Probabilistic Programming *with*

PyMC3

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Probabilistic Programming

Stochastic language "primitives"

Distribution over values:

```
X ~ Normal(μ, σ)
x = X.random(n=100)
```

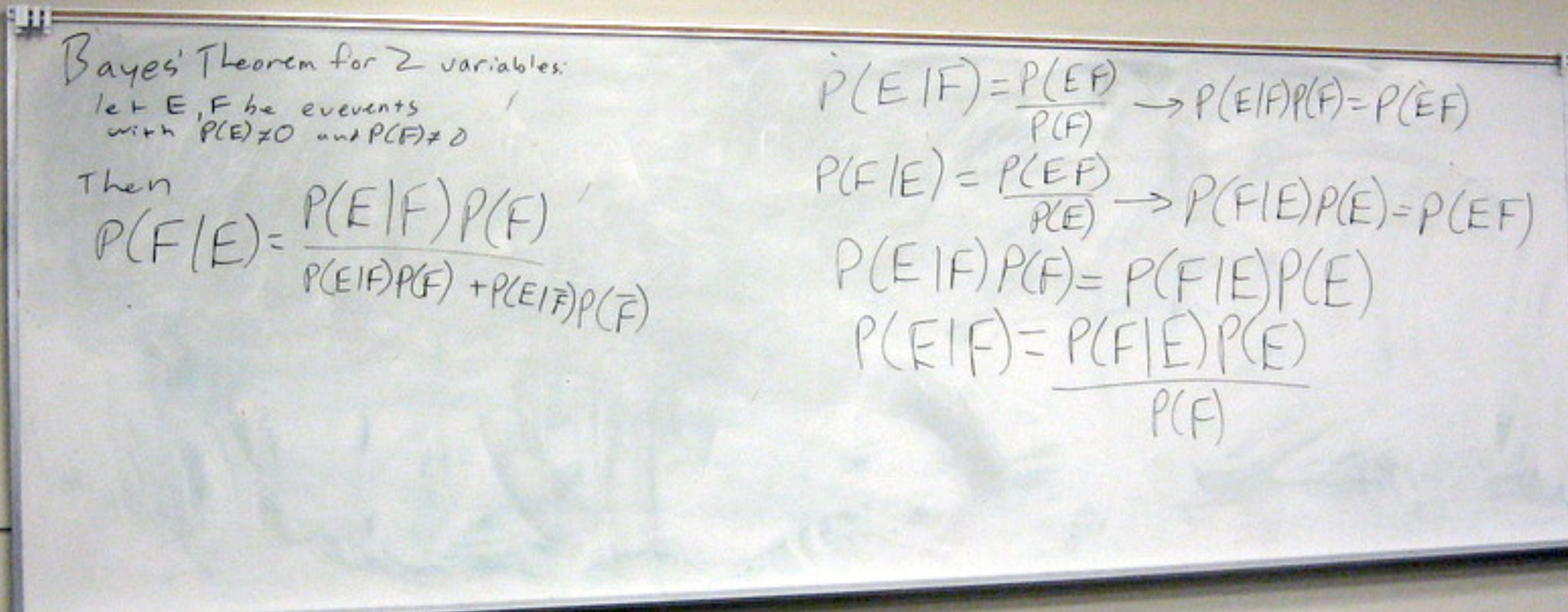
Distribution over functions:

```
Y ~ GaussianProcess(mean_func(x), cov_func(x))
y = Y.predict(x2)
```

Conditioning:

```
p ~ Beta(1, 1)
z ~ Bernoulli(p) # z|p
```

Bayesian Inference



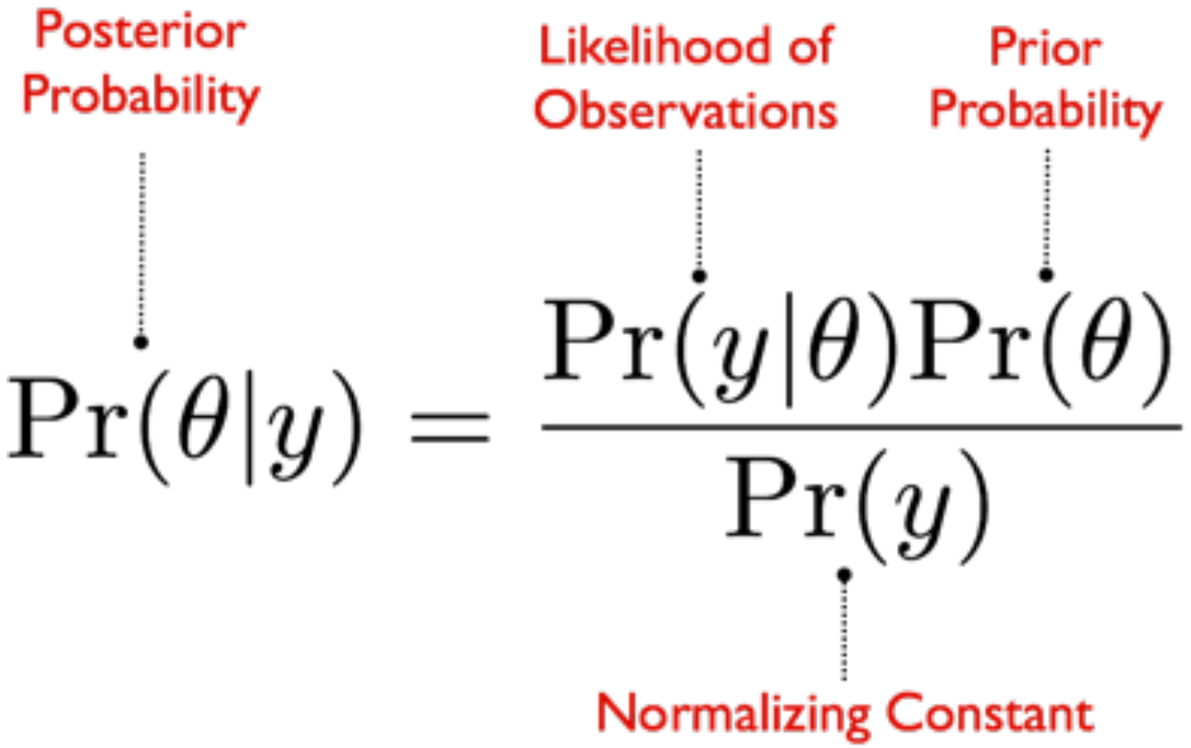
Inverse Probability

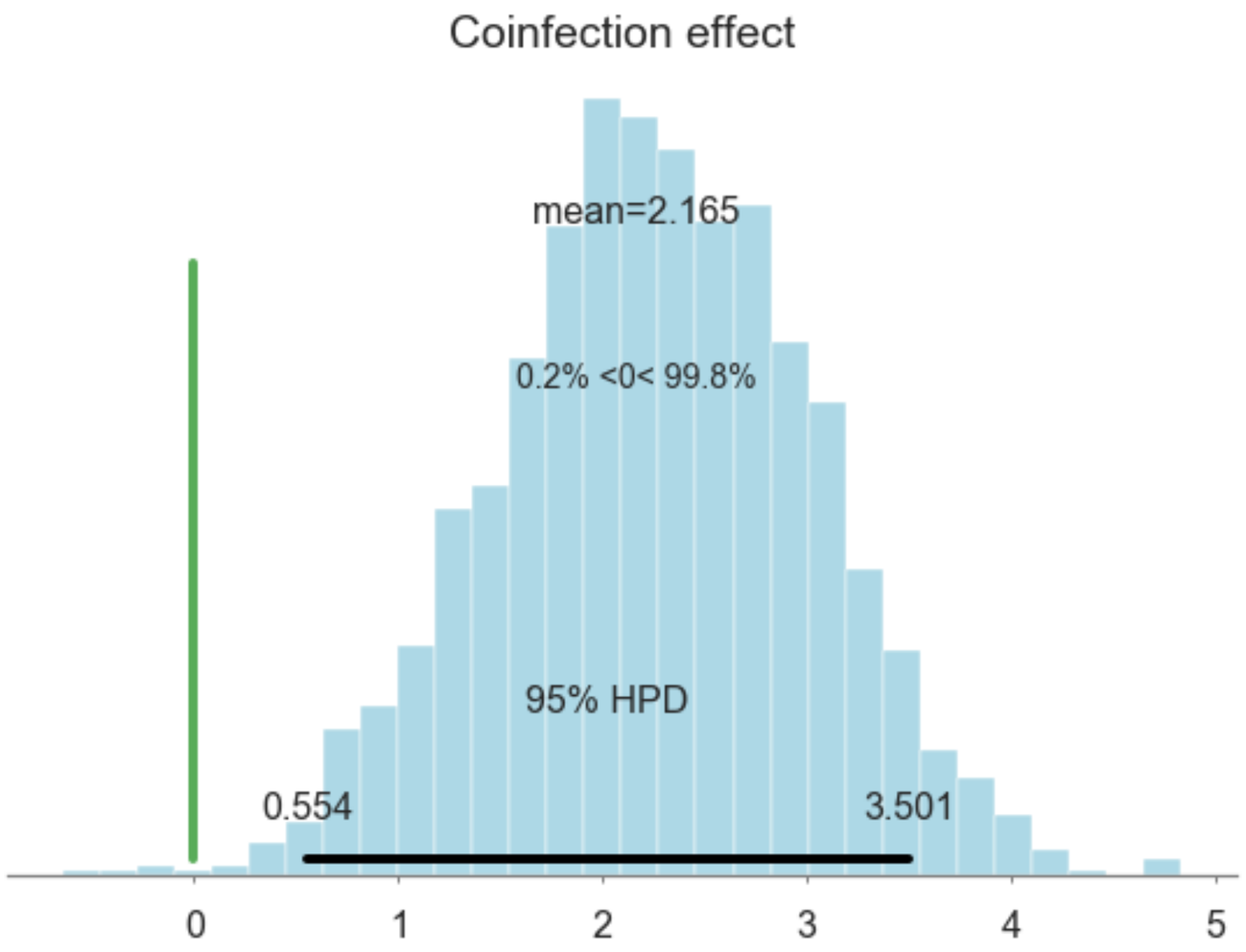
$$Pr(\theta|y)$$

Why Bayes?

“The Bayesian approach is attractive because it is **useful**. Its usefulness derives in large measure from its simplicity. Its simplicity allows the investigation of **far more complex models** than can be handled by the tools in the classical toolbox.”

—Link and Barker 2010


Posterior Probability
Likelihood of Observations
Prior Probability
$\Pr(\theta|y) = \frac{\Pr(y|\theta)\Pr(\theta)}{\Pr(y)}$
Normalizing Constant


Coinfection effect
mean=2.165
0.2% <0< 99.8%
95% HPD
0.554
3.501
0
1
2
3
4
5

Probabilistic Programming

in three easy steps

Encode a Probability Model⚐

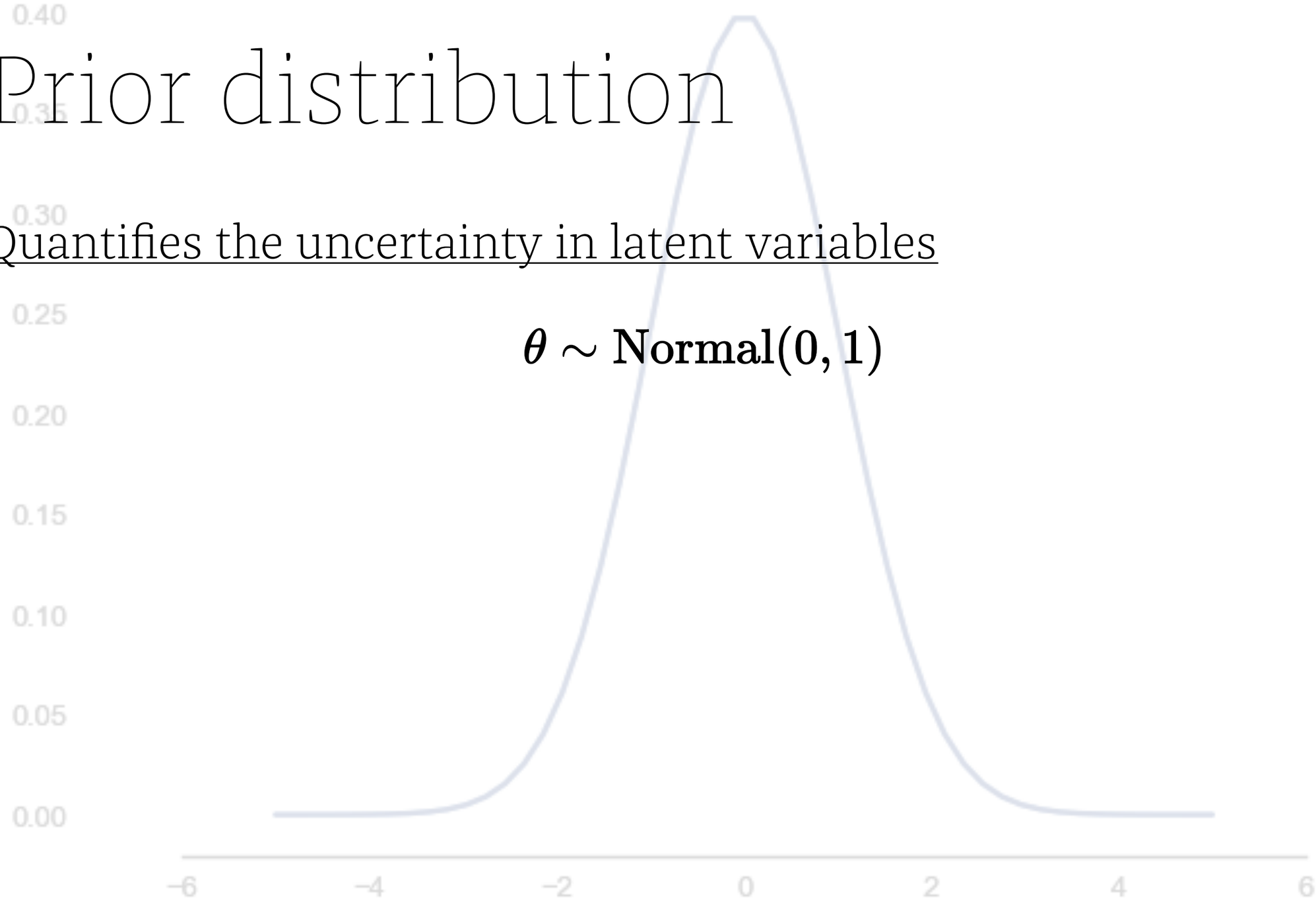
1

⚐ in Python

Prior distribution

Quantifies the uncertainty in latent variables

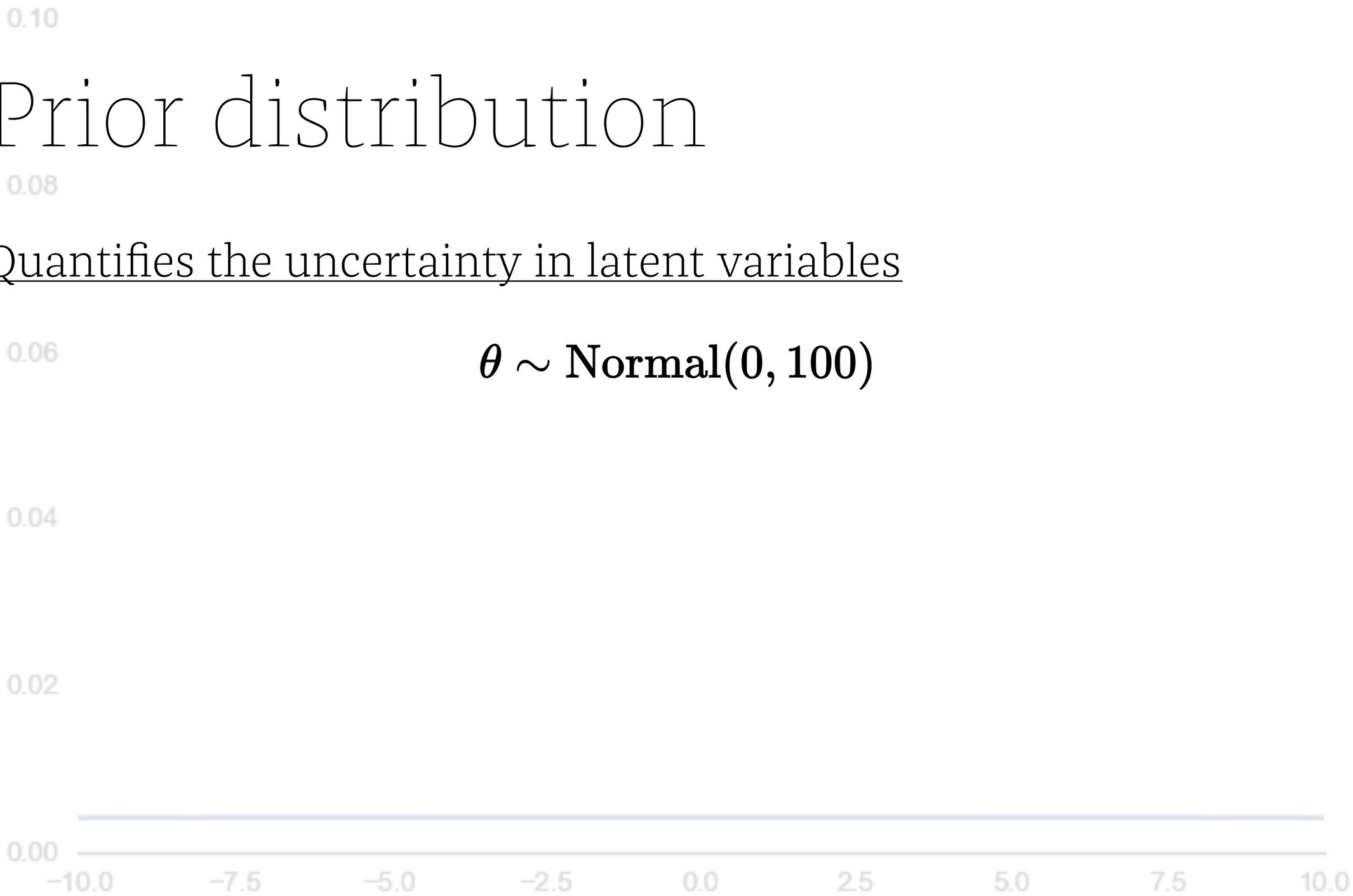
$$\theta \sim \mathbf{Normal}(0, 1)$$



Prior distribution

Quantifies the uncertainty in latent variables

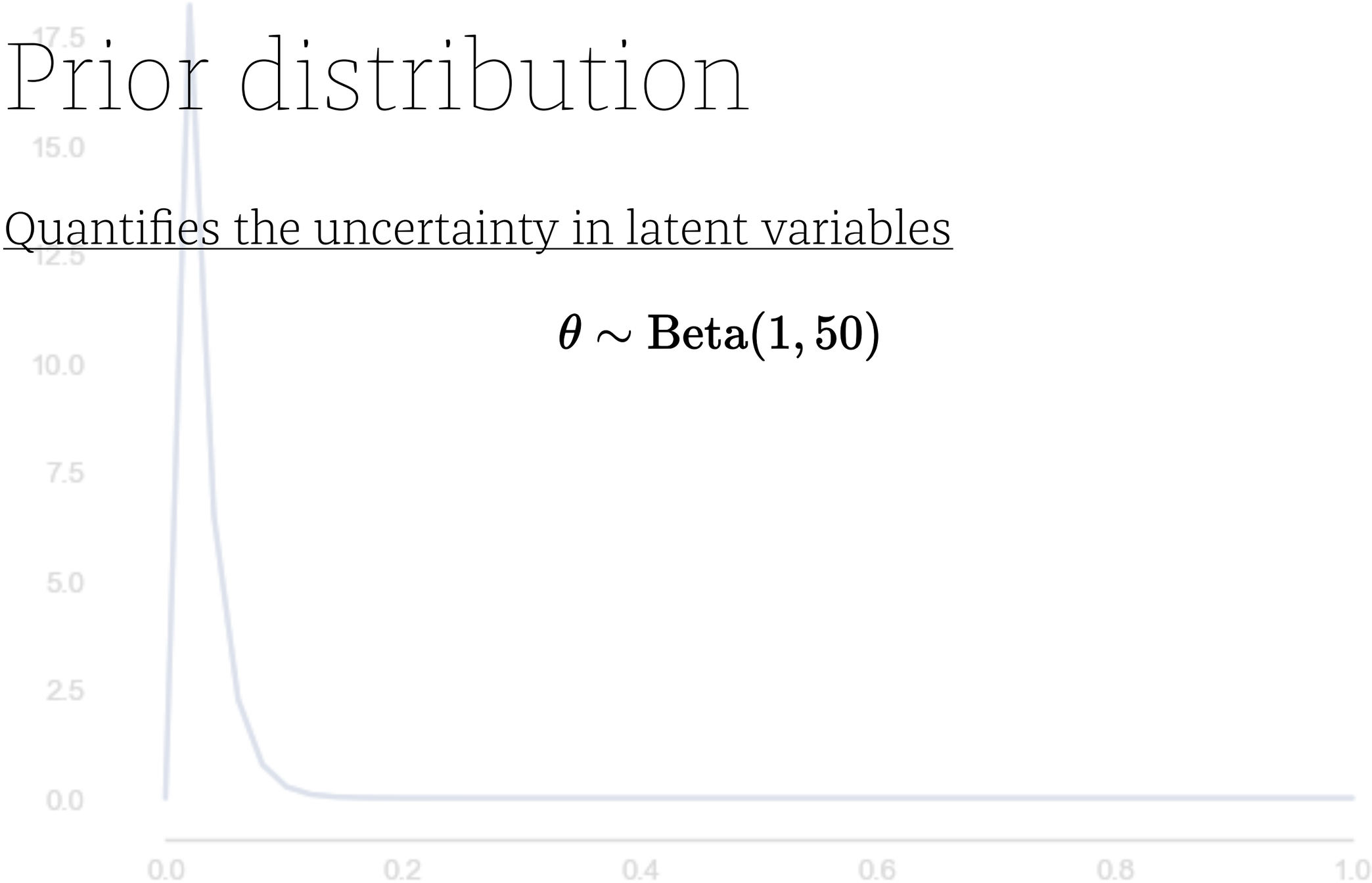
$$\theta \sim \mathbf{Normal}(0, 100)$$



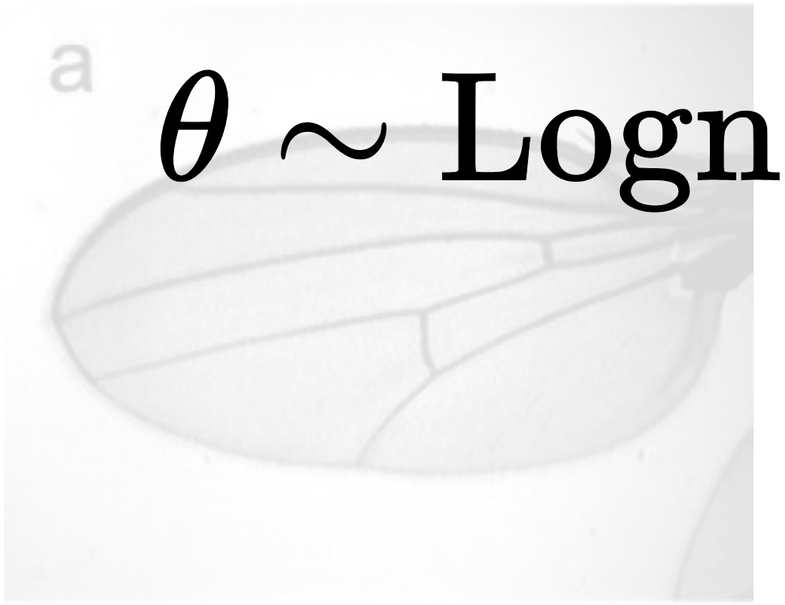
Prior distribution

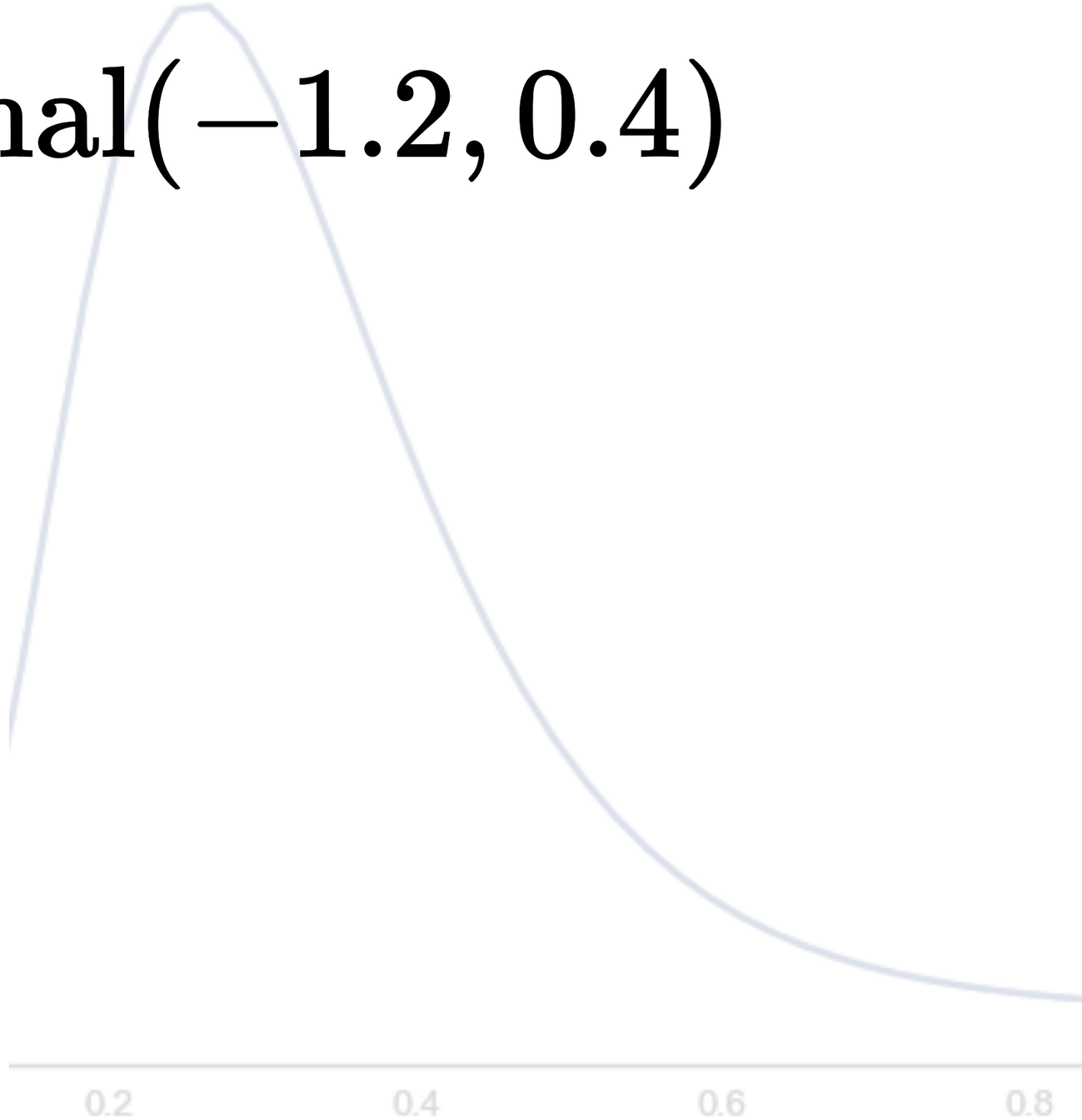
Quantifies the uncertainty in latent variables

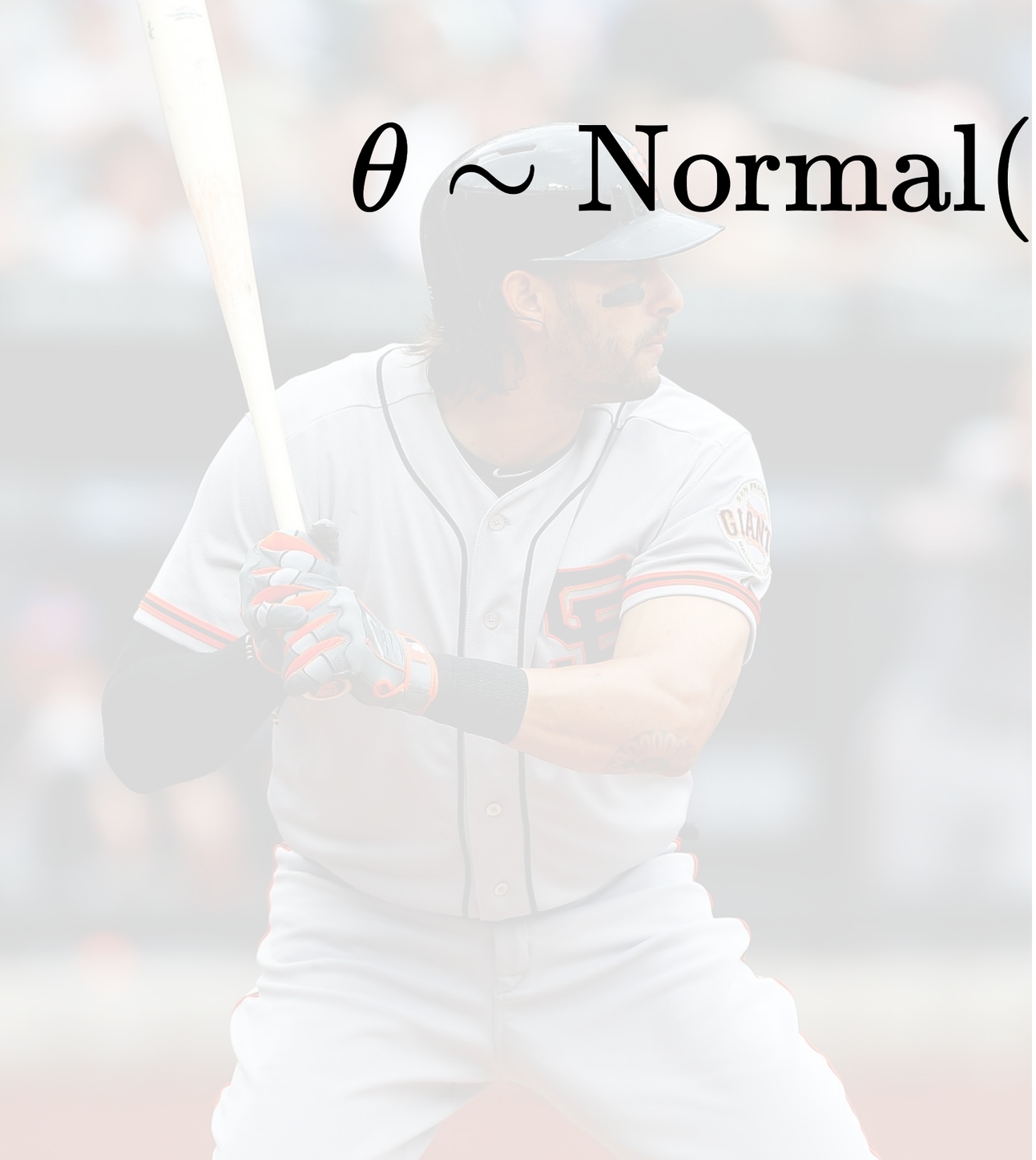
$$\theta \sim \mathbf{Beta}(1, 50)$$



$$\theta \sim \text{Lognormal}(-1.2, 0.4)$$







$$\theta \sim \text{Normal}(0.261, 0.034)$$

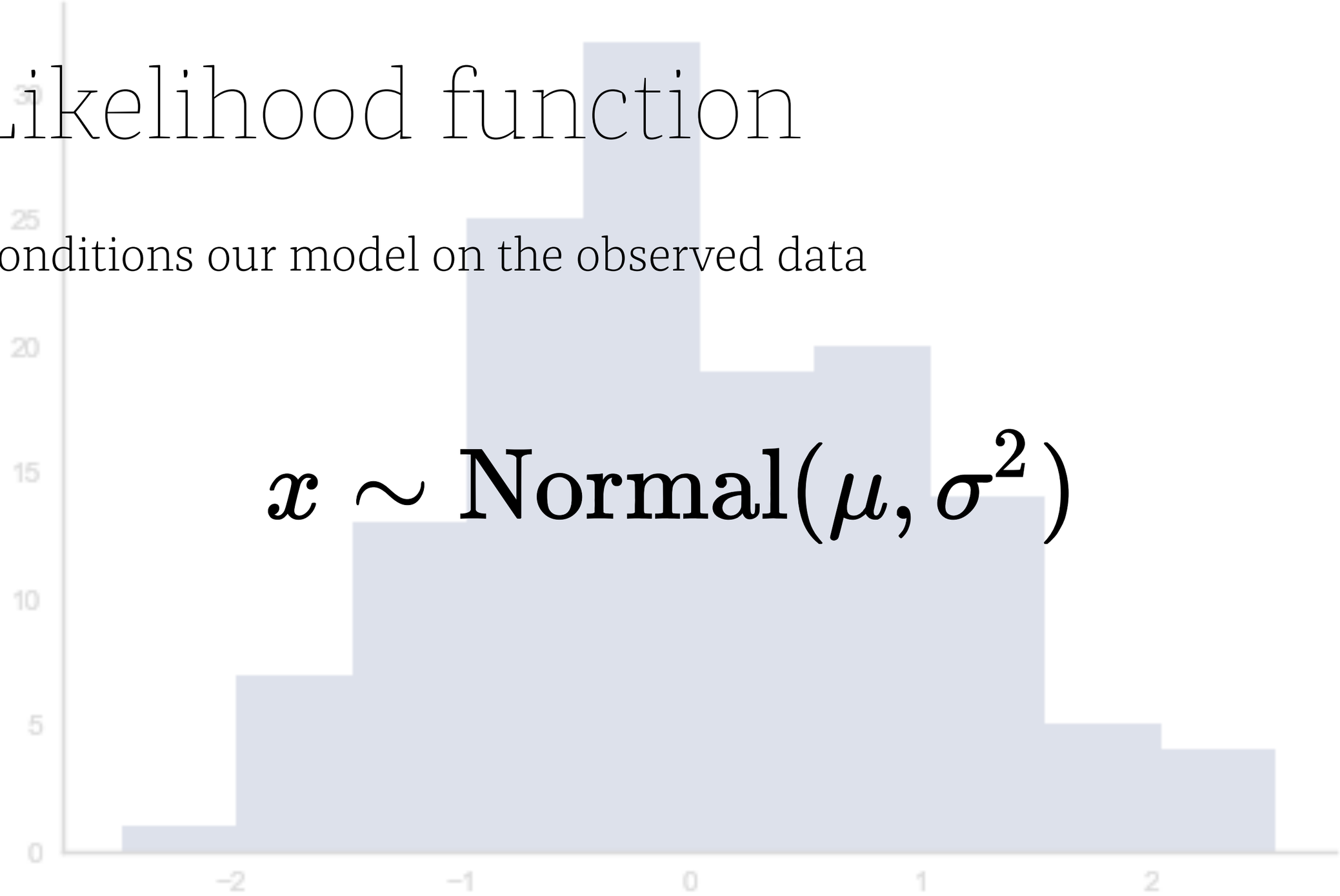
Likelihood function

Conditions our model on the observed data

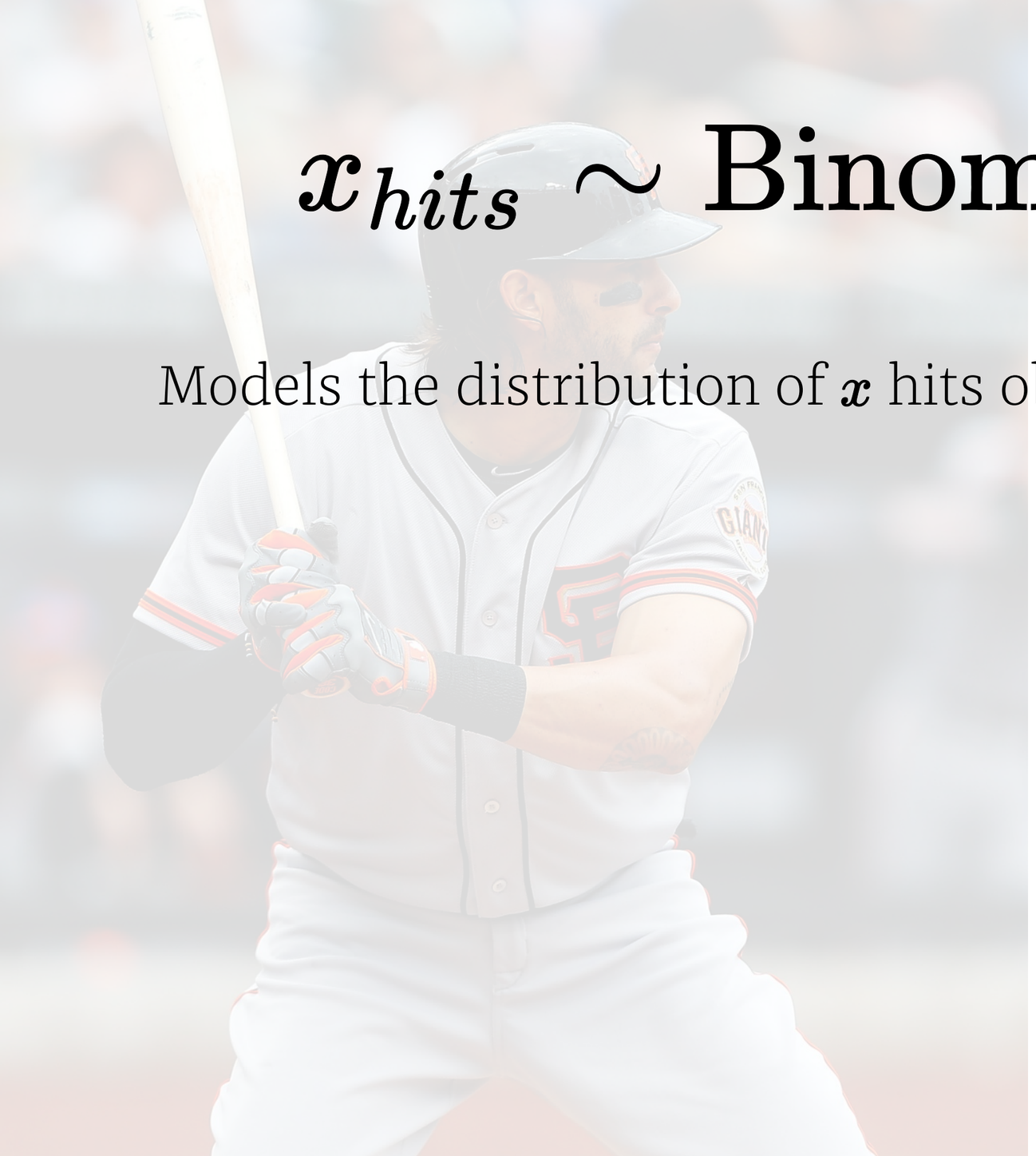
$$Pr(y|\theta)$$

Likelihood function

Conditions our model on the observed data

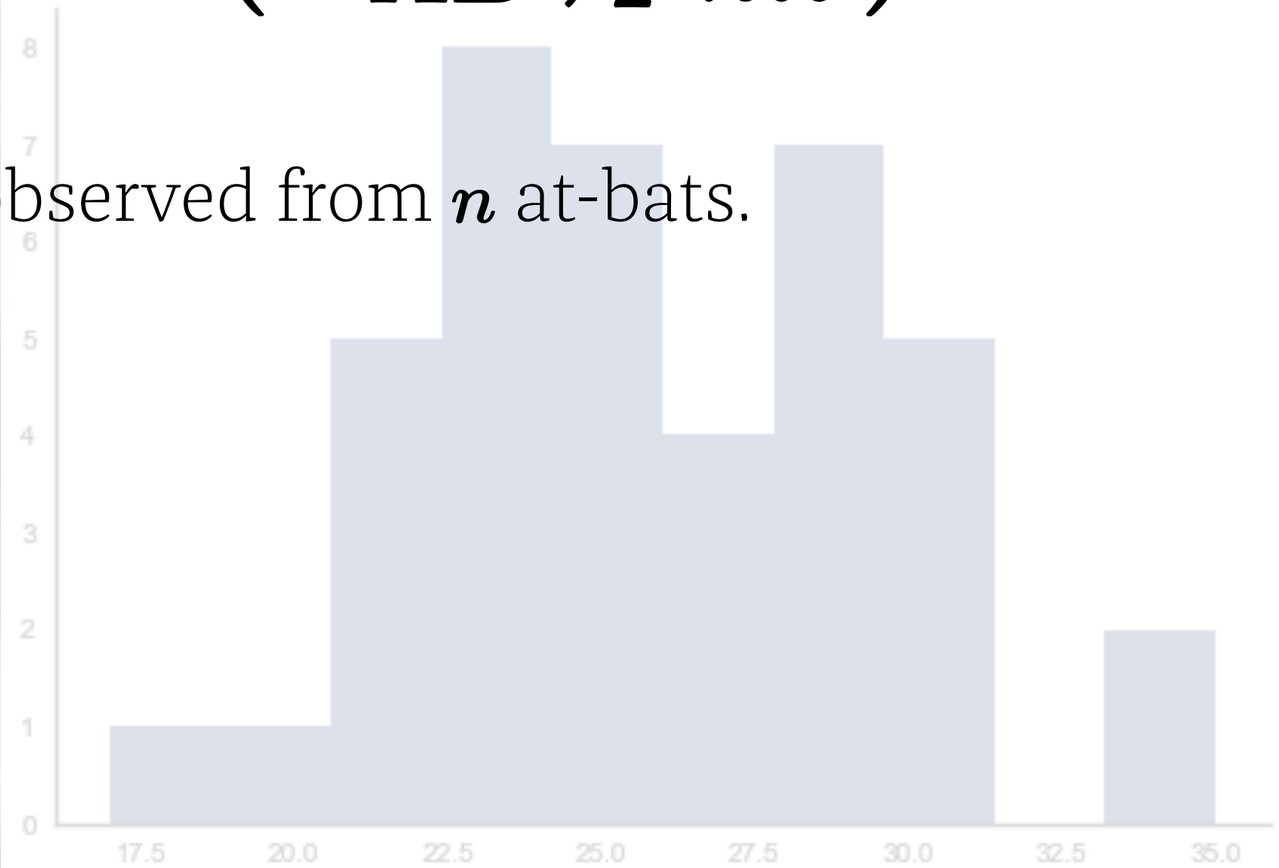


$$x \sim \mathbf{Normal}(\mu, \sigma^2)$$



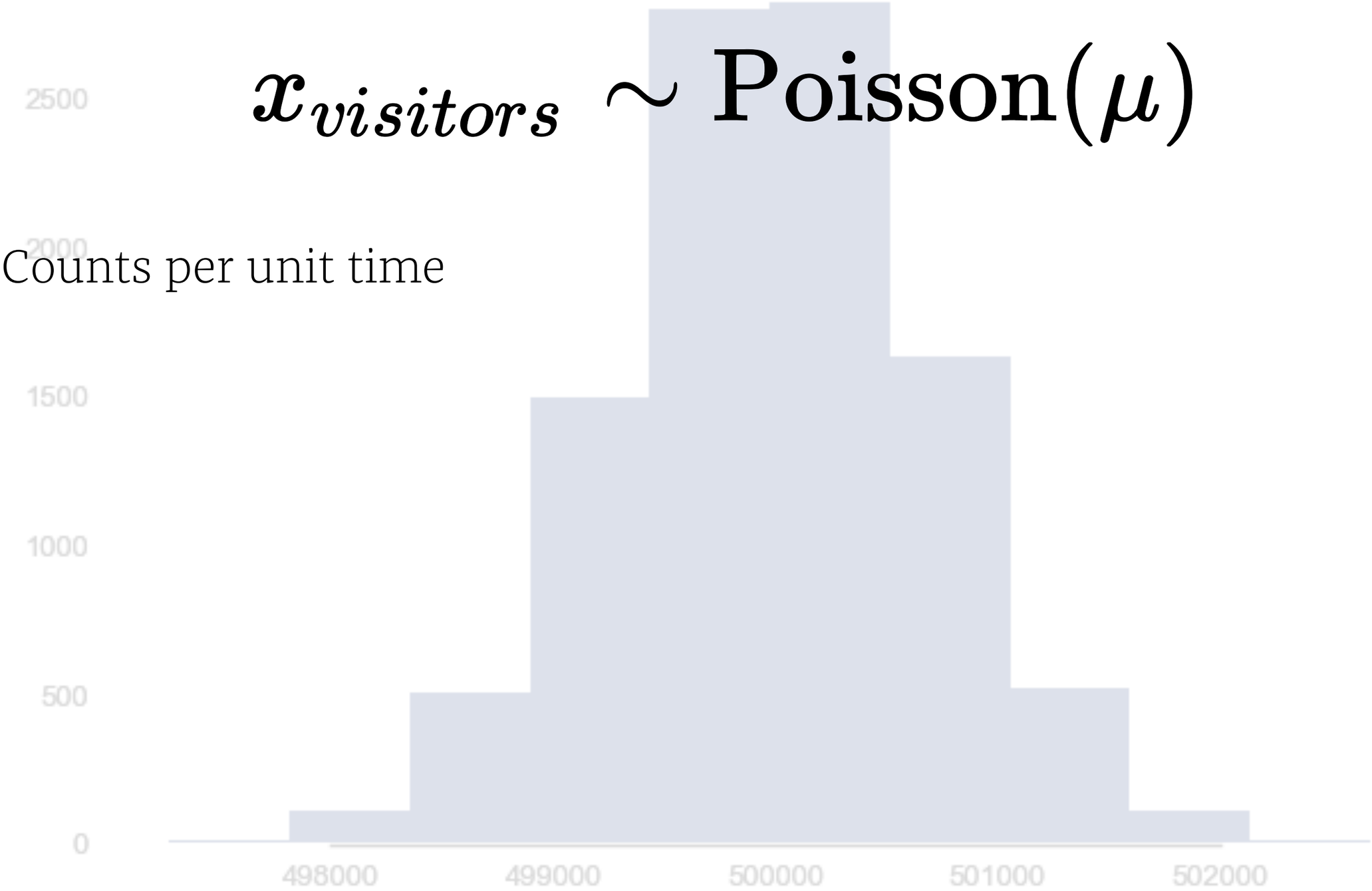
$$x_{hits} \sim \text{Binomial}(n_{AB}, p_{hit})$$

Models the distribution of x hits observed from n at-bats.



$$x_{visitors} \sim \text{Poisson}(\mu)$$

Counts per unit time



Infer Values

for latent variables

2

Posterior distribution

$$Pr(\theta|y) \propto Pr(y|\theta)Pr(\theta)$$

Posterior distribution

$$Pr(\theta|y) = \frac{Pr(y|\theta)Pr(\theta)}{Pr(y)}$$

Posterior distribution

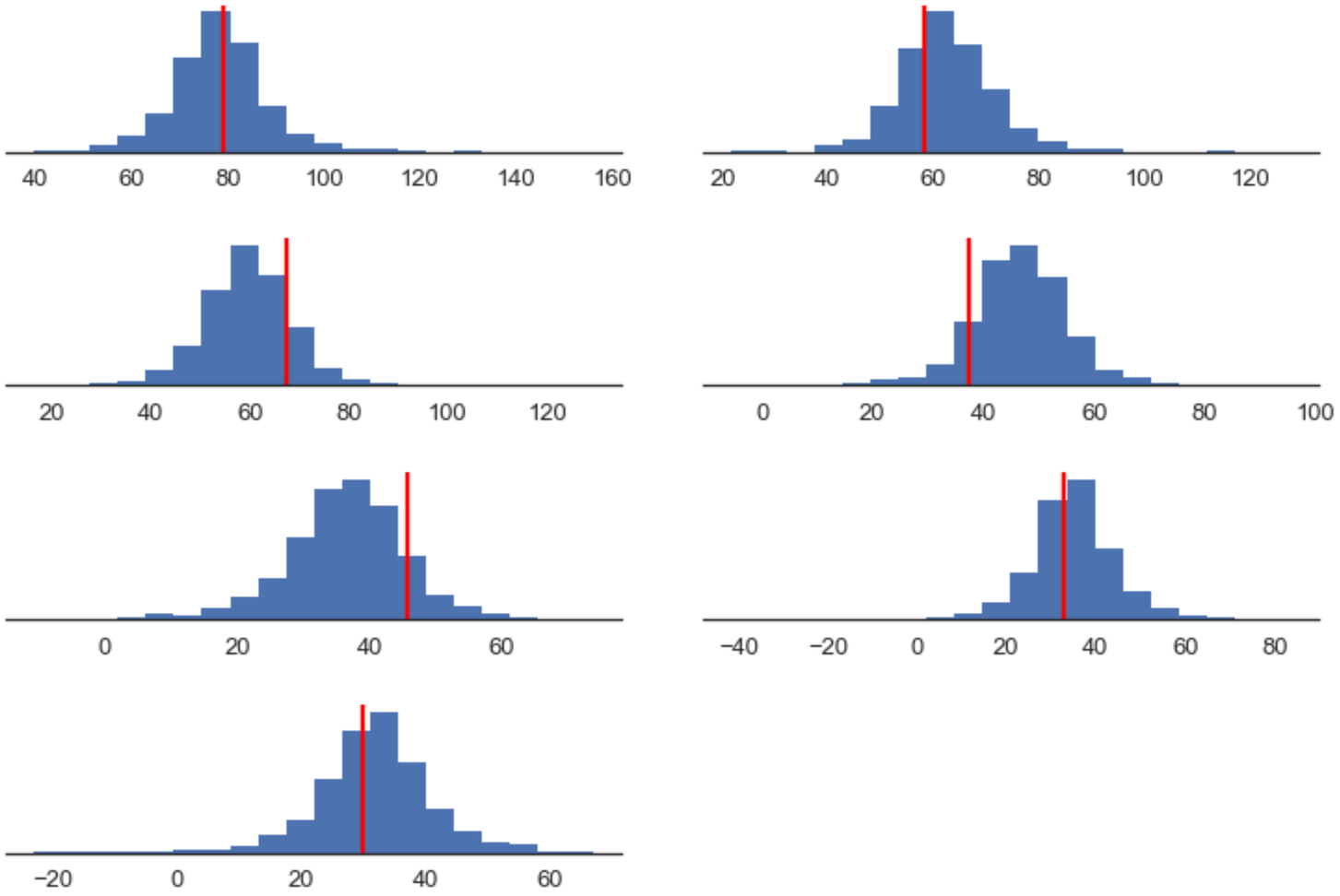
$$Pr(\theta|y) = \frac{Pr(y|\theta)Pr(\theta)}{\int_\theta Pr(y|\theta)Pr(\theta)d\theta}$$

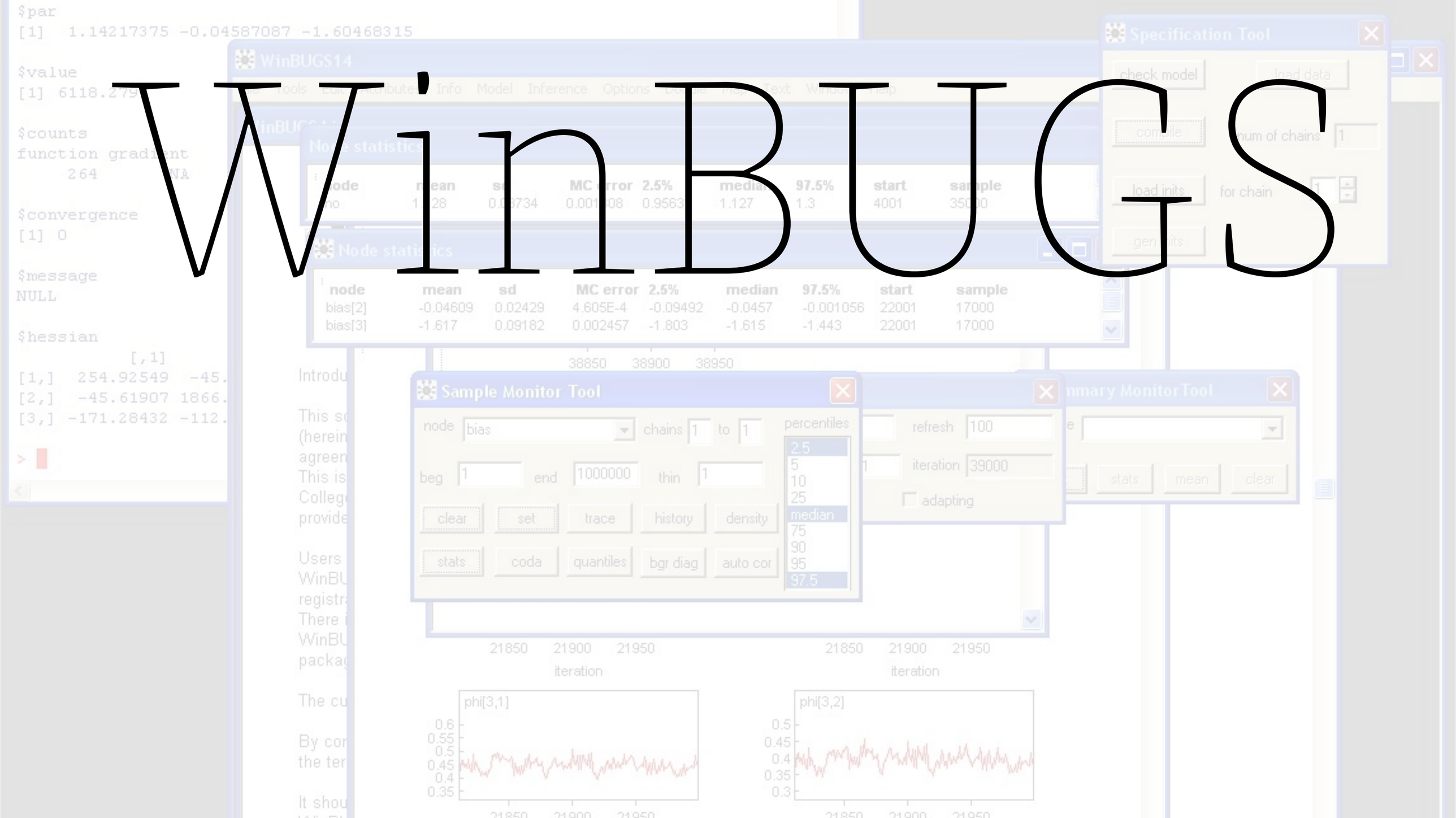
Probabilistic programming **abstracts** the inference procedure

Check your Model

3

Model checking




WinBUGS
$par
[1] 1.14217375 -0.04587087 -1.60468315
$value
[1] 6118.279
$counts
function gradient
264 NA
$convergence
[1] 0
$message
NULL
$hessian
[,1]
[1,] 254.92549 -45.
[2,] -45.61907 1866.
[3,] -171.28432 -112.
WinBUGS14
Specification Tool
check model
load data
compile
num of chains 1
load inits
for chain 1
gen inits
Node statistics
node mean sd MC error 2.5% median 97.5% start sample
bias[2] -0.04609 0.02429 4.605E-4 -0.09492 -0.0457 -0.001056 22001 17000
bias[3] -1.617 0.09182 0.002457 -1.803 -1.615 -1.443 22001 17000
Sample Monitor Tool
node bias
chains 1 to 1
beg 1
end 1000000
thin 1
percentiles
2.5
5
10
25
median
75
90
95
97.5
clear
set
trace
history
density
stats
coda
quantiles
bgr diag
auto cor
refresh 100
iteration 39000
adapting
stats
mean
clear
38850 38900 38950
21850 21900 21950
iteration
phi[3,1]
phi[3,2]
0.6
0.55
0.5
0.45
0.4
0.35
0.3

```
$par
[1]  1.14217375 -0.04587087 -1.60468315

$value
[1] 6118.279

$counts
function gradient
     264       NA

$convergence
[1] 0

$message
NULL

$hessian
           [,1]
[1,]  254.92549  -45.
[2,]  -45.61907 1866.
[3,] -171.28432 -112.

>
```

WinBUGS14

File Tools Edit Attributes Info Model Inference Options Doodle Map Text Window Help

Node statistics

node	mean	sd	MC error	2.5%	median	97.5%	start	sample
rho	1.128	0.08734	0.001308	0.9563	1.127	1.3	4001	35000

Node statistics

node	mean	sd	MC error	2.5%	median	97.5%	start	sample
bias[2]	-0.04609	0.02429	4.605E-4	-0.09492	-0.0457	-0.001056	22001	17000
bias[3]	-1.617	0.09182	0.002457	-1.803	-1.615	-1.443	22001	17000

Specification Tool

check model | load data | compile | num of chains 1 | load inits | for chain 1 | gen inits

Sample Monitor Tool

node bias | chains 1 to 1 | beg 1 | end 1000000 | thin 1

clear | set | trace | history | density | stats | coda | quantiles | bgr diag | auto cor

percentiles: 2.5, 5, 10, 25, median, 75, 90, 95, 97.5

refresh 100 | iteration 39000 | adapting

stats | mean | clear

38850 38900 38950

21850 21900 21950 iteration

21850 21900 21950 iteration

phi[3,1]

0.6 0.55 0.5 0.45 0.4 0.35

phi[3,2]

0.5 0.45 0.4 0.35 0.3

Introdu

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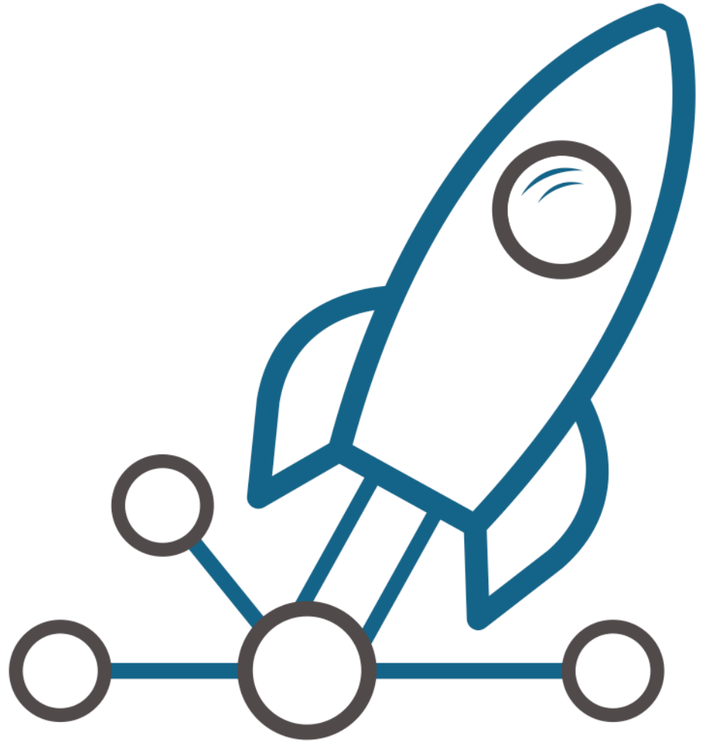
```
model {
      for (j in 1:J){
        y[j] ~ dnorm (theta[j], tau.y[j])
        theta[j] ~ dnorm (mu.theta, tau.theta)
        tau.y[j] <- pow(sigma.y[j], -2)
      }
      mu.theta ~ dnorm (0.0, 1.0E-6)
      tau.theta <- pow(sigma.theta, -2)
      sigma.theta ~ dunif (0, 1000)
    }
```

PyMC3

- ☞ started in 2003
- ☞ PP framework for fitting arbitrary probability models
- ☞ based on Theano
- ☞ implements "next generation" Bayesian inference methods
- ☞ NumFOCUS sponsored project 🎉👯



github.com/pymc-devs/pymc3

Calculating Gradients in Theano

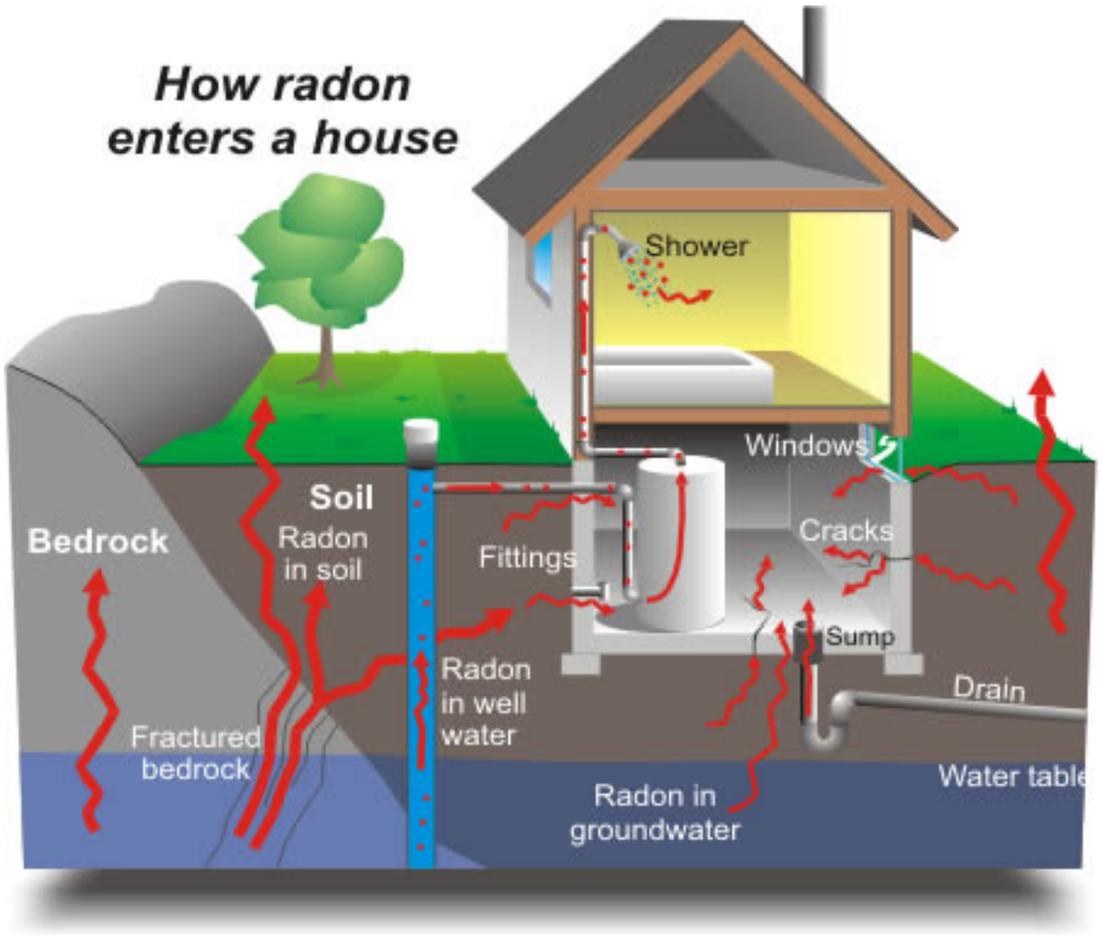
```
>>> from theano import function, tensor as tt
>>> x = tt.dmatrix('x')
>>> s = tt.sum(1 / (1 + tt.exp(-x)))
>>> gs = tt.grad(s, x)
>>> dlogistic = function([x], gs)
>>> dlogistic([[3, -1],[0, 2]])
array([[ 0.04517666,  0.19661193],
       [ 0.25      ,  0.10499359]])
```

Calculating Gradients in Theano

```
>>> from theano import function, tensor as tt
>>> x = tt.dmatrix('x')
>>> s = tt.sum(1 / (1 + tt.exp(-x)))
>>> gs = tt.grad(s, x)
>>> dlogistic = function([x], gs)
>>> dlogistic([[3, -1],[0, 2]])
array([[ 0.04517666,  0.19661193],
       [ 0.25      ,  0.10499359]])
```

Example: Radon exposure*

* Gelman et al. (2013) Bayesian Data Analysis


How radon enters a house
Shower
Windows
Soil
Radon in soil
Bedrock
Fittings
Cracks
Sump
Radon in well water
Drain
Fractured bedrock
Water table
Radon in groundwater

Unpooled model

Model radon in each county independently.

$$y_i = \alpha_{j[i]} + \beta x_i + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma)$$

where $j = 1, \ldots, 85$ (counties)

Priors

```
with Model() as unpooled_model:

    α = Normal('α', 0, sd=1e5, shape=counties)
    β = Normal('β', 0, sd=1e5)
    σ = HalfCauchy('σ', 5)
```

```
>>> type(β)
pymc3.model.FreeRV
```

```
>>> type(β)
pymc3.model.FreeRV
>>> β.distribution.logp(-2.1).eval()
array(-12.431863999839544)
```

```
>>> type(β)
pymc3.model.FreeRV
>>> β.distribution.logp(-2.1).eval()
array(-12.43186399839954)
>>> β.random(size=4)
array([ -10292.91760326,   22368.53416626,
         124851.2516102,   44143.62513182]])
```

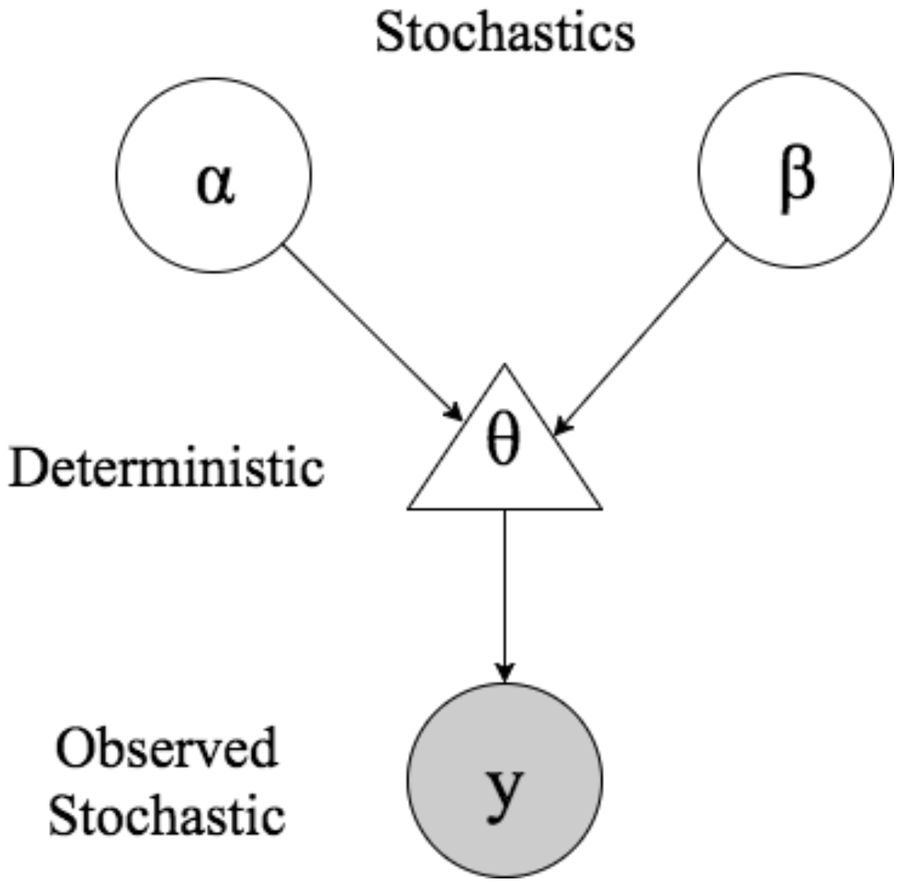
Transformed variables

```
with unpooled_model:

    θ = α[county] + β*floor
```

Likelihood

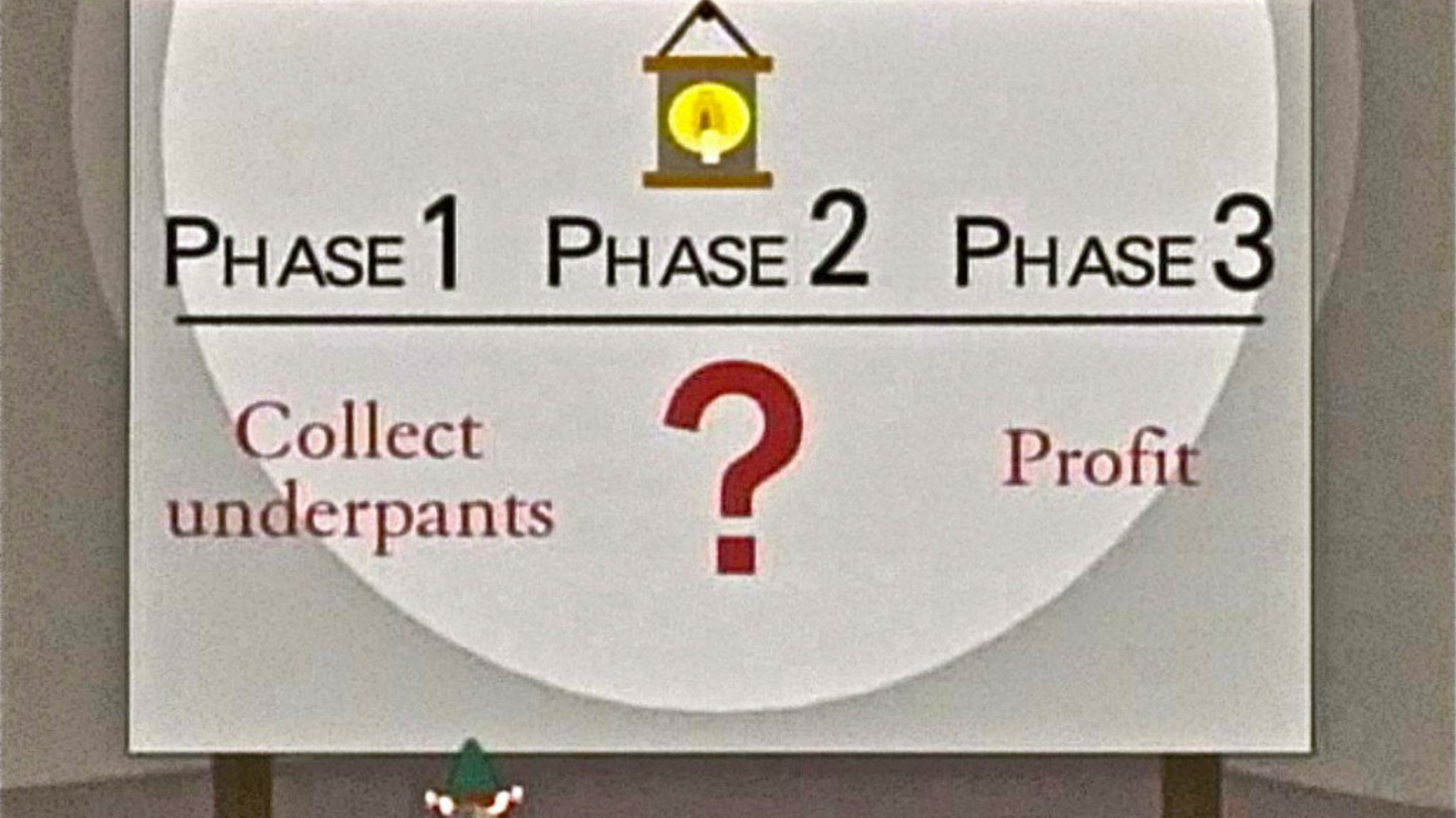
```
with unpooled_model:

    y = Normal('y', θ, sd=σ, observed=log_radon)
```

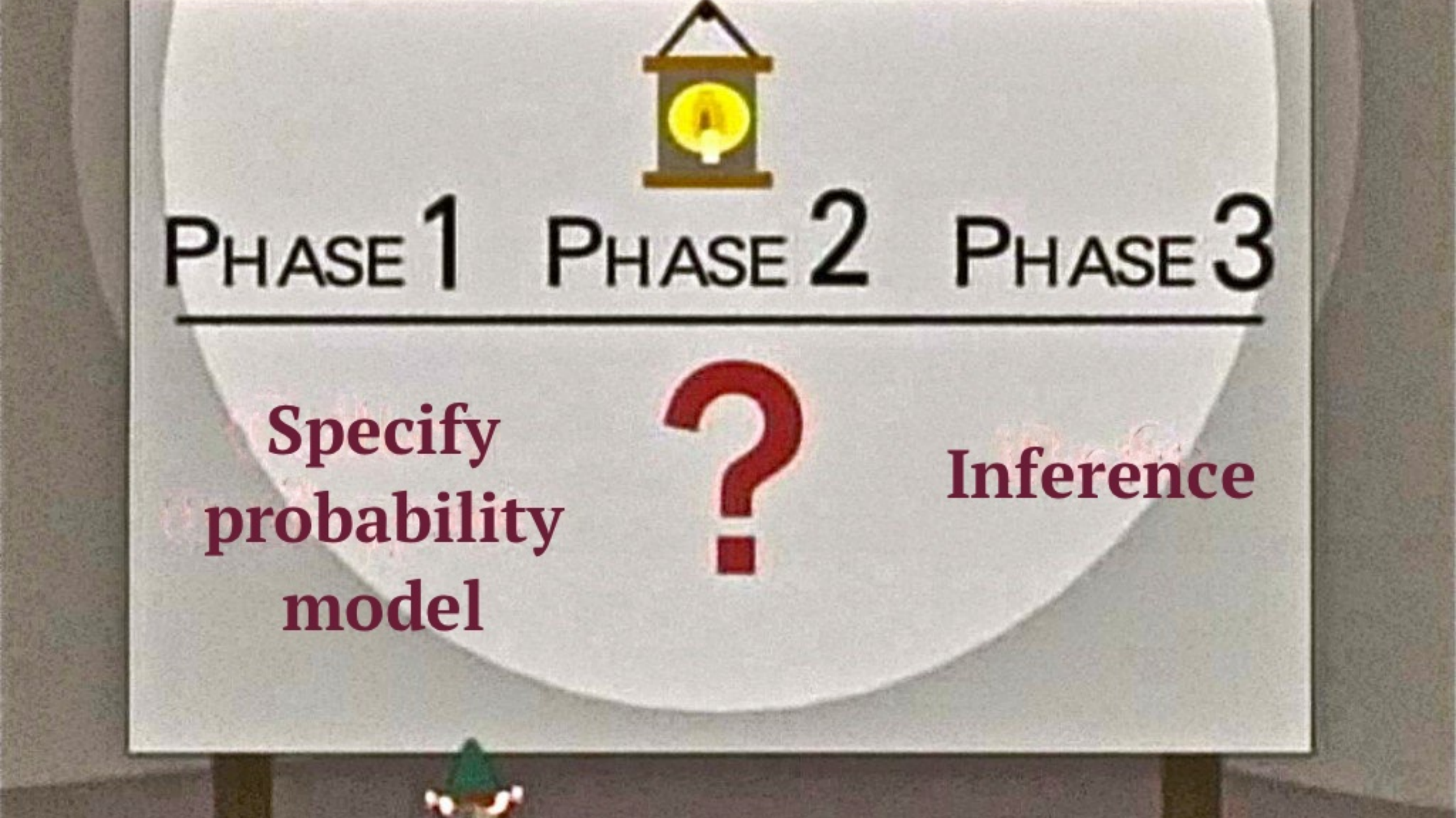
Model graph



Calculating Posteriors

$$Pr(\theta|y) \propto Pr(y|\theta)Pr(\theta)$$


PHASE 1
PHASE 2
PHASE 3
Collect underpants
?
Profit


PHASE 1
PHASE 2
PHASE 3
Specify probability model
?
Inference

Bayesian approximation

- ☞ Maximum a posteriori (MAP) estimate
- ☞ Laplace (normal) approximation
- ☞ Rejection sampling
- ☞ Importance sampling
- ☞ Sampling importance resampling (SIR)
- ☞ Approximate Bayesian Computing (ABC)

MCMC

Markov chain Monte Carlo simulates a **Markov chain** for which some function of interest is the **unique, invariant, limiting** distribution.

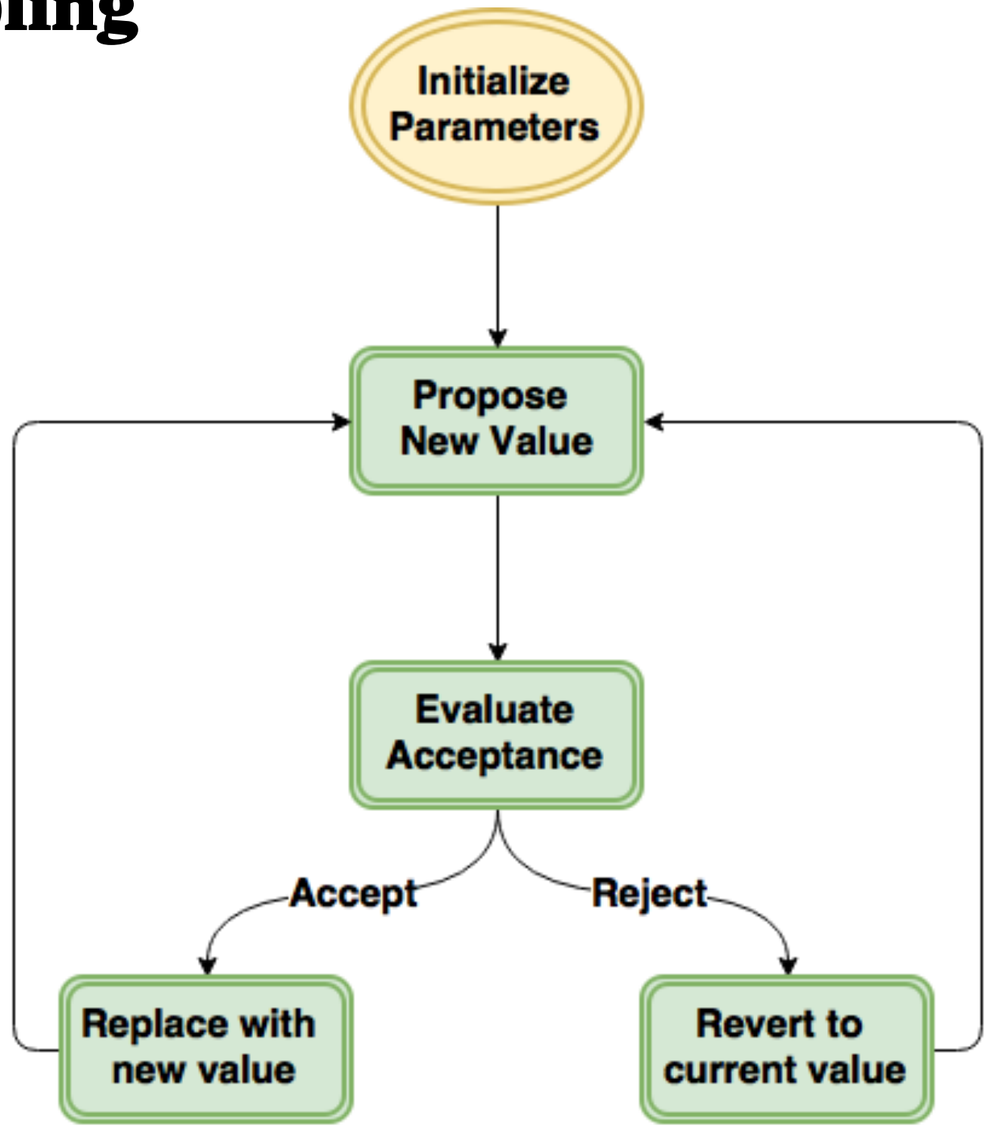
MCMC

Markov chain Monte Carlo simulates a **Markov chain** for which some function of interest is the **unique, invariant, limiting** distribution.

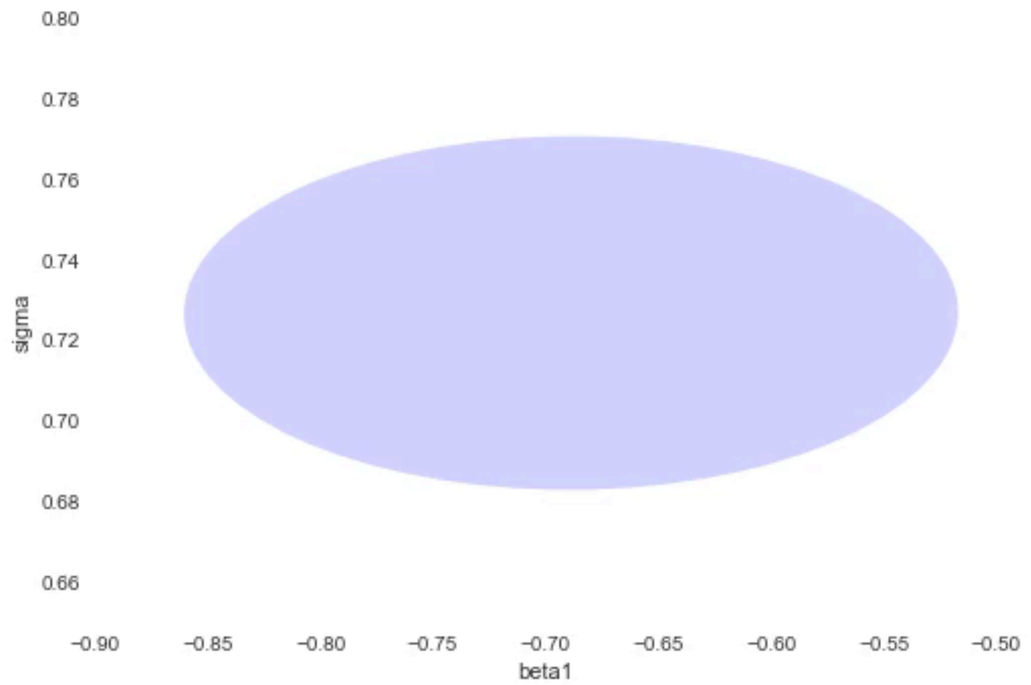
This is guaranteed when the Markov chain is constructed that satisfies the **detailed balance equation**:

$$\pi(x)Pr(y|x) = \pi(y)Pr(x|y)$$

Metropolis sampling



Metropolis sampling**



** 2000 iterations, 1000 tuning

Hamiltonian Monte Carlo

Uses a physical analogy of a frictionless particle moving on a hyper-surface

Requires an auxiliary variable to be specified

☞ position (unknown variable value)

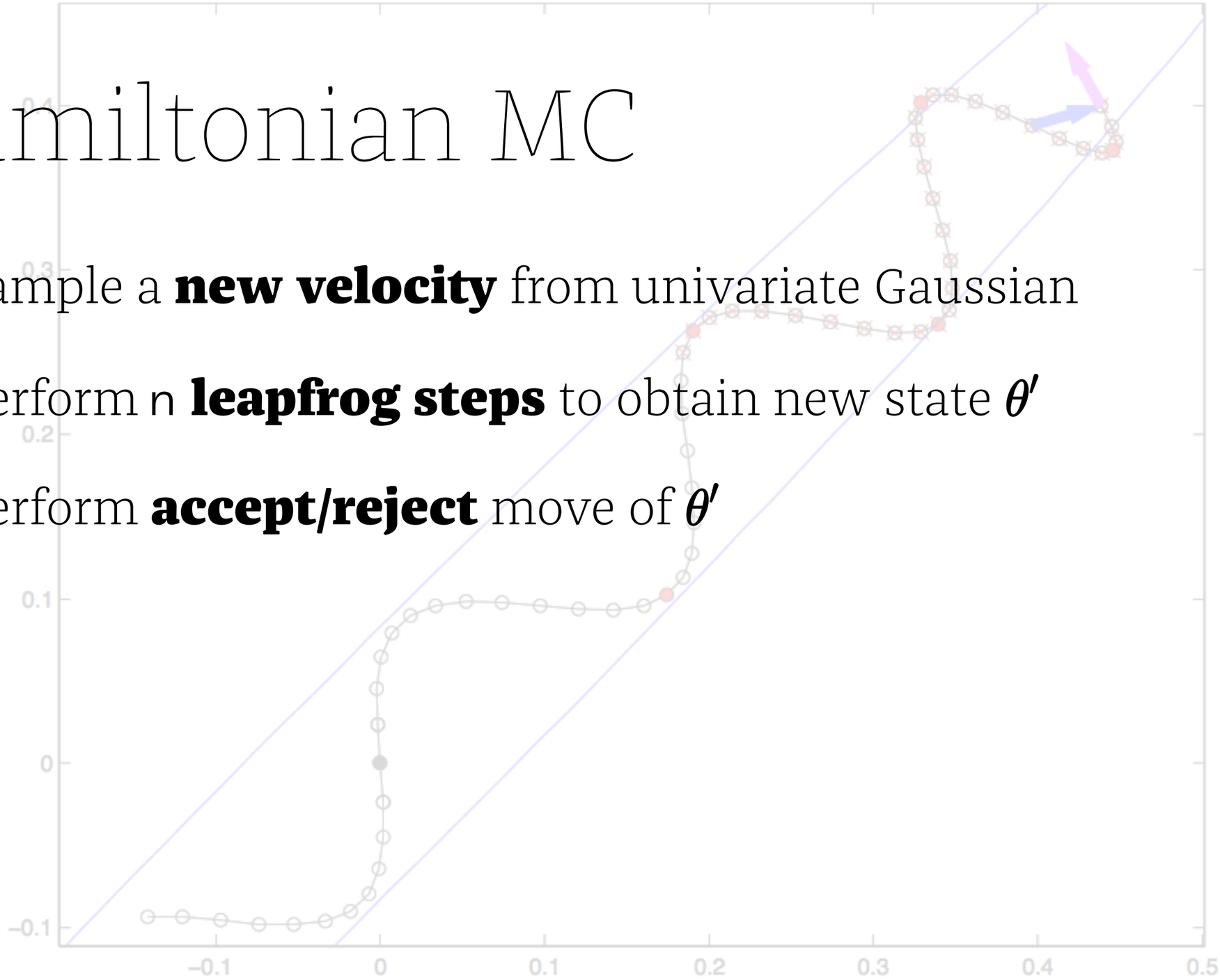
☞ momentum (auxiliary)

Hamiltonian MC

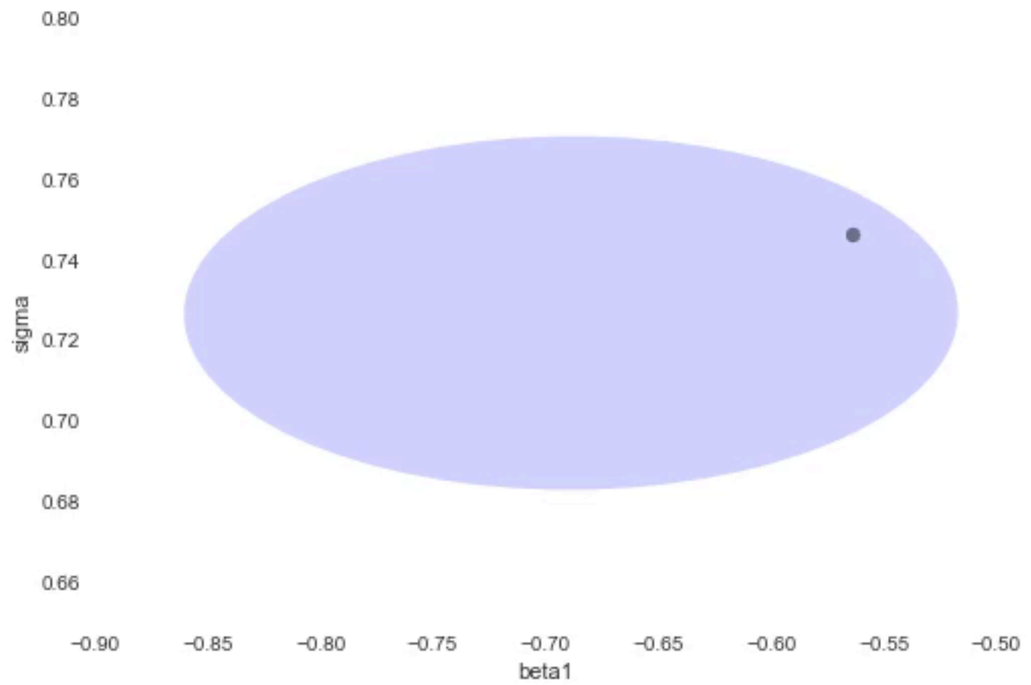
① Sample a **new velocity** from univariate Gaussian

② Perform n **leapfrog steps** to obtain new state θ'

③ Perform **accept/reject** move of θ'



Hamiltonian MC**



** 2000 iterations, 1000 tuning

No U-Turn Sampler (NUTS)

Hoffmann and Gelman (2014)

```
    sigma_y = HalfCauchy('sigma_y',5)

    # Expected value
    y_hat = a[county]

    # Data likelihood
    y_like = Normal('y_like', mu=y_hat, sd=sigma_y, observed=log_radon)
```

In [ ]:
```
with model:
    samples = sample(draws=1000, n_init=20000)
```

Start Recording

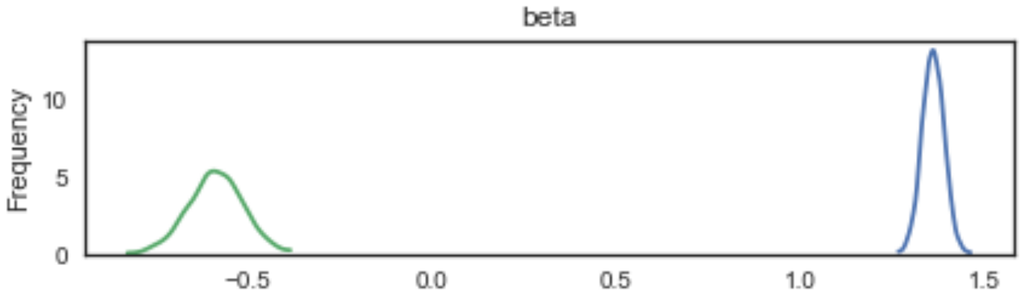
Varying intercept model

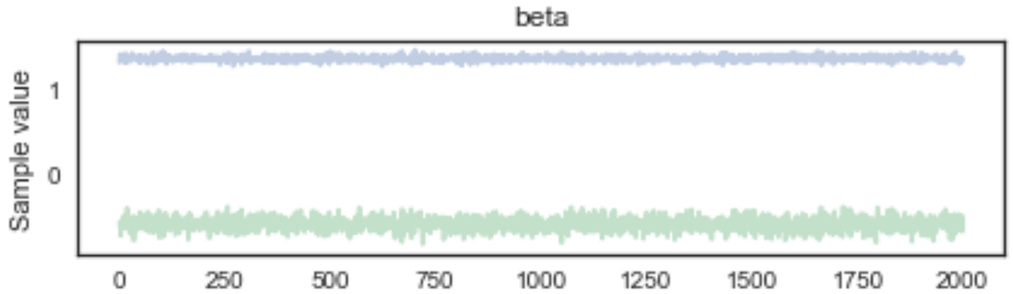
This model allows intercepts to vary across county, according to a random effect.

$$y_i = \alpha_{j[i]} + \beta x_i + \epsilon_i$$

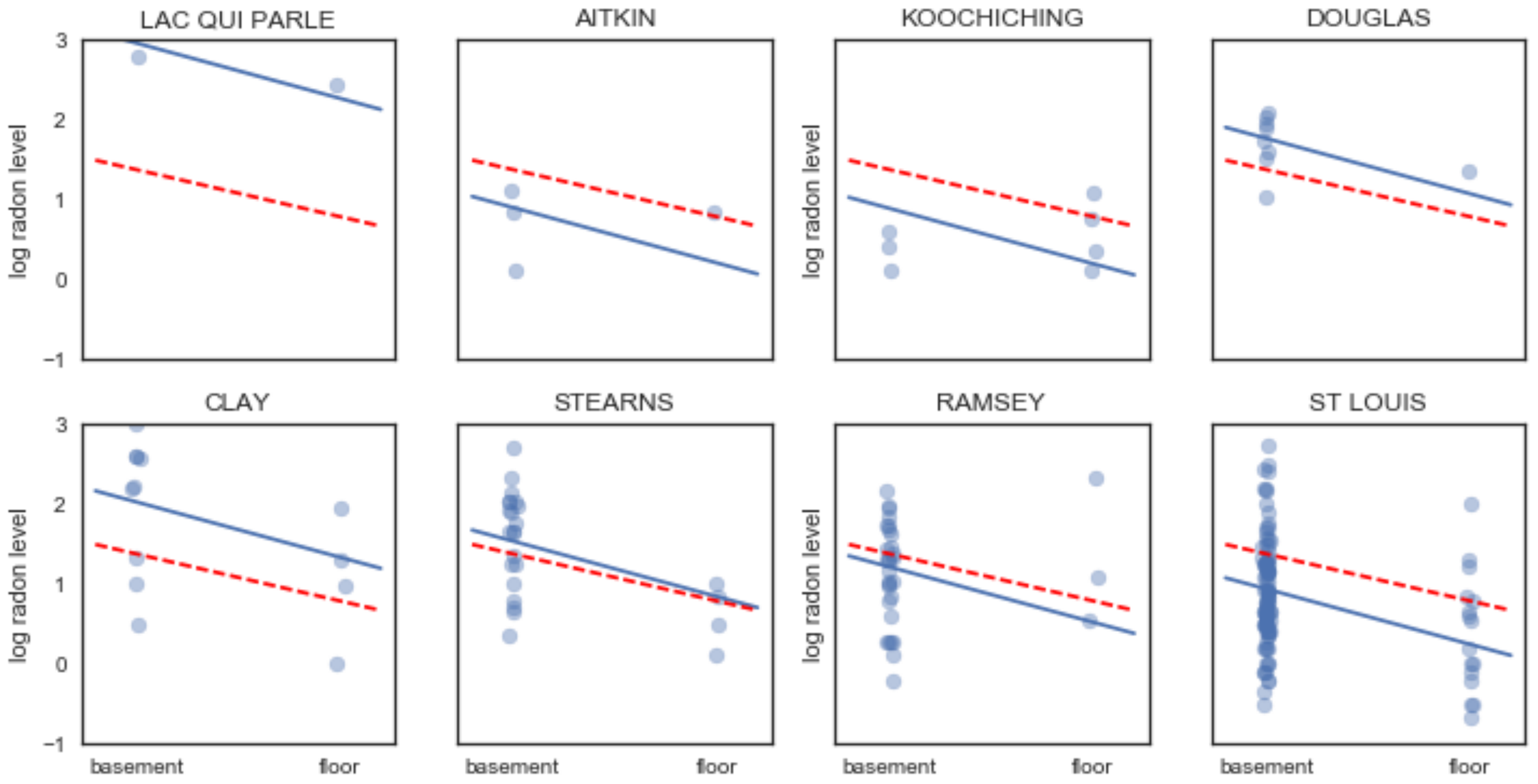
where

$$\epsilon_i \sim N(0, \sigma_y^2)$$

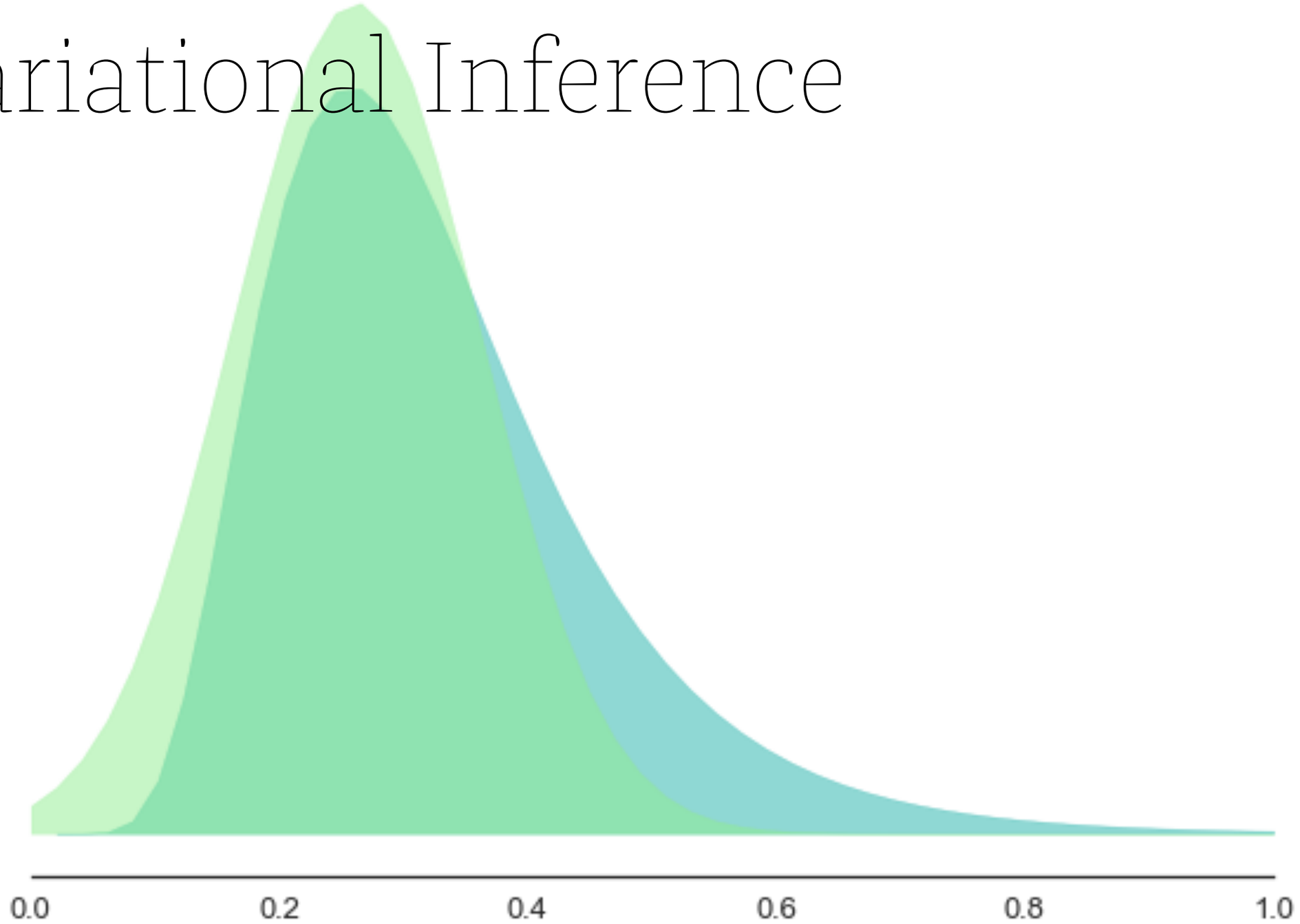




	mean	sd	mc_error	hpd_2.5	hpd_97.5
beta__0	1.362390	0.029348	0.000673	1.306512	1.420500
beta__1	-0.587654	0.073564	0.001590	-0.733906	-0.442381


LAC QUI PARLE
AITKIN
KOOCHICHING
DOUGLAS
CLAY
STEARNS
RAMSEY
ST LOUIS
log radon level
3
2
1
0
−1
basement
floor

Variational Inference



Variational Inference

Variational inference minimizes the **Kullback-Leibler divergence**

$$\mathbb{KL}(q(\theta) \parallel p(\theta \mid y)) = \int q(\theta, \phi) \frac{q(\theta, \phi)}{p(\theta|y)} d\theta$$

$$\Rightarrow \mathbb{E}_q \left(\log \left(\frac{q(\theta)}{p(\theta \mid y)} \right) \right)$$

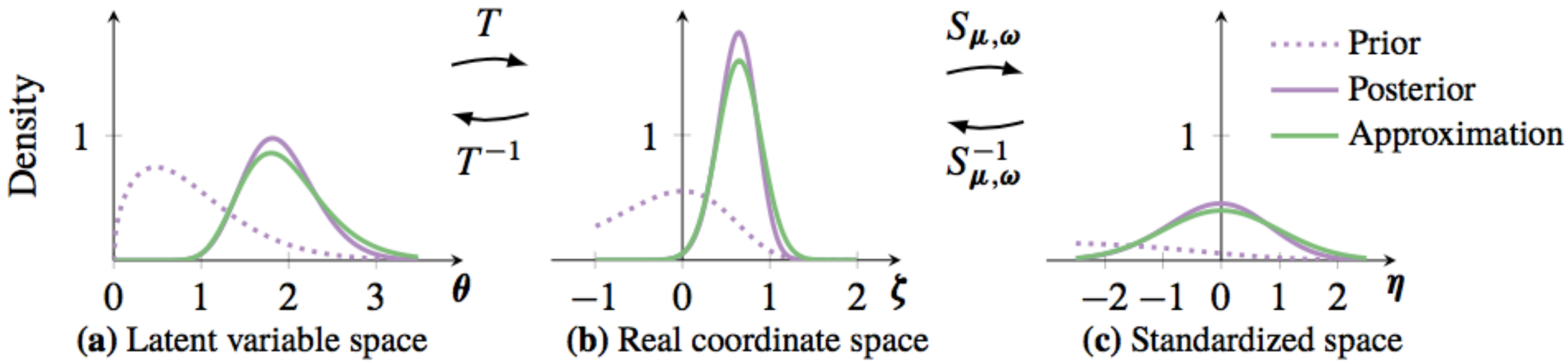
from approximate distributions, but we can't calculate the true posterior distribution.

Evidence Lower Bound

(ELBO)

$$\mathbb{KL}(q(\theta) \parallel p(\theta \mid \mathcal{D})) = -(\underbrace{\mathbb{E}_q(\log p(\mathcal{D}, \theta)) - \mathbb{E}_q(\log q(\theta))}_{\textbf{ELBO}}) + \log p(\mathcal{D})$$

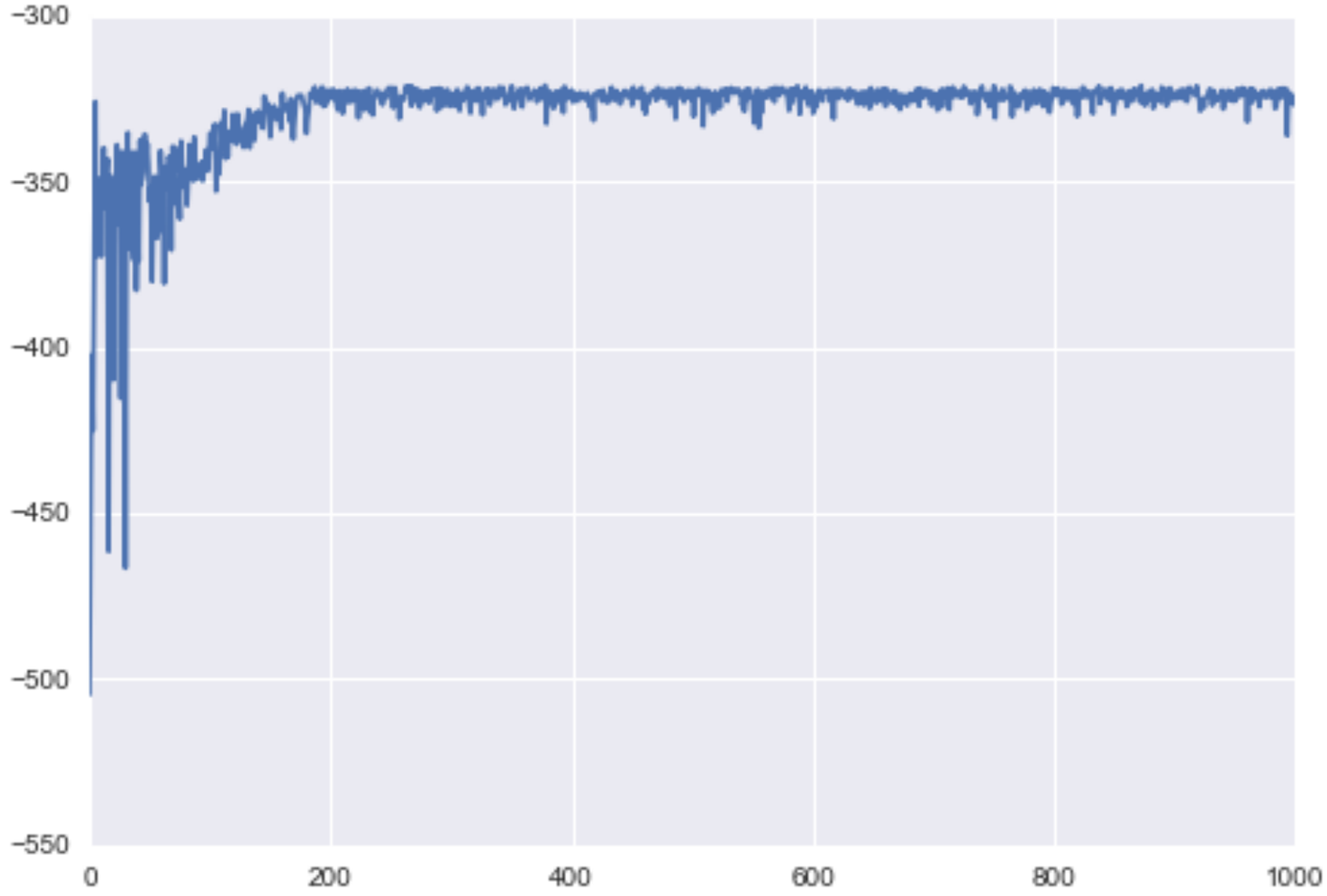
ADVI*



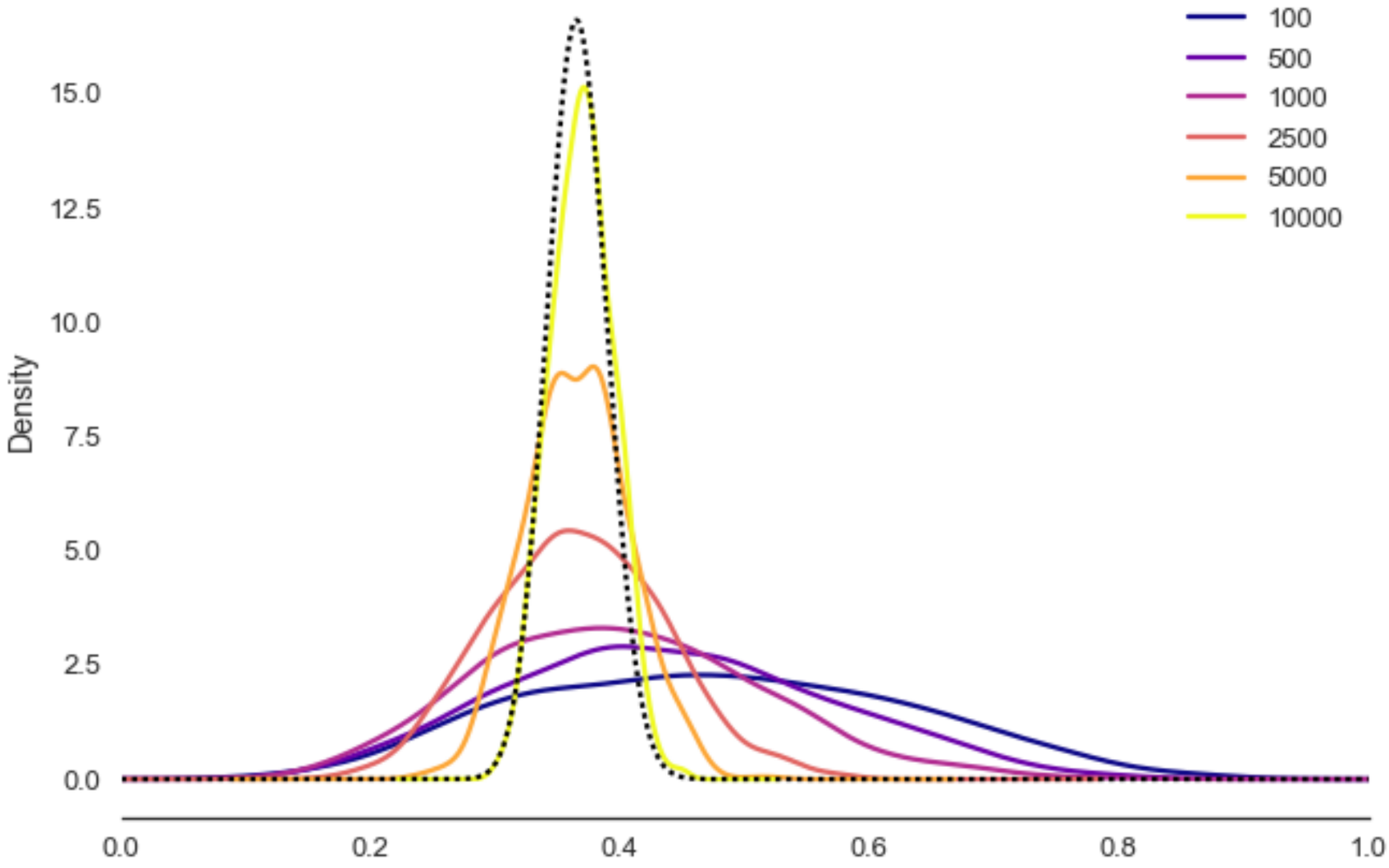
(a) Latent variable space (b) Real coordinate space (c) Standardized space

* Kucukelbir, A., Tran, D., Ranganath, R., Gelman, A., & Blei, D. M. (2016, March 2). Automatic Differentiation Variational Inference. arXiv.org.

Maximizing the ELBO



Estimating `Beta(147, 255)` **posterior**



```
with partial_pooling:

    approx = fit(n=100000)
```

```
Average Loss = 1,115.5: 100%|██████████| 100000/100000 [00:13<00:00, 7690.51it/s]
Finished [100%]: Average Loss = 1,115.5
```

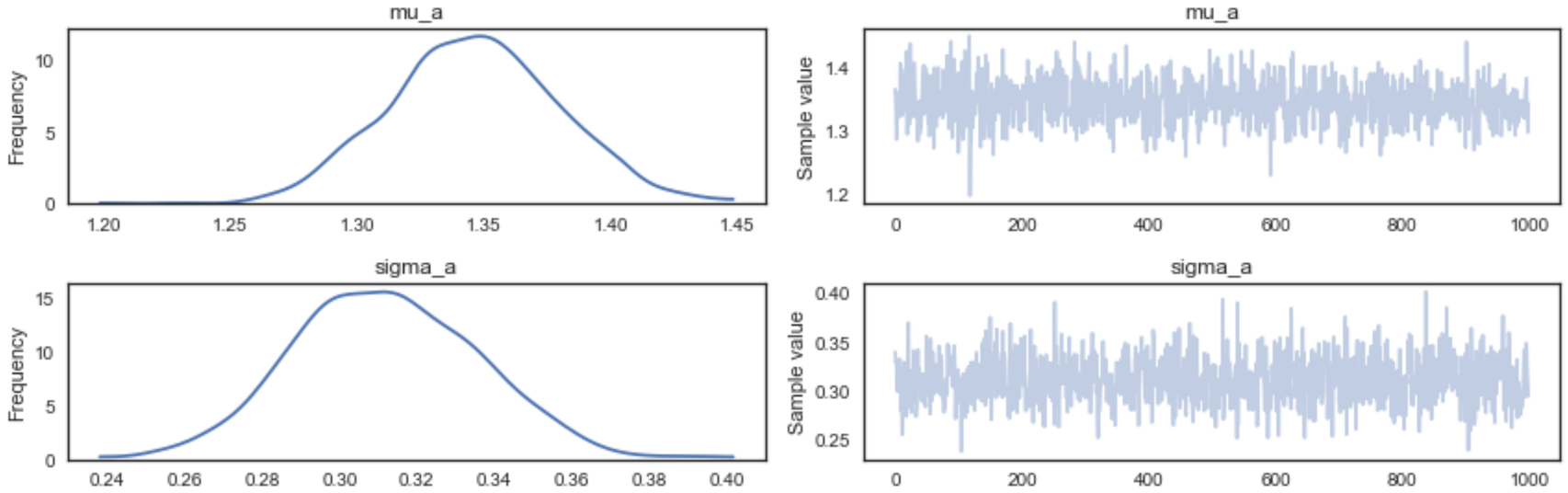
```
with partial_pooling:

    approx = fit(n=100000)
```

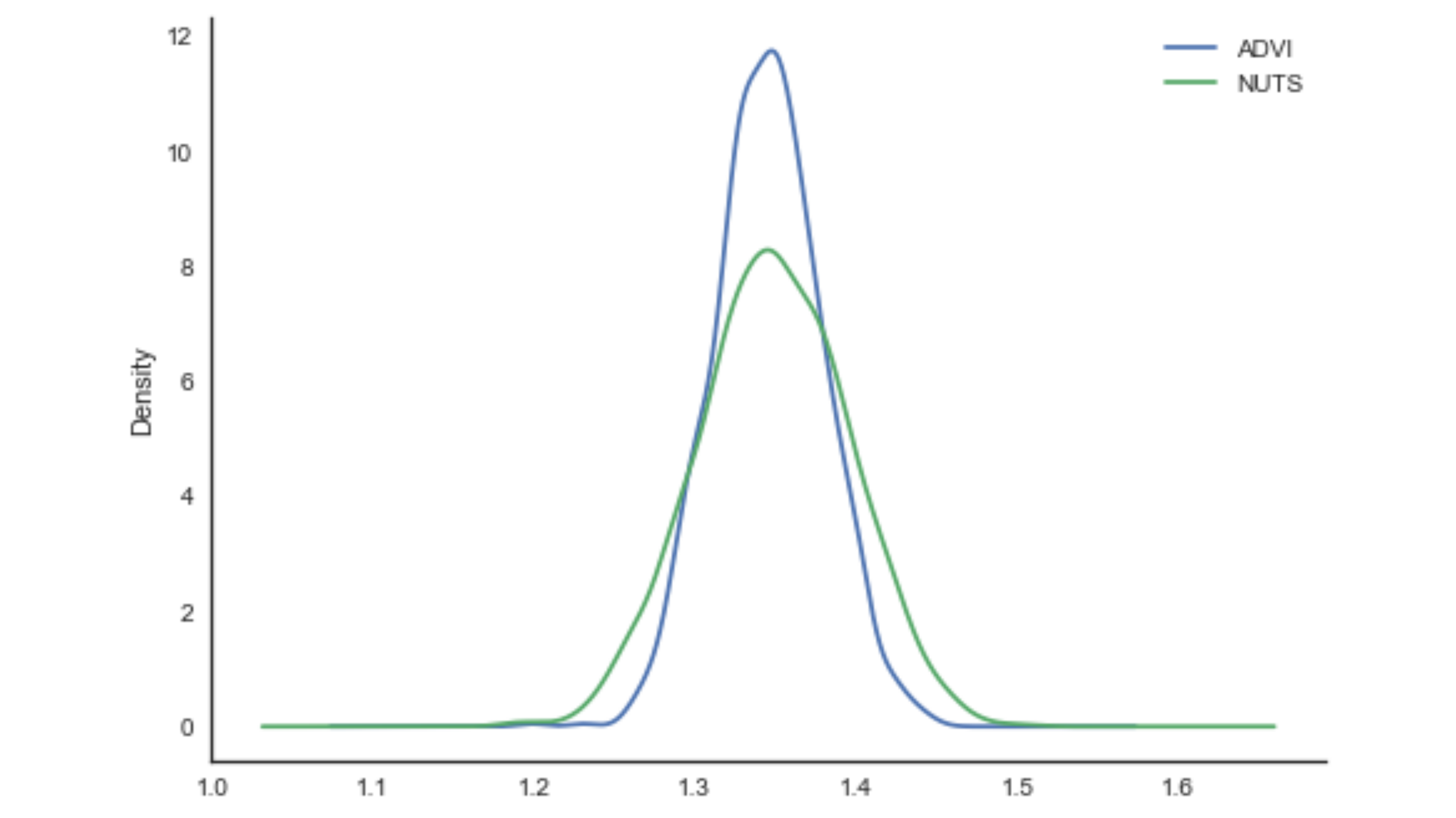
```
Average Loss = 1,115.5: 100%|██████████| 100000/100000 [00:13<00:00, 7690.51it/s]
Finished [100%]: Average Loss = 1,115.5
```

```
>>> approx
```

```
<pymc3.variational.approximations.MeanField at 0x119aa7c18>
```

```
with partial_pooling:

    approx_sample = approx.sample(1000)

traceplot(approx_sample, varnames=['mu_a', 'σ_a'])
```




ADVI
NUTS
Density
12
10
8
6
4
2
0
1.0
1.1
1.2
1.3
1.4
1.5
1.6

New PyMC3 Features

- ☞ Gaussian processes
- ☞ Elliptical slice sampling
- ☞ Sequential Monte Carlo methods
- ☞ Time series models

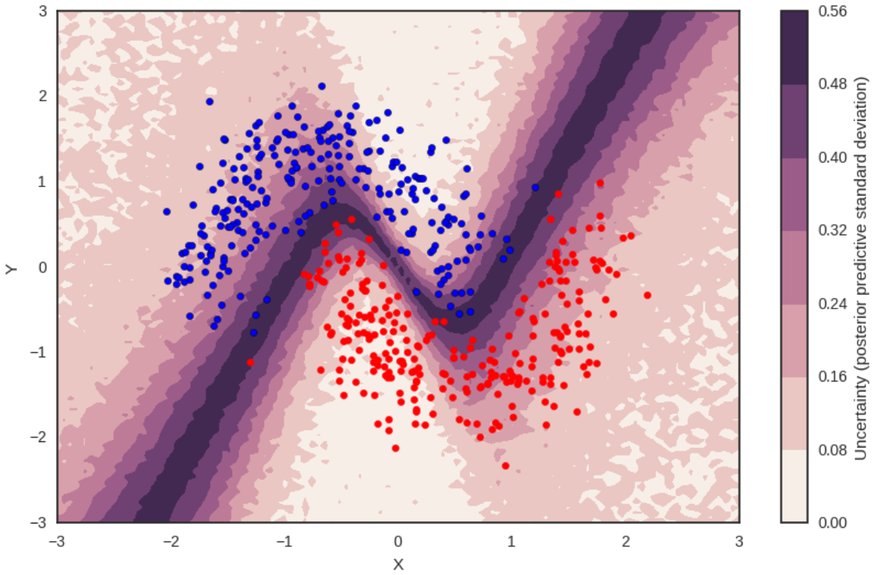
Convolutional variational autoencoder[♌]

```
import keras

class Decoder:

    ...

    def decode(self, zs):

        keras.backend.theano_backend._LEARNING_PHASE.set_value(np.uint8(0))

        return self._get_dec_func()(zs)
```

[♌] Taku Yoshioka (c) 2016

```
with pm.Model() as model:
    # Hidden variables
    zs = pm.Normal('zs', mu=0, sd=1,
                   shape=(minibatch_size, dim_hidden),
                   dtype='float32')

    # Decoder and its parameters
    dec = Decoder(zs, net=cnn_dec)

    # Observation model
    xs_ = pm.Normal('xs_', mu=dec.out.ravel(), sd=0.1,
                    observed=xs_t.ravel(), dtype='float32')
```

Bayesian Deep Learning in PyMC3✧



✧ Thomas Wiecki 2016

```
with pm.Model() as neural_network:
    # Weights from input to hidden layer
    weights_in_1 = pm.Normal('w_in_1', 0, sd=1,
                             shape=(X.shape[1], n_hidden),
                             testval=init_1)

    # Weights from 1st to 2nd layer
    weights_1_2 = pm.Normal('w_1_2', 0, sd=1,
                            shape=(n_hidden, n_hidden),
                            testval=init_2)

    # Weights from hidden layer to output
    weights_2_out = pm.Normal('w_2_out', 0, sd=1,
                              shape=(n_hidden,),
                              testval=init_out)

    # Build neural-network using tanh activation function
    act_1 = pm.math.tanh(pm.math.dot(ann_input,
                                     weights_in_1))
    act_2 = pm.math.tanh(pm.math.dot(act_1,
                                     weights_1_2))
    act_out = pm.math.sigmoid(pm.math.dot(act_2,
                                          weights_2_out))

    # Binary classification -> Bernoulli likelihood
    out = pm.Bernoulli('out',
                       act_out,
                       observed=ann_output)
```

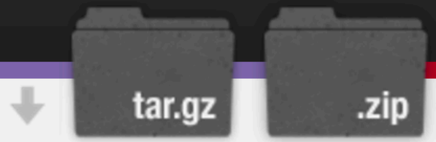
The Future

- ☞ Operator Variational Inference
- ☞ Normalizing Flows
- ☞ Riemannian Manifold HMC
- ☞ Stein variational gradient descent
- ☞ ODE solvers

Jupyter Notebook Gallery

GLM-rolling-regression.ipynb	DOC Add missing examples, f
GLM.ipynb	Change signature of get_data
GP-covariances.ipynb	updates to documentation, ac
GP-introduction.ipynb	updates to documentation, ac
GP-slice-sampling.ipynb	make notebook compatible
GP-smoothing.ipynb	DOC Reformat GP notebooks.
LKJ.ipynb	WIP: Update LKJ notebook to
Model Comparison.ipynb	fix computation of d_se introd
PyMC3_tips_and_heuristic.ipynb	Formatting docs (#2127)
SMC2_gaussians.ipynb	SMC experimental (#2045)
api_quickstart.ipynb	Added OO interface to api_qu
bayesian_neural_network_advi.ip...	MAINT More casting fixes. Ma
bayesian_neural_network_opvi-a...	Changed fit method calls to fu
convolutional_vae_keras_advi.ipy...	Update notebook following Ke
cox_model.ipynb	DOC tidy notebooks (#1535)
dawid-skene.ipynb	Change signature of get_data
dependent_density_regression.ip...	Fix math in DDR example
dp_mix.ipynb	Add NUTS and NormalMixture

Probabilistic Programming & Bayesian Methods for Hackers



An intro to Bayesian methods and probabilistic programming from a computation/understanding-first, mathematics-second point of view.

Prologue

The PyMC3 Team

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