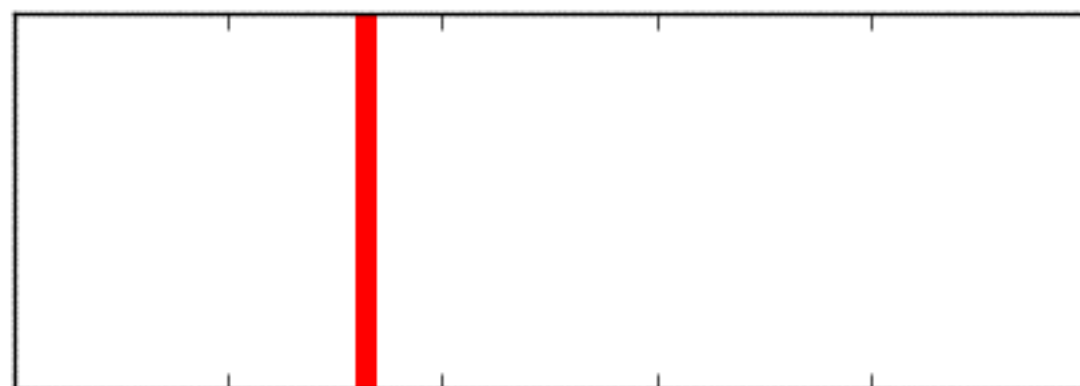
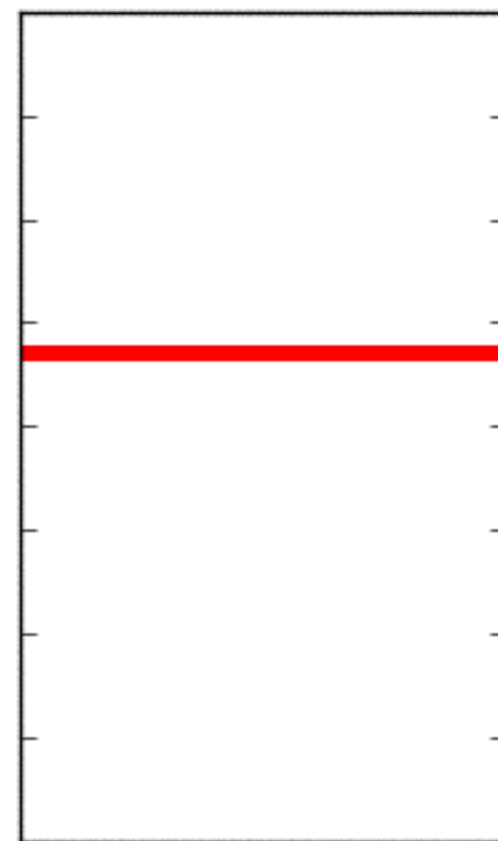
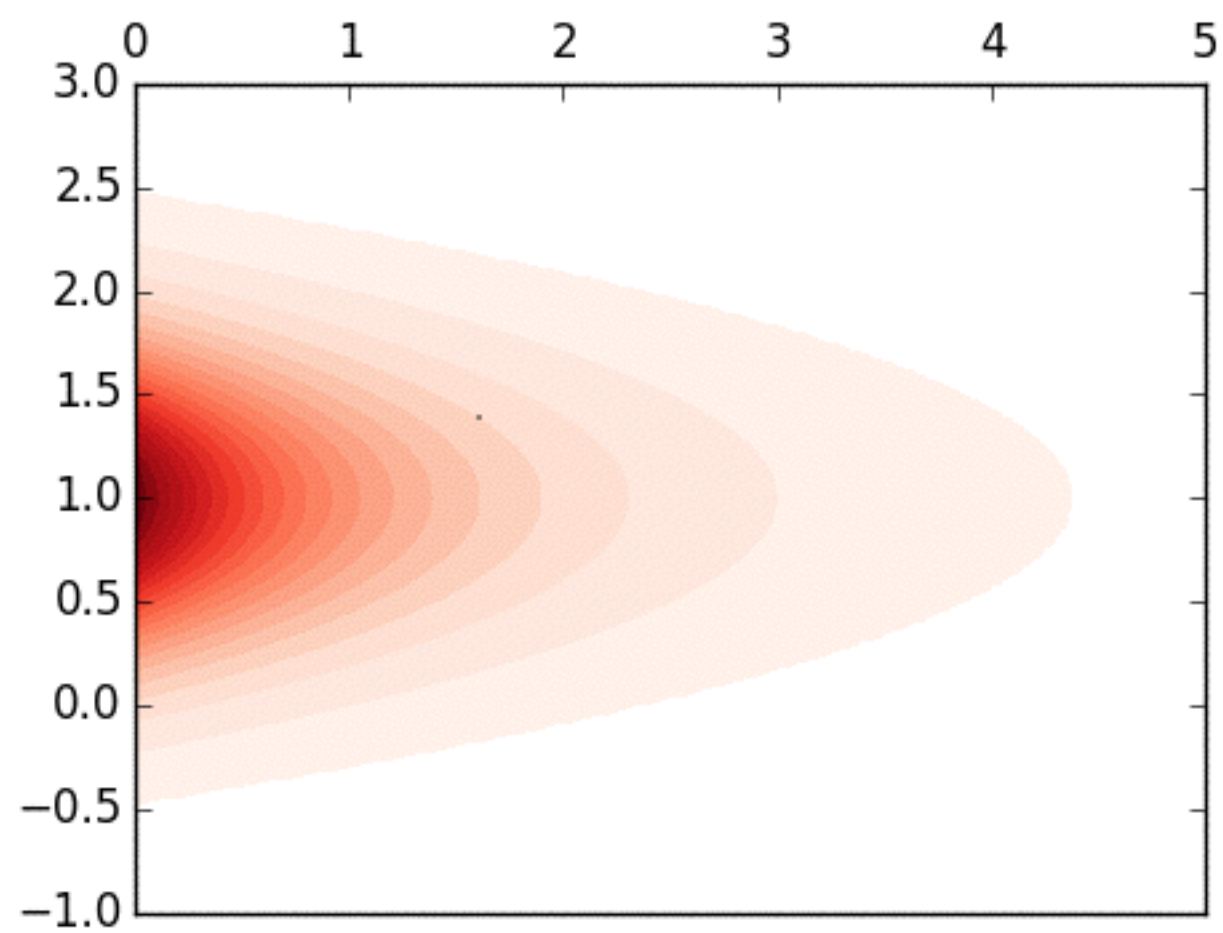


# Sampling Overview

- “Sample” = “Generate values with given distribution”
  - Easy: distribution written down analytically
  - Harder: can only evaluate distribution for given parameter choice

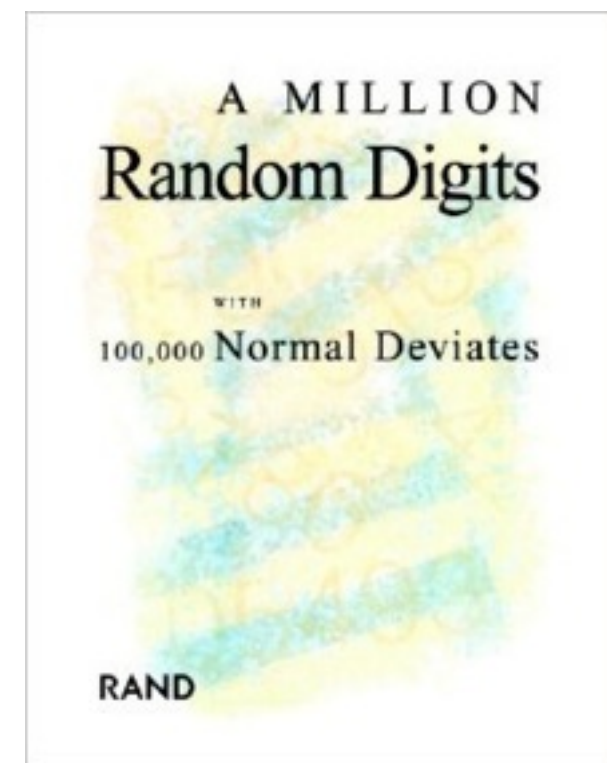
# Sampling Motivation

- Simulate systems
- Short-cut to expectations if you hate maths
- Approximate & characterize distributions
  - Estimate distributions mean, std, etc.
  - Make constraint plots
  - Compare with other data



# Direct Sampling

- Simple analytic distribution:  
can generate samples  
pseudo-randomly
- Actually incredibly complicated!
- ```
import scipy.stats  
X = scipy.stats.poisson(5.0)  
x = X.rvs(1000)
```
- Be aware of random seeds



# Direct Sampling

- e.g. approx solution to Lecture 1 homework problem

```
import numpy as np
dice = np.random.randint(20, size=1000000) + 1
dice_cubed = dice**3
print dice_cubed.mean()
```

- Often easier than doing sums/integrals

# Monte Carlo Markov Chains

- Often cannot directly sample from a distribution
- But can evaluate  $P(\underline{x})$  for any given  $\underline{x}$
- Markov chain = memory-less sequence

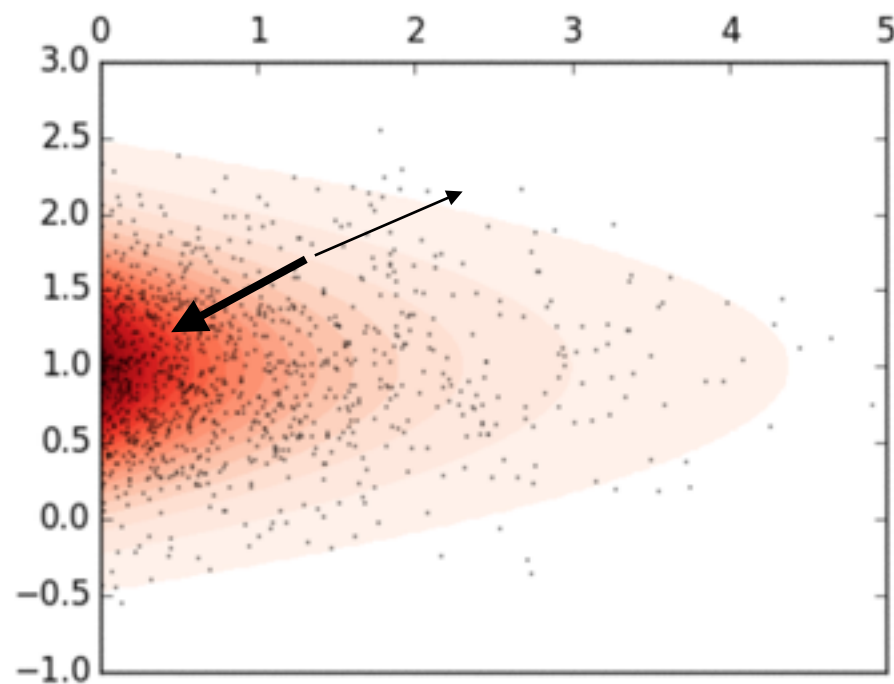
$$x_n = f(x_{n-1})$$

- MCMC: Random generation rule for  $f(x)$  which yields  $x_n$  with stationary distribution  $P(x)$   
i.e. chain histogram tends to  $P$



# MCMC

- Jump around parameter space
- Number of jumps near  $x \sim P(x)$



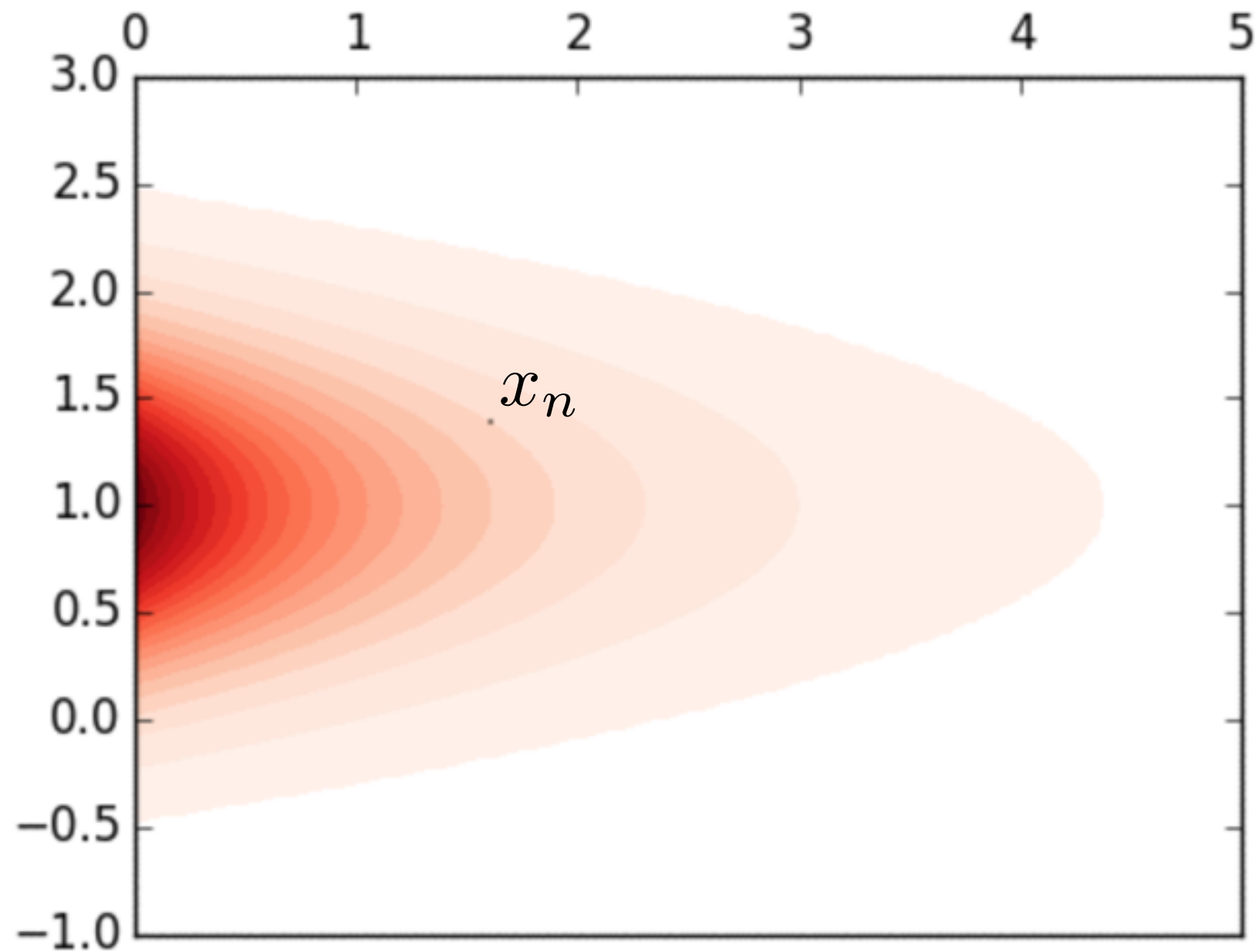
- Standard algorithms:  $x$  = single parameter set  
Advanced algorithms:  $x$  = multiple parameter sets

# Metropolis-Hastings

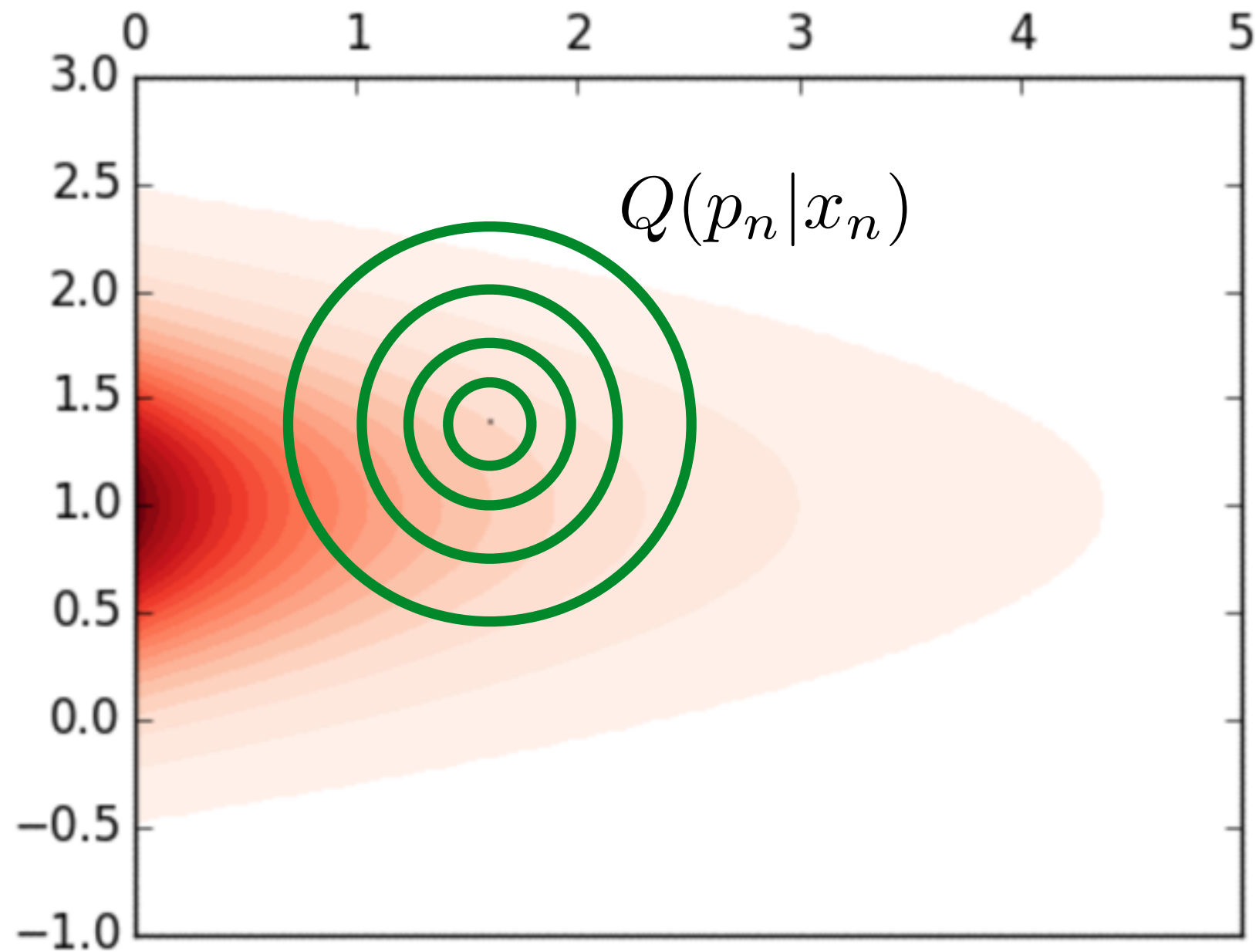
- Given current sample  $x_n$  in parameter space
  - Generate new proposed sample  $p_n \sim Q(p_n|x_n)$
  - For simplest algorithm  $Q(p|x) = Q(x|p)$

$$x_{n+1} = \begin{cases} p_n & \text{with probability } \min\left(\frac{P(p_n)}{P(x_n)}, 1\right) \\ x_n & \text{otherwise} \end{cases}$$

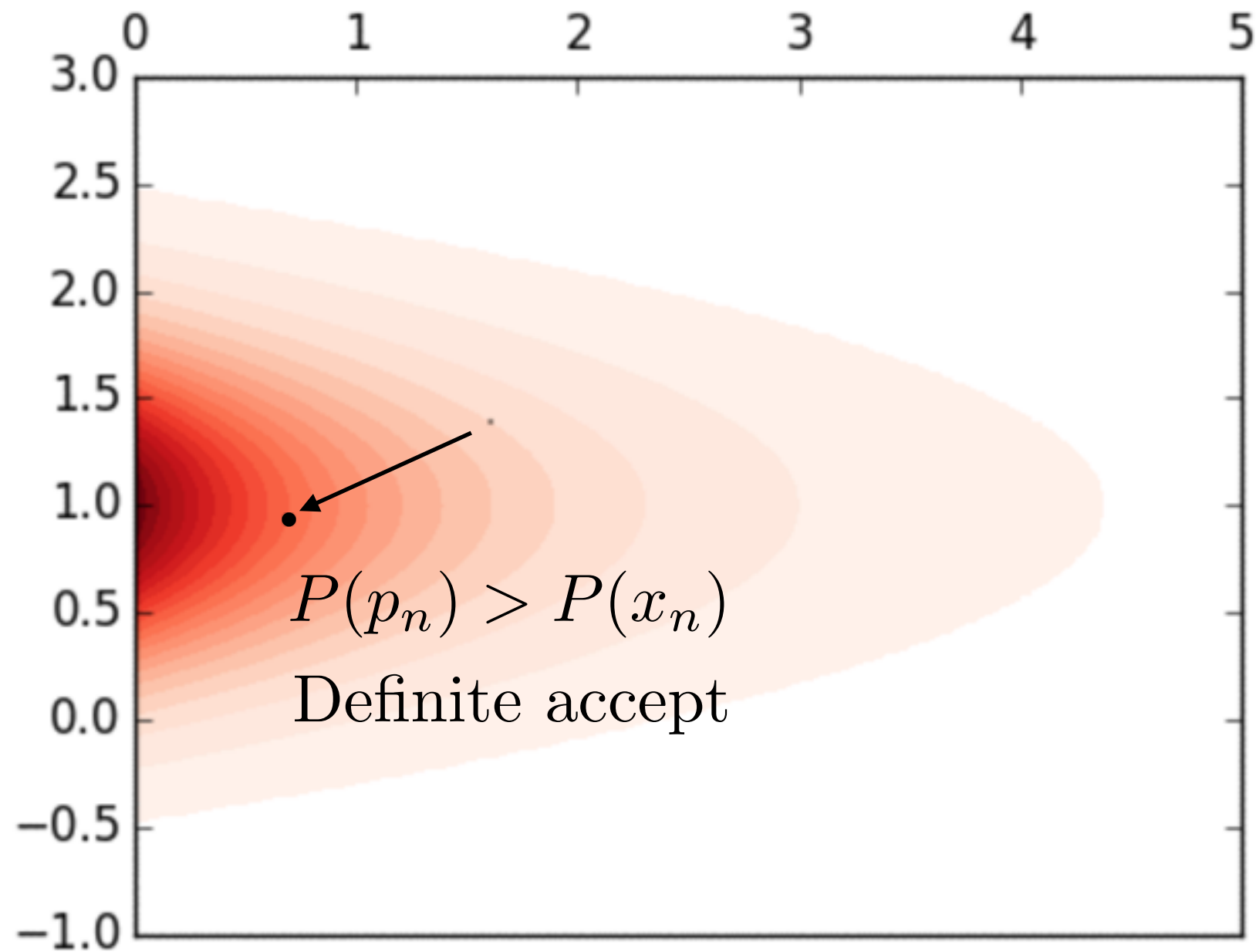
# Metropolis-Hastings



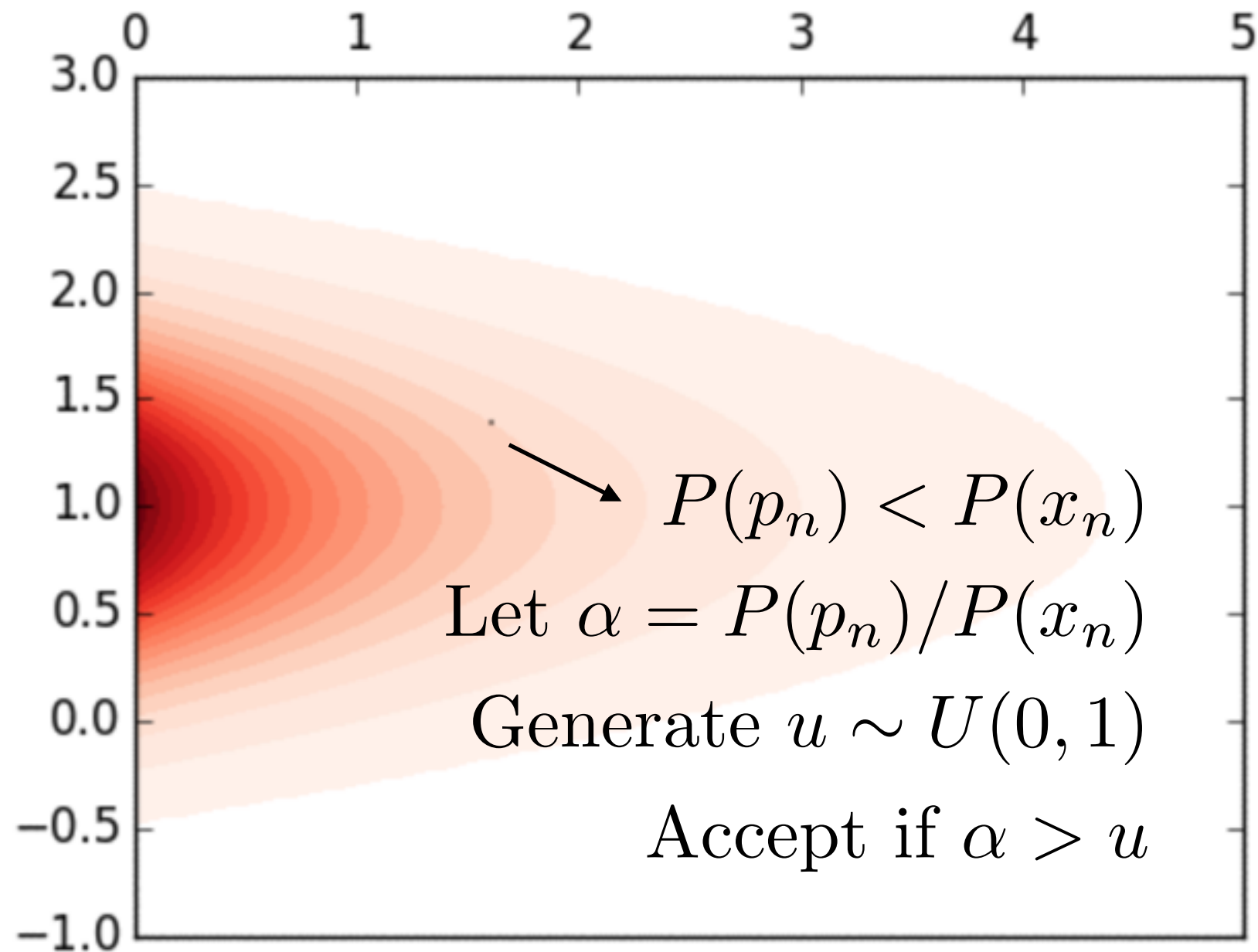
# Metropolis-Hastings



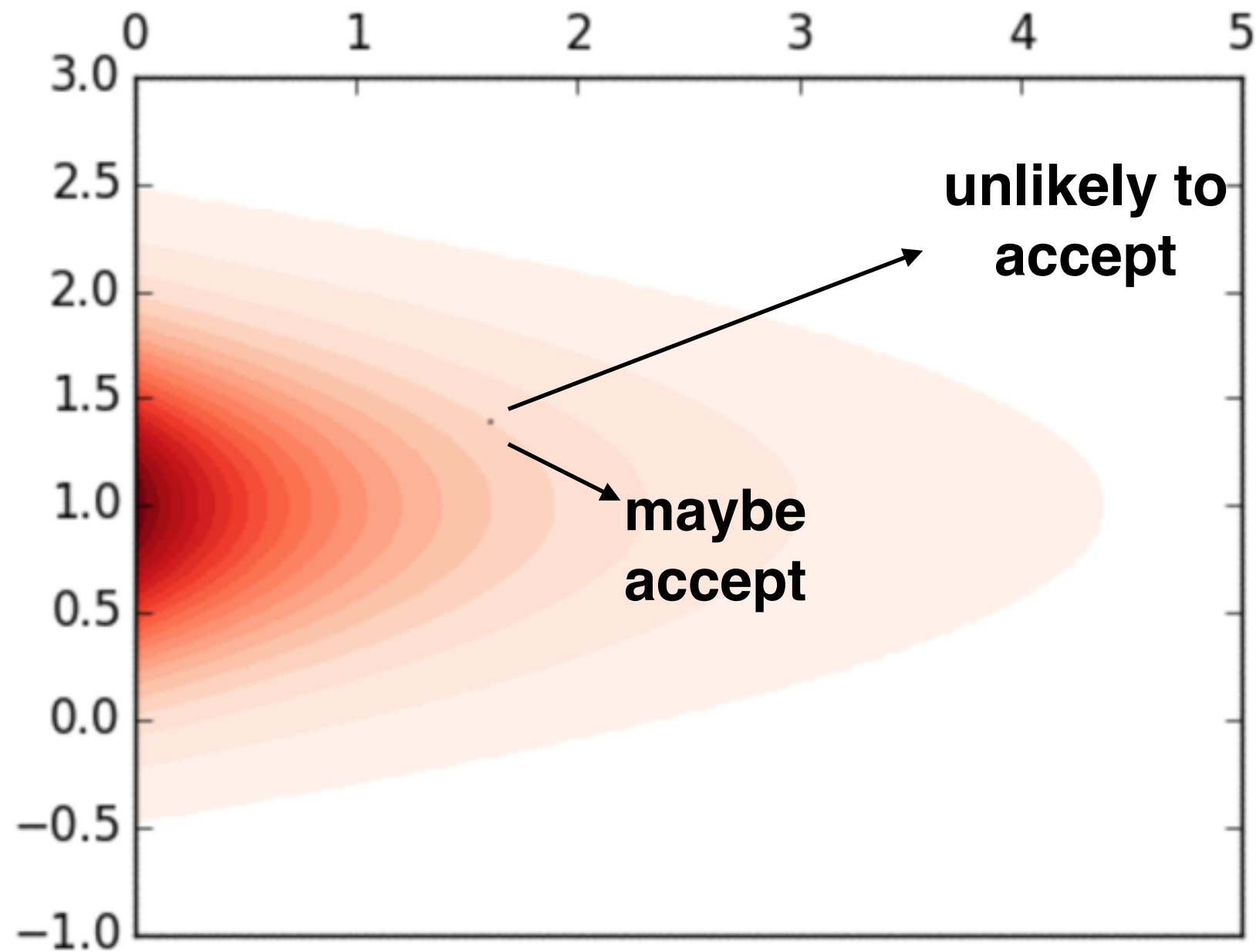
# Metropolis-Hastings



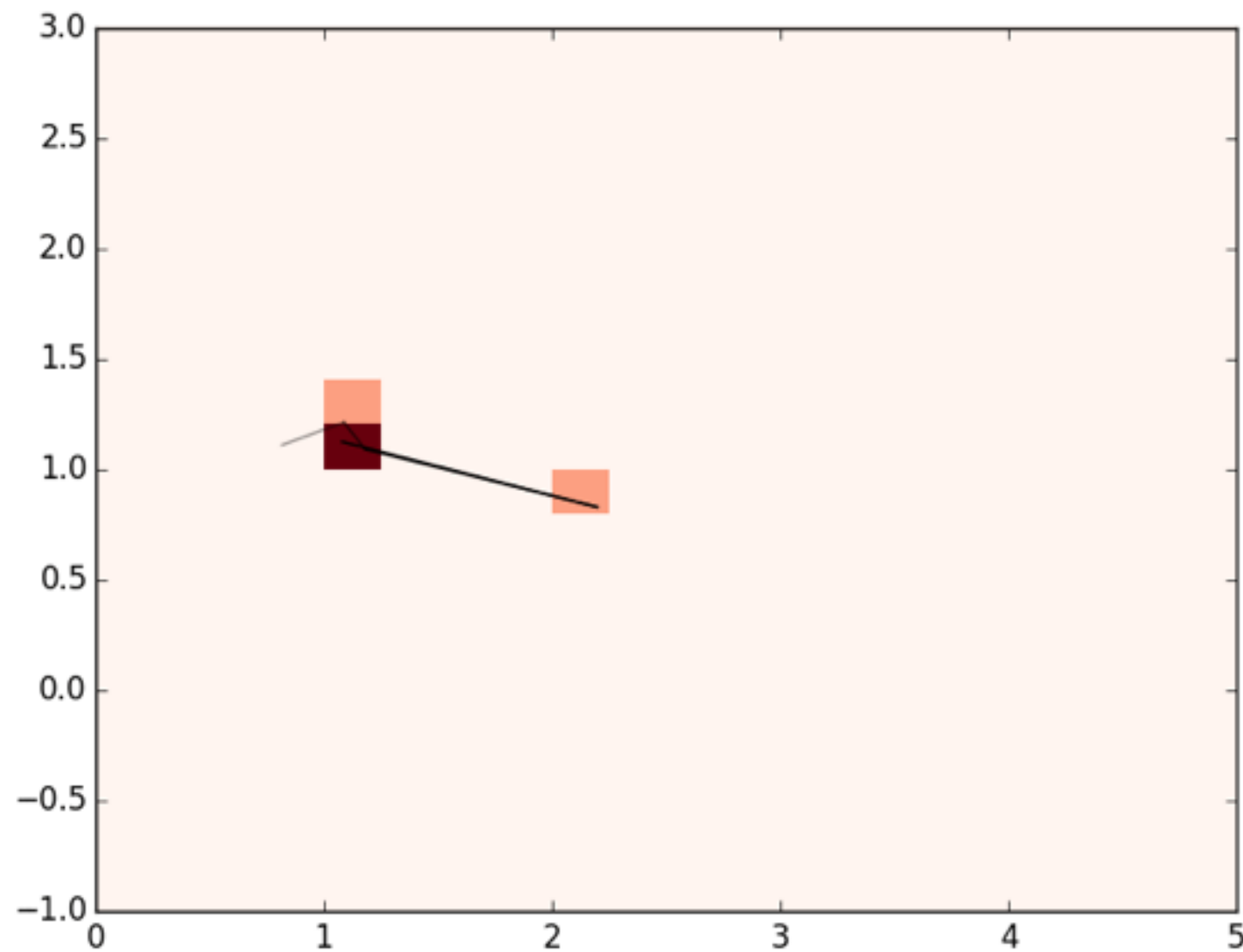
# Metropolis-Hastings



# Metropolis-Hastings



# Metropolis-Hastings



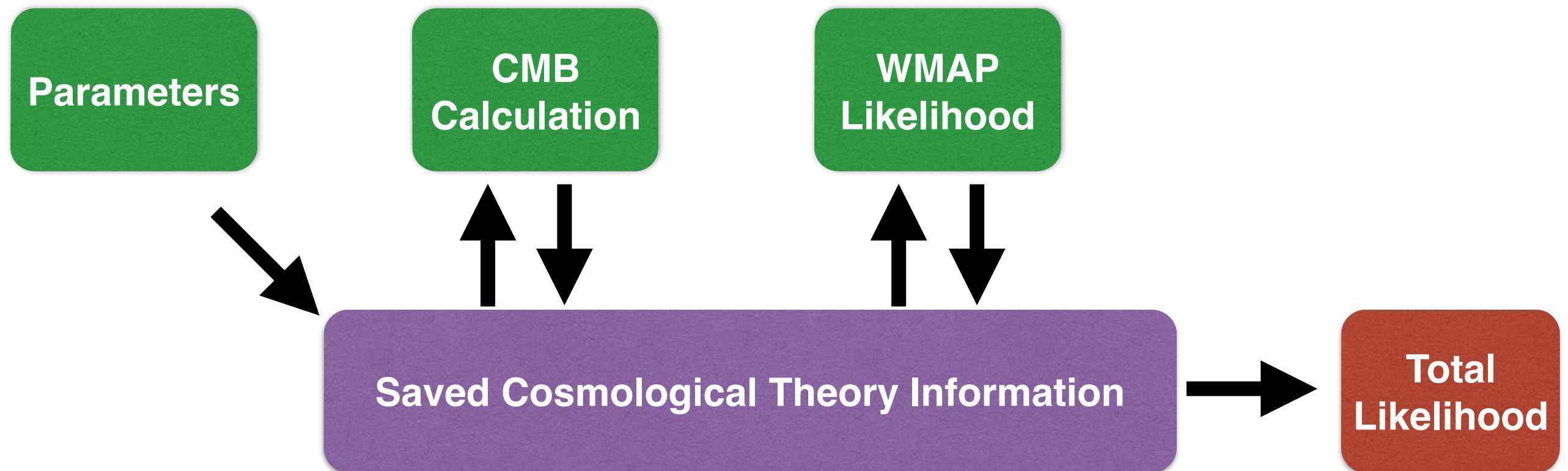


# Metropolis-Hastings Proposal

- MCMC will always converge in  $\infty$  samples
- Proposal function  $Q$  determines efficiency of MCMC
- Ideal proposal has  $\text{cov}(Q) \sim \text{cov}(P)$
- (Multivariate) Gaussian centred on  $x_n$  usually good  
Tune  $\sigma$  (+covariance) to match  $P$
- Ideal acceptance fraction  $\sim 0.2 - 0.3$

# Metropolis Example

- > `cosmosis demos/demo10.ini`
- > #This will take too long! Figure out how to change demo 7 to use Metropolis!



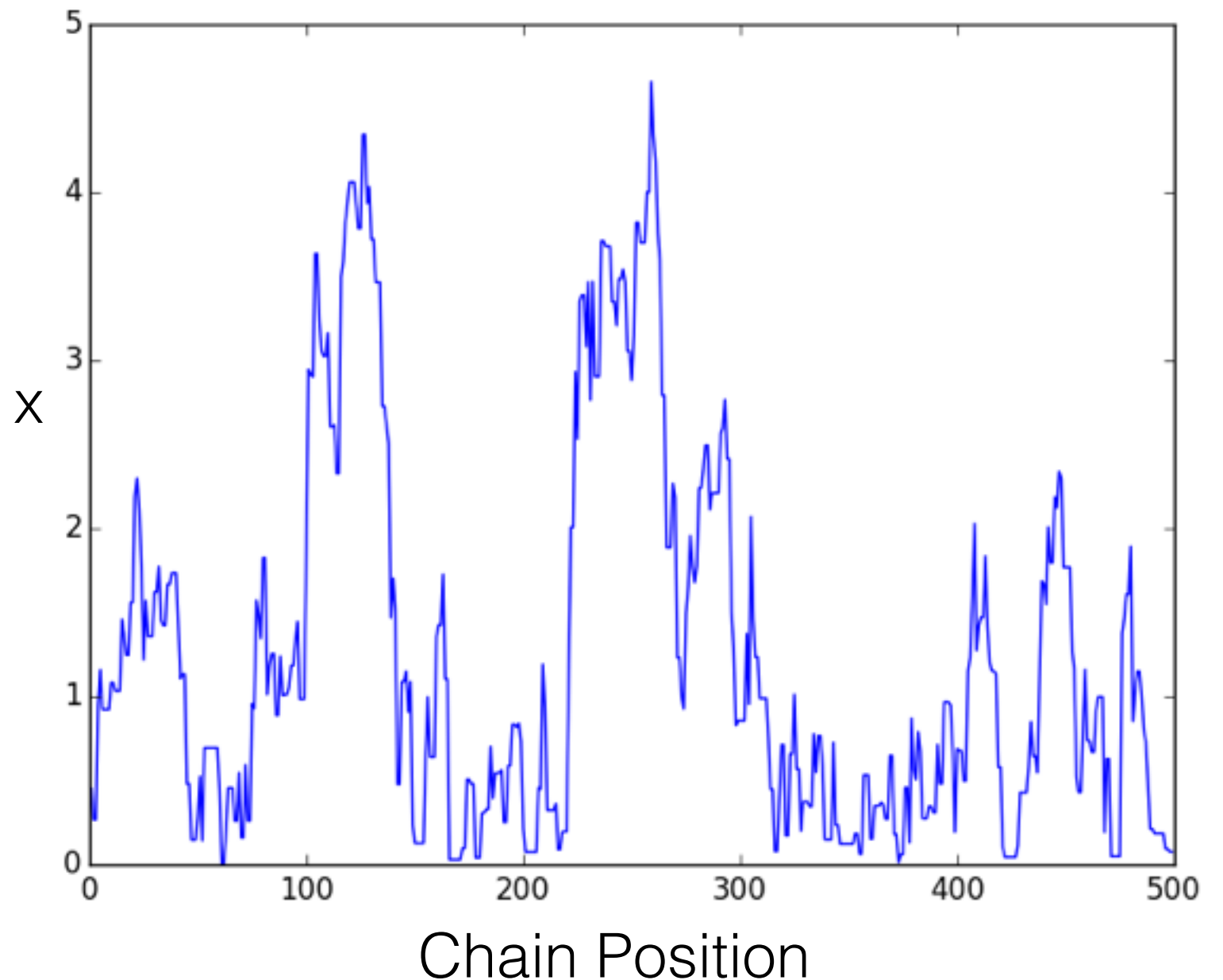
<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo10>

# Metropolis-Hastings Convergence

- Have I taken enough samples?
- Many convergence tests available
  - Easiest is visual!

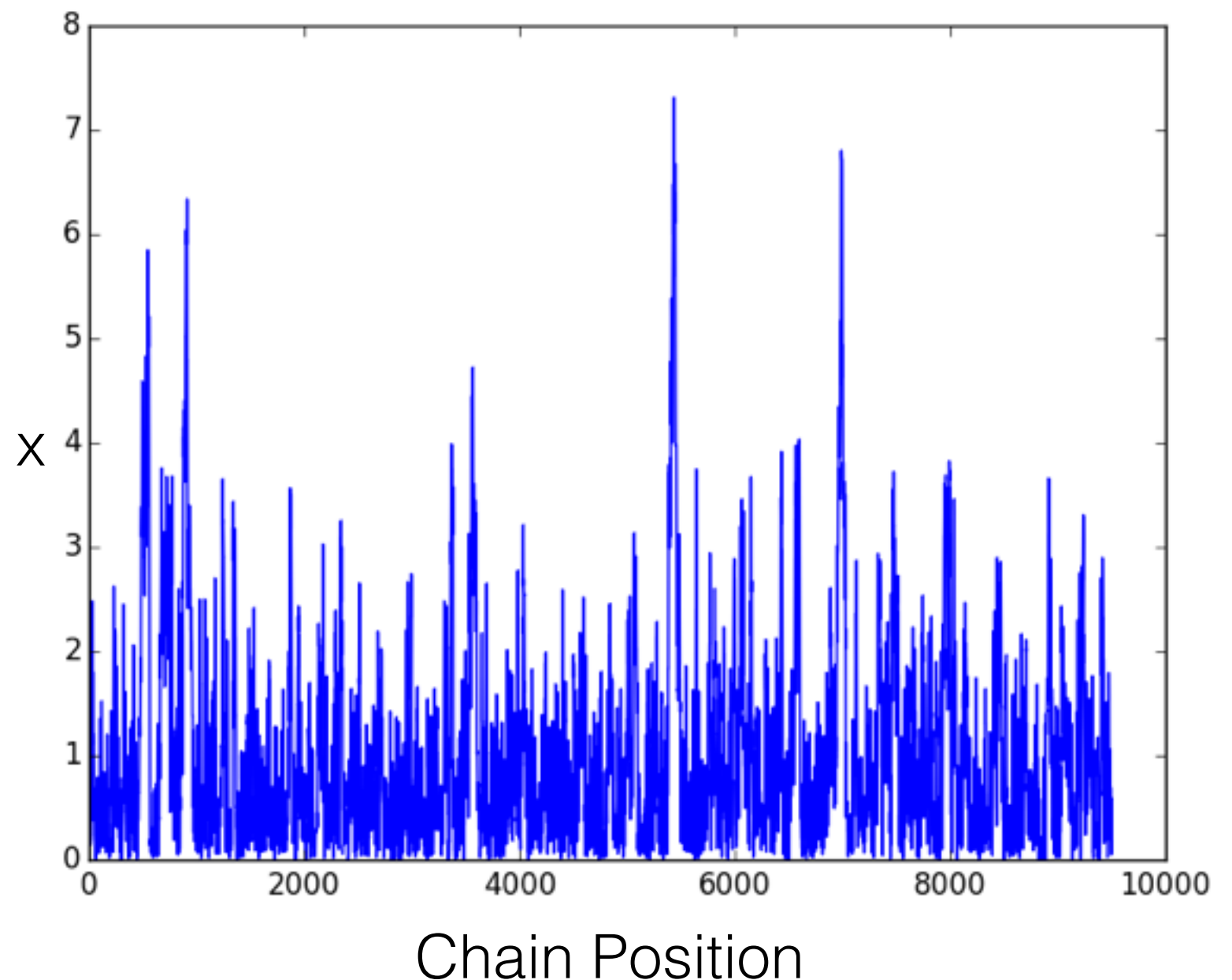
# Metropolis-Hastings Convergence

- Bad Mixing
- Structure and correlations visible



# Metropolis-Hastings Convergence

- Good Mixing
- Looks like noise
- Must be true for all parameters in space

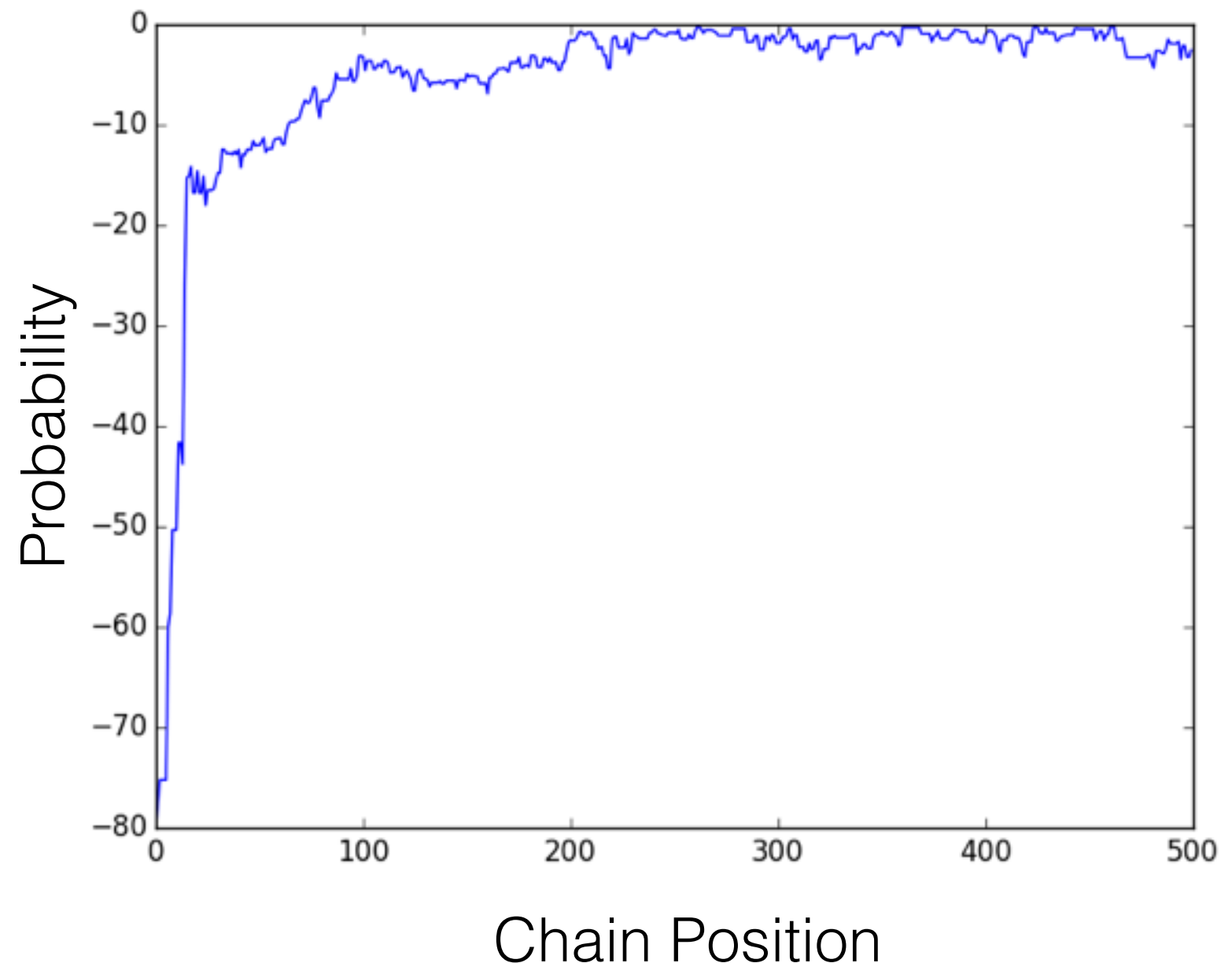


# Metropolis-Hastings Convergence

- Run several chains and compare results
  - $(\text{Variance of means}) / (\text{Mean of variances})$   
Less than e.g. 3%

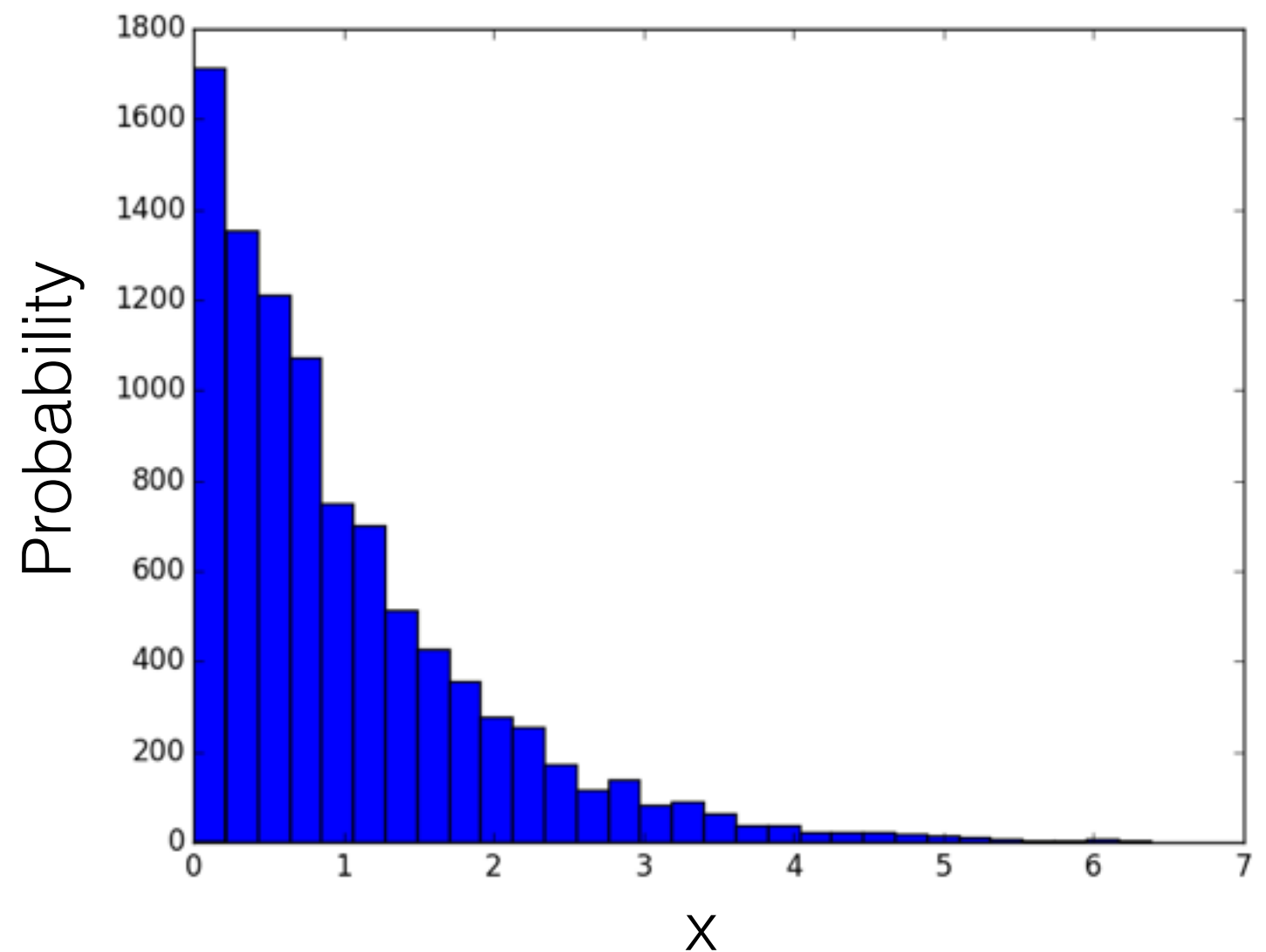
# Metropolis-Hastings Burn in

- Chain will explore peak only after finding it
- Cut off start of chain



# Metropolis-Hastings Analysis

- Probability proportional to chain multiplicity
- Histogram chain, in 1D or 2D
- Can also thin e.g. remove every other sample





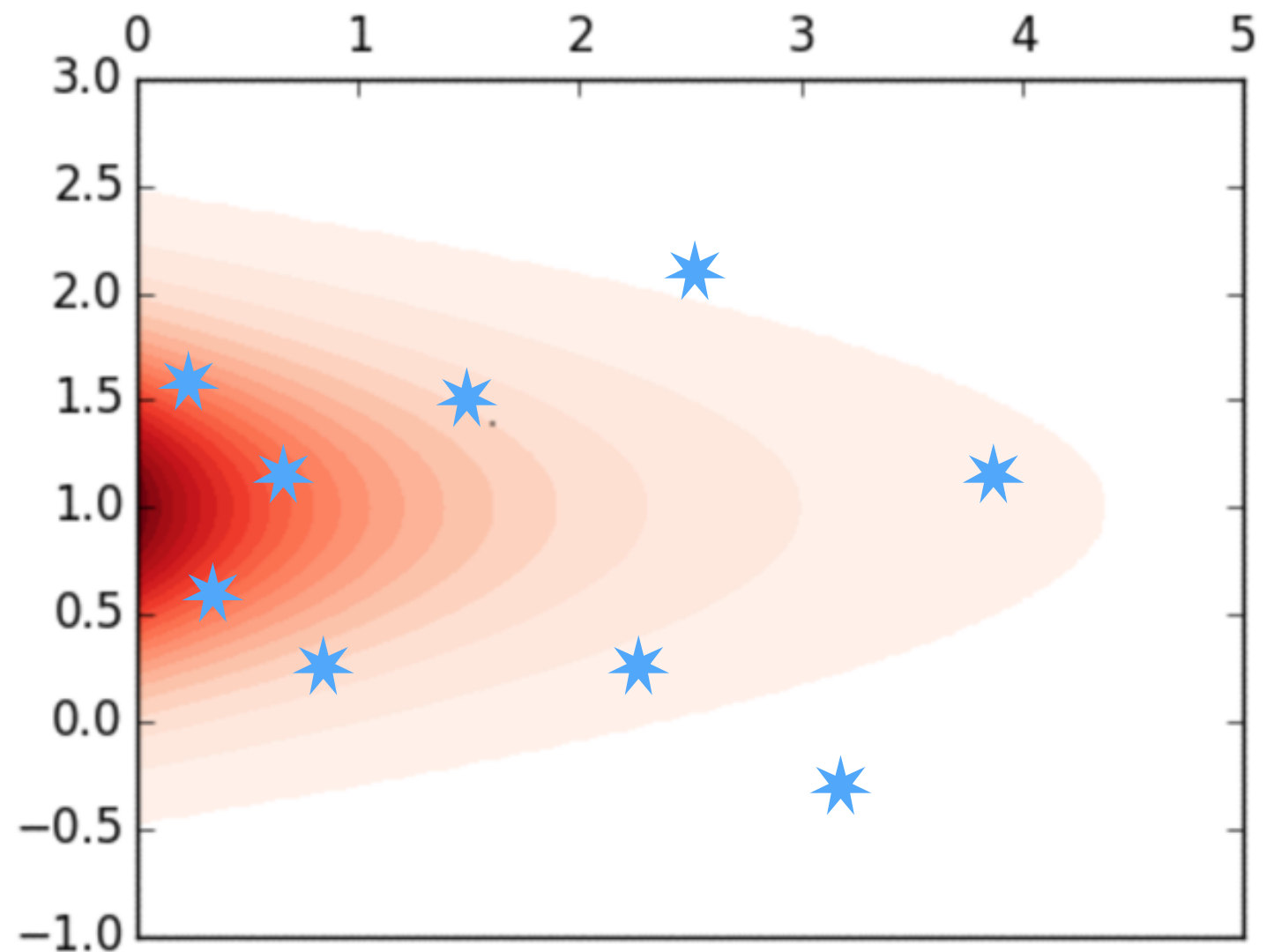
# Metropolis-Hastings Analysis

- Can also get expectations of derived parameters

$$E[f(x)] = \int P(x) f(x) dx \approx \frac{1}{N} \sum_i f(x_i)$$

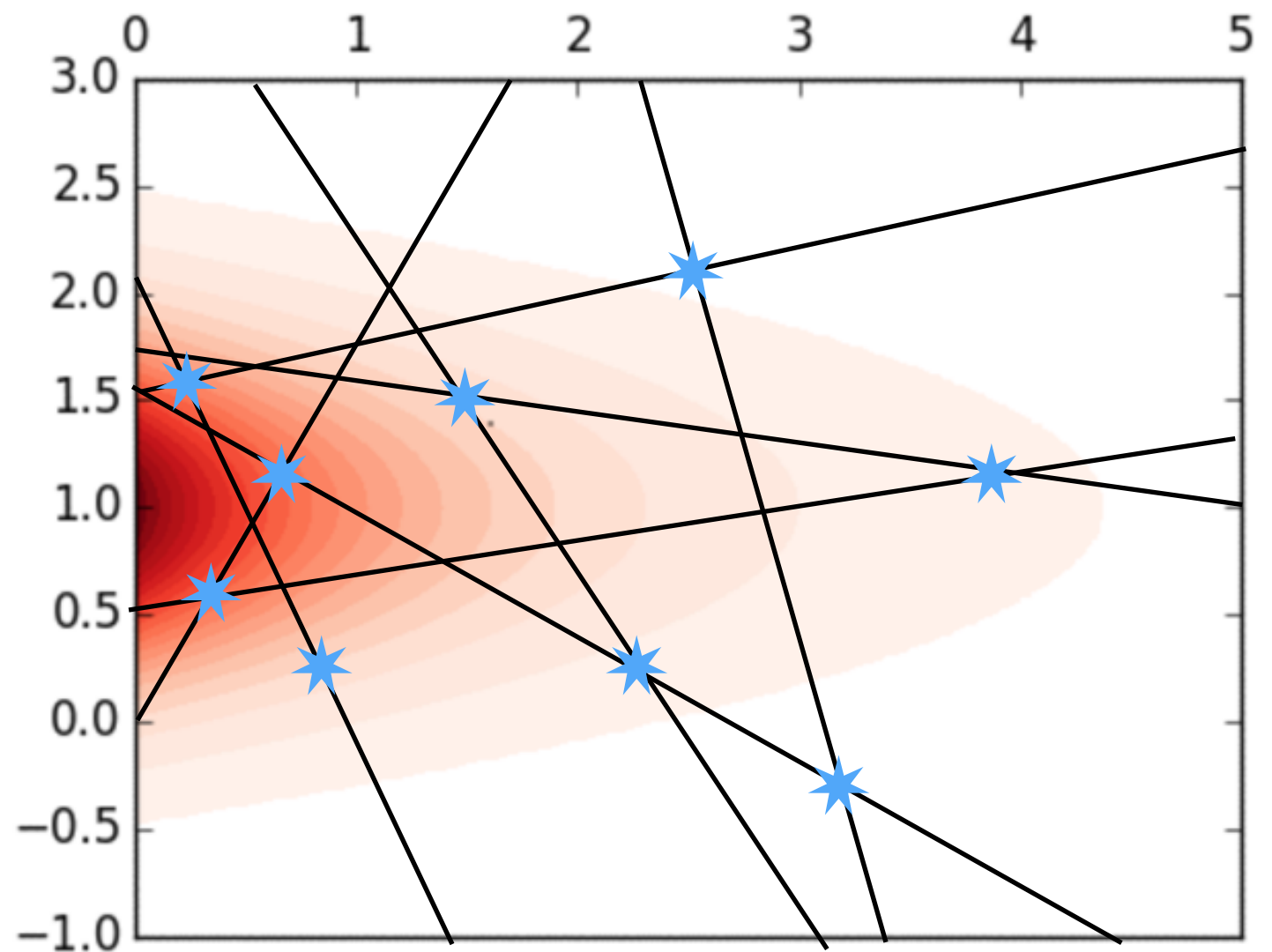
# Emcee Sampling

- Goodman & Weare algorithm
- Group of live “walkers” in parameter space
- Parallel update rule on connecting lines - affine invariant
- Popular in astronomy for nice and friendly python package



# Emcee Sampling

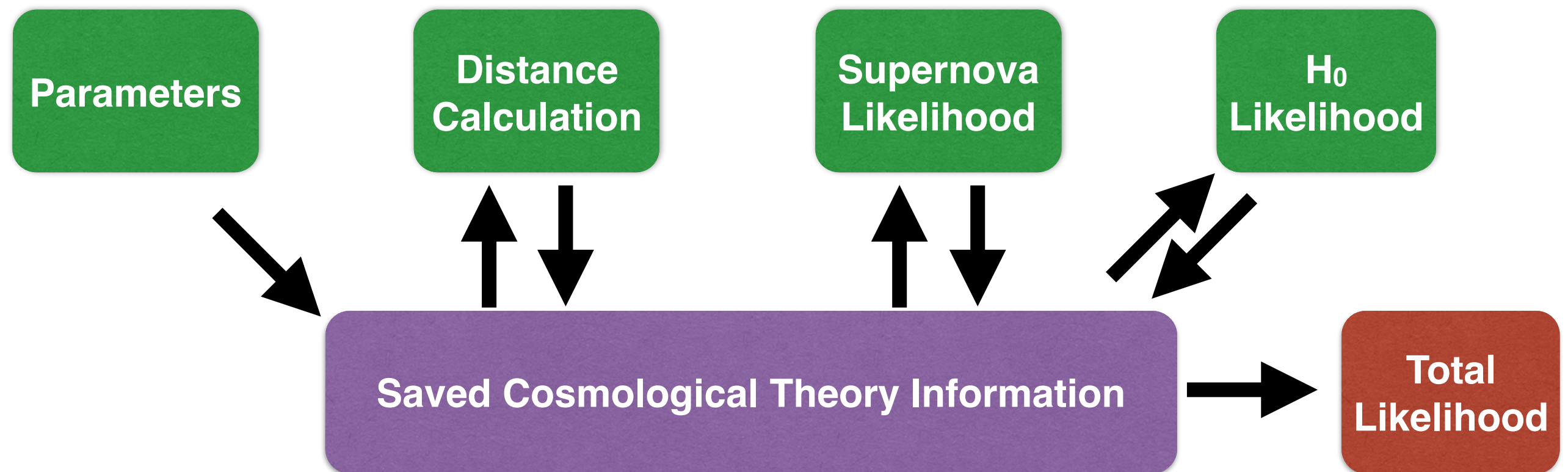
- Goodman & Weare algorithm
- Group of live “walkers” in parameter space
- Parallel update rule on connecting lines - affine invariant
- Popular in astronomy for nice and friendly python package



# Emcee Example

```
> cosmosis demos/demo5.ini
```

```
> postprocess demos/demo5.ini -o plots -p demo5
```



<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo5>

# Model Selection

- Given two models, how can we compare them?
- Simplest approach = compare ML
  - Does not include uncertainty or Occam's Razor
- Recall that all our probabilities have been conditional on the model, as in Bayes:

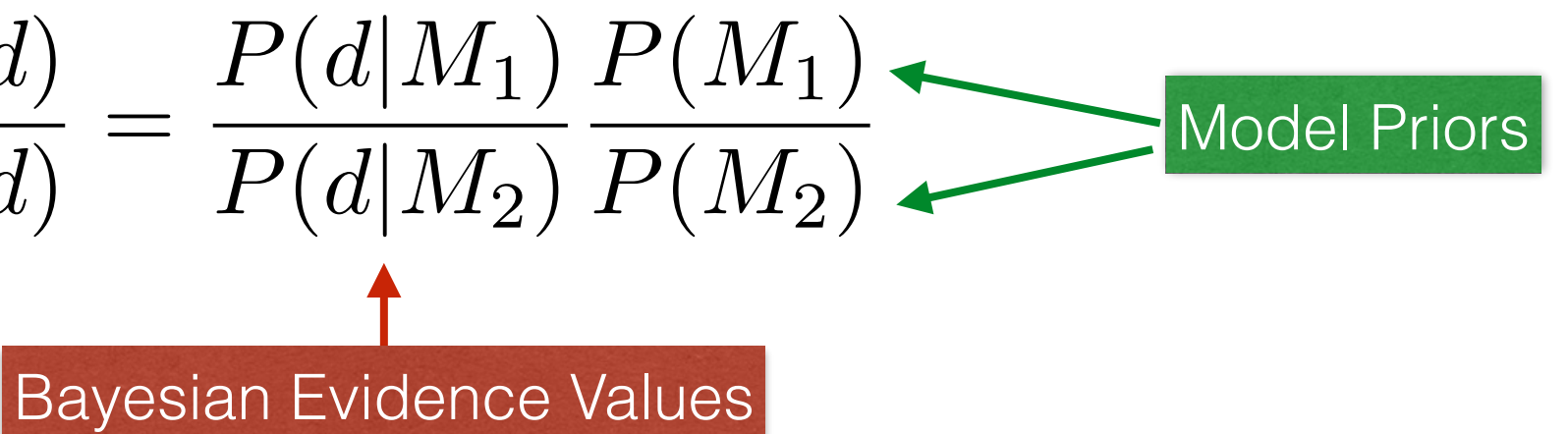
$$P(p|M) = \frac{P(d|pM)P(p|M)}{P(d|M)}$$

# Model Selection: Bayesian Evidence

- Can use Bayes Theorem again, on model level:

$$P(M|d) = \frac{P(d|M)P(M)}{P(d)}$$

- Only really meaningful when comparing models:

$$\frac{P(M_1|d)}{P(M_2|d)} = \frac{P(d|M_1)}{P(d|M_2)} \frac{P(M_1)}{P(M_2)}$$


Bayesian Evidence Values

Model Priors

# Model Selection: Bayesian Evidence

- Likelihood of parameters within model:

$$P(d|pM)$$

- Evidence of model:

$$P(d|p)$$

# Model Selection: Bayesian Evidence

- Evidence is the bit we ignored before when doing parameter estimation
- Given by an integral over prior space

$$P(d|M) = \int P(d|pM)P(p|M)dp$$

- Hard to evaluate - posterior usually small compared to prior



# Model Selection: Evidence Approximations

- Nice evidence approximations for some cases:
  - Savage-Dickey Density ratio  
(for when one model is a subset of another)
  - Akaike information criterion AIC  
Bayesian information criterion BIC  
Work in various circumstances

# Model Selection: Nested Sampling

$$\begin{aligned}\int L(\theta)p(\theta)d\theta &= \int L(X)dX \\ &\approx \sum L_i \delta X_i \\ dX &\equiv P(\theta)d\theta\end{aligned}$$

$X$  = remaining prior volume

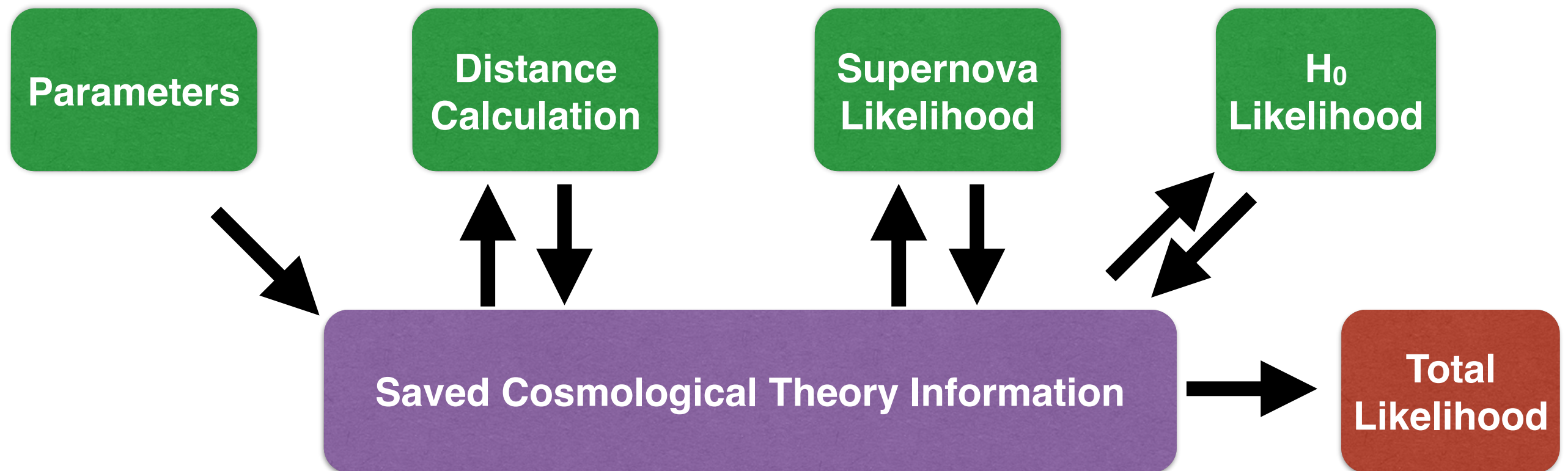
# Model Selection: Nested Sampling

- Also uses ensemble of live points
  - Computes constraints as well as evidence
- Each iteration, replace lowest likelihood point with one higher up
  - By cleverly sampling into envelope of active points
- Multinest software is extremely clever
  - C, F90, Python bindings

# Multineest Example

```
> cosmosis demos/demo9.ini
```

```
> postprocess -o plots -p demo9 demos/demo9.ini  
--extra demos/extra9.py
```



<https://bitbucket.org/joezuntz/cosmosis/wiki/Demo9>

# Exercise

- With a prior  $s \sim N(0.5, 0.1)$  and other priors of your choice, write a Metropolis Hastings sampler to draw from the LMC Cepheid likelihood. Plot 1D and 2D constraints on the parameters.