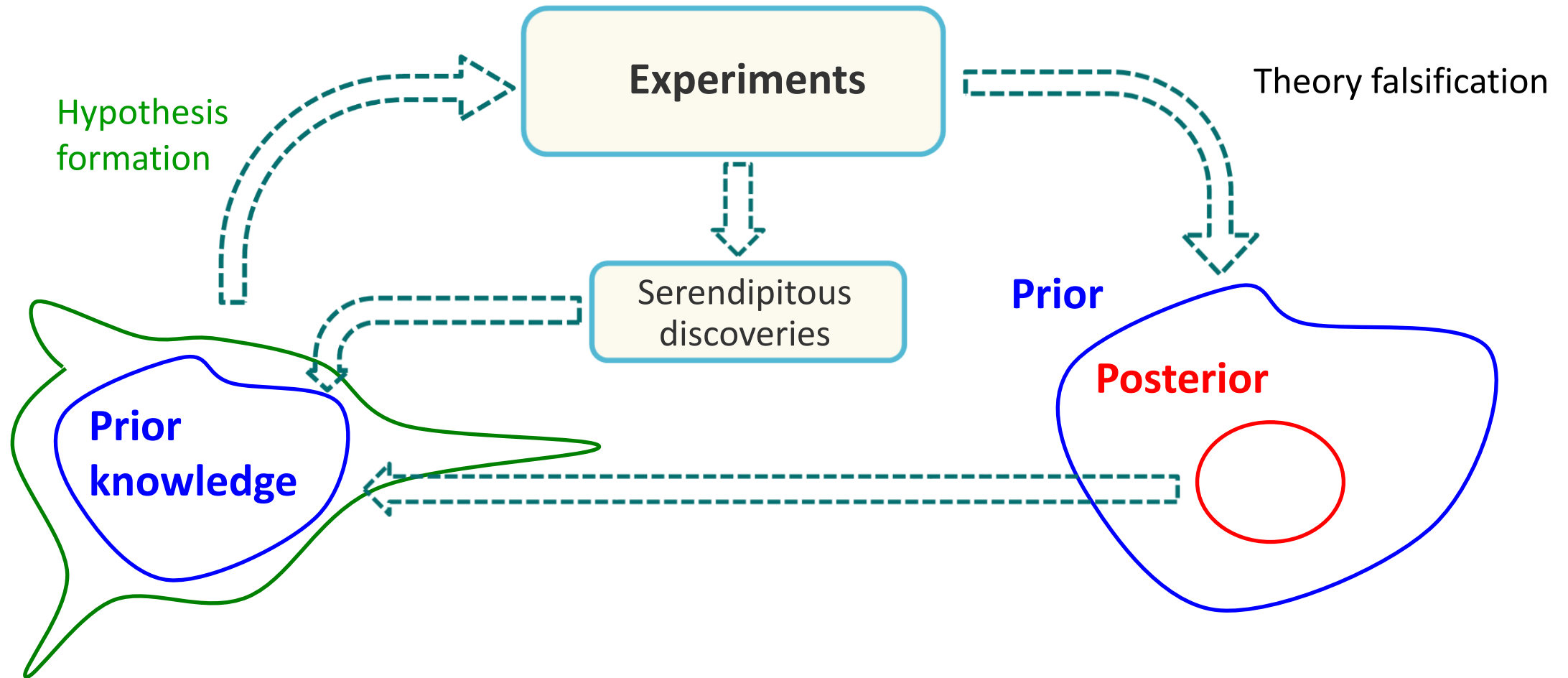


Lecture 27: Bayesian Solutions for (Linear) Real World Problems

Instructor: Sergei V. Kalinin

Where do Bayesian methods fit into R&D?



Rewards:

Policies:

Instrument development:

Hypothesis making:

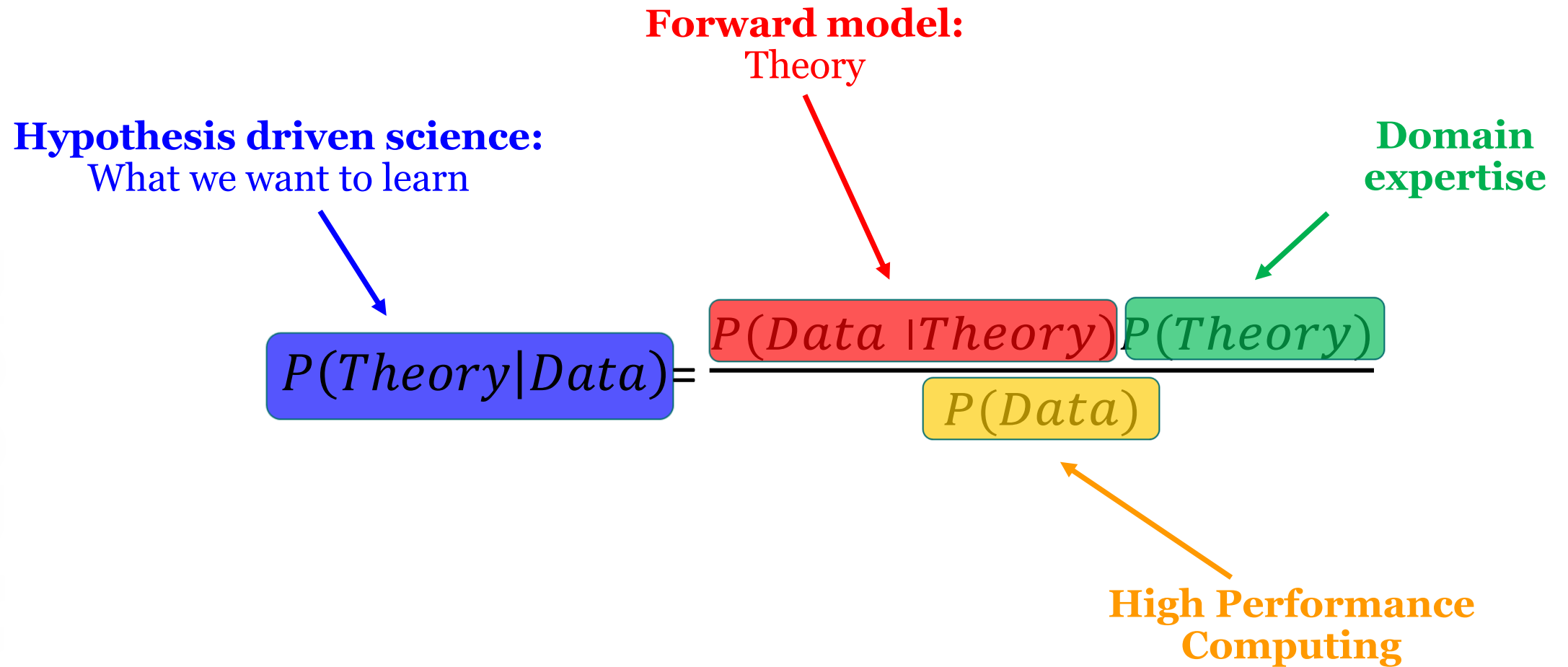
Why are we doing science/R&D?

Exploration-exploitation balance

New tools create new opportunities

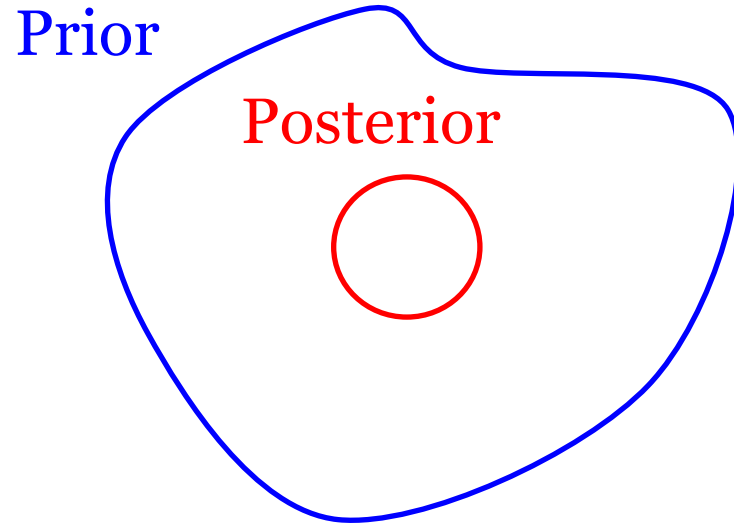
Extrapolation into the unknown

How does it work?

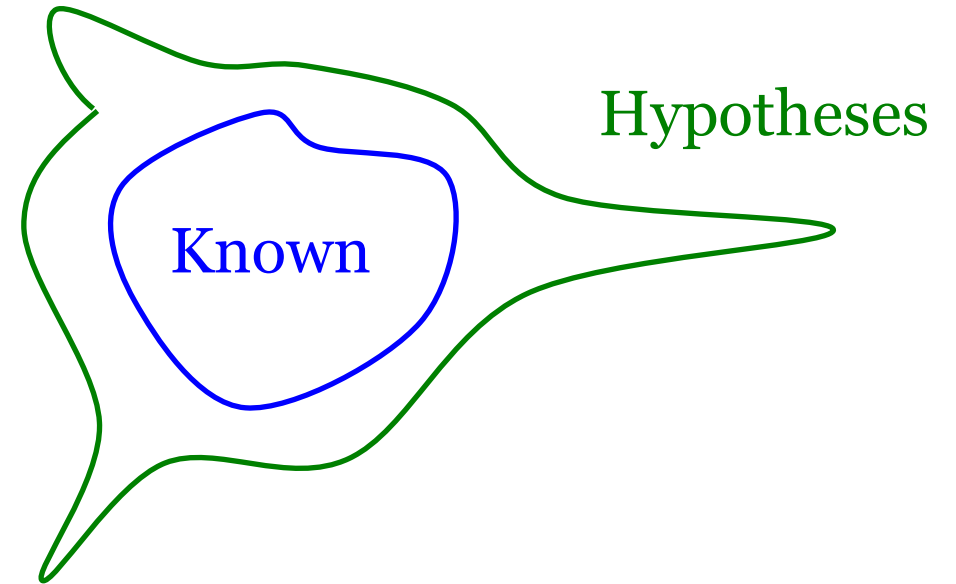


Experimentalists know the priors. Albeit they do not know that they know it, or how to convert them to algorithmic form

What Bayesian Methods (and ML) cannot do?

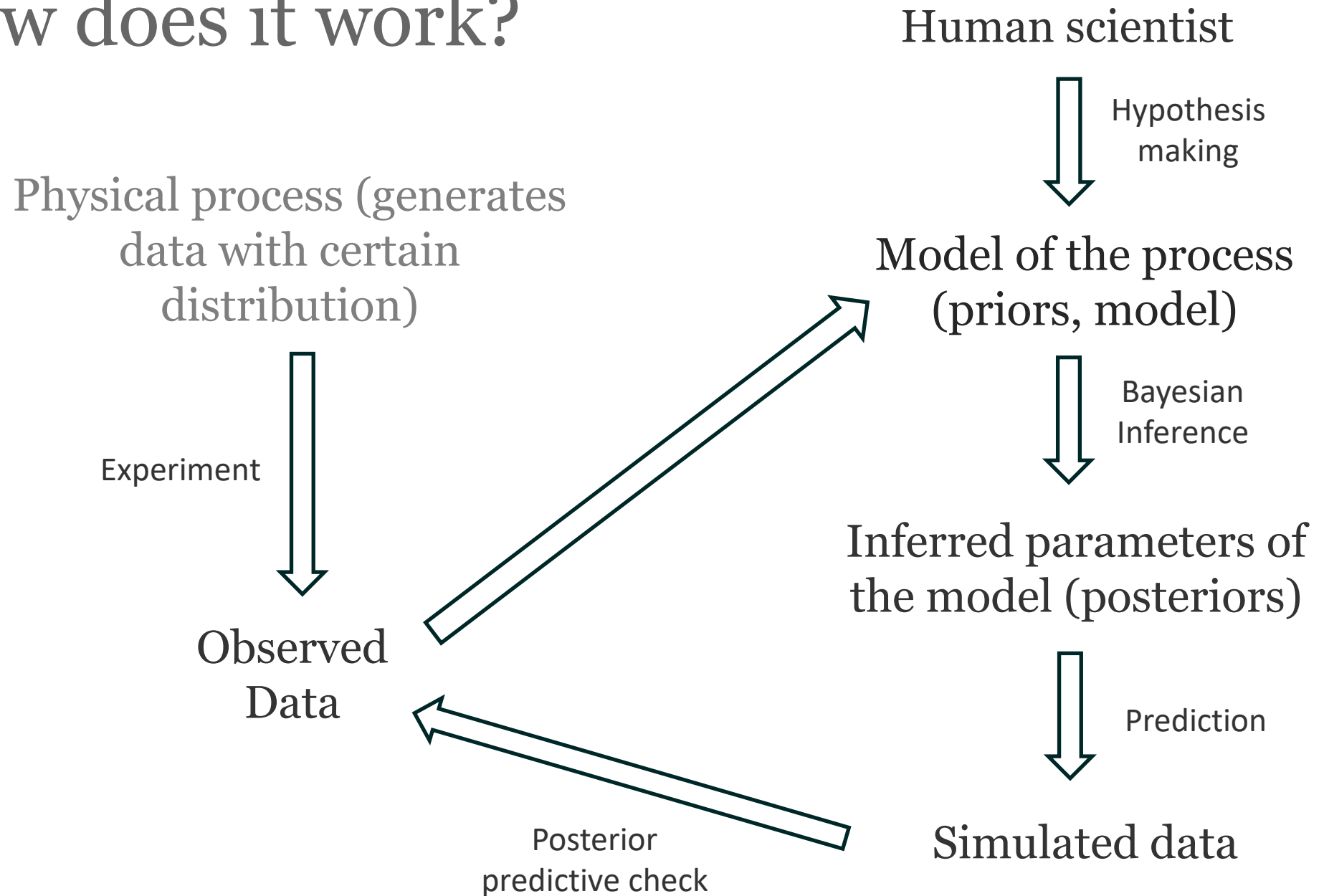


Refinement:
Can be defined as probabilistic model



Hypothesis formation:
How can we do it?

How does it work?



When Bayes is easy

- 1. Beta distribution is conjugate to the Binomial likelihood:** This means that if you have a Binomial likelihood (e.g., flipping coins) and a Beta-distributed prior on the probability of heads, the resulting posterior distribution after observing some data will also be a Beta distribution.
- 2. Gamma distribution is conjugate to the Poisson likelihood:** If you're observing the number of events occurring in fixed intervals of time or space (modeled by a Poisson distribution) and have a Gamma-distributed prior on the rate parameter, the posterior will also be Gamma-distributed.
- 3. Normal distribution is conjugate to itself:** If both the likelihood and the prior are normally distributed, then the posterior will also be normally distributed.

Used to be biggest problem for Bayesian analysis – we **could** only solve simplest problems, or force real world problems into oversimplified frameworks

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

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

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.

Metropolis-Hastings algorithm

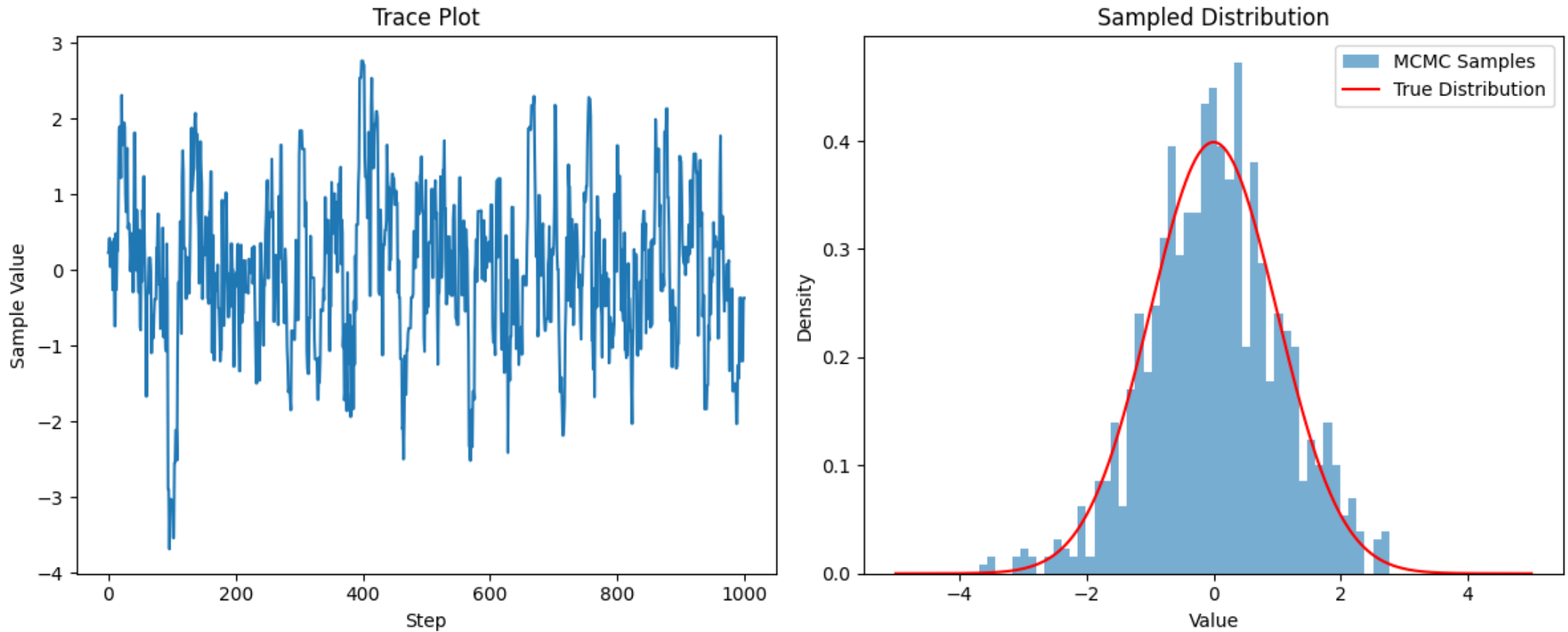
We don't need to evaluate any integral, *we just sample from the distribution many times* (e.g., 50K times) and find (estimate) the posterior mean, middle 95%, etc., from that.

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

$$\theta^{(1)} = \begin{cases} \theta' & \text{with probability } \alpha \\ \theta^{(0)} & \text{with probability } 1 - \alpha \end{cases}$$

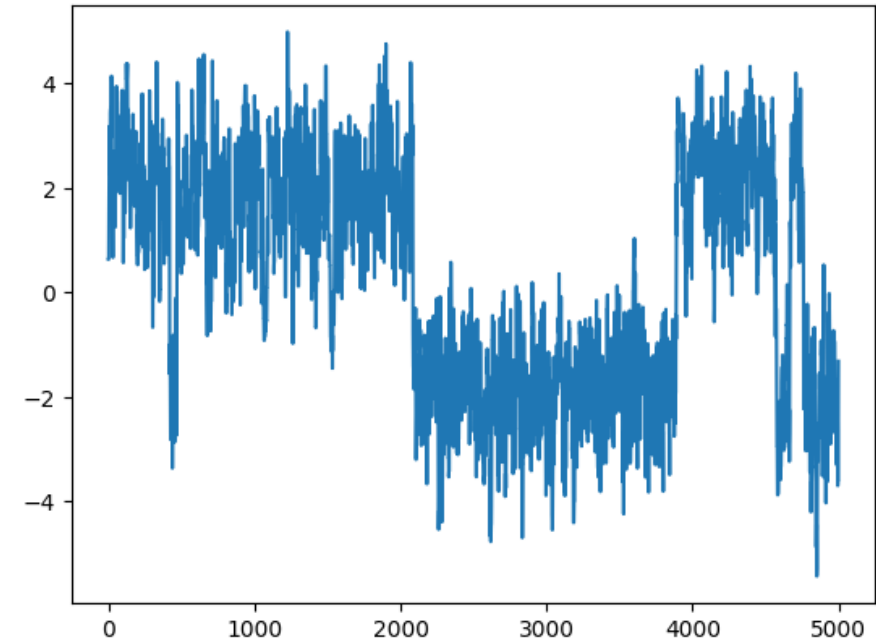
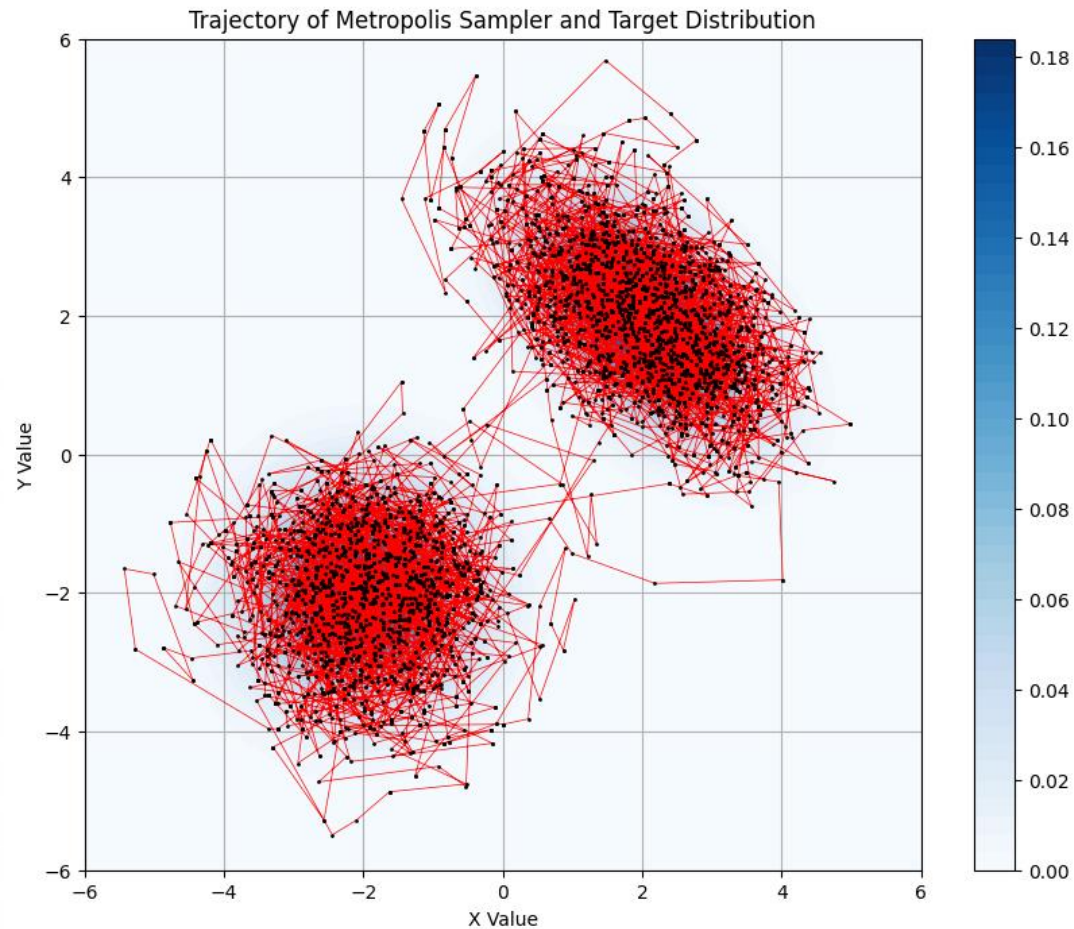
$$\text{where } \alpha = \min \left(1, \frac{\pi(\theta')}{\pi(\theta^{(0)})} \right)$$

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

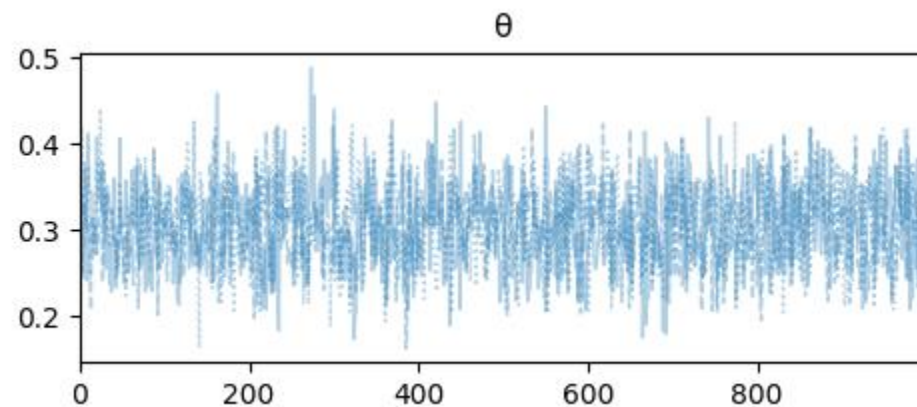
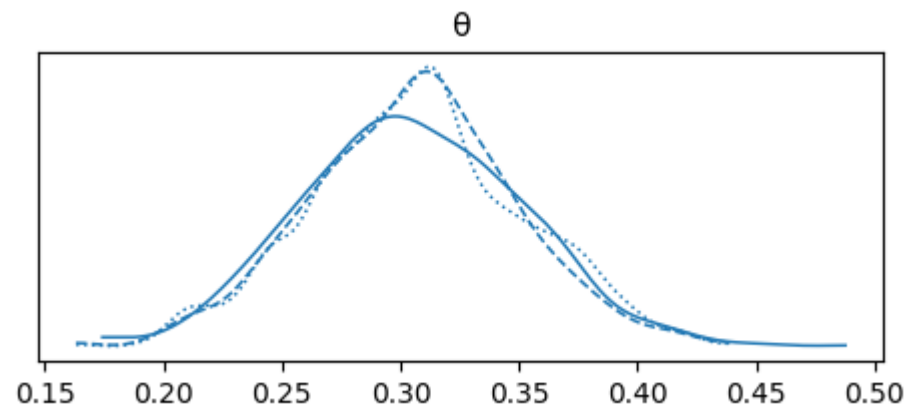
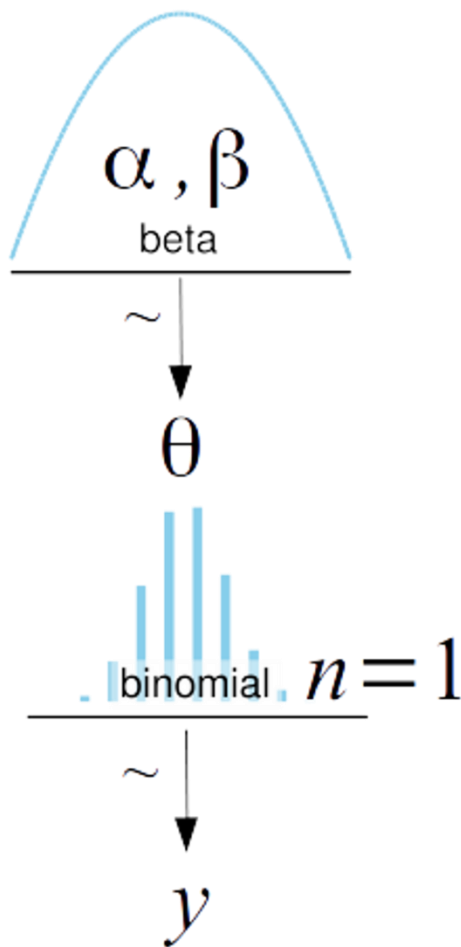
Let's toss a coin!



Colab: 19_PYMC_BayesianEZ.ipynb

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

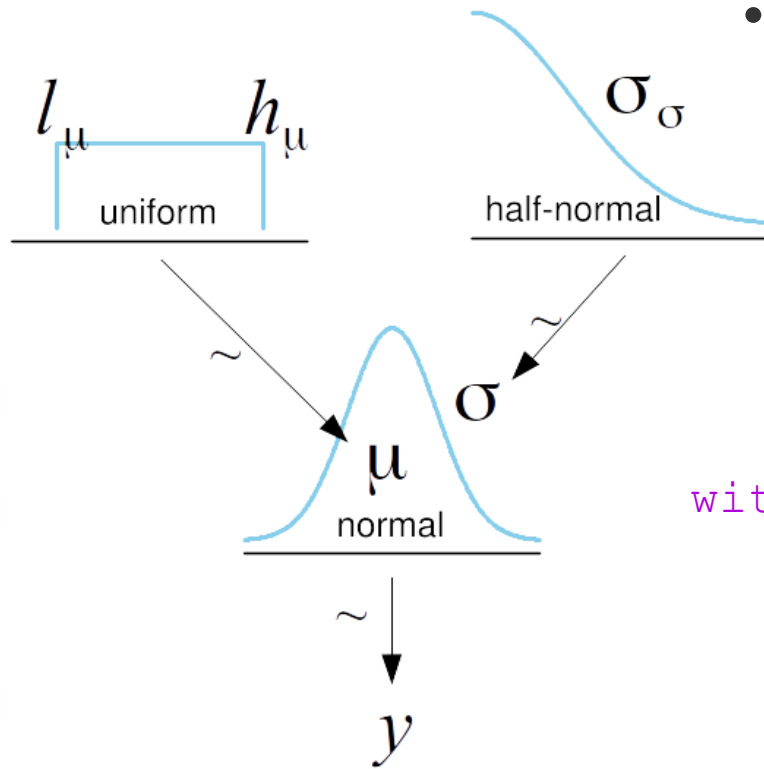
```
with pm.Model() as our_first_model:  
     $\theta$  = pm.Beta('θ', alpha=1., beta=1.)  
    y = pm.Bernoulli('y', p= $\theta$ , observed=data)  
    trace = pm.sample(1000, random_seed=123, chains = 3)
```



Colab: 19_PYMC_BayesianEZ.ipynb

But how do we get physics done?

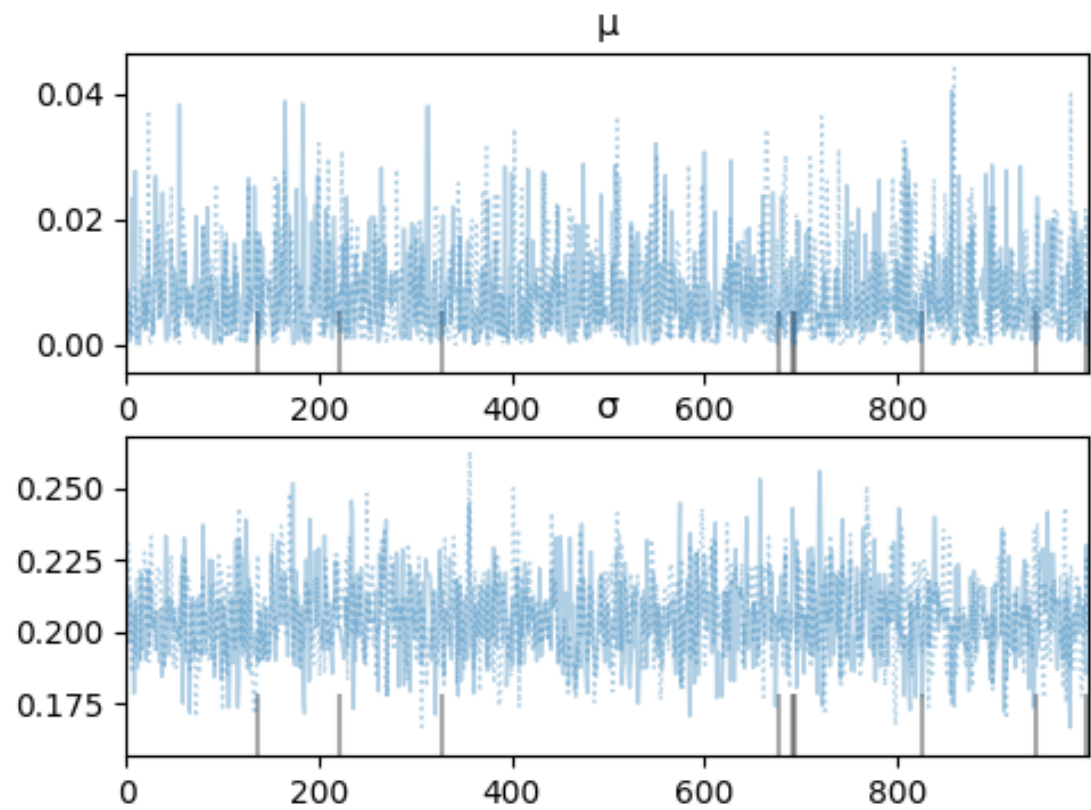
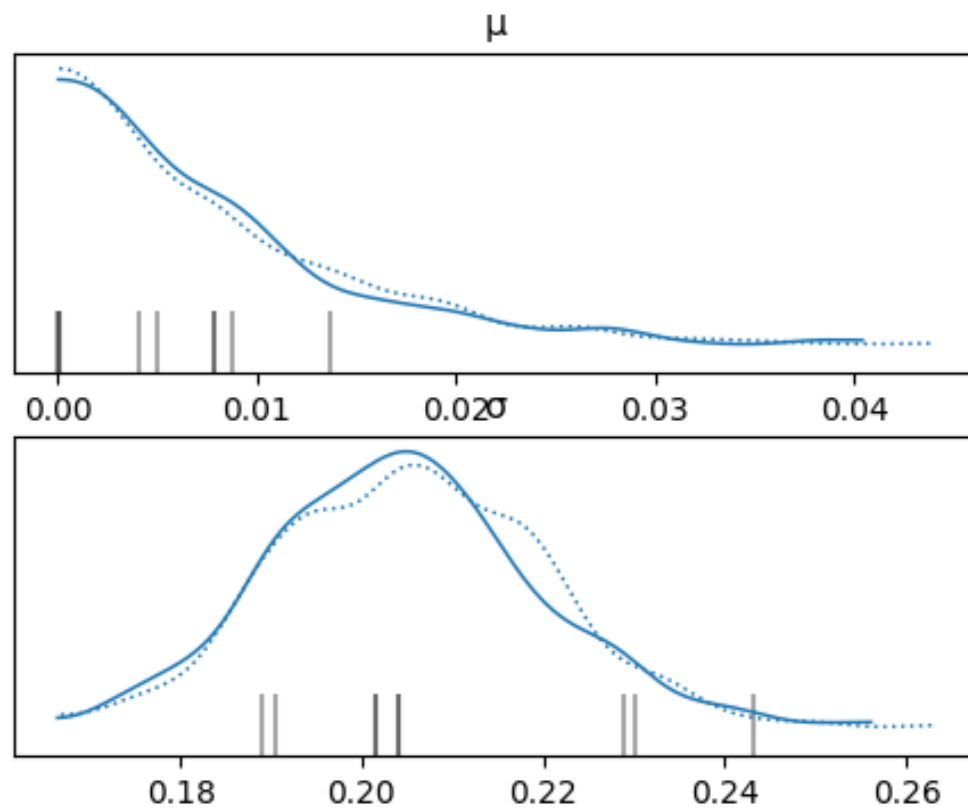
- Imagine that we have some observational data
- Can we say which distribution has it come from?



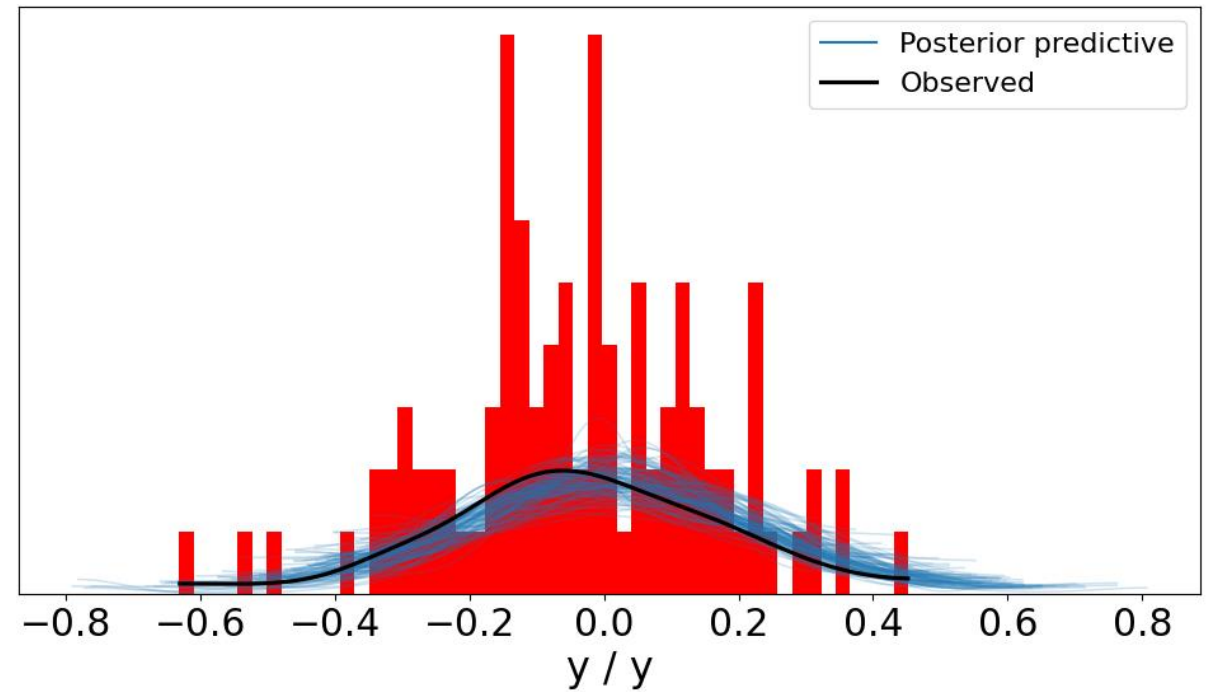
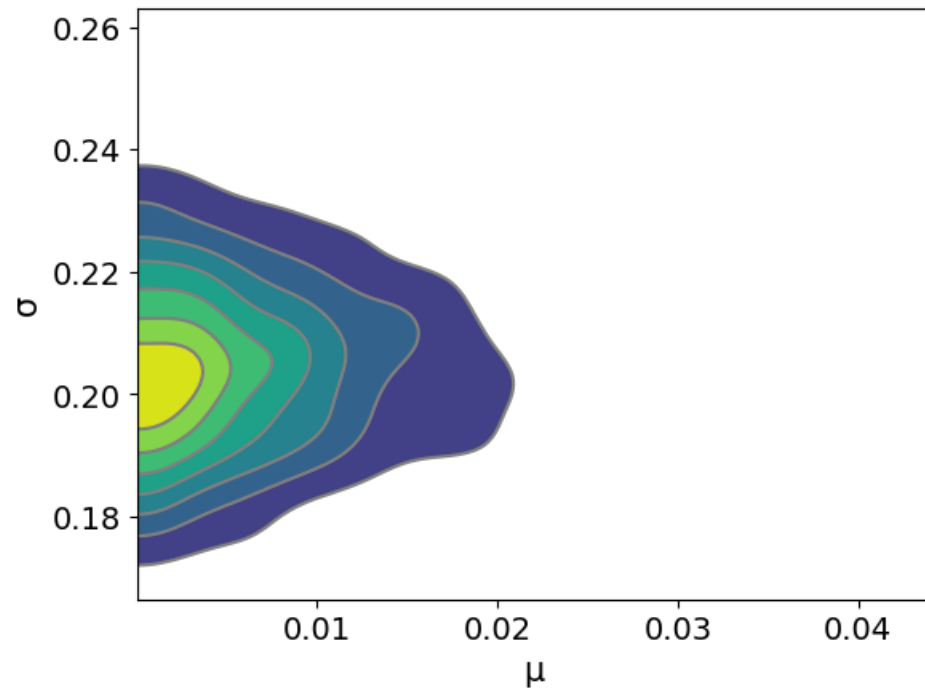
Define Bayesian model!

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


Presto!

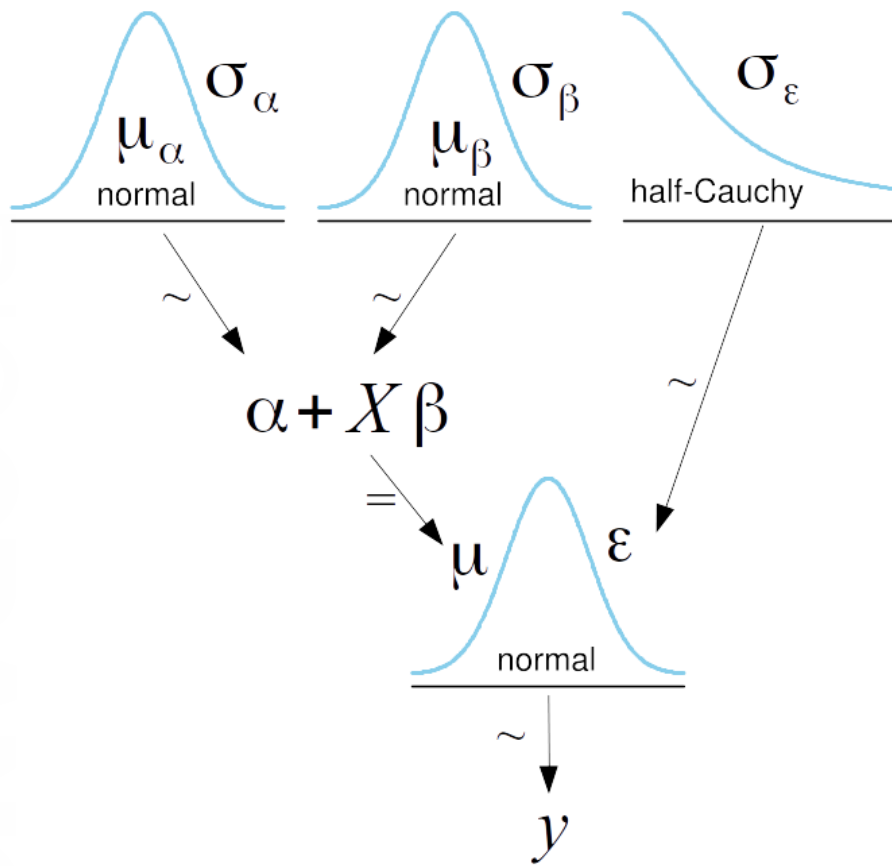


Presto!



Linear regression Bayesian style

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



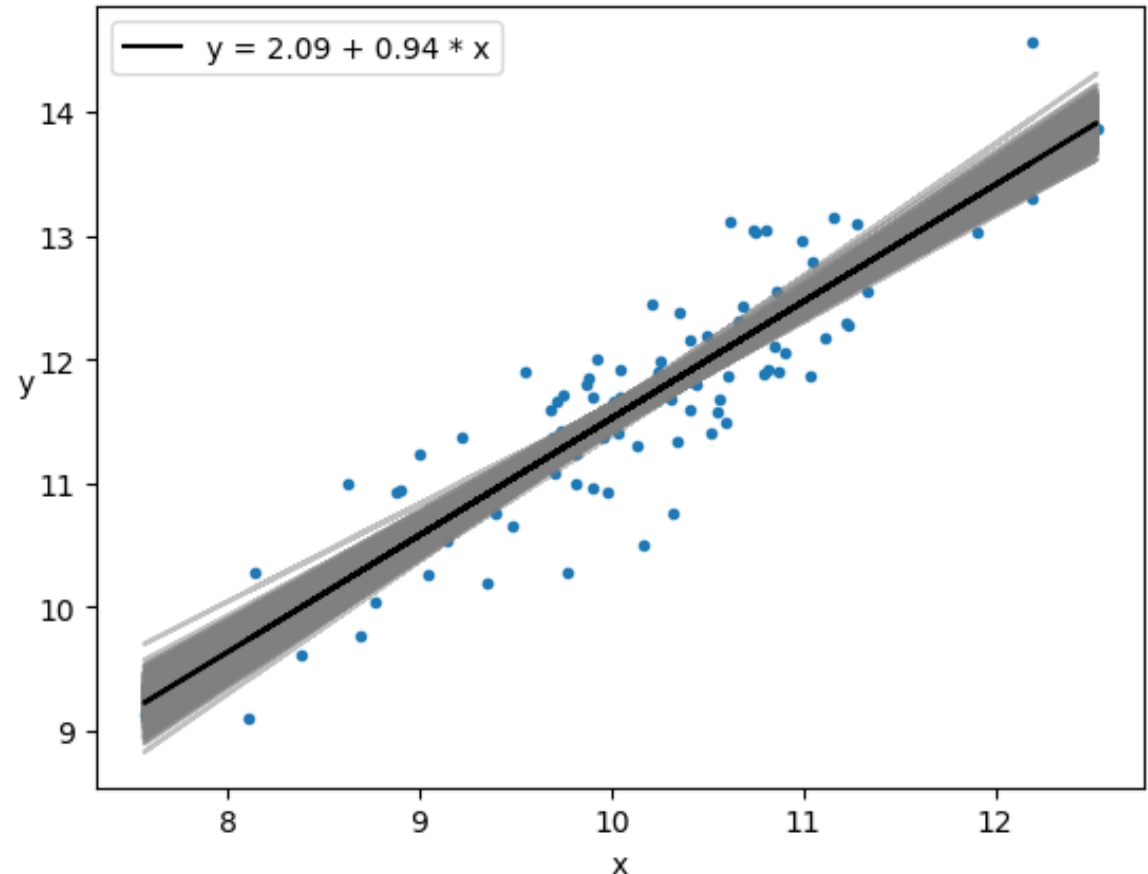
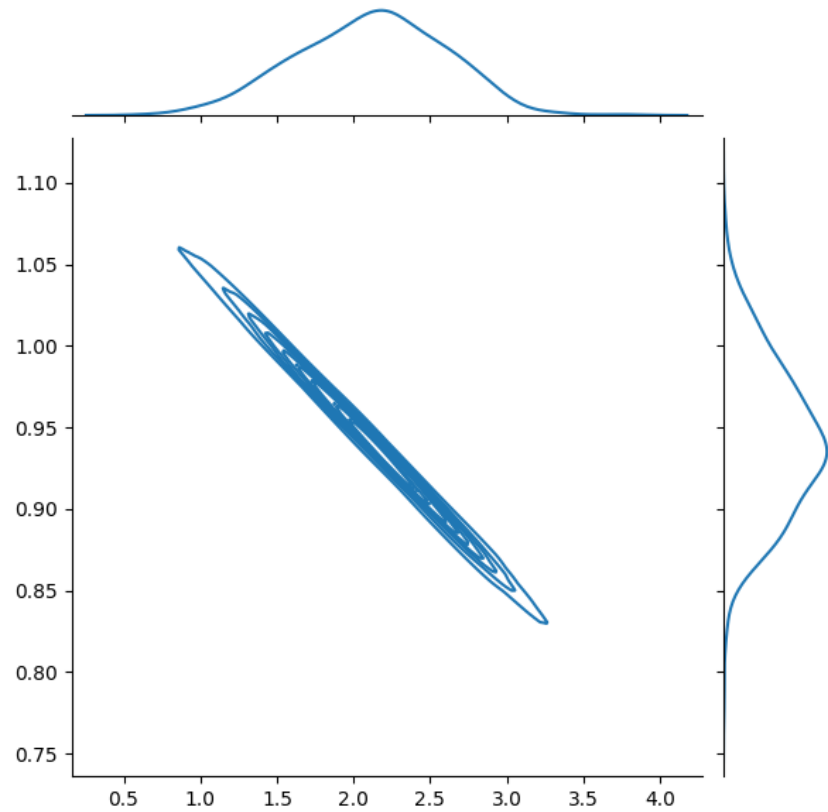
Define Bayesian model!

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

     $\mu$  = pm.Deterministic('μ',  $\alpha$  +  $\beta$  * x)
    y_pred = pm.Normal('y_pred', mu= $\mu$ ,
                       sigma= $\epsilon$ , observed=y)

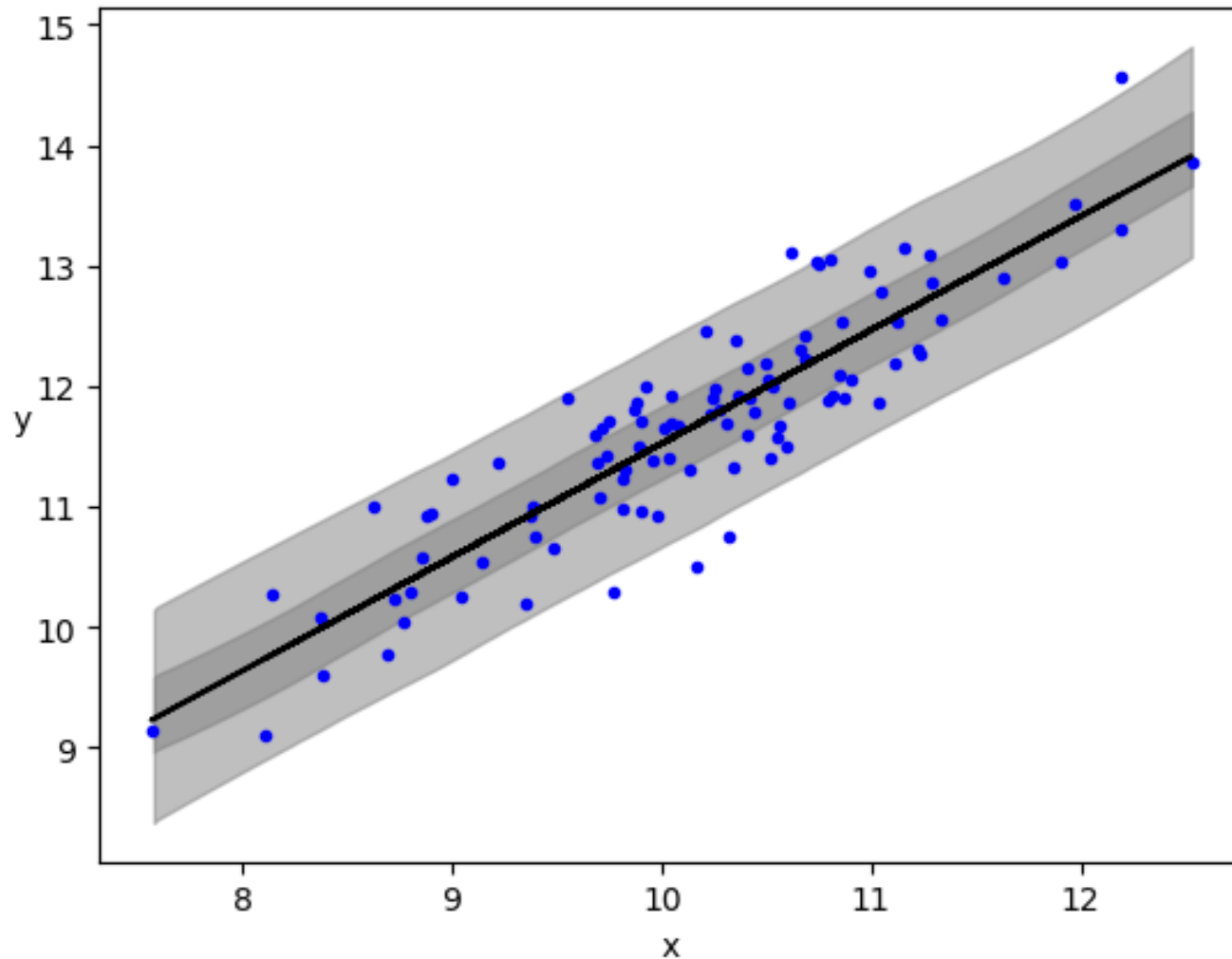
idata_g = pm.sample(2000, tune=2000)
```


The outputs?



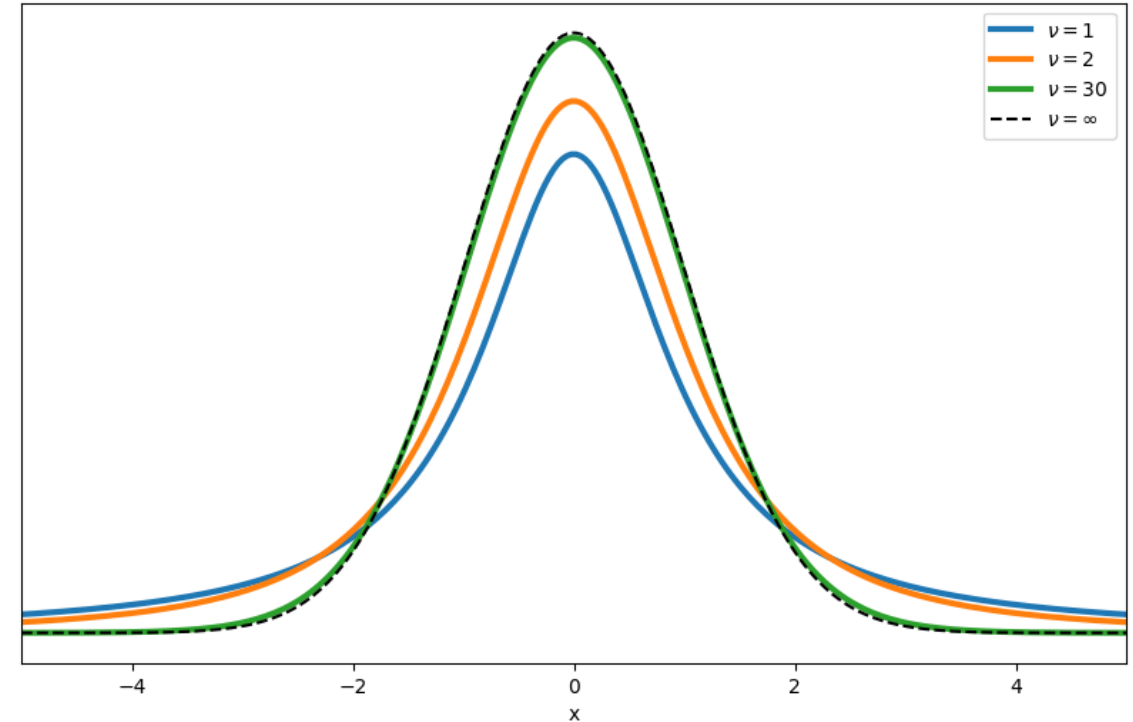
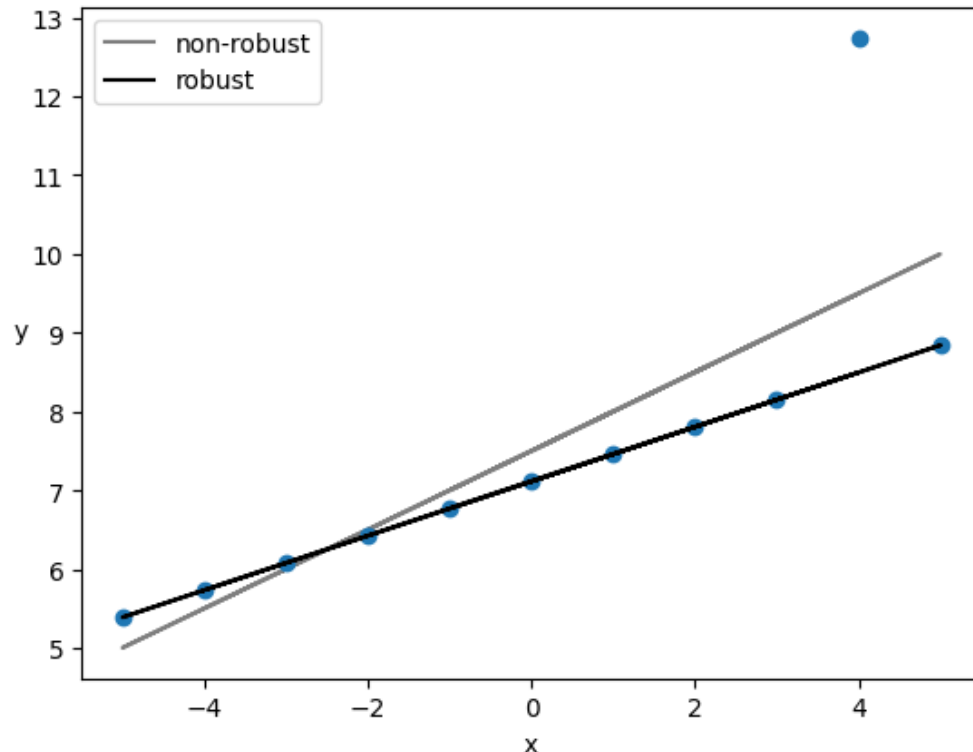
- The output of the Bayesian model will be draws for the slope and offset: families of lines consistent with data
- We can analyze their joint distribution
- And plot these lines

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:
     $\alpha$  = pm.Normal(' $\alpha$ ', mu=y_3.mean(), sigma=1)
     $\beta$  = pm.Normal(' $\beta$ ', mu=0, sigma=1)
     $\epsilon$  = pm.HalfNormal(' $\epsilon$ ', 5)
     $\nu_{\text{_}}$  = pm.Exponential(' $\nu_{\text{_}}$ ', 1/29)
     $\nu$  = pm.Deterministic(' $\nu$ ',  $\nu_{\text{_}}$  + 1)
    y_pred = pm.StudentT('y_pred', mu= $\alpha$  +  $\beta$  * x_3, sigma= $\epsilon$ , nu= $\nu$ , observed=y_3)
    idata_t = pm.sample(2000)
```

Bayesian methods for “impossible” problems

