Introduction to Bayesian Statistics

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SMPE lecture
January 2023

Goal

- How to leverage your knowledge about the system?
- How to check whether it is reasonable or not?
- Given a some observations, how to generate "similar" values? ~~GANs ? No, not today~~

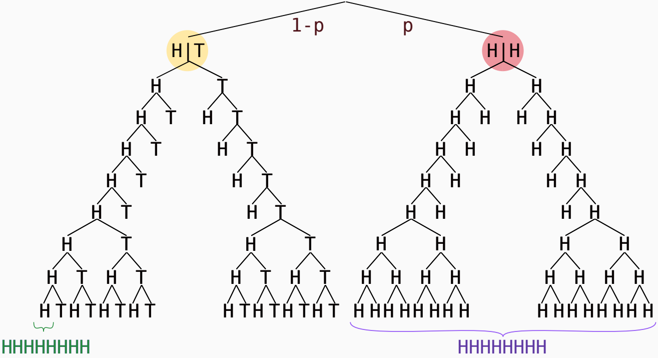
This talk:

1. Brief introduction to Bayesian statistics.
2. Brief introduction to Bayesian sampling with a brief presentation of STAN
3. A brief discussion on model selection

Bayesian Statistics

A first example

Consider a fair coin and two-headed one and pick one at random



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- What is the probability that the coin is the two-headed one ?

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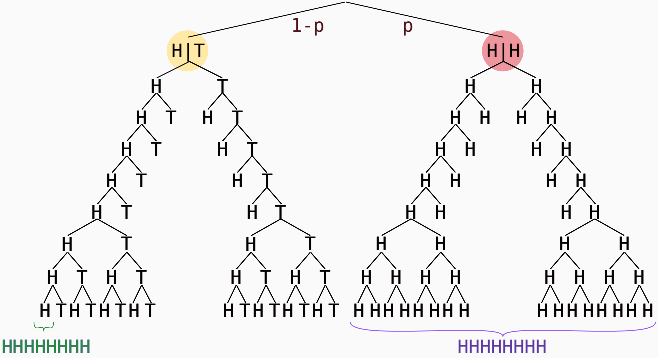

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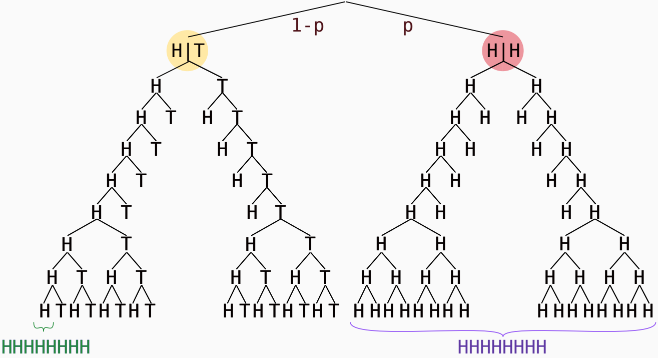
- What is the probability that the coin is the two-headed one ?

$$p[Two - Headed] = \frac{256}{1 + 256} \approx 0.996$$

A first example (continued)

Now let's put the two-headed one in a jar with 999 fair coins...



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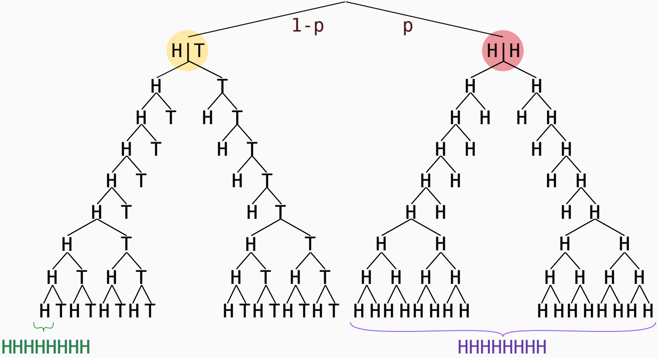

The coin is tossed 8 times. The outcome is a head 8 times in a row.

- What is the probability that the coin is the two-headed one ?

$$p[Two - Headed] = \frac{.001 \times 1}{\frac{1}{256} \times 0.999 + 1 \times .001} \approx 0.204$$

Bayes Rule

Notation

- $p(A)$ = probability that $\boxed{A}$ occurs
- $p(A, B)$ = probability that $\boxed{A \text{ and } B}$ occurs
- $p(A|B)$ = probability that $\boxed{A}$ occurs, given that $\boxed{B}$ occurs

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Conjunction rule

- $p(A, B) = p(A|B)p(B)$
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Bayes rule Equate and divide by $p(B)$

$$\boxed{p(A|B) = \frac{p(B|A)p(A)}{p(B)}}$$

Background on Bayesian Statistics

Model we assume $y \sim \mathcal{M}(\theta, x)$

- θ: Model parameters
- y: Dependent data (response)
- x: Independent data (covariates/predictors/constants)

Examples

- $y \sim \mathcal{N}(\mu, \sigma)$
- $y \sim x^2 + \mathcal{U}(\alpha, \beta)$
- $y \sim \mathcal{N}(\alpha x + \beta, \sigma)$
- $y \sim \mathcal{N}(\alpha \log(x) + \beta, \alpha' x + \beta')$

Everyone: Model data as random

Background on Bayesian Statistics

Bayesians: Data is fixed (observed), model parameters as random

$$p(\theta, y, x) = p(y, \theta, x)$$
$$p(\theta|y, x)p(y, x) = p(y|\theta, x)p(\theta, x)$$

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

$\propto p(y|\theta, x)p(\theta)$ (y, and x are fixed for a given data set)

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Bayes rule $\boxed{\underbrace{p(\theta|y, x)}_{\text{Posterior}} \propto \underbrace{p(y|\theta, x)}_{\text{Likelihood}} \underbrace{p(\theta, x)}_{\text{Prior}}}$ assuming $y \sim \mathcal{M}(\theta, x)$

- Posterior: The answer, probability distributions of parameters
- Likelihood: A (model specific) computable function of the parameters
- Prior: "Initial guess", existing knowledge of the system

The key to building Bayesian models is specifying the likelihood function, same as frequentist.

Head and Tail

> *When spun on edge 250 times, a Belgian 1€ coin came up heads 140 times and tails 110. It looks very suspicious to me. If the coin were unbiased, the chance of getting a result as extreme as that would be less than 7%.*
>
> *– From "The Gardian" quoted by MacKay*
> *in Information Theory, Inference and Learning Algorithms*

- Model: $Y \sim \mathcal{B}(\pi)$
- Data: $y = 1, 0, 1, 1, 0, 0, 1, 1, 1, \ldots$
- $p(y|\pi = 1/2)$
  $= \frac{(140+110)!}{110!140!} . (\frac{1}{2})^{110} . (\frac{1}{2})^{140}$
  ≈ 0.00835

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- Data: $y = 1, 0, 1, 1, 0, 0, 1, 1, 1, \ldots$
- $p(|y| \leq 110 | \pi = 1/2)$
  $= \sum_{k \leq 110} \frac{250!}{k!(250-k)!} \cdot \frac{1}{2^{250}}$
  ≈ 0.033

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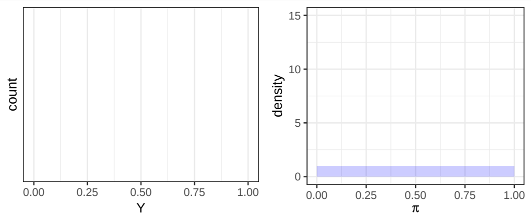

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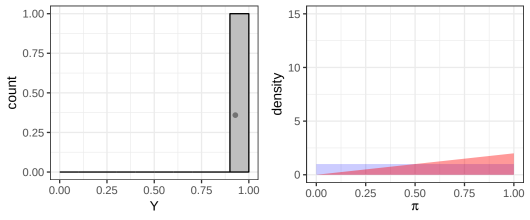

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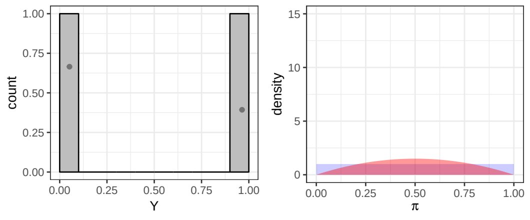

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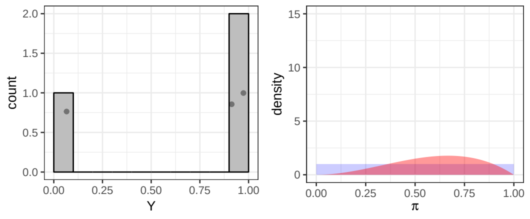

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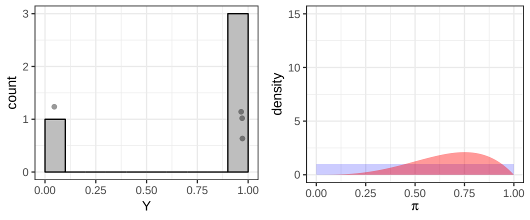

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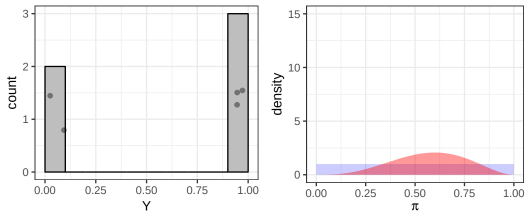

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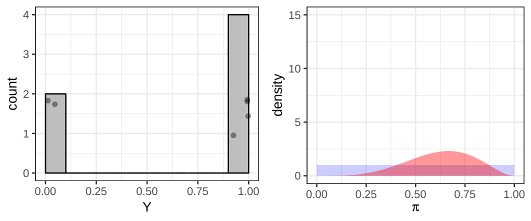

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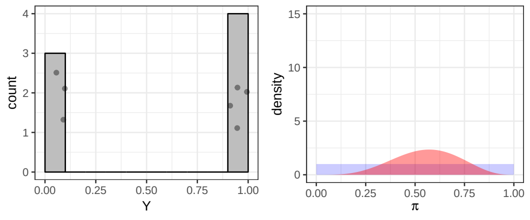

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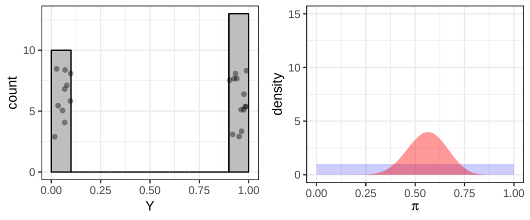

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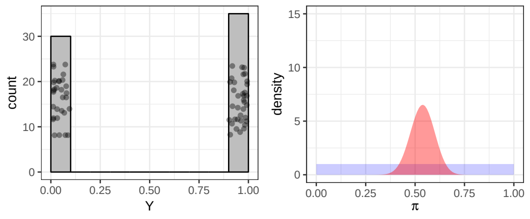

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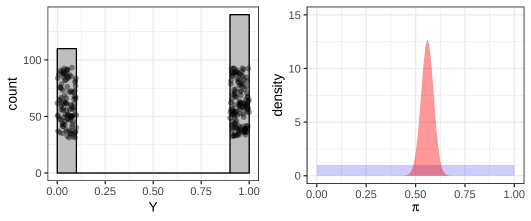

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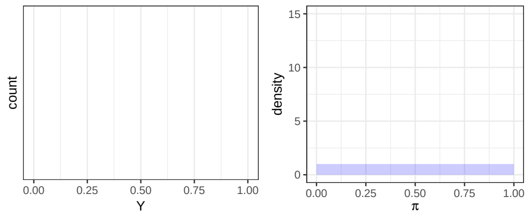

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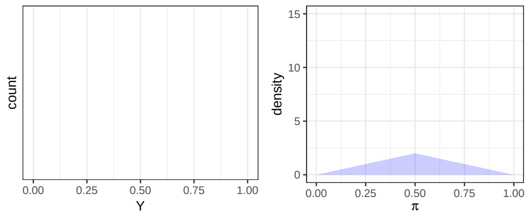

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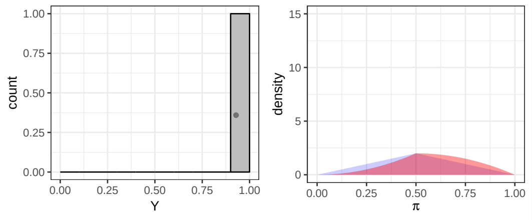

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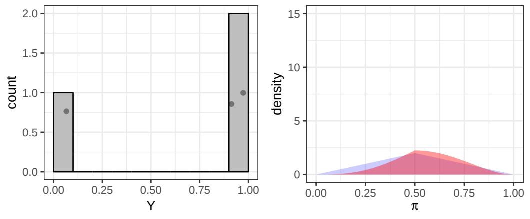

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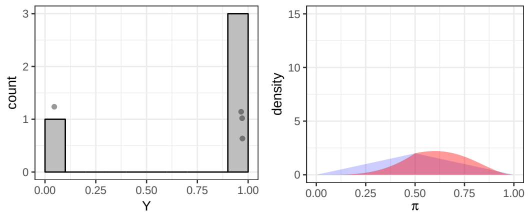

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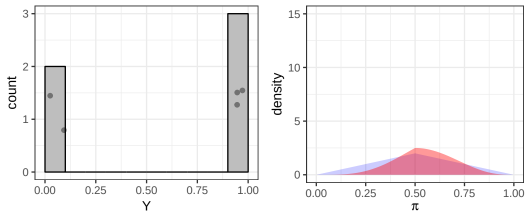

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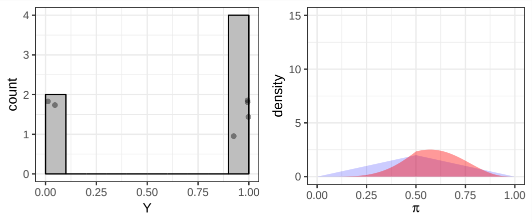
When spun on edge 250 times, a Belgian 1€ coin came up heads 140 times and tails 110. It looks very suspicious to me. If the coin were unbiased, the chance of getting a result as extreme as that would be less than 7%.

– From "The Gardian" quoted by MacKay
in Information Theory, Inference and Learning Algorithms

- Model: $Y \sim \mathcal{B}(\pi)$
- Data: $y = 1, 0, 1, 1, 0, 0, 1, 1, 1, \ldots$
- Prior: $\pi \sim \mathcal{T}(0, 1)$



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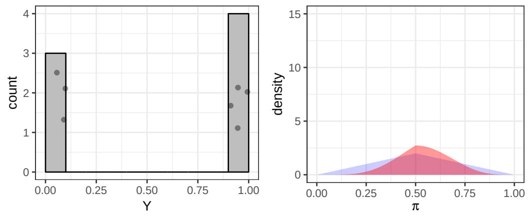

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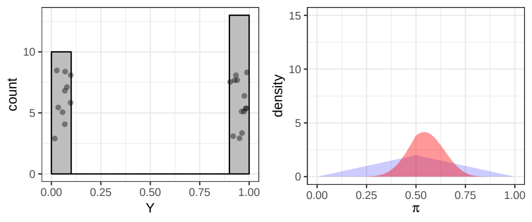

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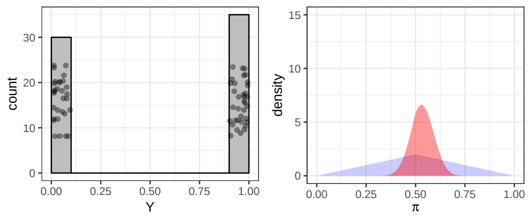

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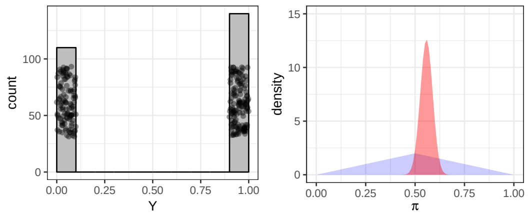

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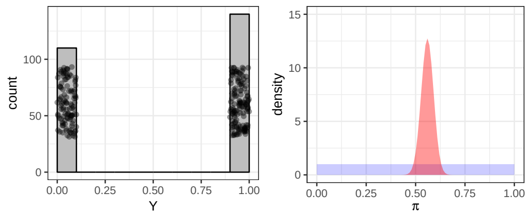

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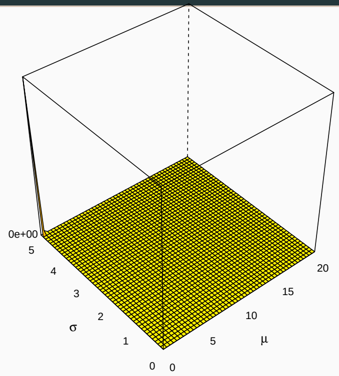
A Simple Gaussian Model

Initial Belief and First Observations

- Model: $Y \sim \mathcal{N}(\mu, \sigma)$
- Prior: $\mu \sim \mathcal{U}(0, 20)$ and $\sigma \sim \mathcal{U}(0, 5)$



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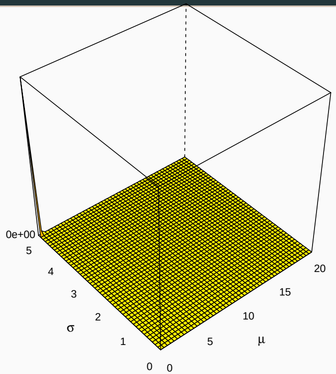



```
set.seed(162);
n=20; mu=12.5; sigma=1.6;
Y=rnorm(n, mean=mu, sd=sigma);
Y
```

```
 [1] 13.899247 12.951346 12.164091 10.869858 13.075777 12.552552 15.446823
 [8] 11.920264 12.849875  9.367122 12.083848 13.852930 12.740590  9.674321
[15] 11.489182 12.195024 13.946985  9.220992 11.821921  9.347013
```

Likelihood for This Model

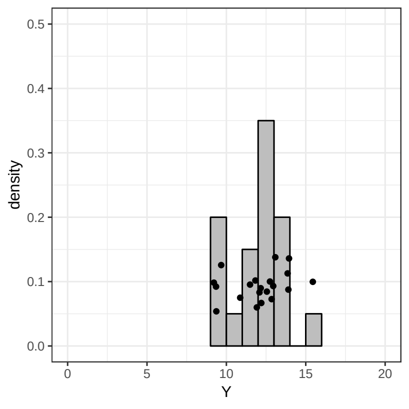
Model: $Y \sim \mathcal{N}(\mu, \sigma)$, hence $p(y|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{y-\mu}{2}\right)^2\right)$

Therefore $p(\mu,\sigma|y) \propto \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{y_i-\mu}{2}\right)^2\right) \cdot \frac{1}{100}$

Exploiting information (Normal model)

```
[1] "Mean: 12.07348806679"
[1] "Standard Deviation: 1.70127707382769"
```

Distribution of observations Y



Posterior distribution

Exploiting information (Normal model)

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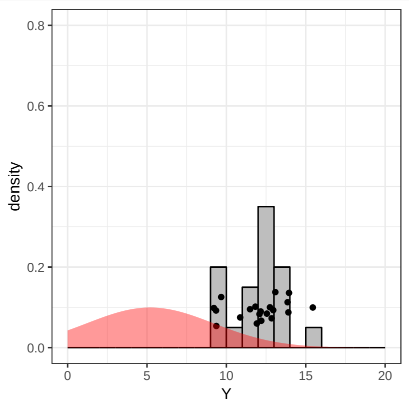

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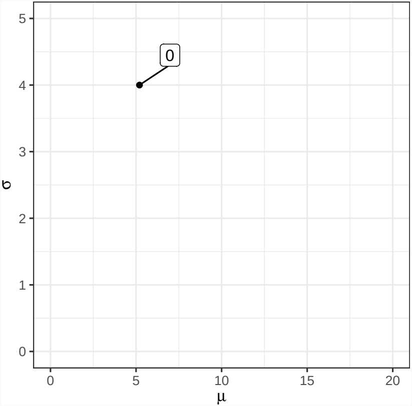

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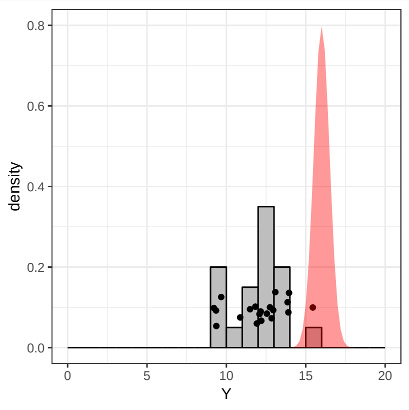

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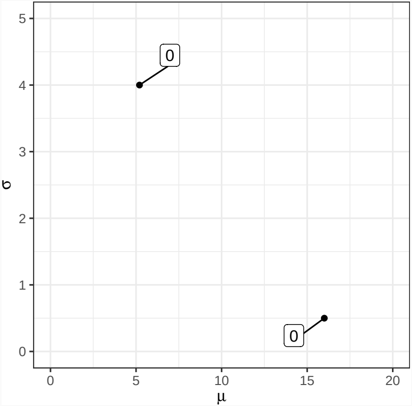

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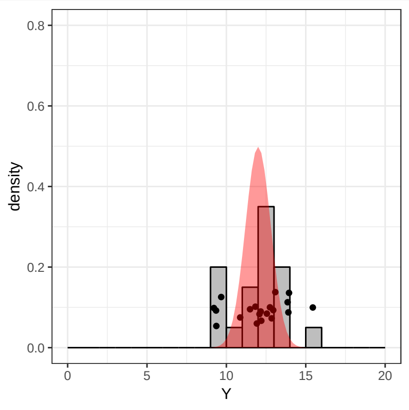

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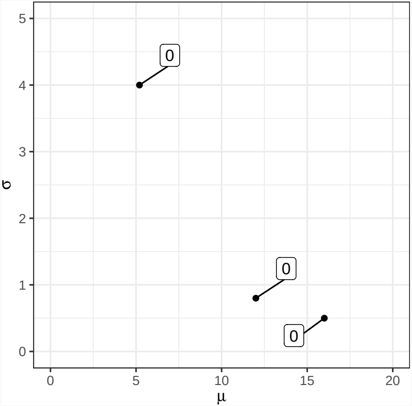

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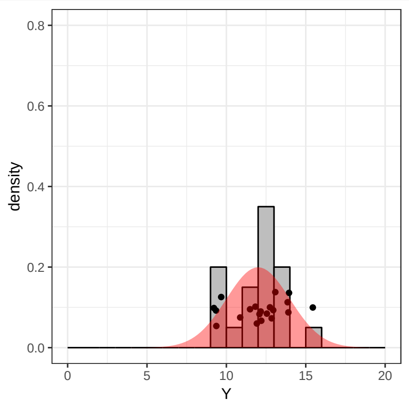

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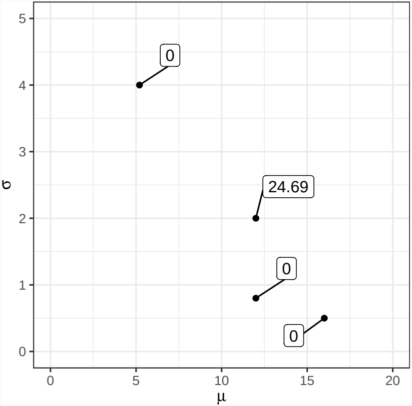

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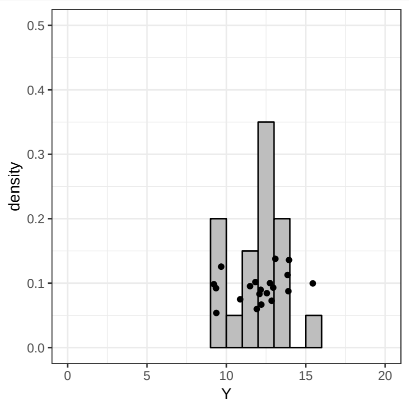

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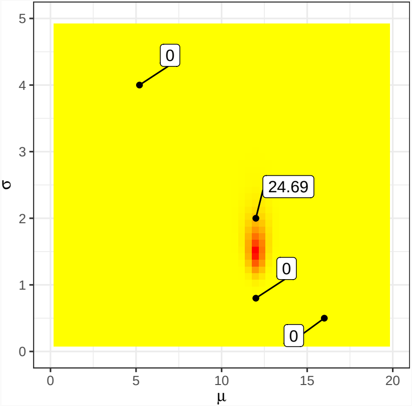

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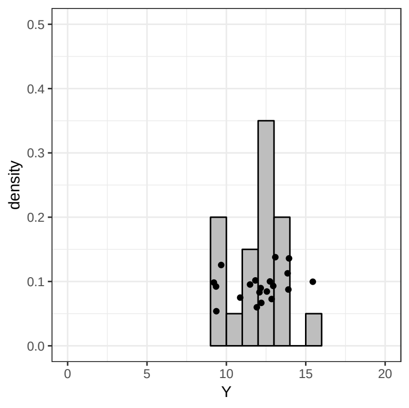
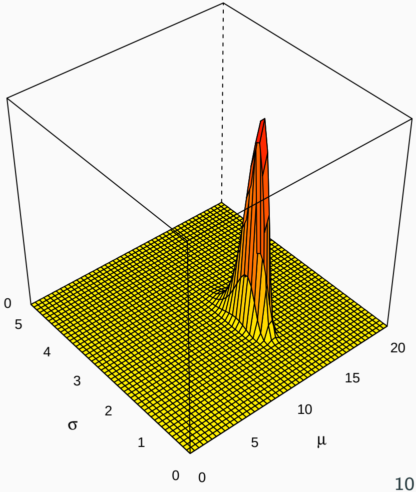


Posterior distribution



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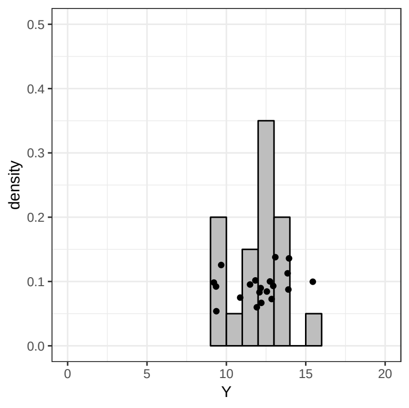
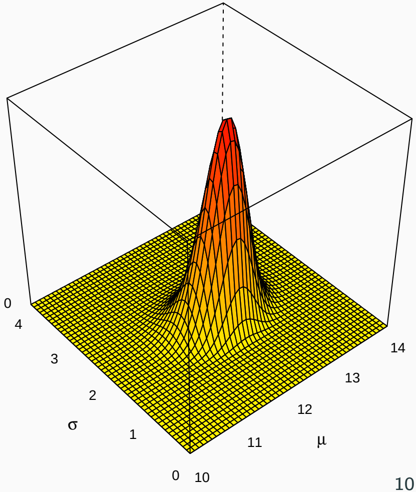
Distribution of observations Y



Posterior distribution (Zoom)



Single point estimate (Normal model)

```
[1] "Mean: 12.07348806679"
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```

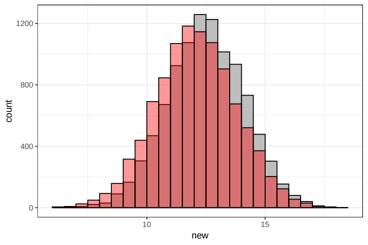
$$p(\mu, \sigma | y) \propto \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{y_i - \mu}{2}\right)^2\right) \cdot \frac{1}{100}$$

- *Machine Learning*: Maximum Likelihood $|y$
  - $\mu_{MLE} = \frac{1}{n}\sum_{i=1}^{n} y_i$
  - $\sigma_{MLE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \mu_{MLE})^2}$
- *Frequentist*: ensure $\mathbb{E}[\mu_F] = \mu$ and $\mathbb{E}[\sigma_F^2] = \sigma^2$
  - $\mu_F = \frac{1}{n}\sum_{i=1}^{n} y_i$
  - $\sigma_F = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(y_i - \mu_F)^2}$
- *Bayesian*: sample the posterior

Generating new data

- θ: unknown parameter ($\mu = 12.5$, $\sigma = 1.6$)
- y: observation
- $\hat{\theta}$: single point estimate of θ ($\mu \approx 12.07$, $\sigma \approx 1.7$)
- $\tilde{y}$: future observations

Generating $\tilde{y}$ from $\hat{\theta}$



(does not account for the uncertainty on $\hat{\theta}$)

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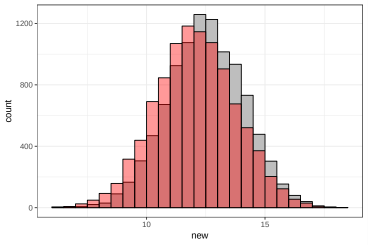
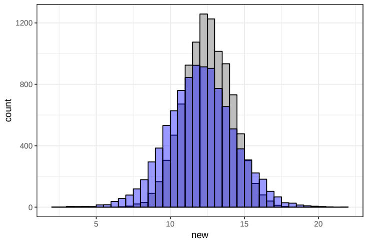


(does not account for the uncertainty on $\hat{\theta}$)

Generating $\tilde{y}$ from many $\tilde{\theta}|y$



Noise on y + uncertainty on θ

Influence of the prior

Take away messages:

1. With enough data, reasonable people converge.
2. If any $p(\theta) = 0$, no data will change that
   - Sometimes imposing $p(\theta) = 0$ is nice (e.g., $\theta > 0$)
3. An uninformative prior is better than a wrong highly (supposedly) informative prior.
4. With conjugate priors, calculus of the likelihood is possible Otherwise, the normalization is a huge pain

Computing confidence intervals, high density regions, expectation of complex functions... Samples are easier to use than distributions.

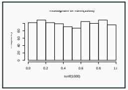
BUGS: Bayesian inference Using Gibbs Sampling

$$\boxed{\underbrace{p(\theta|y,x)}_{\text{Posterior}} \propto \underbrace{p(y|\theta,x)}_{\text{Likelihood}} \underbrace{p(\theta,x)}_{\text{Prior}}}$$

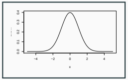
Bayesian Sampling

Generating random number: direct method

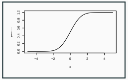
- Input:
  - $\mathcal{U}(0,1)$



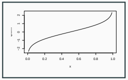
  - A target density f_Y



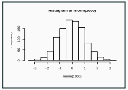
- 3 *Easy* steps:
  1. Compute $F_Y(t) = \int_{-\infty}^{t} f_Y(y).dy$



  2. Compute the inverse F_Y^{-1}



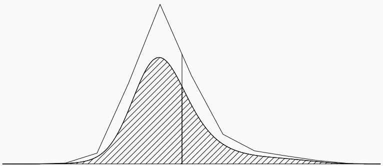
  3. Apply F_Y^{-1} to your uniform numbers



Step 1 is generally quite complicated. The *prior* makes it *even worse*.

Multi-dimensional densities: just as complicated unless the law has a very particular structure

Rejection method



Assume we have M and g, s.t. $p(\theta|y) \leq Mg(\theta)$

- Draw $\theta \sim g$ and accept with probability $\dfrac{p(\theta|y)}{Mg(\theta)}$

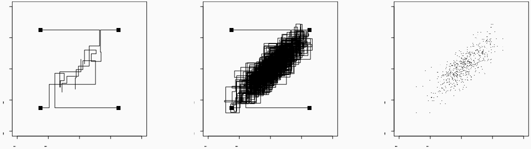
Works well if Mg is a good approximation of $p(.|y)$

Issues:

- p is multiplied by the prior. Where is the max? Which g, which M?
- Is the landscape flat, hilly, spiky?
- Rejection can be quite inefficient ($\rightsquigarrow$ Importance sampling)

Monte Carlo Markov Chain simulation

Dimension by dimension (Gibbs sampler): $\theta_j^t \sim p(.|\theta_{-j}^{t-1}, y)$



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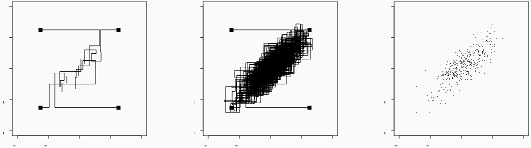


Metropolis-Hasting: Jumping distribution J

- $\theta^* \sim J(\theta^{t-1}) \quad r = \dfrac{p(\theta^*|y)}{p(\theta^{t-1}|y)} \quad \theta^t = \begin{cases} \theta^* & \text{with proba. } \min(r, 1) \\ \theta^{t-1} & \text{otherwise} \end{cases}$

Look for high density areas

- Highly skewed (short/long-tail) or multi-modal are problematic
- Transformation, reparameterization, auxiliary variables, simulated tempering, ...
- Trans-dimensional Markov chains: the dimension of the parameter space can change from one iteration to the next

Hamiltonian Monte-Carlo

Try to eliminate the random walk inefficiency

- Add a momentum variable ϕ_j for each component θ_j and move to the right direction

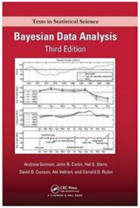
Hamiltonian Monte-Carlo combines MCMC with deterministic optimization methods

- Leapfrog: L steps of $\varepsilon/2$ ($L\varepsilon \approx 1$)
- No U-turn Sampler (NUTS): adapt step sizes locally, the trajectory continues until it turns around

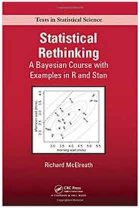
What is Stan?

A probabilistic programming language implementing full Bayesian statistical inference with MCMC sampling (NUTS, HMC) and penalized maximum likelihood estimation with optimization (L-BFGS)

Stanislaw Ulam, namesake of Stan and co-inventor of Monte Carlo methods shown here holding the Fermiac, Enrico Fermi's physical Monte Carlo simulator for neutron diffusion



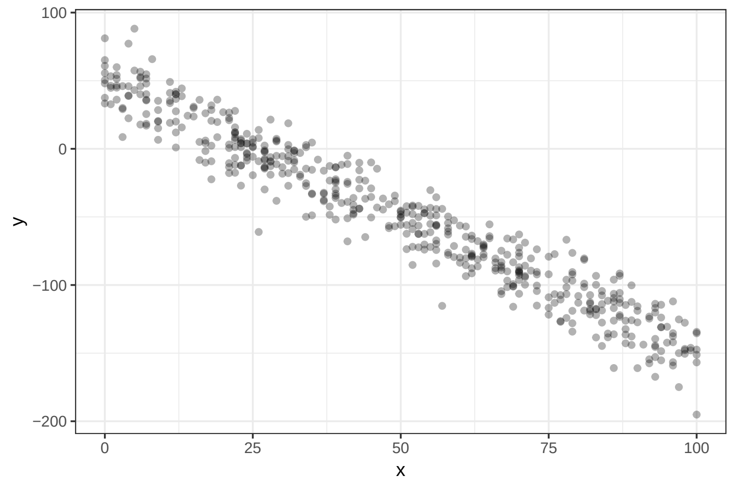
Bayesian Data Analysis,
Gelman et al., 2013



Bayesian Course with examples in R and Stan,
Richard McElreath, 2015

A simple example

```
ggplot(df, aes(x, y))+geom_point(alpha=0.3) + theme_bw()
```



A natural model

Model $y \sim \mathcal{N}(\alpha x + \beta, \sigma^2)$

Prior

- $\alpha \sim \mathcal{N}(0, 10)$
- $\beta \sim \mathcal{N}(0, 10)$
- $\sigma \sim \mathcal{N}(0, 10)^+$

A STAN model

```
library(rstan)

modelString = "data { // the observations
    int<lower=1> N; // number of points
    vector[N] x;
    vector[N] y;
}
parameters { // what we want to find
    real intercept;
    real coefficient;
    real<lower=0> sigma; // indication: sigma cannot be negative
}
model {
    // We define our priors
    intercept   ~ normal(0, 10); // We know that all the parameters follow a normal distri
    coefficient ~ normal(0, 10);
    sigma       ~ normal(0, 10);

    // Then, our likelihood function
    y ~ normal(coefficient*x + intercept, sigma);
}
"
sm = stan_model(model_code = modelString)
```

Running STAN

```
data = list(N=nrow(df),x=df$x,y=df$y)
fit = sampling(sm,data=data, iter=500, chains=8)

SAMPLING FOR MODEL 'ea4b5a288cf5f1d87215860103a9026e' NOW (CHAIN 1).
Chain 1: Gradient evaluation took 7.6e-05 seconds
Chain 1: 1000 transitions using 10 leapfrog steps per transition would take 0.76 seconds.
Chain 1: Iteration:   1 / 500 [  0%]  (Warmup)
Chain 1: Iteration:  50 / 500 [ 10%]  (Warmup)
Chain 1: Iteration: 100 / 500 [ 20%]  (Warmup)
Chain 1: Iteration: 150 / 500 [ 30%]  (Warmup)
Chain 1: Iteration: 200 / 500 [ 40%]  (Warmup)
Chain 1: Iteration: 250 / 500 [ 50%]  (Warmup)
Chain 1: Iteration: 251 / 500 [ 50%]  (Sampling)
Chain 1: Iteration: 300 / 500 [ 60%]  (Sampling)
Chain 1: Iteration: 350 / 500 [ 70%]  (Sampling)
Chain 1: Iteration: 400 / 500 [ 80%]  (Sampling)
Chain 1: Iteration: 450 / 500 [ 90%]  (Sampling)
Chain 1: Iteration: 500 / 500 [100%]  (Sampling)
Chain 1:  Elapsed Time: 0.101632 seconds (Warm-up)
Chain 1:                0.044023 seconds (Sampling)
Chain 1:                0.145655 seconds (Total)

SAMPLING FOR MODEL 'ea4b5a288cf5f1d87215860103a9026e' NOW (CHAIN 2).
Chain 2: Gradient evaluation took 2e-05 seconds
Chain 2: 1000 transitions using 10 leapfrog steps per transition would take 0.2 seconds.
Chain 2: Iteration:   1 / 500 [  0%]  (Warmup)
```

Inspecting results

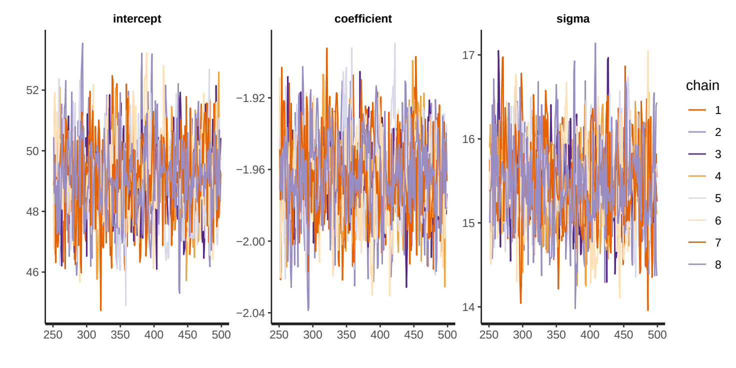
```
print(fit)
```

```
               mean se_mean   sd     2.5%      25%      50%      75%    97.5%
intercept     49.12    0.04 1.31    46.53    48.24    49.13    50.00    51.68
coefficient   -1.96    0.00 0.02    -2.01    -1.98    -1.96    -1.95    -1.92
sigma         15.48    0.01 0.48    14.56    15.15    15.47    15.79    16.44
lp__       -1630.71    0.04 1.14 -1633.61 -1631.32 -1630.42 -1629.85 -1629.36
            n_eff Rhat
intercept     997 1.00
coefficient   979 1.00
sigma        1057 1.00
lp__          840 1.01

Samples were drawn using NUTS(diag_e) at Wed May 22 22:30:52 2019.
For each parameter, n_eff is a crude measure of effective sample size,
and Rhat is the potential scale reduction factor on split chains (at
convergence, Rhat=1).
```

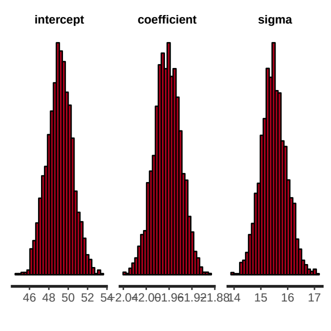
Checking Convergence

```
stan_trace(fit)
```

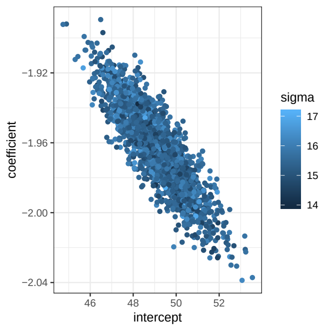


Looking at samples

```
stan_hist(fit)
```




```
ggplot(as.data.frame(rstan::extract(fit)))
    geom_point(aes(x=intercept, y=coefficie
```



This allows to define credibility regions (or intervals).

A catch on model selection

Remember overfitting ?

What's a good model ? A model with a small prediction error...

- Adding parameters in a linear regression always improve the Residual Standard Error, hence the R^2.
- Yet we would like to have few parameters (parsimony, Occam's razor)

How do we distinguish "true" parameters from "false" ones ?

Intuitively:

- Non-significant β should go to 0
- The RSE should be penalized by the number of parameters

Option 1:

Let's consider several alternative models $M_1, M_2, \ldots$

BIC $(M) = k \ln(n) - 2\ln(\widehat{L(M)})$, where

- $\hat{L}$ is the maximized value of the likelihood function
- n is the number of observations
- k is the number of parameters

Option 1: Prior on the Models

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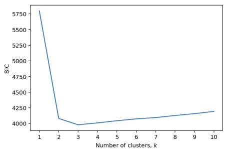
Bayesian argument:

- Uniform prior over alternative models
- When n is large the BIC is proportional to $-\log(p(M_i|Y))$
  - Choose the model with the smaller BIC!!



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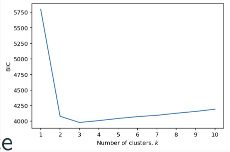

AIC $(M) = 2k - 2\ln(\hat{L})$

- Based on information theory and KL divergence
- Asymptotic too

Option 2:

Wait! If I have $X_1, ..., X_k$ parameters, there are 2^k models.

- Heuristic 1: add parameters one after the other
- Heuristic 2: peel the model

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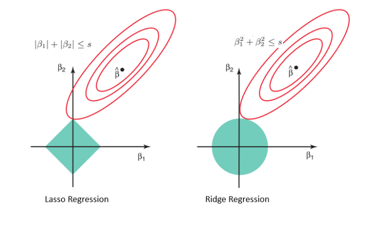
When we just don't know which parameters should be kept, an other option would be to penalize large coefficients

Lasso Min. $\sum_i (\beta.x_i - y_i)^2 + \lambda \sum_k |\beta_k|$ **Ridge** Min. $\sum_i (\beta.x_i - y_i)^2 + \lambda \sum_k \beta_k^2$



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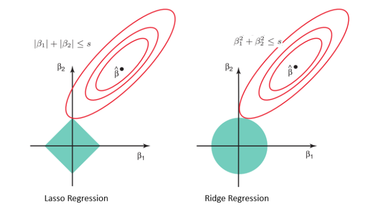
Lasso Min. $\sum_i (\beta.x_i - y_i)^2 + \lambda \sum_k |\beta_k|$
Exponential prior with parameter λ for β

Ridge Min. $\sum_i (\beta.x_i - y_i)^2 + \lambda \sum_k \beta_k^2$
Gaussian prior with variance $1/\lambda$ for β



Standard linear regression can be seen as a uniform (improper) prior

Wrap-up

Truth vs. Myths

Where Blayesian sampling fails:

- ~~Cover the space~~ (e.g., high dimensions)
- ~~Uninformed far away density spikes~~ (mixtures requires informative models and priors)
- ~~High quantiles/rare events~~

Informative priors and starting points are difficult to come up with.

- Much more expensive than "simple" Likelihood optimization, which is also why machine learning techniques are so popular

Where it helps:

- Captures "correlations"
- Robust expectation estimation (1 simulation = very biased)
- Exploit all your knowledge about the system
- Uncertainty quantification with Monte Carlo