Machine Learning + Statistics: Better Together Than Apart

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https://github.com/dhuppenkothen/cargese2018_tutorials

All models are wrong,
but some are useful.

— George Box

Iterative Understanding of Nature

Iterative Understanding of Nature

- Experimental Design

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- Experimental Design
- Data Collection

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- Model Formulation

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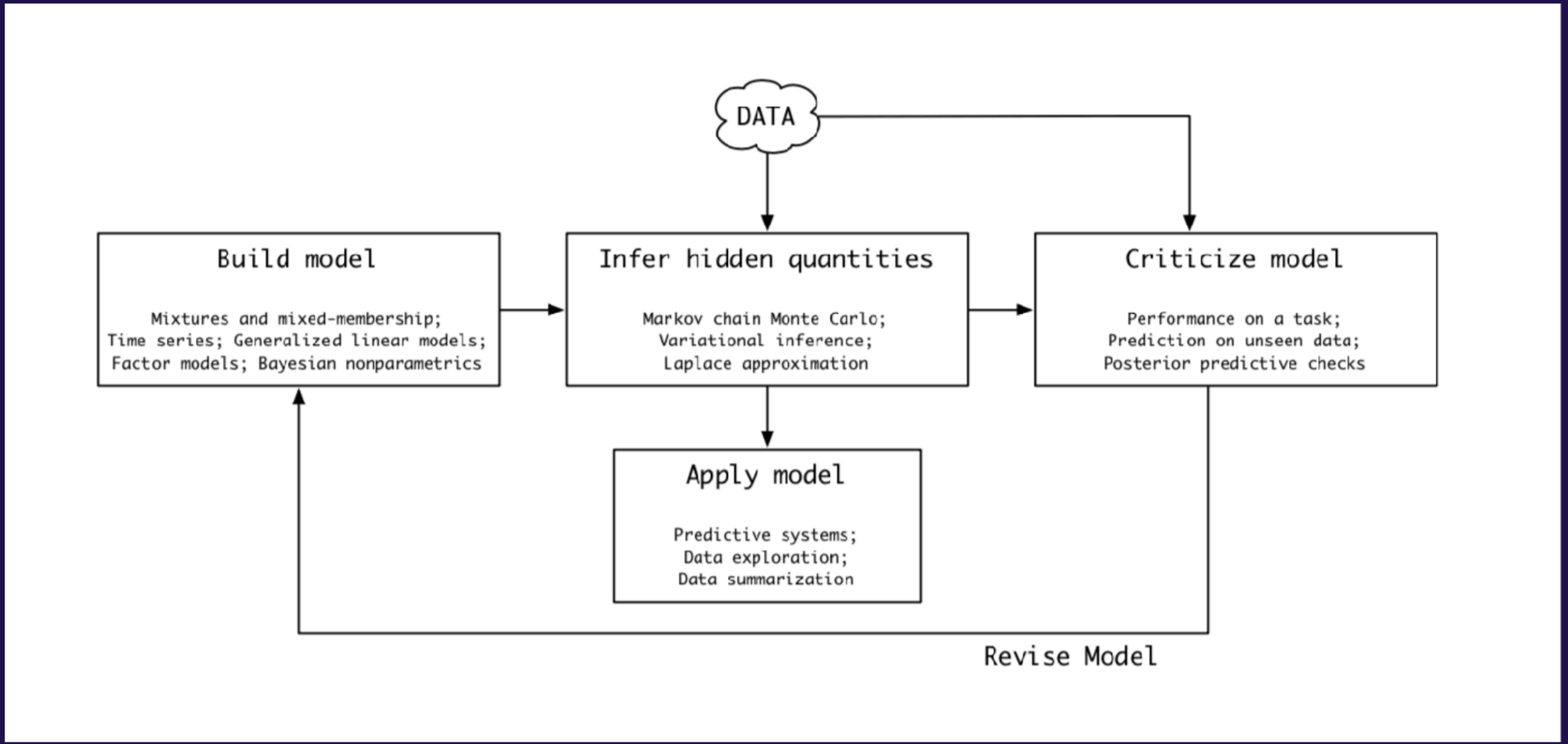

DATA
Build model
Mixtures and mixed-membership;
Time series; Generalized linear models;
Factor models; Bayesian nonparametrics
Infer hidden quantities
Markov chain Monte Carlo;
Variational inference;
Laplace approximation
Criticize model
Performance on a task;
Prediction on unseen data;
Posterior predictive checks
Apply model
Predictive systems;
Data exploration;
Data summarization
Revise Model

Blei (2014)

Building + Revising Models

Building + Revising Models Part III

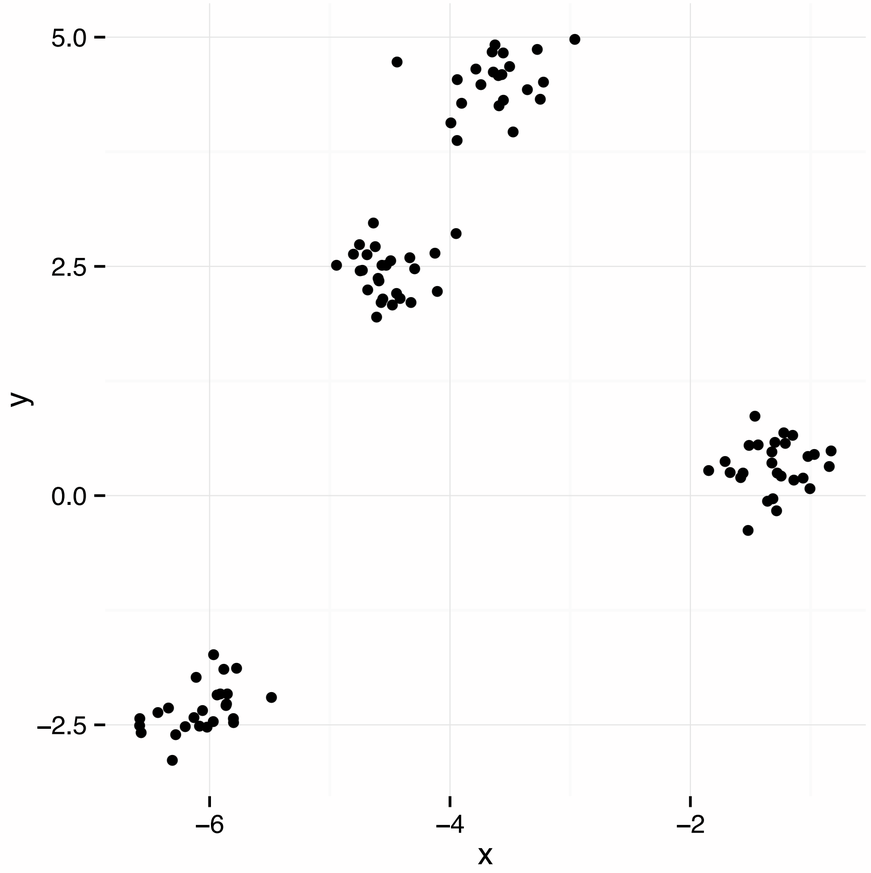
Building + Revising Models Part III (sort of)

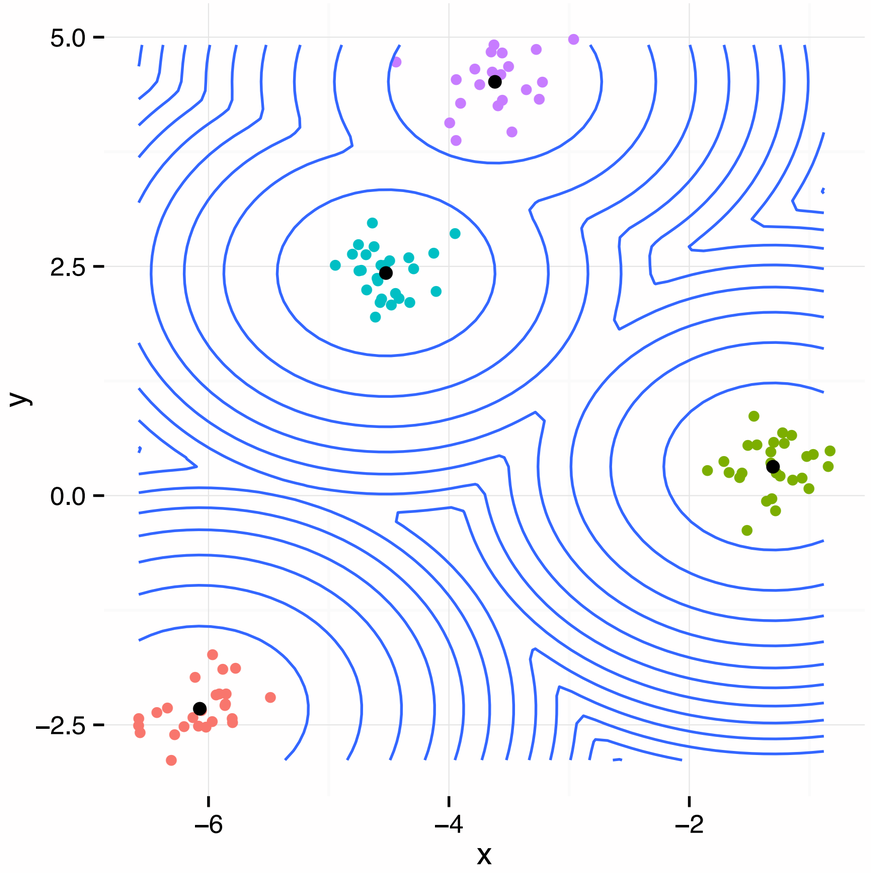
Wednesday: Bayesian Hierarchical Models

Yesterday: Machine Learning

Today: Both!

Gaussian Mixture Models





Blei (2014)

(1) The Generative Process

1. Draw mixture proportions $\theta \sim \text{Dirichlet}(\alpha)$
2. For each mixture component k, draw $\mu_k \sim \mathcal{N}(0, \sigma^2)$
3. For each data point i:
   a. Draw mixture assignment $z_i \mid \theta \sim \text{Discrete}(\theta)$
   b. Draw data point $x_i \mid z_i, \mu \sim \mathcal{N}(\mu_{z_i}, 1)$

(2) The Joint Probability Distribution

$$p(\theta, \mu, z, x \mid \sigma_0^2, \alpha) = p(\theta \mid \alpha) \prod_{k=1}^{K} p(\mu_k \mid \sigma_0^2) \prod_{i=1}^{N} (p(z_i \mid \theta) p(x_i \mid z_i, \mu, z_i))$$

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cluster proportions

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cluster proportions

Gaussian means

cluster assignments

data points

(2) The Joint Probability Distribution

Dirichlet

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cluster proportions

Gaussian means

cluster assignments

data points

(2) The Joint Probability Distribution

Dirichlet Normal

$$p(\theta, \mu, z, x \mid \sigma_0^2, \alpha) = p(\theta \mid \alpha) \prod_{k=1}^{K} p(\mu_k \mid \sigma_0^2) \prod_{i=1}^{N} (p(z_i \mid \theta) p(x_i \mid z_i, \mu, z_i))$$

cluster proportions

Gaussian means

cluster assignments

data points

(2) The Joint Probability Distribution

Dirichlet Normal Discrete

$$p(\theta, \mu, z, x \mid \sigma_0^2, \alpha) = p(\theta \mid \alpha) \prod_{k=1}^{K} p(\mu_k \mid \sigma_0^2) \prod_{i=1}^{N} (p(z_i \mid \theta) p(x_i \mid z_i, \mu, z_i))$$

cluster proportions

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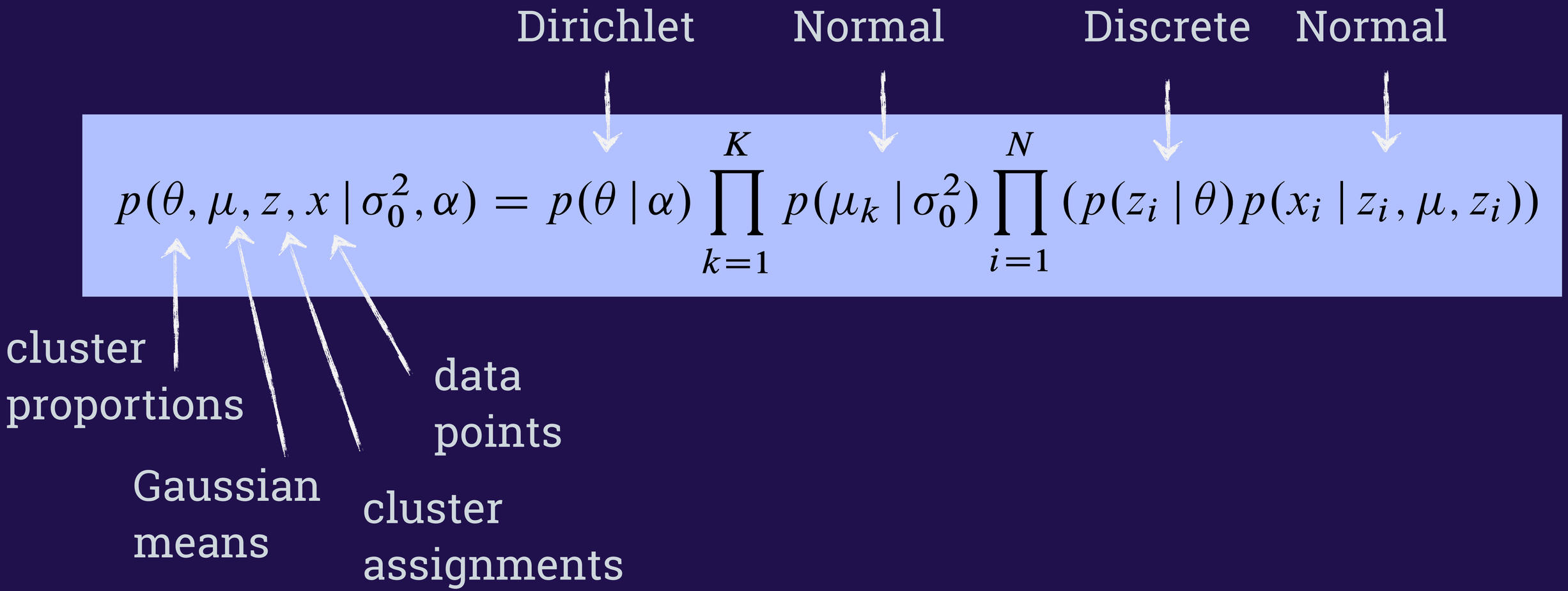


(3) The Probabilistic Graphical Model

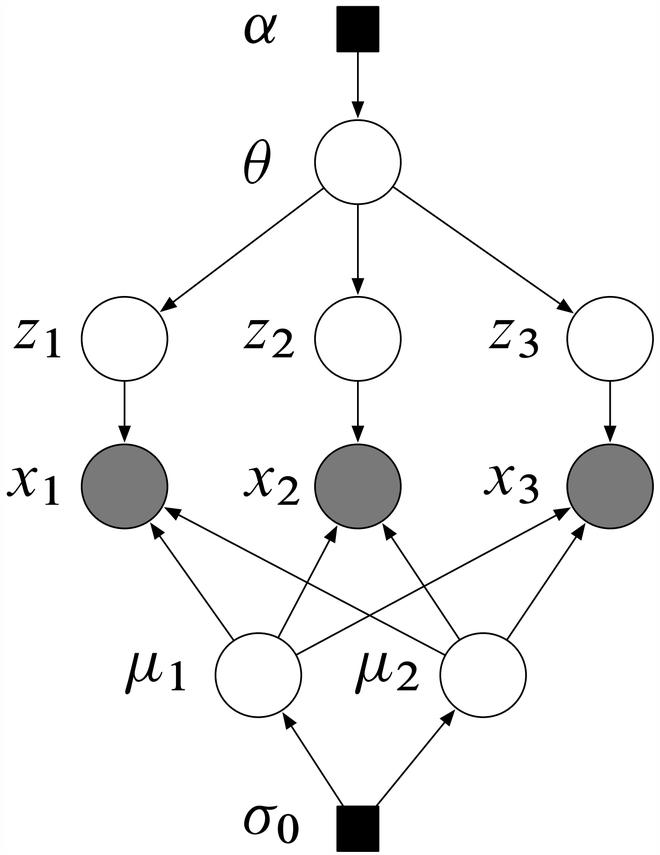
Exercise: Can you draw a graphical model for the Gaussian Mixture Model?

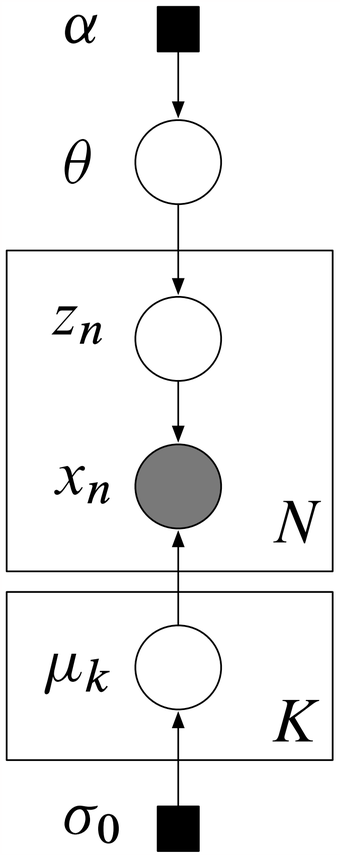
Blei (2014)

(3) The Probabilistic Graphical Model

Blei (2014)

(3) The Probabilistic Graphical Model





$\sim \text{Dirichlet}_K(\alpha)$

$\sim \text{Discrete}(\theta)$

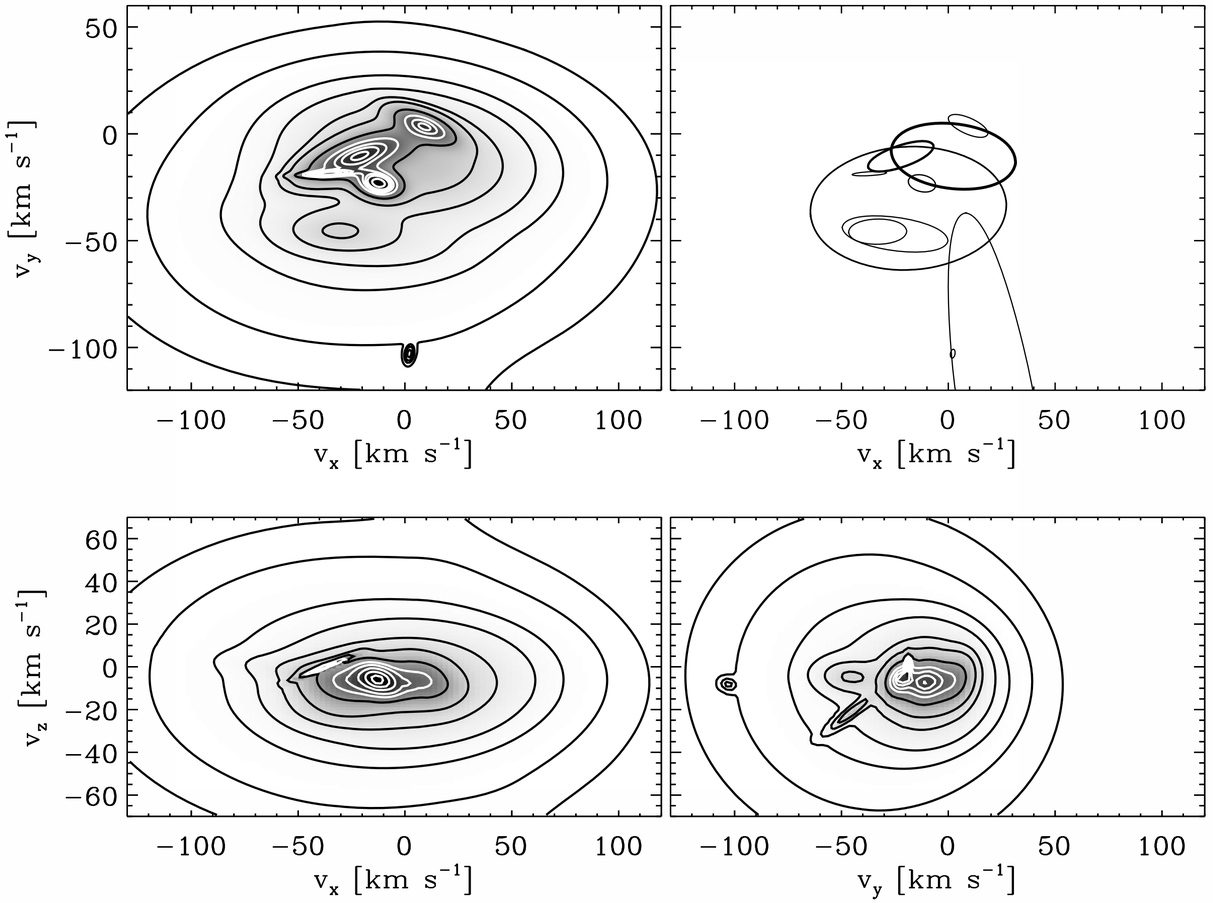
$\sim \mathcal{N}(\mu_{z_n}, \sigma^2)$

$\sim \mathcal{N}(0, \sigma_0^2)$

Blei (2014)

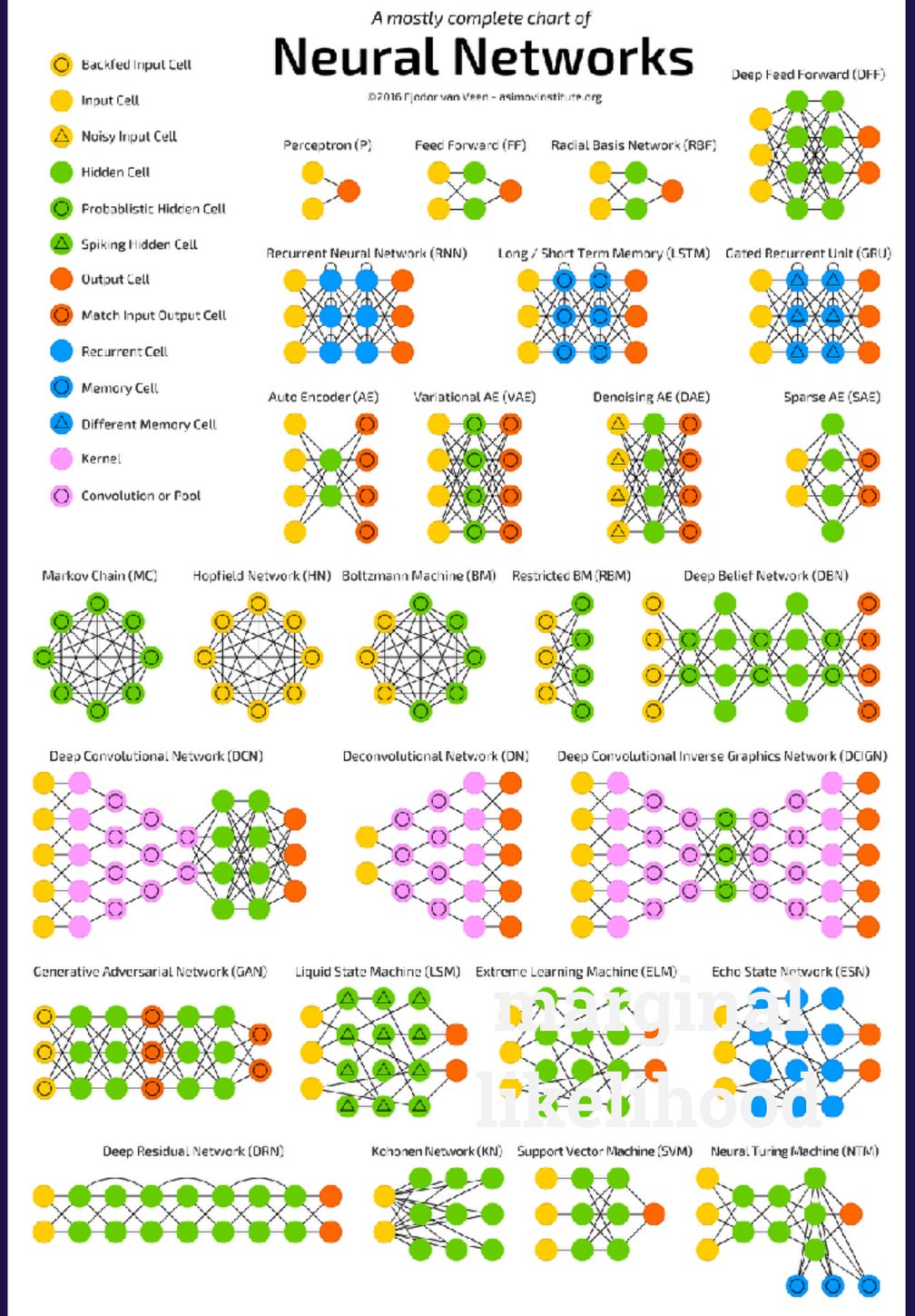
Measurement Uncertainties?
Missing Data?

Extreme Deconvolution



Bovy et al (2009)

Neural Networks + Probabilistic Models



Fjodor van Veen; https://towardsdatascience.com/the-mostly-complete-chart-of-neural-networks-explained-3fb6f2367464

https://playground.tensorflow.org

Using Neural Networks as Emulators

posterior

likelihood

prior

$$P(\theta \mid x) = \frac{P(x \mid \theta) P(\theta)}{P(x)}$$

marginal likelihood

black box
simulator
~~likelihood~~

posterior

prior

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marginal
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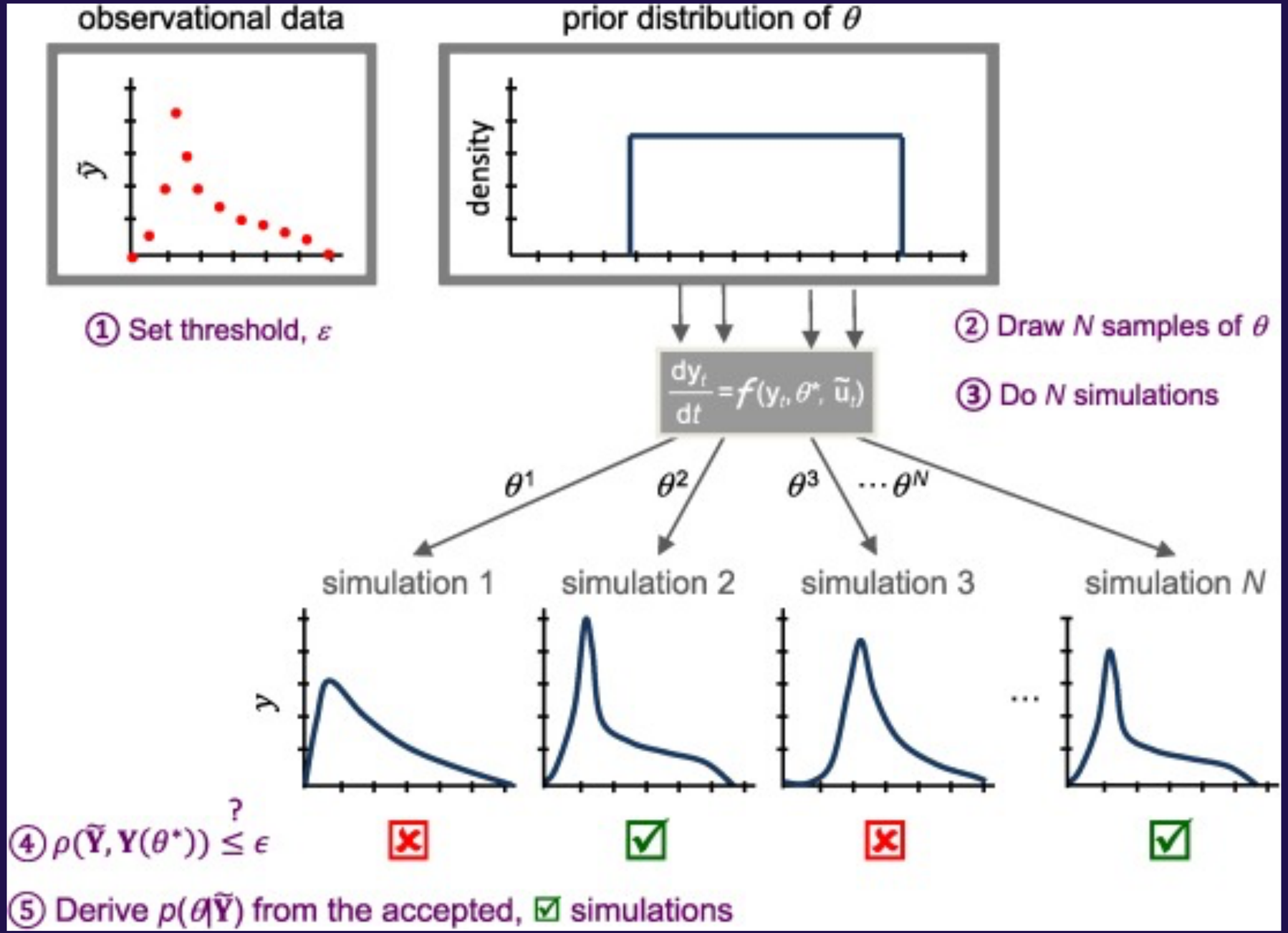
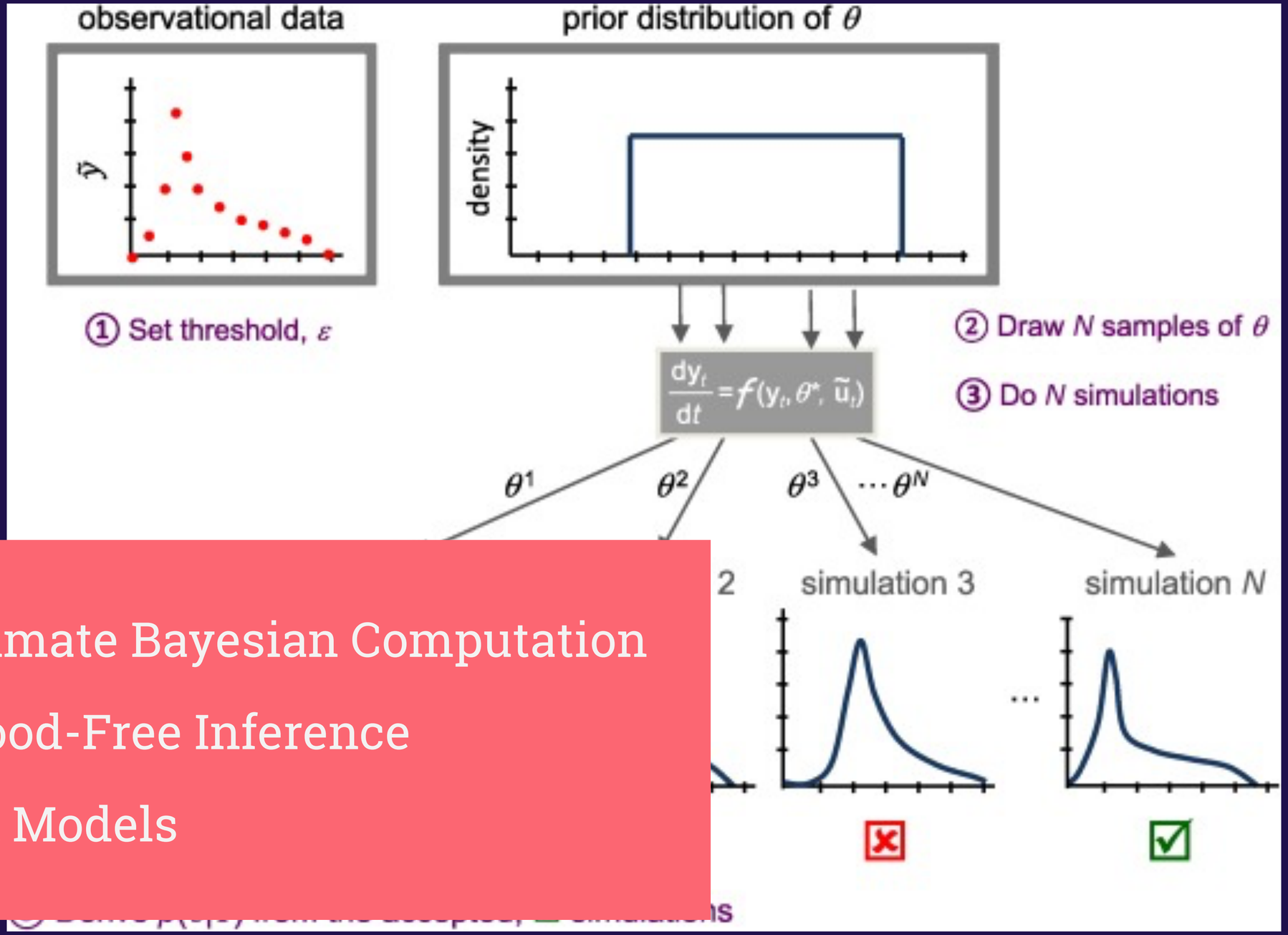
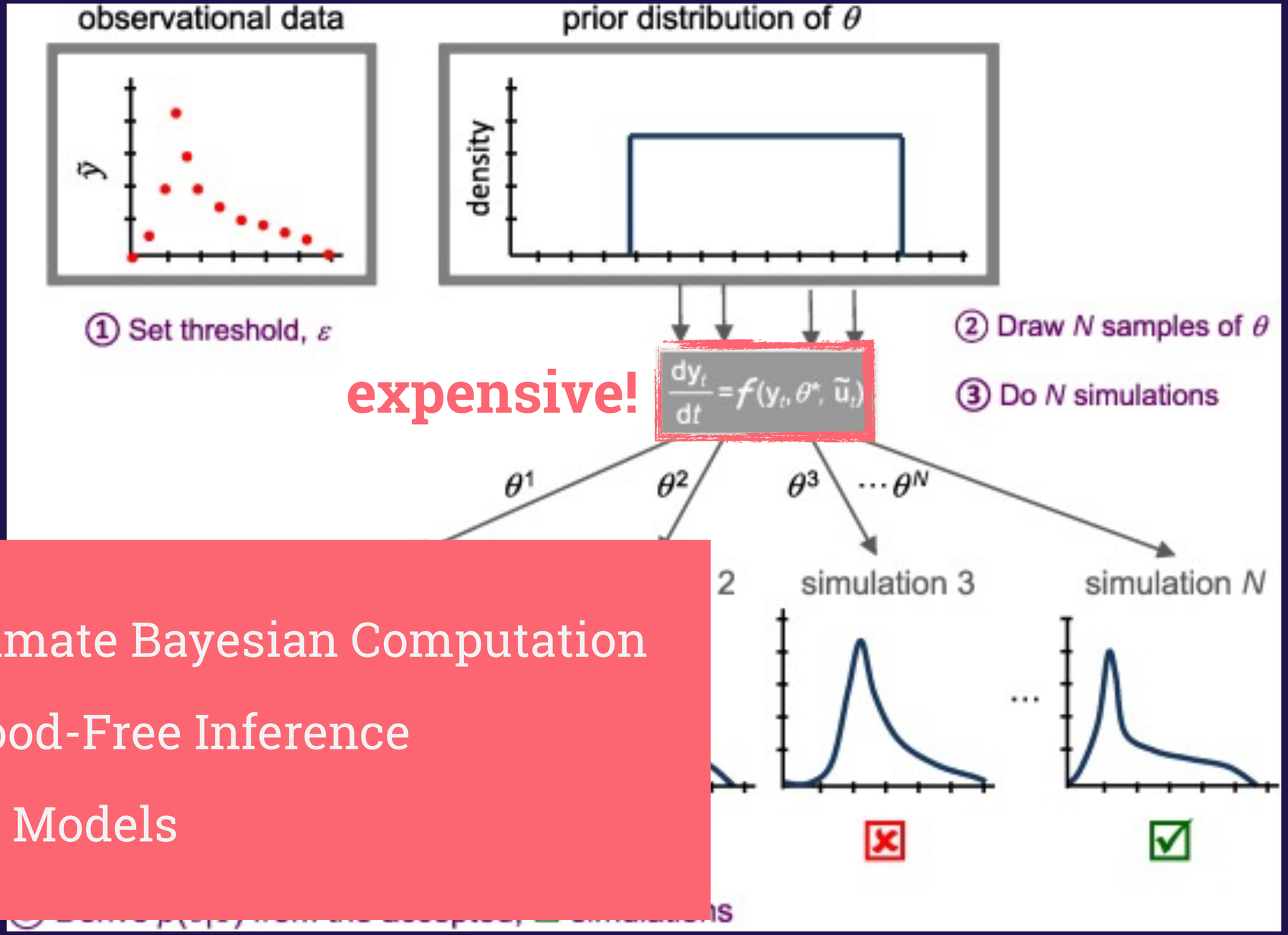

observational data
prior distribution of θ
density
① Set threshold, ε
② Draw N samples of θ
③ Do N simulations
dy_t/dt = f(y_t, θ*, ũ_t)
θ1
θ2
θ3
⋯ θN
simulation 1
simulation 2
simulation 3
simulation N
④ ρ(Ỹ, Y(θ*)) ≤ ε ?
⑤ Derive p(θ|Ỹ) from the accepted, ☑ simulations



Approximate Bayesian Computation

Likelihood-Free Inference

Implicit Models



Approximate Bayesian Computation

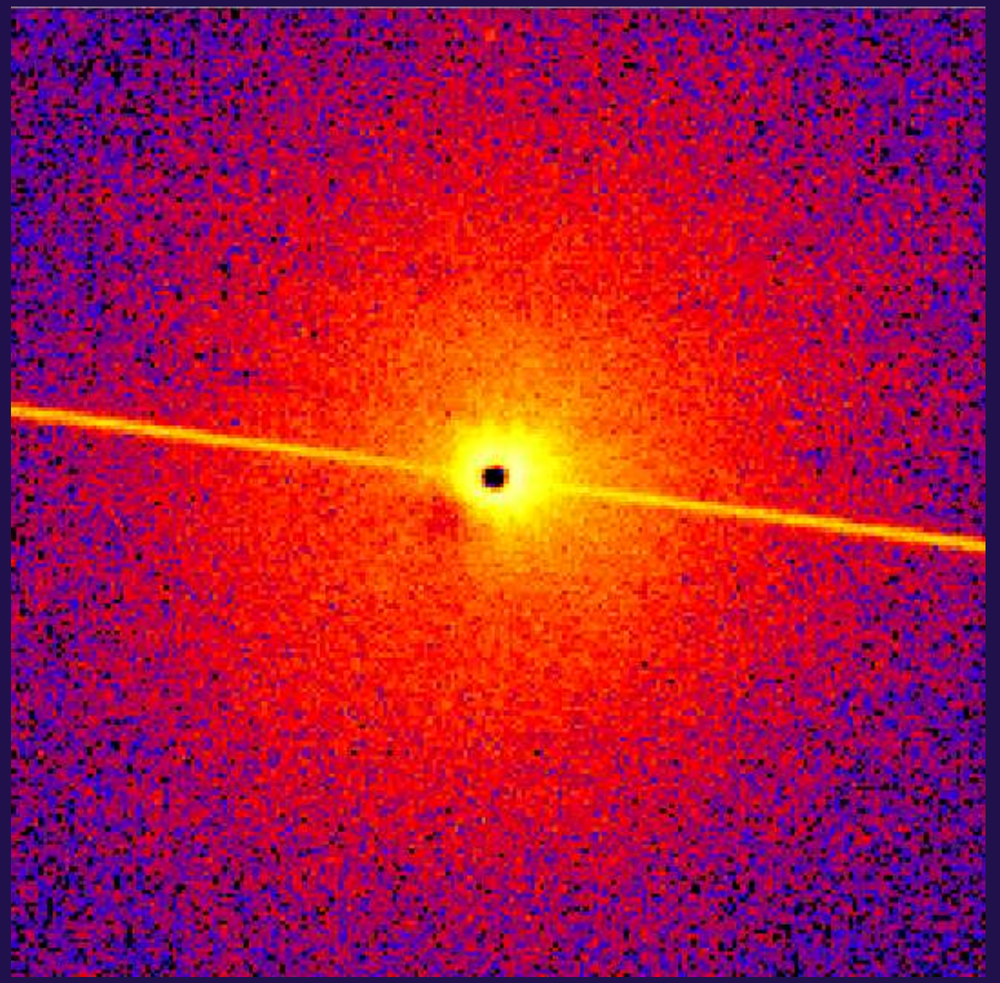
Likelihood-Free Inference

Implicit Models

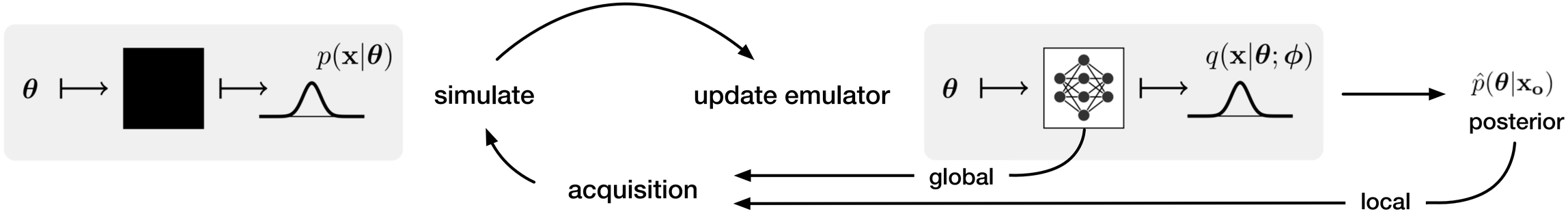
data analysis

data collection

physics



Lueckmann et al (2018)



also see: Brehmer et al (2018): Mining gold from implicit models to improve likelihood-free inference, Brehmer et al (2018): A Guide to Constraining Effective Field Theories with Machine Learning

Probabilistic Programming

pymc3

```
# setup model
model = pm.Model()
with model:
    # cluster sizes
    p = pm.Dirichlet('p', a=np.array([1., 1., 1.]), shape=k)
    # ensure all clusters have some points
    p_min_potential = pm.Potential('p_min_potential', tt.switch


    # cluster centers
    means = pm.Normal('means', mu=[0, 0, 0], sd=15, shape=k)
    # break symmetry
    order_means_potential = pm.Potential('order_means_potential
                                         tt.switch(means[1]-mea
                                         + tt.switch(means[2]-m

    # measurement error
    sd = pm.Uniform('sd', lower=0, upper=20)

    # latent cluster of each observation
    category = pm.Categorical('category',
                              p=p,
                              shape=ndata)

    # likelihood for each observed value
    points = pm.Normal('obs',
                       mu=means[category],
                       sd=sd,
                       observed=data)
```

```
# fit model
with model:
    step1 = pm.Metropolis(vars=[p, sd, means])
    step2 = pm.ElemwiseCategorical(vars=[category], values=[0,
    tr = pm.sample(10000, step=[step1, step2])
```

also:

- STAN
- Edward
- Tensorflow Probability

Exercise (if time): Write the chocolate productivity hierarchical model from the tutorial in a PyMC3 model

Model Interpretation + Critiquing

(see also Blei (2014))

Assess the fitness of the model

- How good is your model in general?
- Where does it fail in particular?

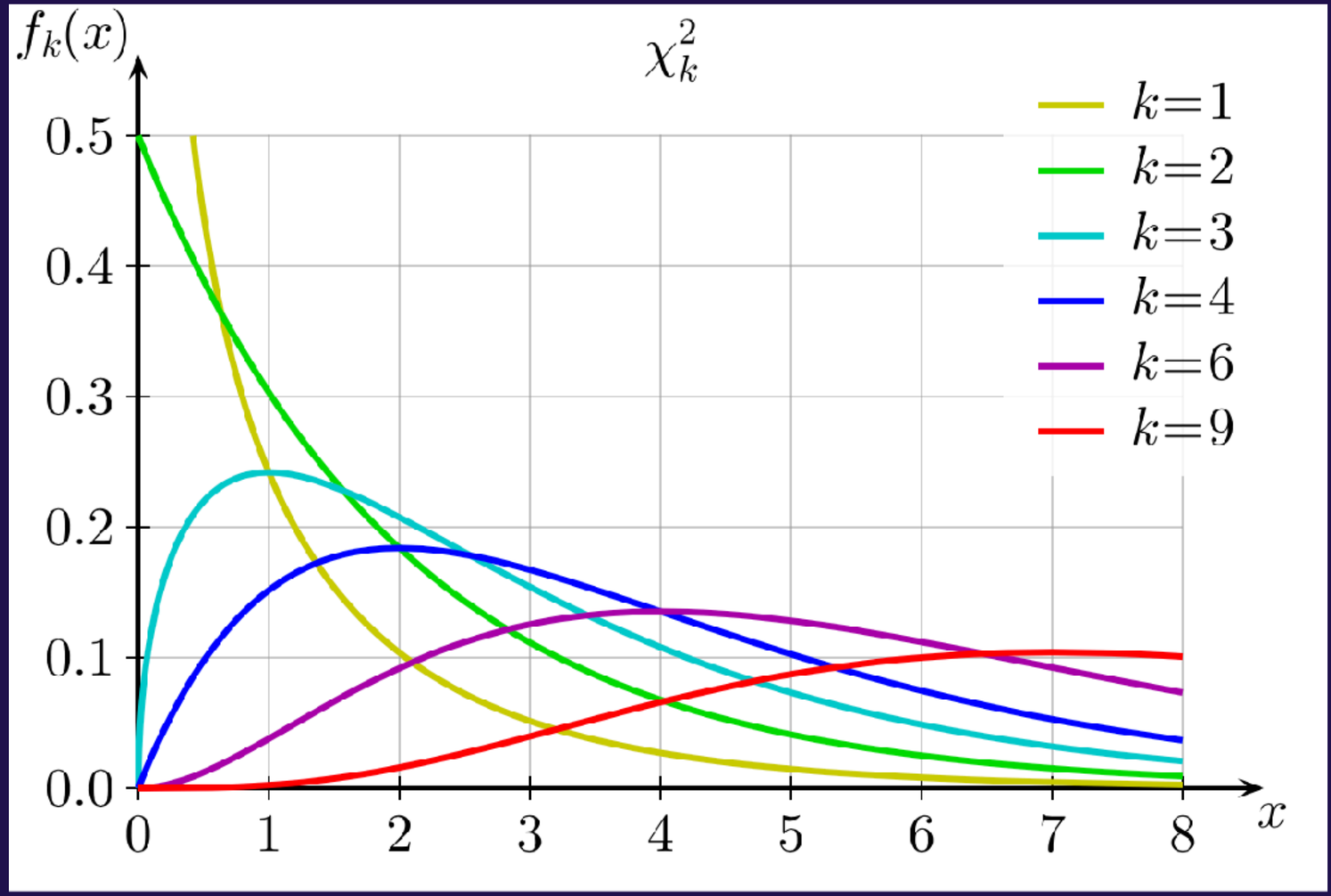
Be pragmatic about your models + inference

Goodness of Fit

$$\mathscr{L}(\theta) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - m(x_i, \theta))^2$$

distributed as χ^2 with *n-k* degrees of freedom

Goodness of Fit



key concept: confront the model's posterior predictive distribution with the observed data

Posterior Predictive Distribution

$$p(\theta \mid \mathbf{y}, I) \propto p(\mathbf{y} \mid \theta, I) p(\theta \mid I)$$

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Predictive Sample Re-use (cross-validation)

- Evaluate model assumption
- can also compare different sampling algorithms!

Posterior Predictive Checks

Is my model good enough in ways that matter?

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T(y) is adaptable to the needs of the practicioner!

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- Critique your models!