Lecture 19: Bayesian EZ

Instructor: Sergei V. Kalinin

Probability of data is generally intractable

- Prior information $p(\theta)$ on parameters θ
- Likelihood of data given parameter values $f(x|\ \theta)$

Problem for physics/theory

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

Outside knowledge

Problem for computation

$$f(x) = \int_{-\infty}^{\infty} f(x|\theta)p(\theta)d\theta$$

To use Bayesian methods, we need to be able to evaluate the denominator, which is the integral of the numerator over the parameter space. In general, this integral is very hard to evaluate.

Solution: Markov Chain Monte Carlo

We don't need to evaluate any integral, *we just sample from the distribution many times* (e.g., 50K times) and find (estimate) the posterior mean, middle 95%, etc., from that.

Metropolis-Hastings:

- An algorithm that generates a sequence
  $\{\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \ldots\}$ from a Markov Chain whose stationary distribution is $\pi(\theta)$ (i.e., the posterior distribution)
- Fast computers and recognition of this algorithm has allowed Bayesian estimation to develop.

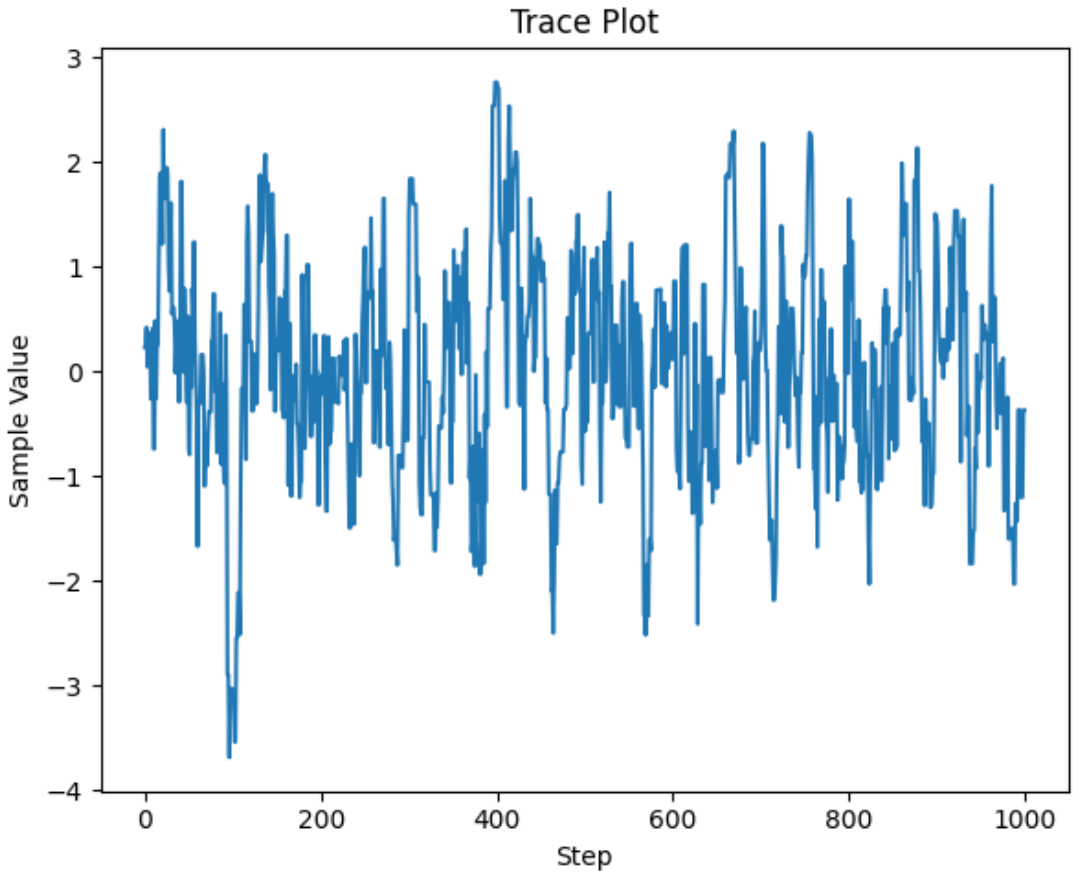
From Jeff Witmer, Introduction to Bayesian Statistics, slides 24 February 2016

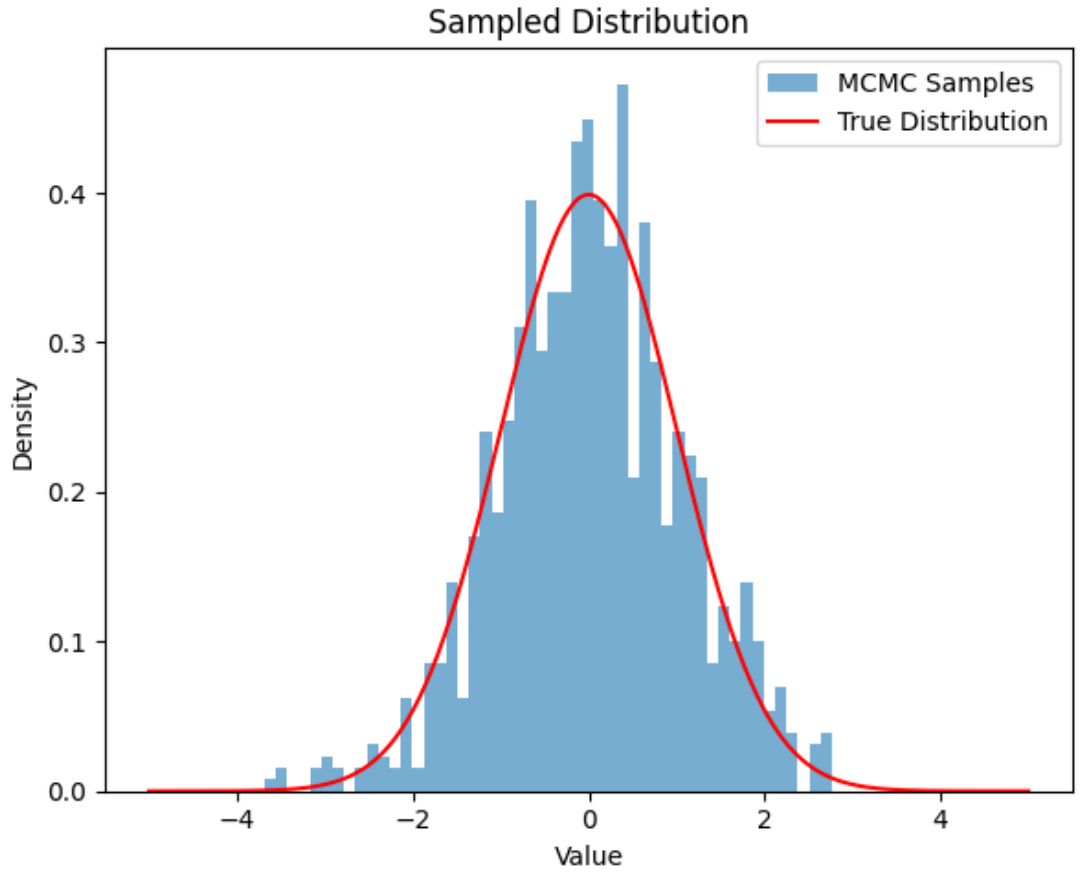
Metropolis-Hastings algorithm

- Initial value $\theta^{(0)}$ to start the Markov Chain
- Propose new value
- Accepted value: θ'

$$\theta^{(1)} = \begin{cases} \theta' \text{ with probability } \alpha \\ \theta^{(0)} \text{ with probability } 1 - \alpha \end{cases} \qquad \text{where } \alpha = \min\left(1, \frac{\pi(\theta')}{\pi(\theta^{(0)})}\right)$$

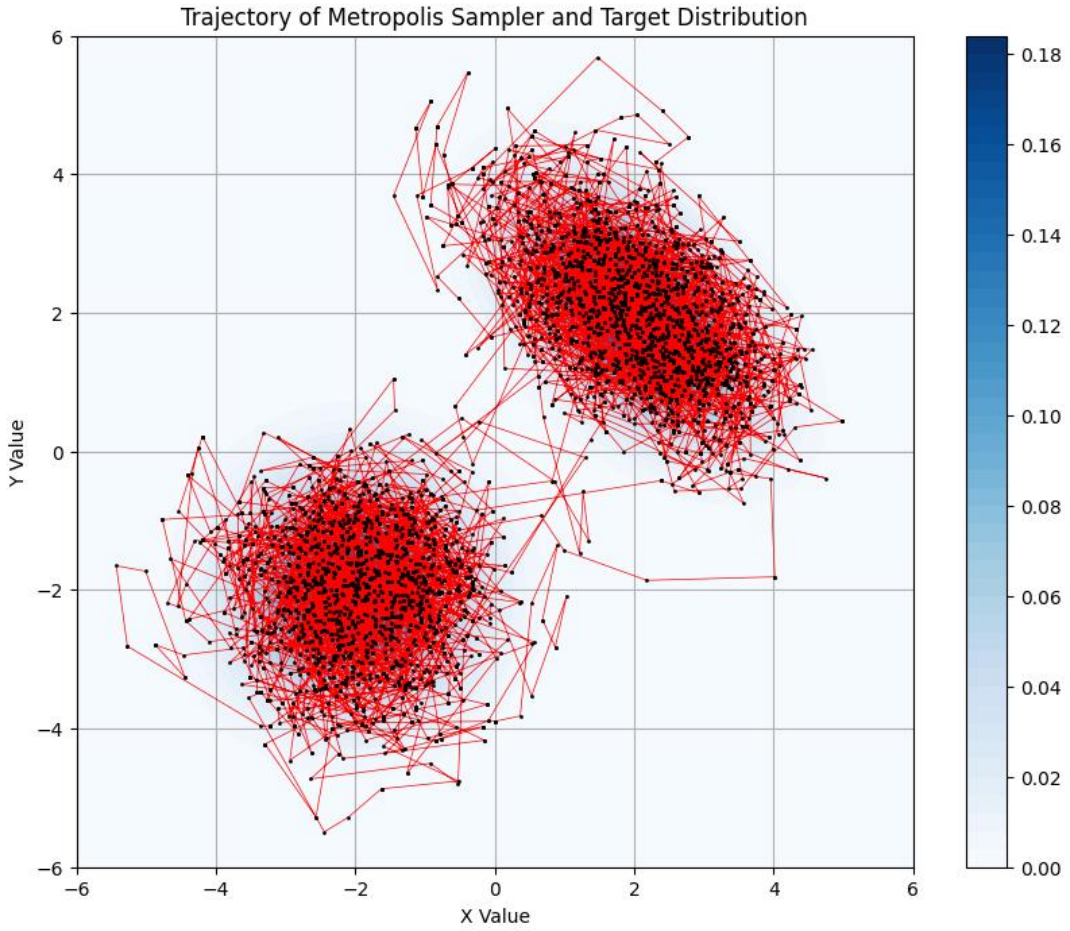
Sampling 1D Gaussian

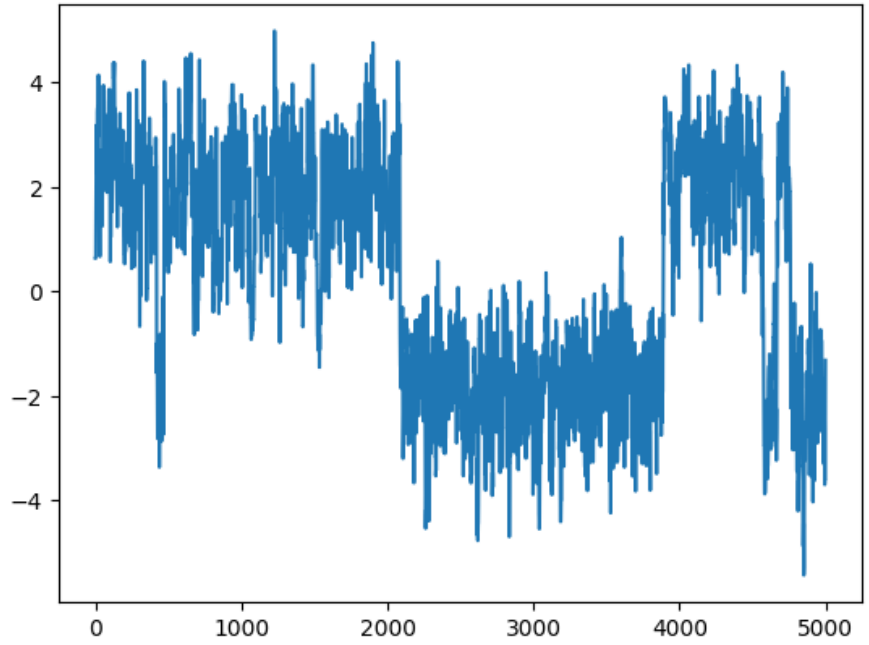




We can calculate any function of the posterior by summing over the trace

Sampling 2D Gaussian





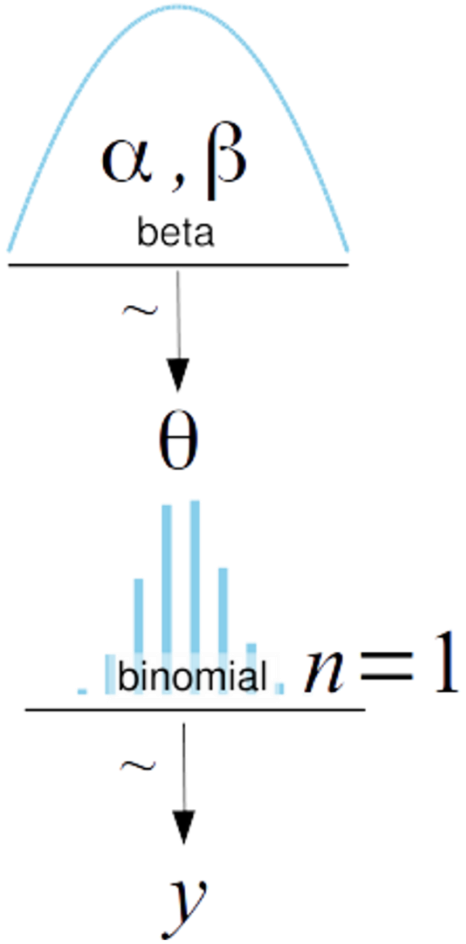
MCMC Solvers:

- BUGS – Bayes Using Gibbs Sampling
- JAGS – Just Another Gibbs Sampler
- Stan – uses Hamiltonian Monte Carlo
- NUTS – No U-Turn Sampler

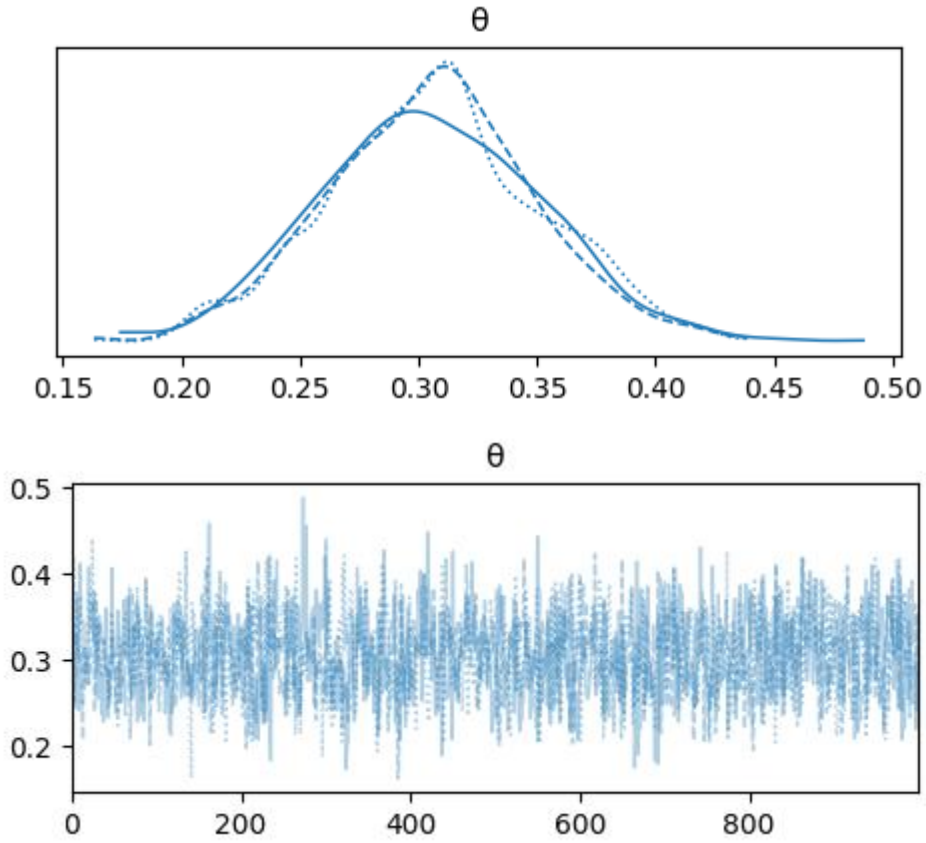
Let’s toss a coin!

Colab: 19_PYMC_BayesianEZ.ipynb

Let's toss a coin (with a PYMC)!



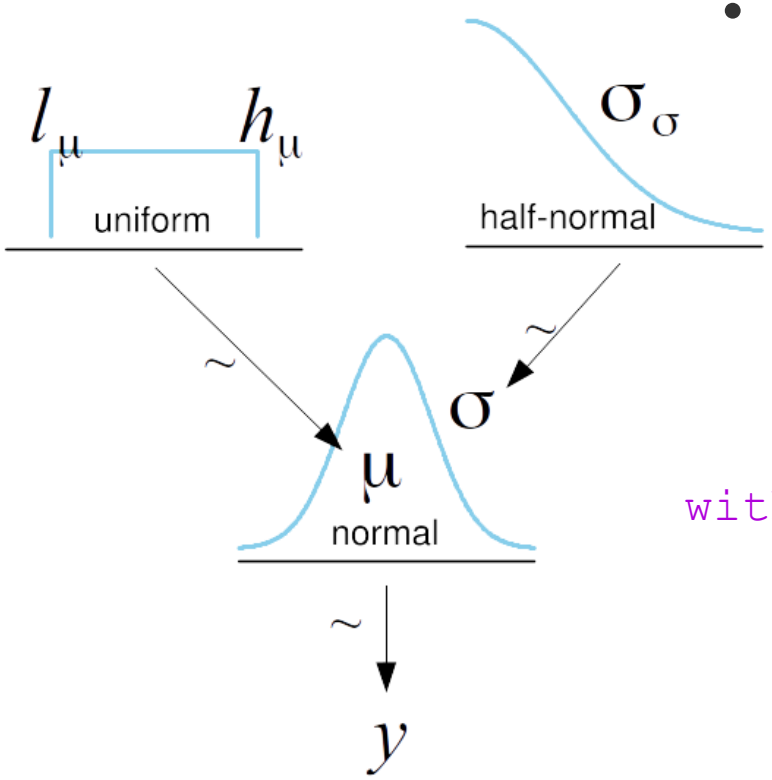

```
with pm.Model() as our_first_model:
    θ = pm.Beta('θ', alpha=1., beta=1.)
    y = pm.Bernoulli('y', p=θ, observed=data)
    trace = pm.sample(1000, random_seed=123, chains = 3)
```



Colab: 19_PYMC_BayesianEZ.ipynb

But how do we get physics done?

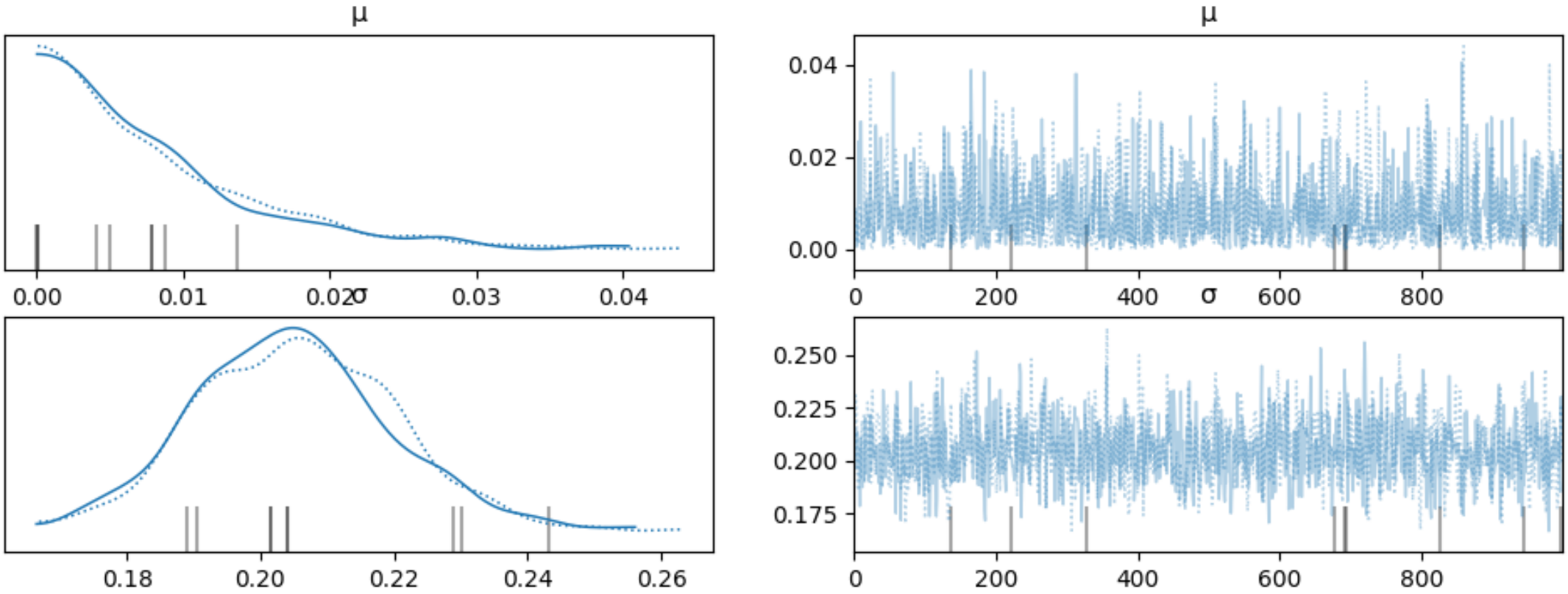
- Imagine that we have some observational data
- Can we say which distribution has it come from?



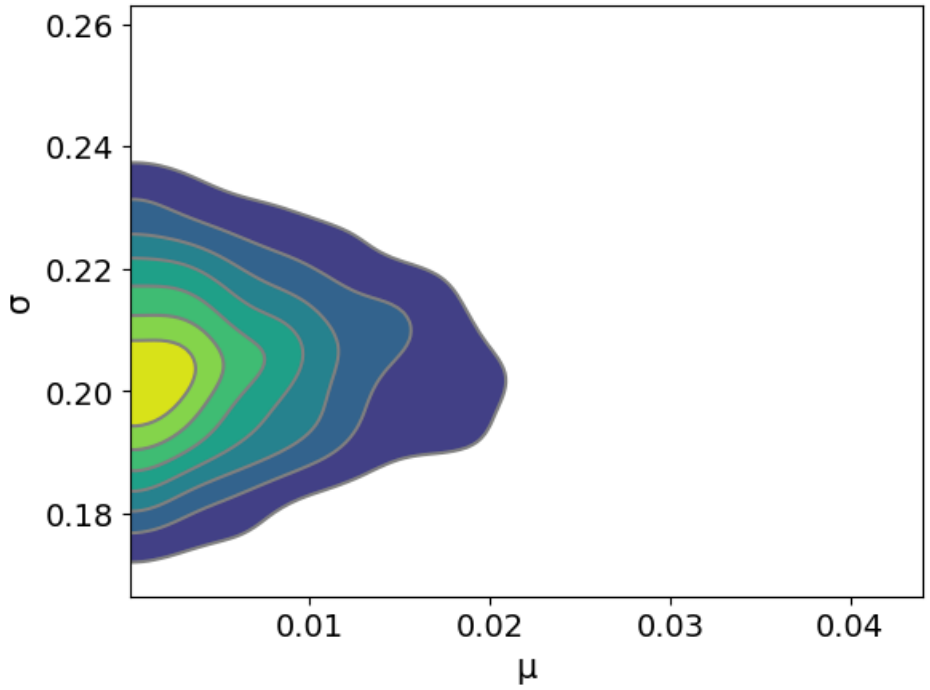
Define Bayesian model!

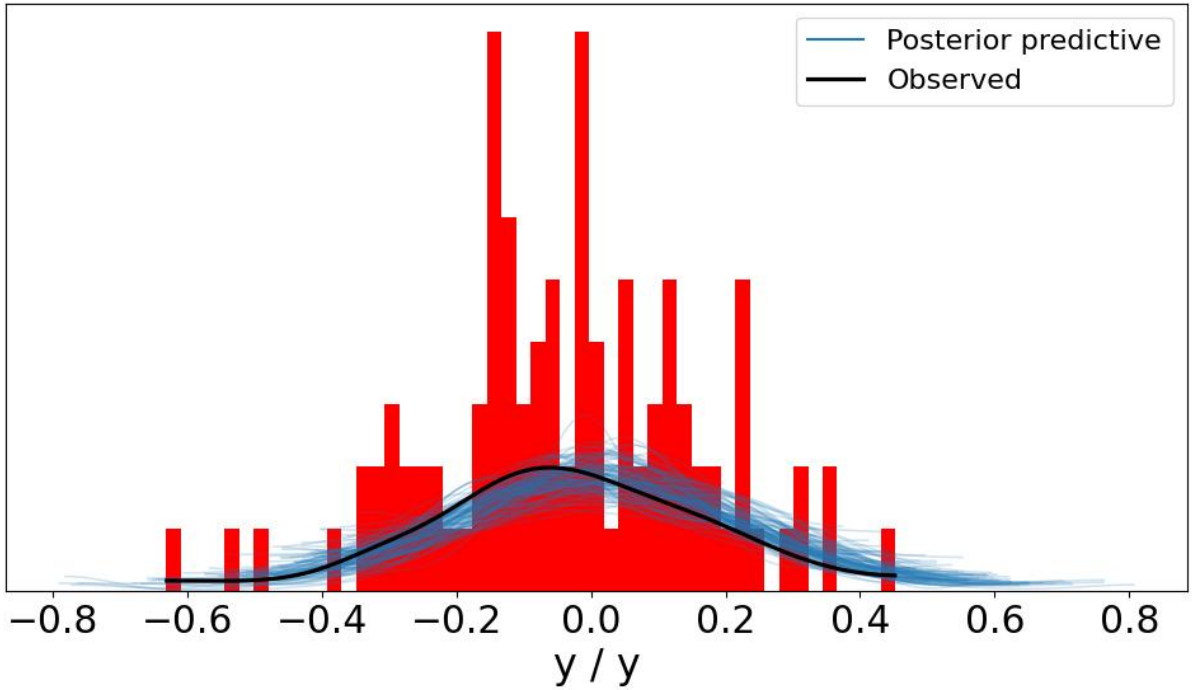
```
with pm.Model() as model_g:
    μ = pm.Uniform('μ', lower=0, upper=2)
    σ = pm.HalfNormal('σ', sigma=1)
    y = pm.Normal('y', mu=μ, sigma=σ, observed=arr)
    idata_g = pm.sample(1000)
```

Presto!


μ
0.00
0.01
0.02
0.03
0.04
σ
0.18
0.20
0.22
0.24
0.26
μ
0.04
0.02
0.00
0
200
400
σ
600
800
0.250
0.225
0.200
0.175
0
200
400
600
800

Presto!

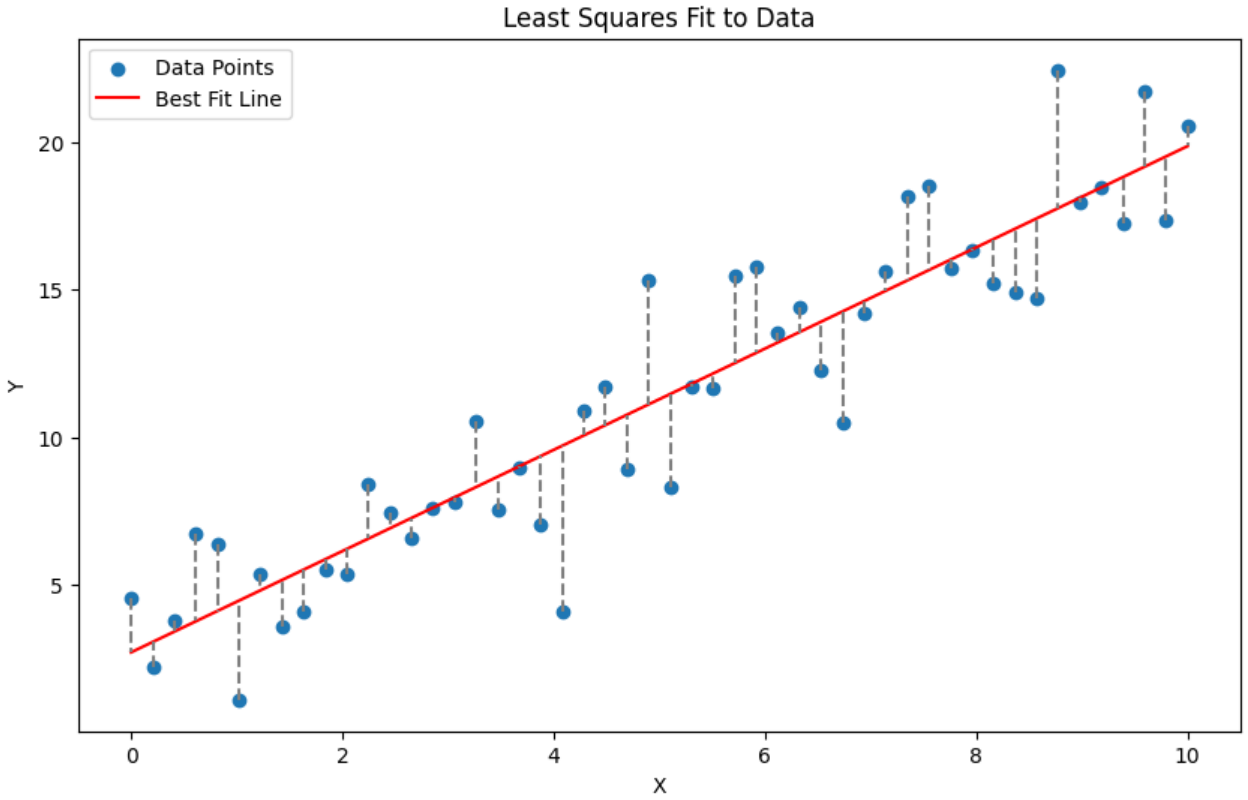

0.26
0.24
0.22
0.20
0.18
σ
0.01
0.02
0.03
0.04
μ


Posterior predictive
Observed
−0.8
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8
y / y

Let's start linear!

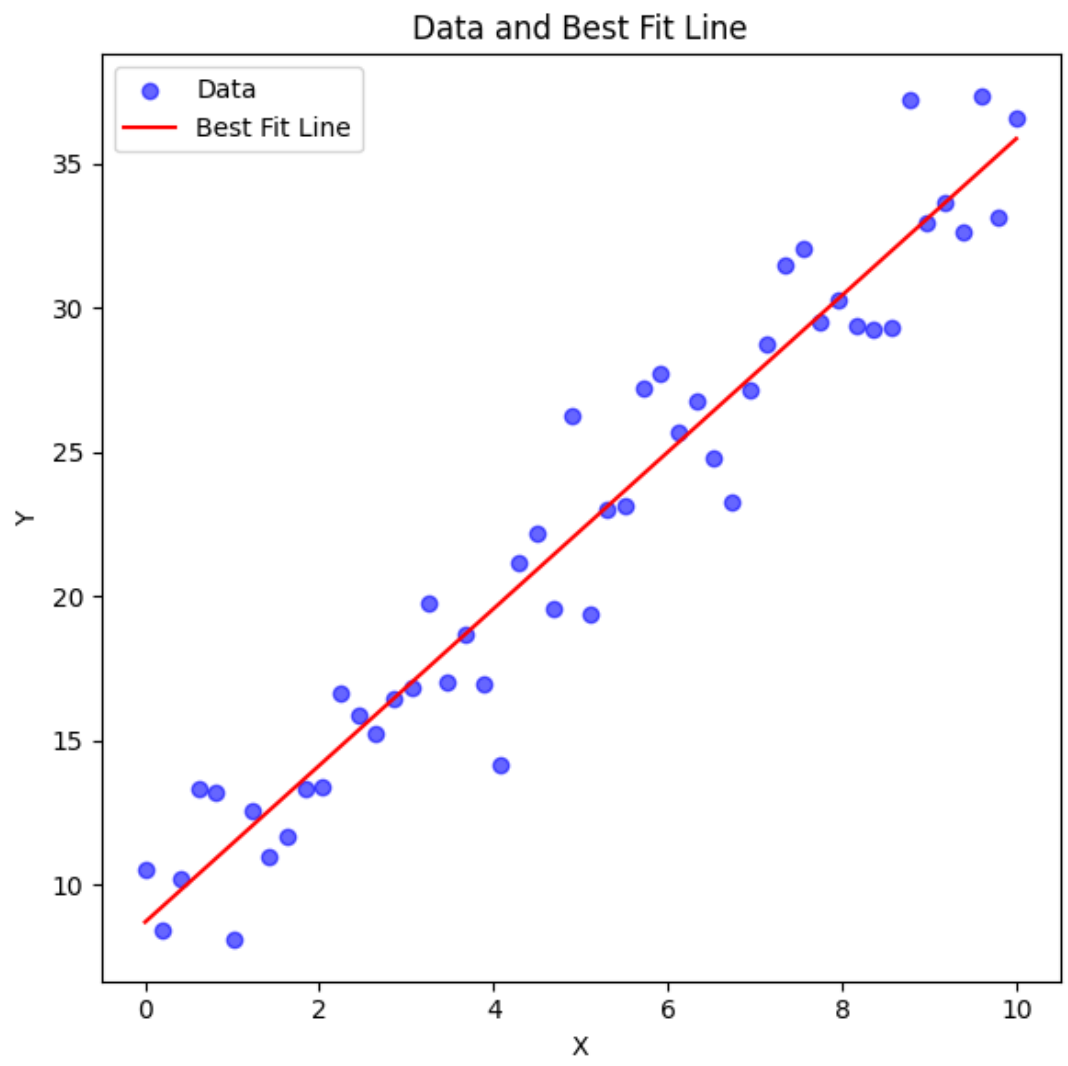
Least Squares Fitting: a method to determine the best-fitting line through a set of points.

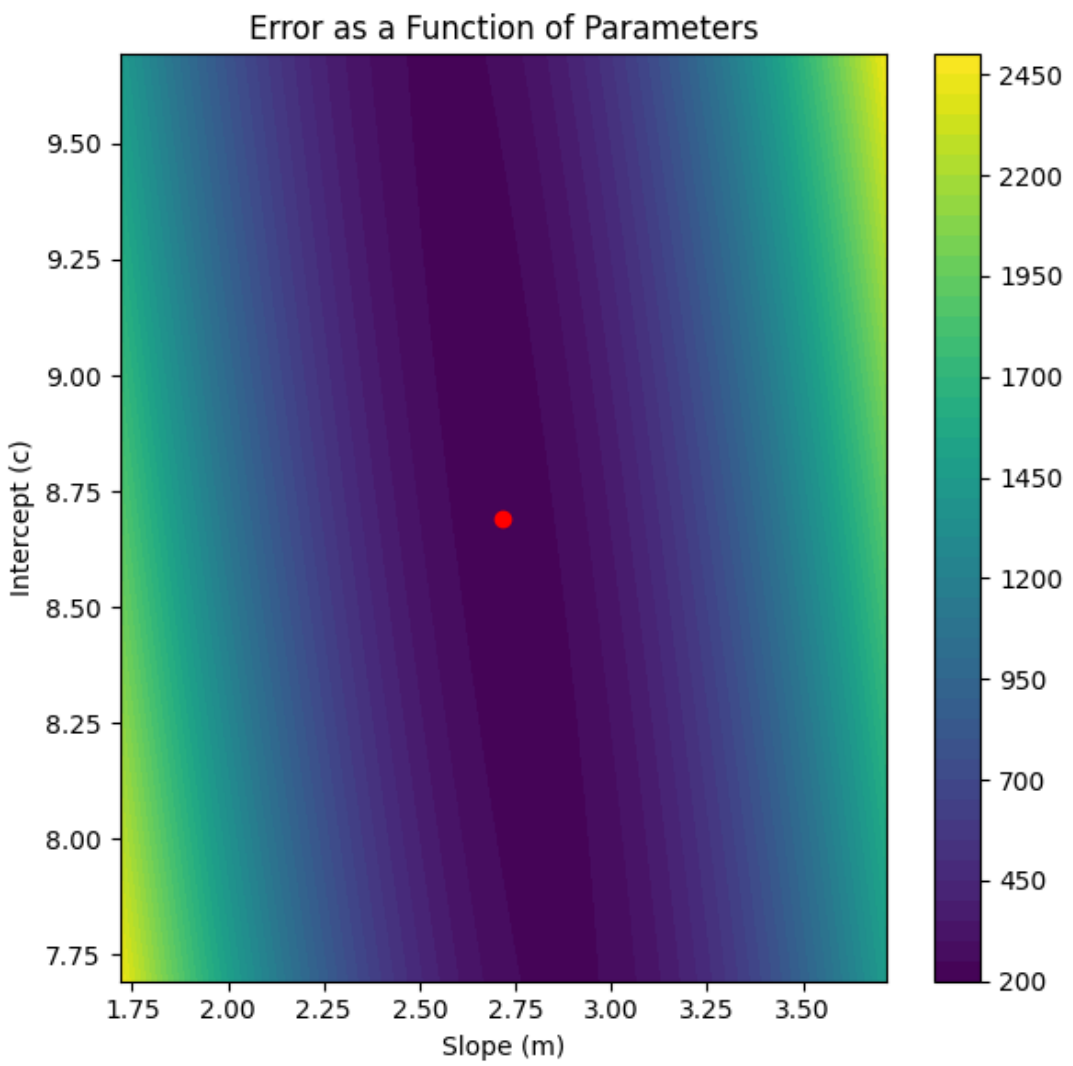
Objective: Minimize the sum of the squares of the differences (residuals) between observed and predicted values.



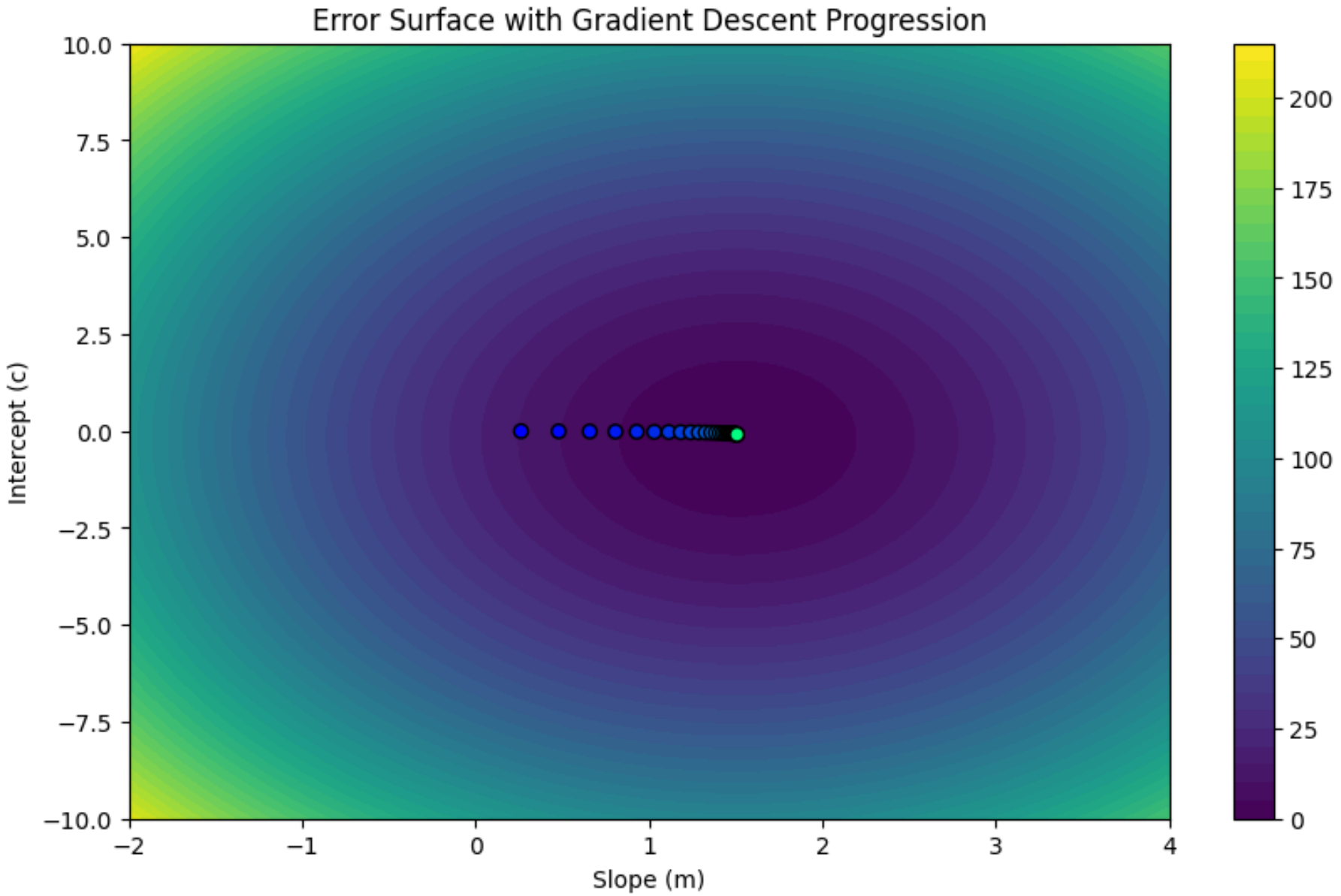
- We have data, meaning collection of points (x_i, y_i)
- We choose function, here $y = a + b\,x$
- We calculate total error, $L(a,b) = \sum((y_i - (a + b\,x_i))^2)$
- We find parameters **a, b** for which **L(a,b)** is minimal

Let’s start linear!

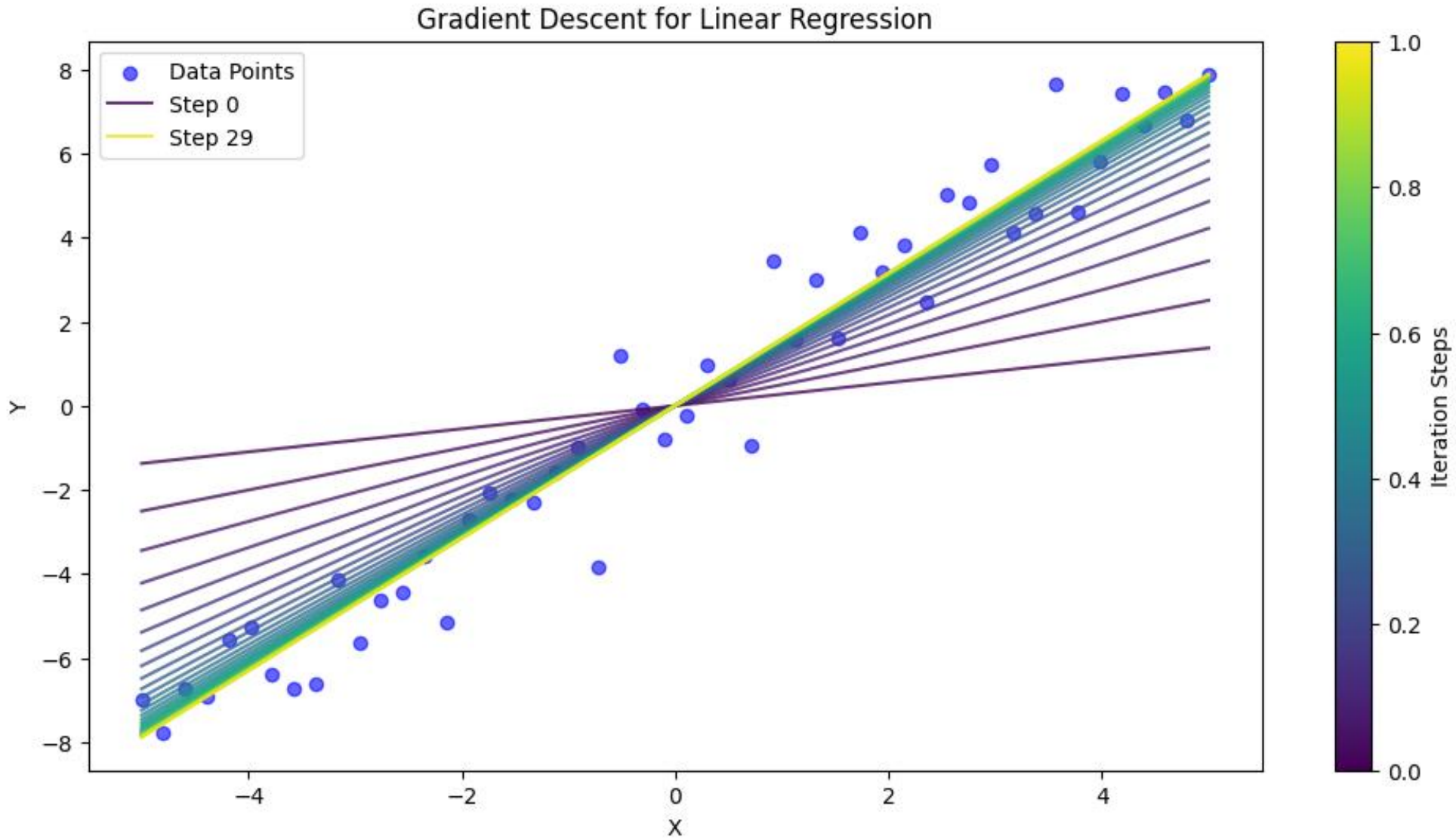




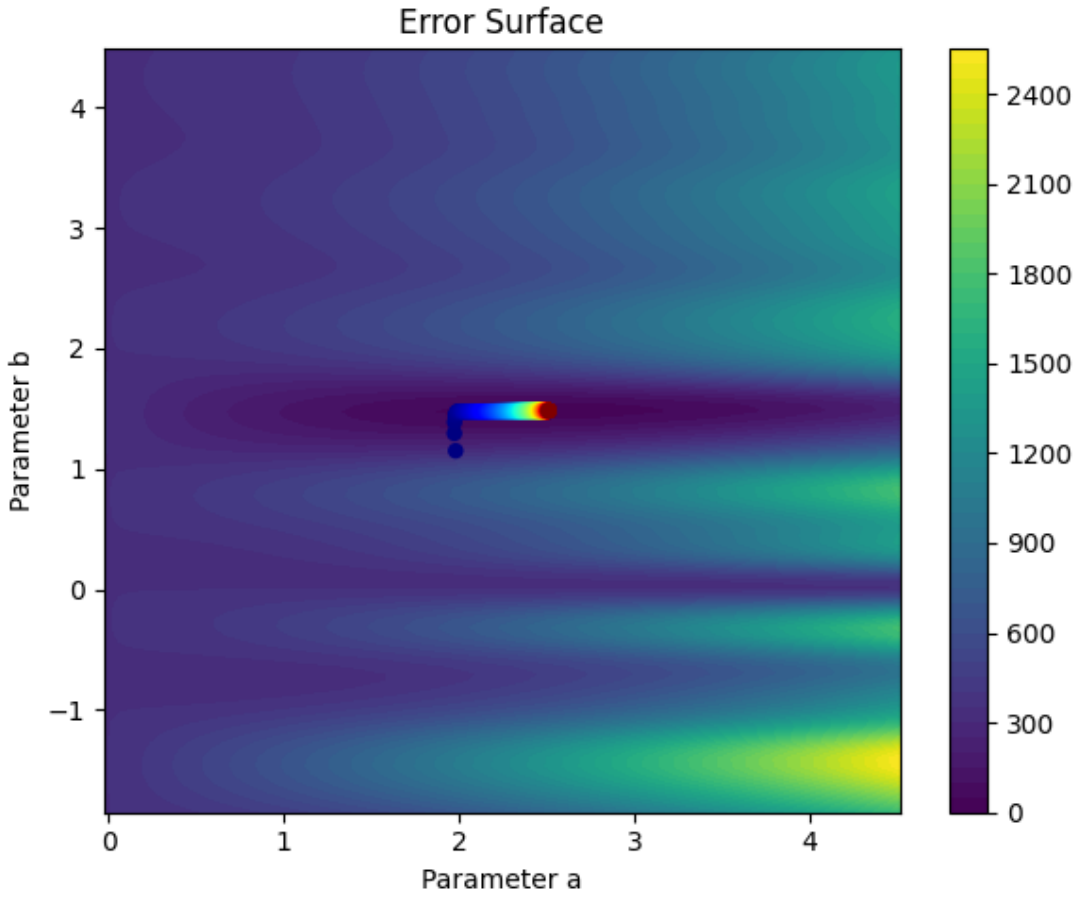
Finding minimum with gradient descent

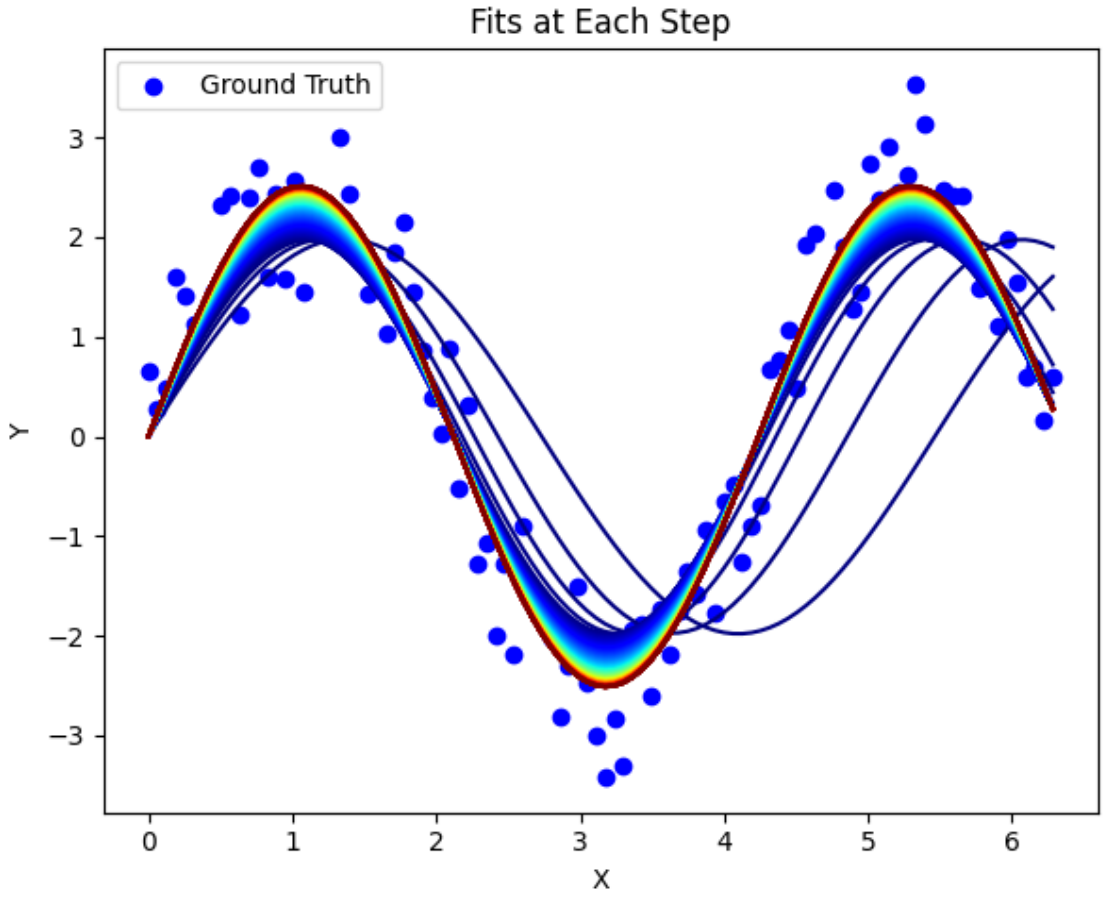


Finding minimum with gradient descent

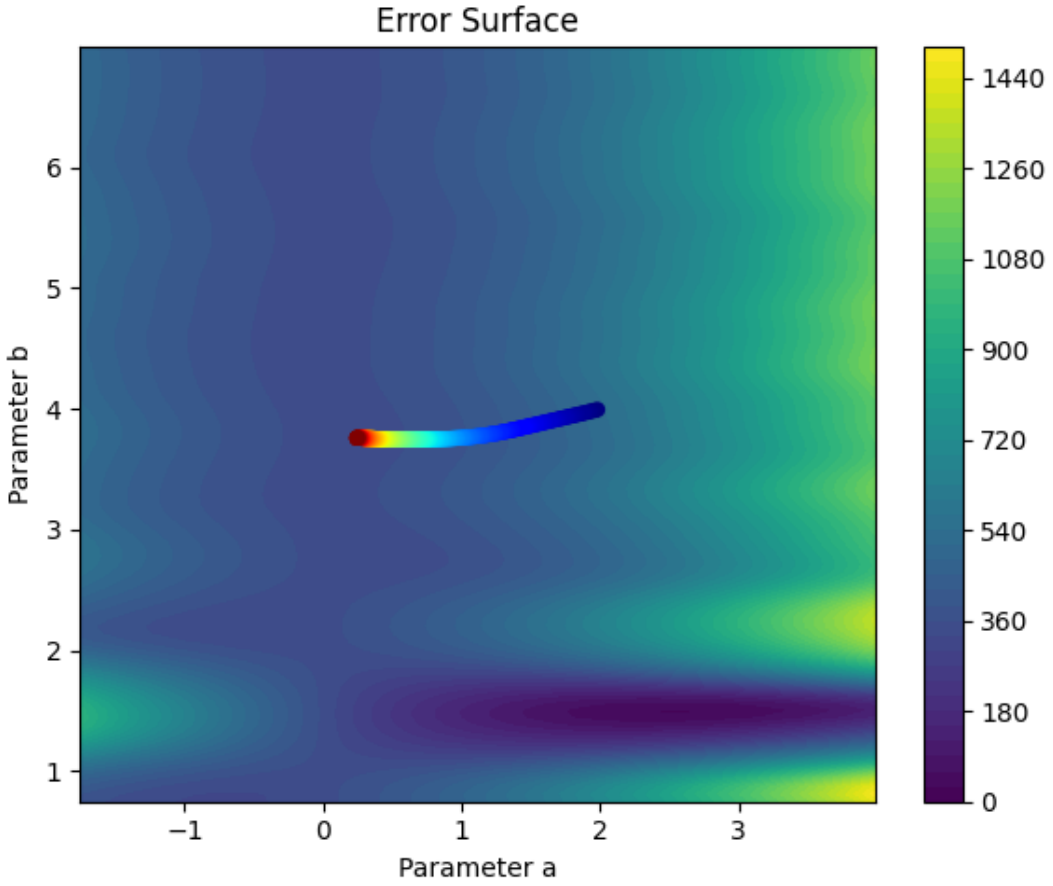


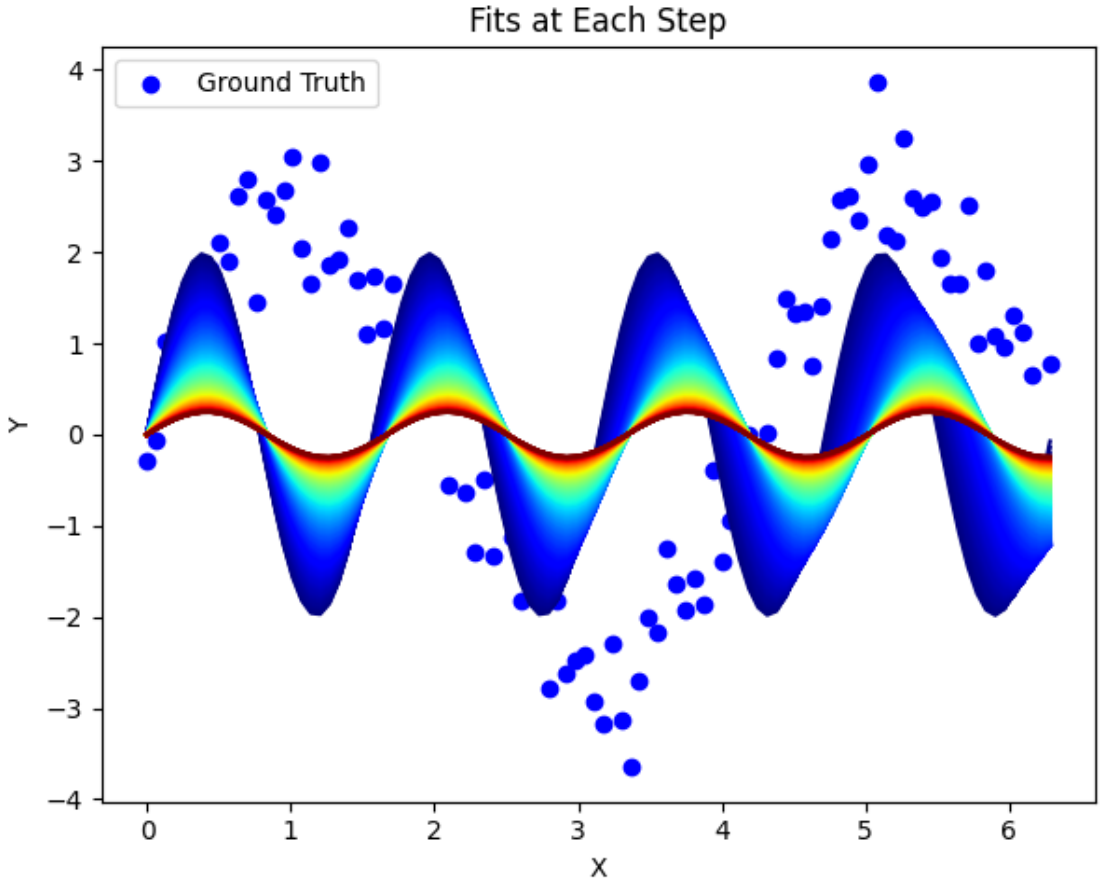
The sine that works





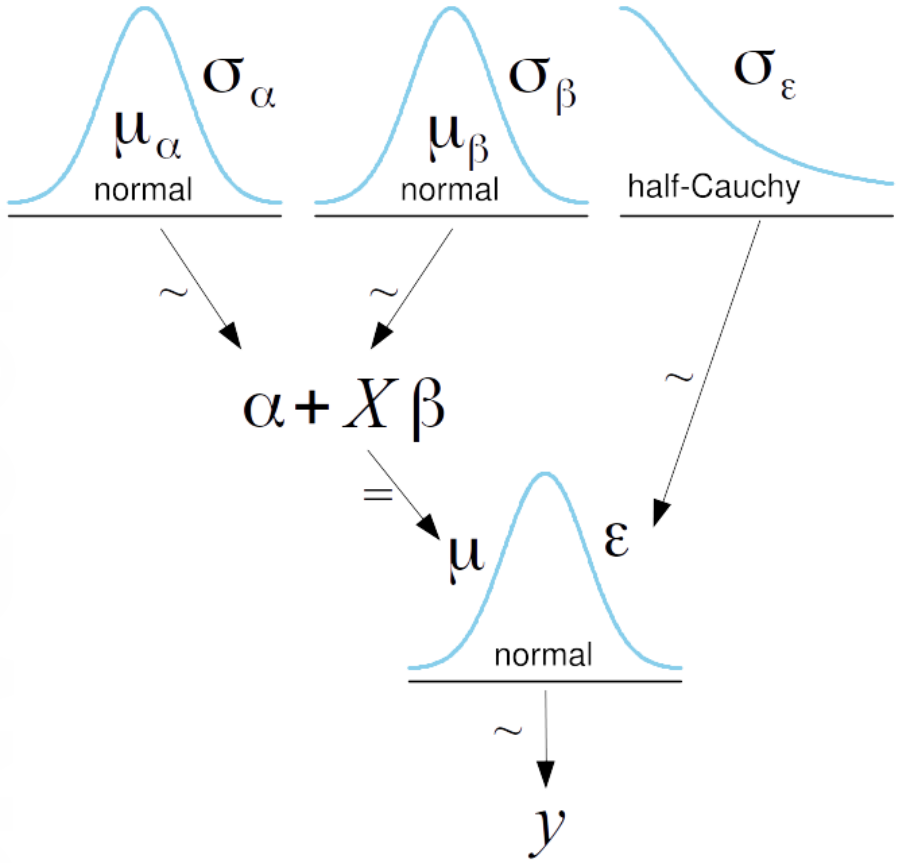
The sine that doesn't





Linear regression Bayesian style

- Imagine that we have some observational data
- Can we fit it by linear function?



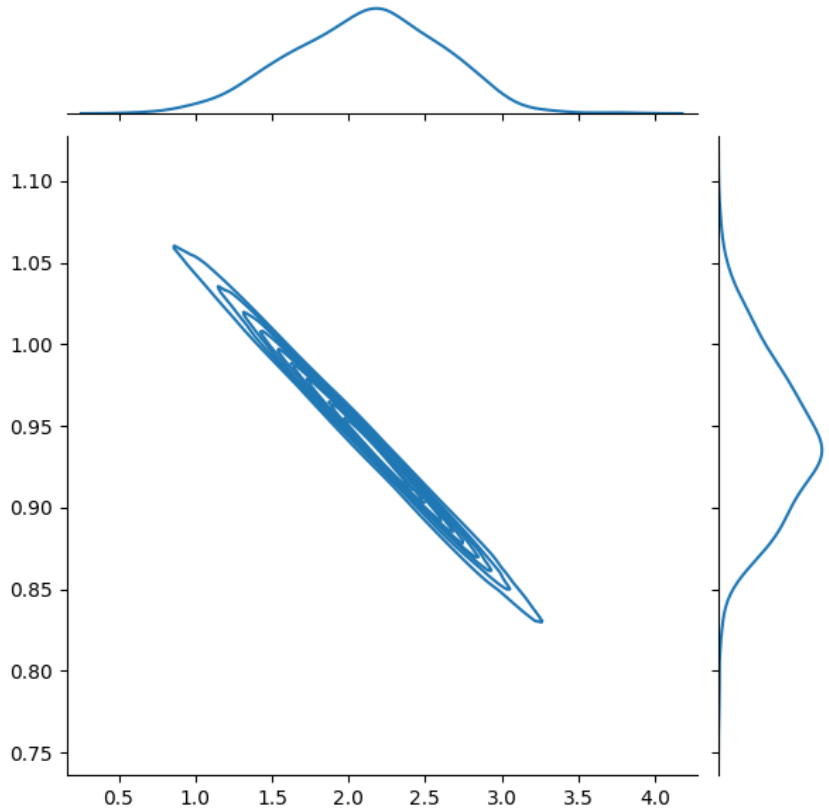
Define Bayesian model!

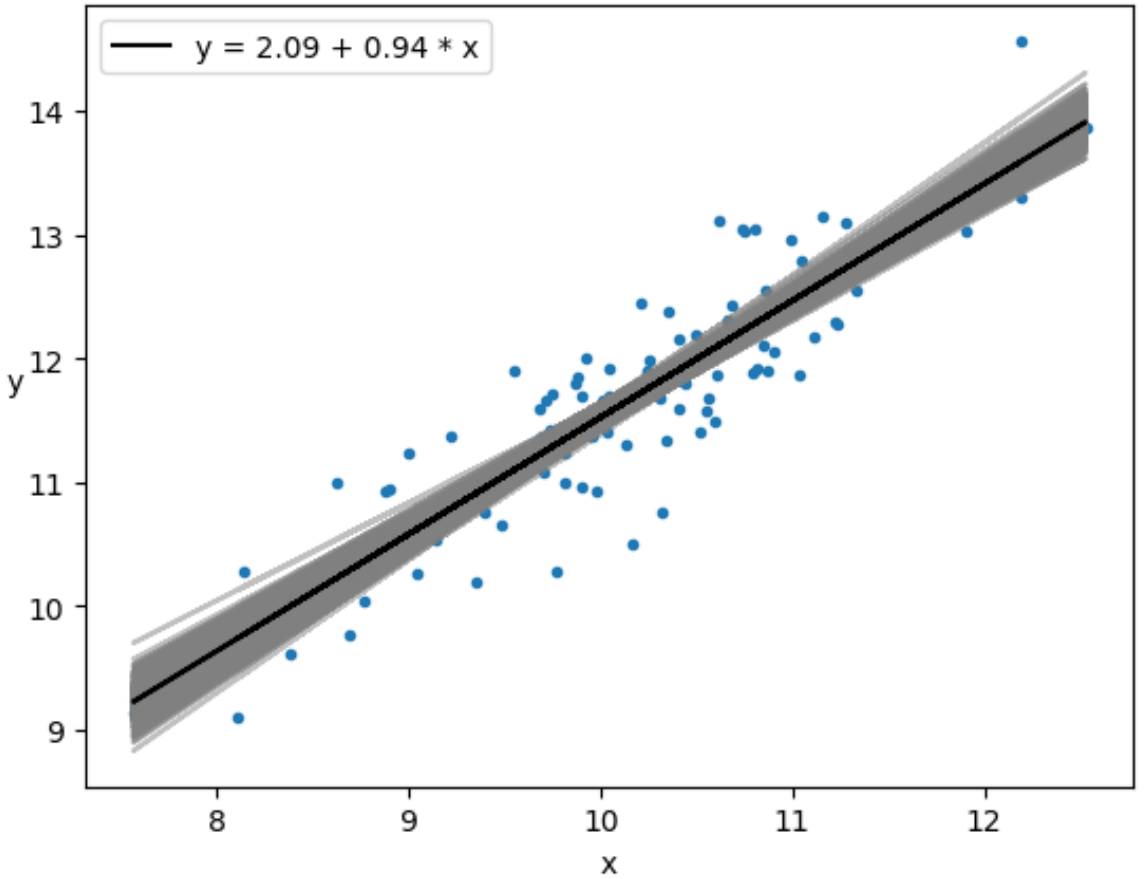
```
with pm.Model() as model_g:
    α = pm.Normal('α', mu=0, sigma=10)
    β = pm.Normal('β', mu=0, sigma=1)
    ϵ = pm.HalfCauchy('ϵ', 5)

    μ = pm.Deterministic('μ', α + β * x)
    y_pred = pm.Normal('y_pred', mu=μ,
                       sigma=ϵ, observed=y)

    idata_g = pm.sample(2000, tune=2000)
```

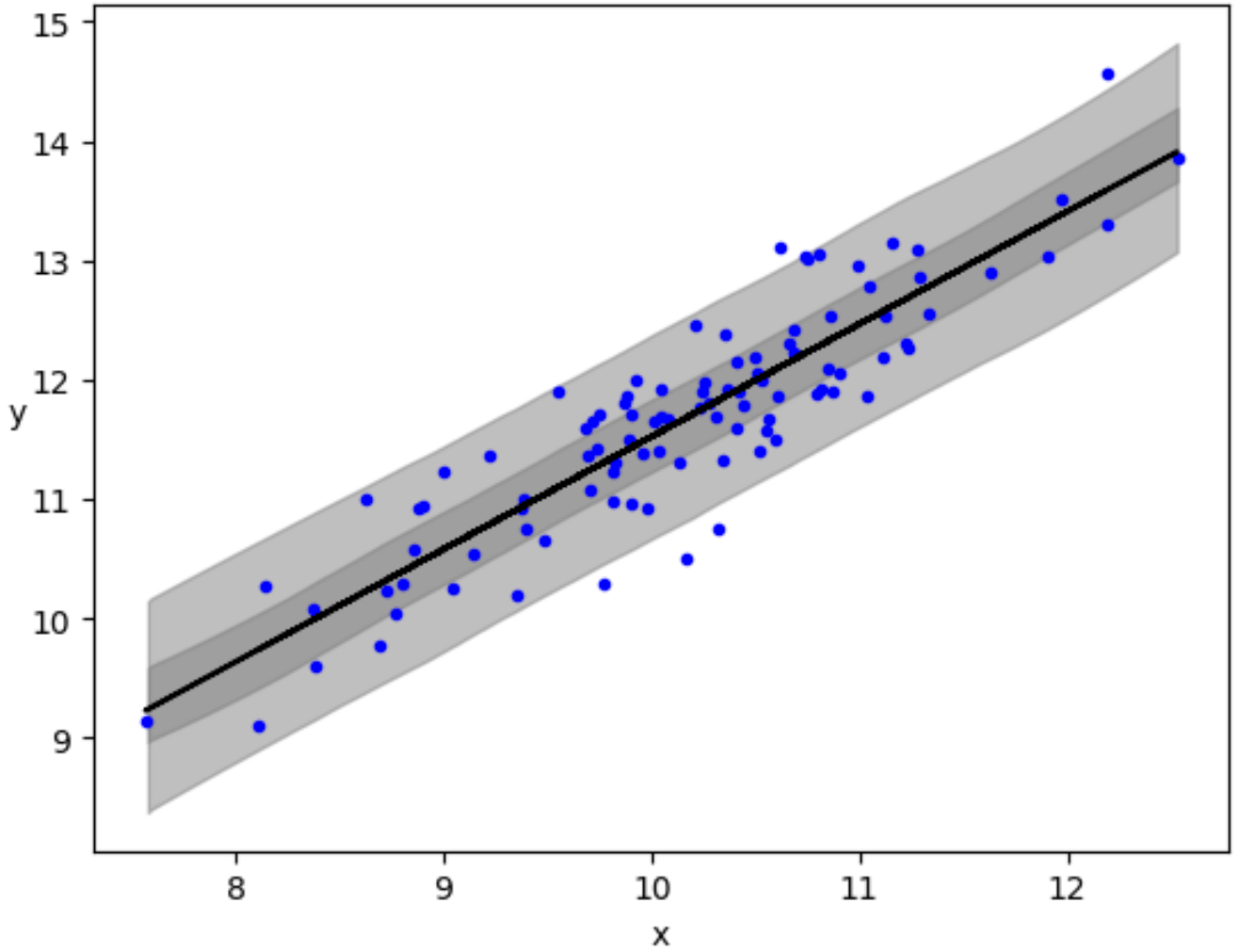
The outputs?





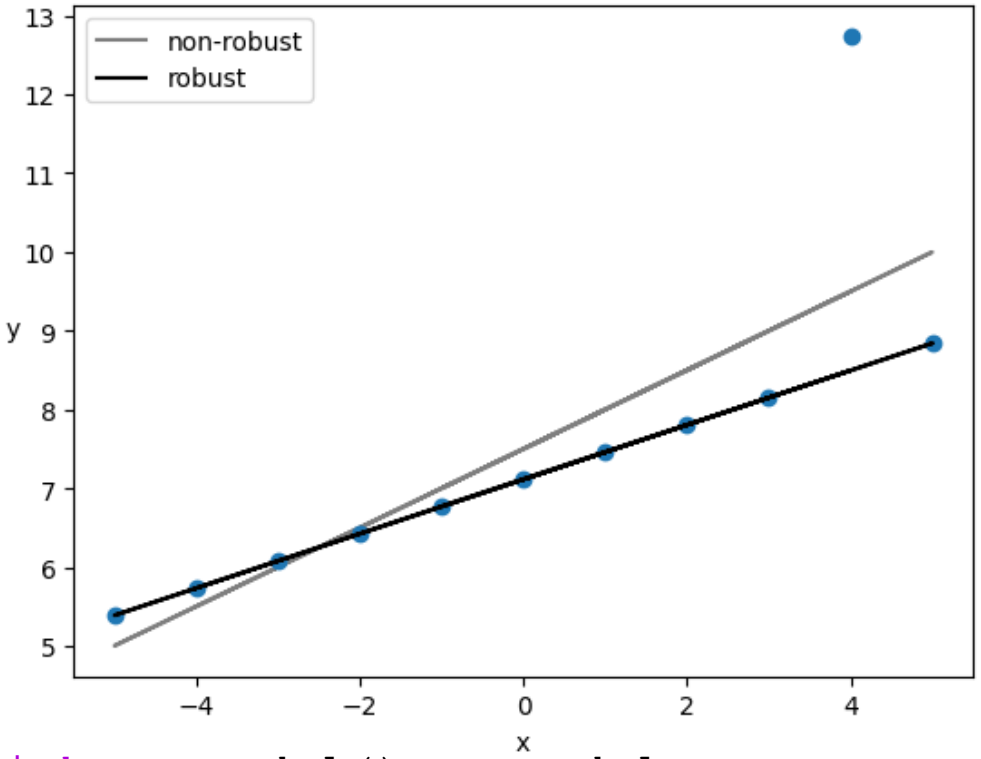
- The output of the Bayesian model will be draws for the slope and offset: families of lines consistent with data
- We can analyze their joint distribution
- And plot these lines

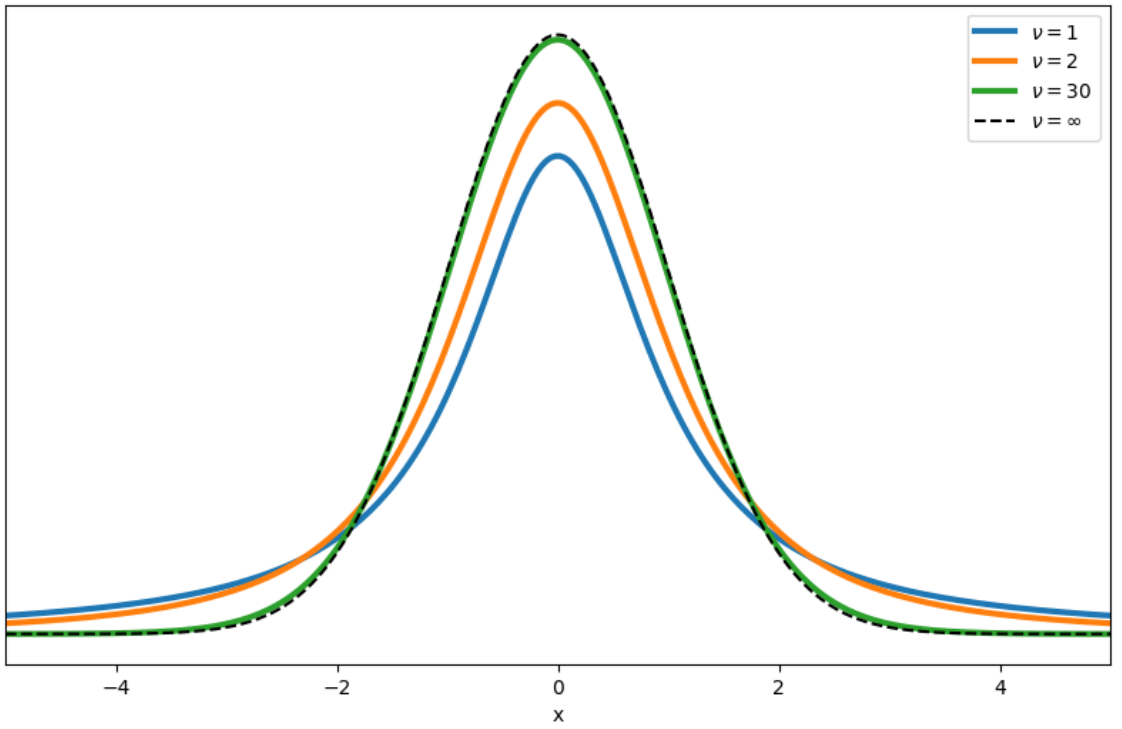
How do we decide if the “data is reasonable”?



- That’s what the posterior predictive checks are for!

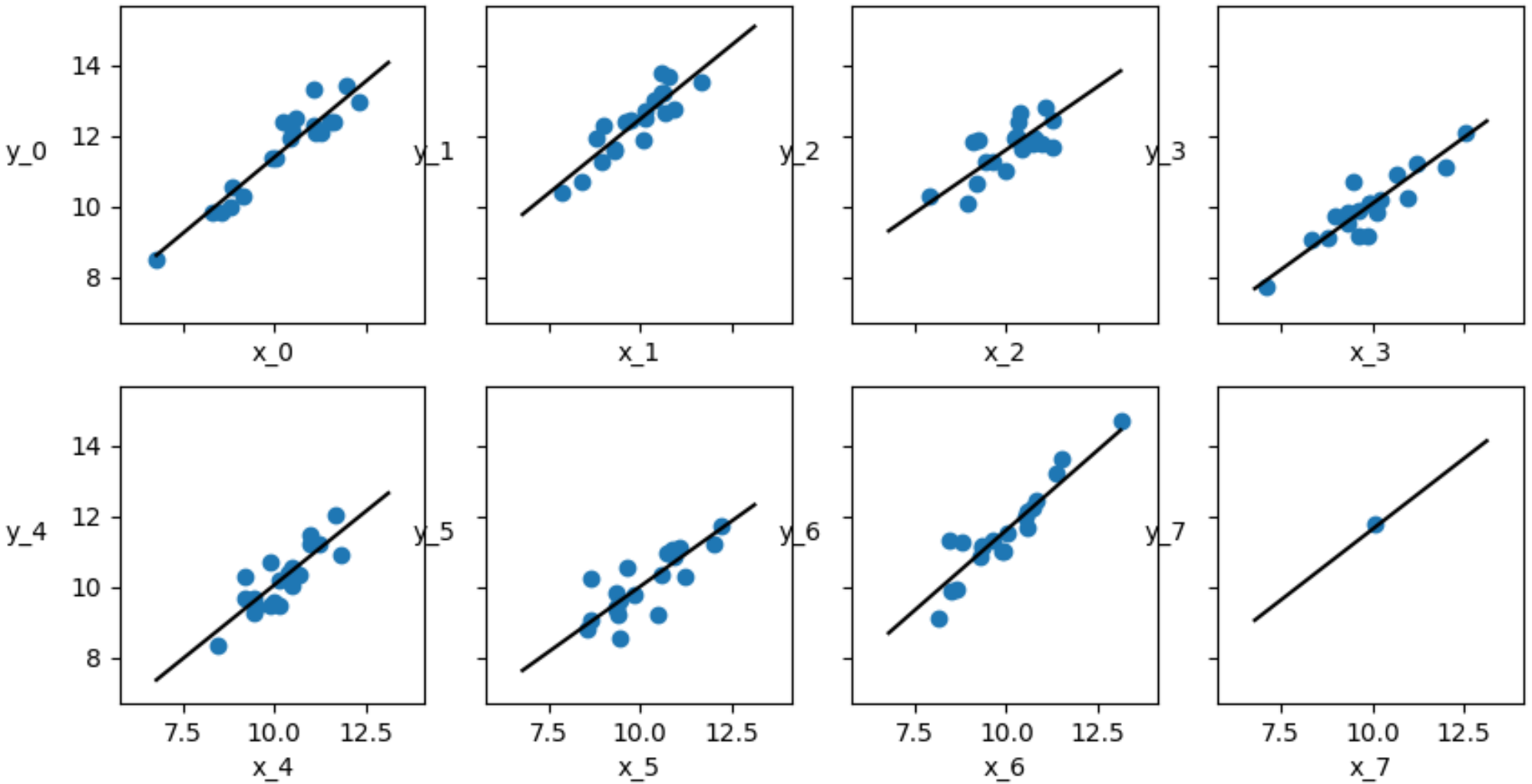
Bayesian methods for “impossible” problems






```
with pm.Model() as model_t:
    α = pm.Normal('α', mu=y_3.mean(), sigma=1)
    β = pm.Normal('β', mu=0, sigma=1)
    ϵ = pm.HalfNormal('ϵ', 5)
    ν_ = pm.Exponential('ν_', 1/29)
    ν = pm.Deterministic('ν', ν_ + 1)
    y_pred = pm.StudentT('y_pred', mu=α + β * x_3,sigma=ϵ, nu=ν, observed=y_3)
    idata_t = pm.sample(2000)
```

Bayesian methods for “impossible” problems



Decision making: ROPE

- We construct an interval (ROPE) around the hypothesis and a decision can be made by comparing the intervals of HDI (94% credible interval) and ROPE.
- Decision rules for different criteria are listed in “Bayesian Analysis with Python” by Osvaldo Martin