Bayesian Learning

Lecture 1 - The Bayesics and Bernoulli data

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Course overview

- Course **webpage**. Course **syllabus**.
- Modes of teaching:
  - Lectures (Mattias Villani and Per Sidén)
  - Mathematical exercises (Per Sidén)
  - Computer labs (Per Sidén and lab assistants)
- **Modules**:
  - The **Bayesics**, single- and multiparameter models
  - **Regression** and **Classification models**
  - **Advanced models** and **Posterior Approximation** methods
  - **Model Inference and evaluation** and **Variable Selection**
- **Examination**
  - Lab reports
  - Computer exam

Lecture overview

- The likelihood function
- Bayesian inference
- Bernoulli model

Likelihood function - Bernoulli trials

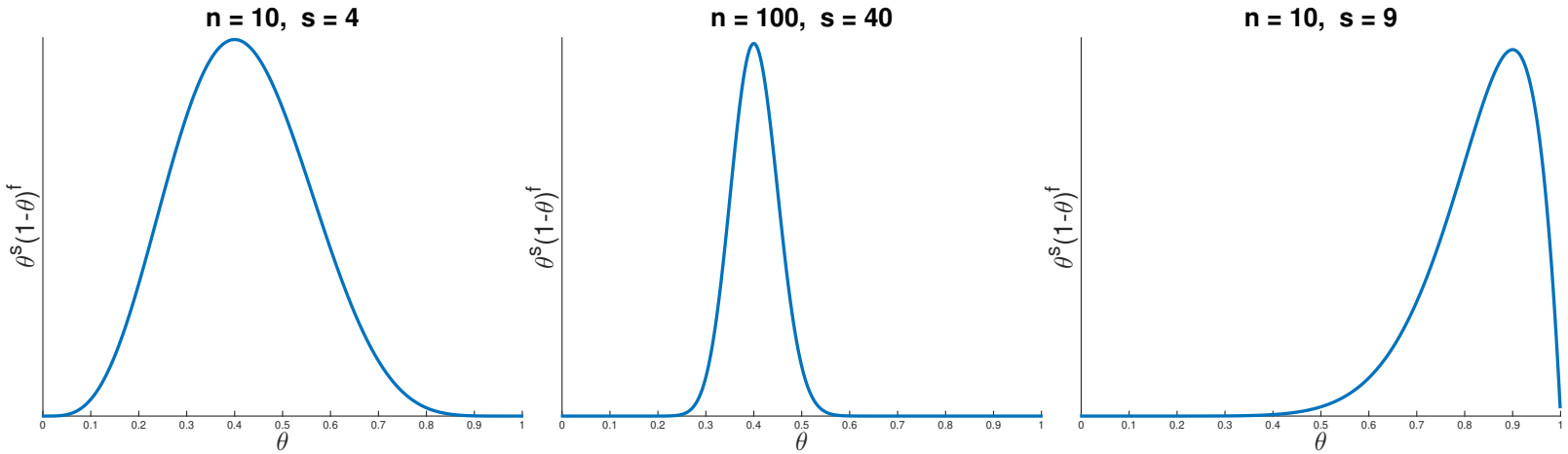
- **Bernoulli trials**:

$$X_1, ..., X_n|\theta \overset{iid}{\sim} Bern(\theta).$$

- **Likelihood** from $s = \sum_{i=1}^{n} x_i$ successes and $f = n - s$ failures.

$$p(x_1, ..., x_n|\theta) \quad = \quad p(x_1|\theta) \cdots p(x_n|\theta) = \theta^s(1-\theta)^f$$

- **Maximum likelihood estimator** $\hat{\theta}$ maximizes $p(x_1, ..., x_n|\theta)$.
- Given the data $x_1, ..., x_n$, plot $p(x_1, ..., x_n|\theta)$ as a function of θ.



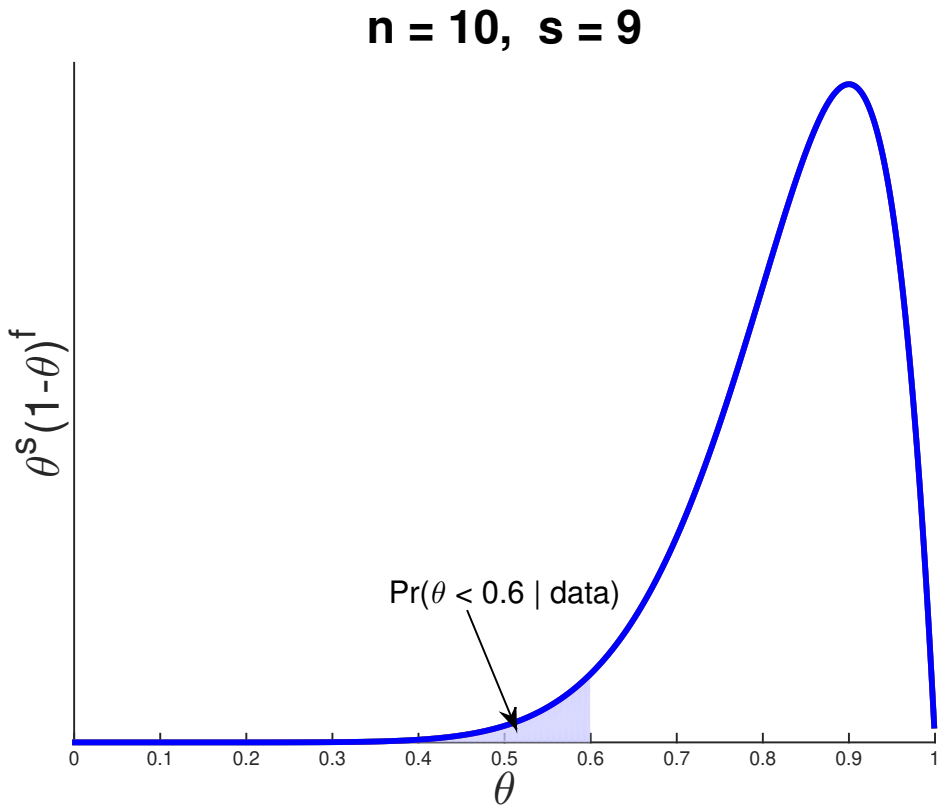
The likelihood function

- Say it out loud:

  The likelihood function is
  the probability of the observed data
  considered as a function of the parameter.

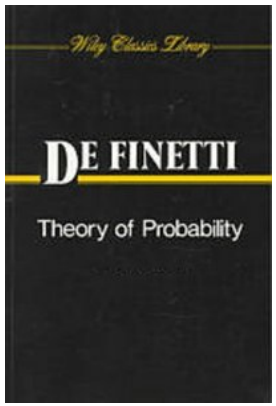
- The symbol $p(x_1, ..., x_n|\theta)$ plays two different roles:
- **Probability distribution** for the data.
  - The data $\mathbf{x} = (x_1, ..., x_n)$ are random.
  - θ is fixed.
- **Likelihood function** for the parameter
  - The data $\mathbf{x} = (x_1, ..., x_n)$ are fixed.
  - $p(x_1, ..., x_n|\theta)$ is function of θ.

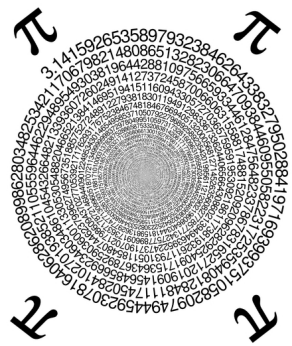
Probabilities from the likelihood?



Uncertainty and subjective probability

- $\Pr(\theta < 0.6|\text{data})$ only makes sense if θ is random.
- But θ may be a fixed natural constant?
- **Bayesian: doesn't matter if θ is fixed or random.**
- Do **You** know the value of θ or not?
- $p(\theta)$ reflects Your knowledge/**uncertainty** about θ.
- **Subjective probability**.
- The statement $\Pr(10\text{th decimal of } \pi = 9) = 0.1$ makes sense.





Bayesian learning

- **Bayesian learning** about a model parameter θ:
  - state your **prior** knowledge as a probability distribution $p(\theta)$.
  - collect **data** $\mathbf{x}$ and form the **likelihood** function $p(\mathbf{x}|\theta)$.
  - **combine** prior knowledge $p(\theta)$ with data information $p(\mathbf{x}|\theta)$.
- **How to combine** the two sources of information?

Bayes' theorem

Learning from data - Bayes' theorem

- How to update from prior $p(\theta)$ to posterior $p(\theta|Data)$?
- Bayes' theorem for events A and B

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

- Bayes' Theorem for a model parameter θ

$$p(\theta|Data) = \frac{p(Data|\theta)p(\theta)}{p(Data)}.$$

- It is the prior $p(\theta)$ that takes us from $p(Data|\theta)$ to $p(\theta|Data)$.
- A probability distribution for θ is extremely useful.
  Predictions. Decision making.
- No prior - no posterior - no useful inferences - no fun.

Medical diagnosis

- A = {Very rare disease}, B ={Positive medical test}.
- $p(A) = 0.0001$. $p(B|A) = 0.9$. $p(B|A^c) = 0.05$.
- Probability of being sick when test is positive:

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)} = \frac{p(B|A)p(A)}{p(B|A)p(A) + p(B|A^c)p(A^c)} \approx 0.0018.$$

- Probably not sick, but 18 times more probable now.

- Morale: If you want $p(A|B)$ then $p(B|A)$ does not tell the whole story. The prior probability $p(A)$ is also very important.

"You can't enjoy the Bayesian omelette without breaking the Bayesian eggs"
Leonard Jimmie Savage

The normalizing constant is not important

- Bayes theorem

$$p(\theta|Data) = \frac{p(Data|\theta)p(\theta)}{p(Data)} = \frac{p(Data|\theta)p(\theta)}{\int_\theta p(Data|\theta)p(\theta)d\theta}.$$

- Integral $p(Data) = \int_\theta p(Data|\theta)p(\theta)d\theta$ can make you cry.
- $p(Data)$ **is just a constant** so that $p(\theta|Data)$ integrates to one.
- Example: $x \sim N(\mu, \sigma^2)$

$$p(x) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2\right].$$

- We may write

$$p(x)| \propto \exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2\right].$$

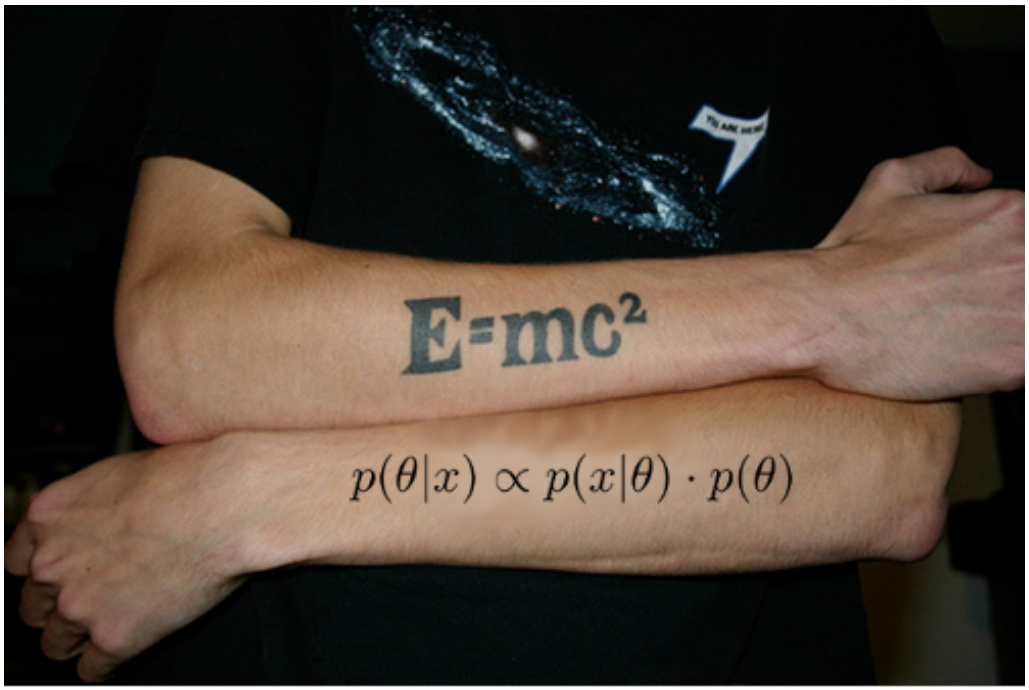
Great theorems make great tattoos

- All you need to know:

$$p(\theta|Data) \propto p(Data|\theta)p(\theta)$$

or

$$\text{Posterior} \propto \text{Likelihood} \cdot \text{Prior}$$



Bernoulli trials - Beta prior

- **Model**

$$x_1, \ldots, x_n | \theta \overset{iid}{\sim} \text{Bern}(\theta)$$

- **Prior**

$$\theta \sim \text{Beta}(\alpha, \beta)$$

$$p(\theta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1} \quad \text{for } 0 \leq \theta \leq 1.$$

- **Posterior**

$$\begin{aligned} p(\theta | x_1, \ldots, x_n) &\propto p(x_1, \ldots, x_n | \theta) p(\theta) \\ &\propto \theta^s (1-\theta)^f \theta^{\alpha-1}(1-\theta)^{\beta-1} \\ &= \theta^{s+\alpha-1}(1-\theta)^{f+\beta-1}. \end{aligned}$$

- Posterior is proportional to the $\text{Beta}(\alpha+s, \beta+f)$ density.
- The prior-to-posterior mapping:

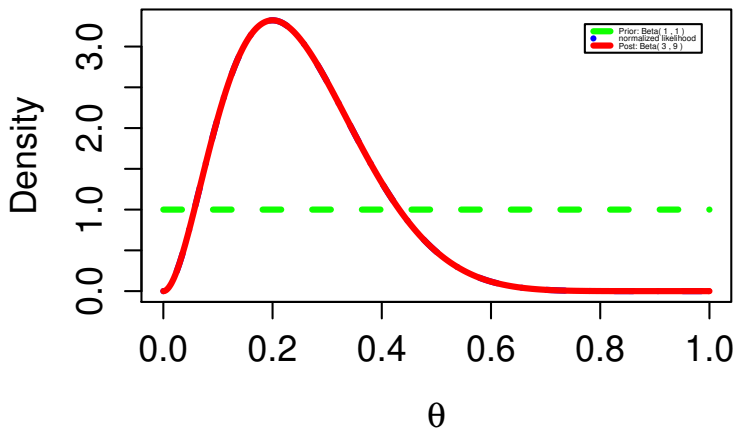
$$\theta \sim \text{Beta}(\alpha, \beta) \overset{x_1, \ldots, x_n}{\Longrightarrow} \theta | x_1, \ldots, x_n \sim \text{Beta}(\alpha+s, \beta+f)$$

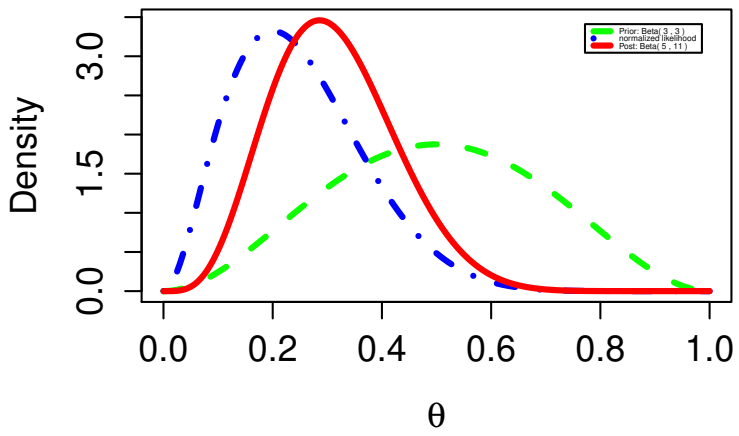
Bernoulli example: spam emails

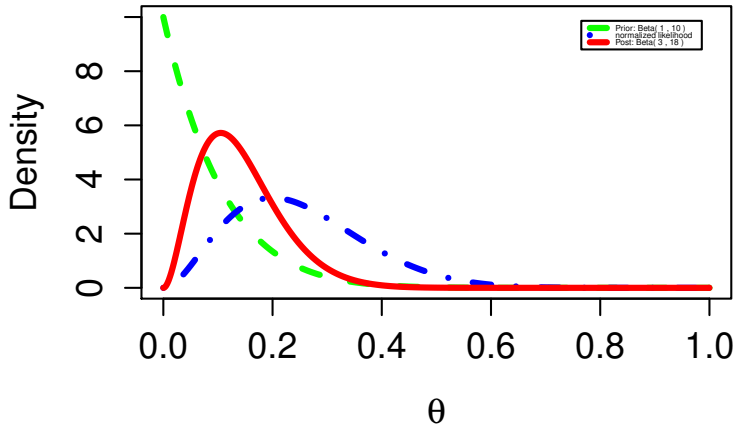
- George has gone through his collection of 4601 e-mails.
- He classified 1813 of them to be spam.
- Let $x_i = 1$ if i:th email is spam.
- **Model**: $x_i|\theta \overset{iid}{\sim} \text{Bern}(\theta)$
- **Prior**: $\theta \sim \text{Beta}(\alpha, \beta)$.
- **Posterior**

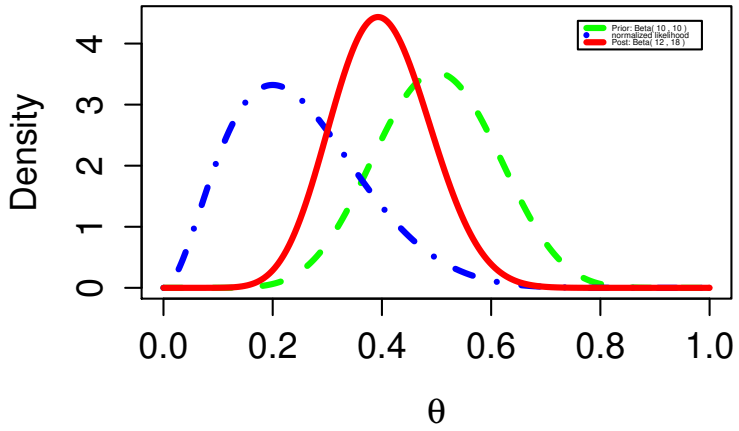
$$\theta|x \sim \text{Beta}(\alpha + 1813, \beta + 2788)$$

Spam data (n=10) - Prior is influential

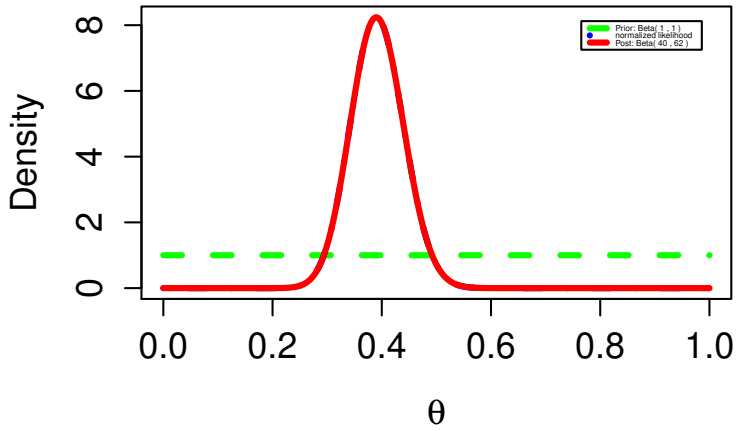


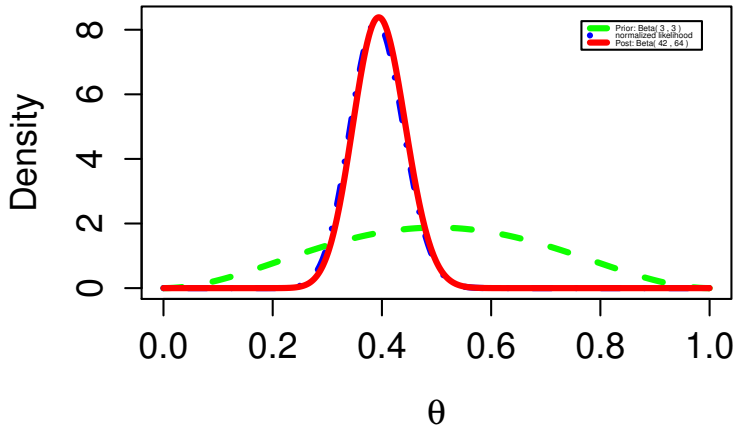


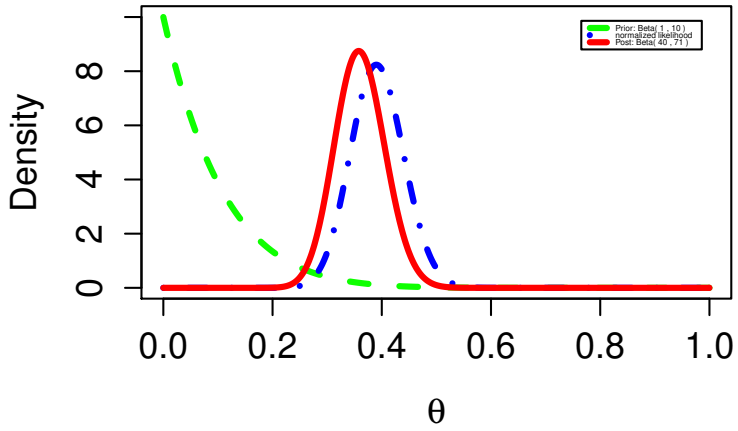


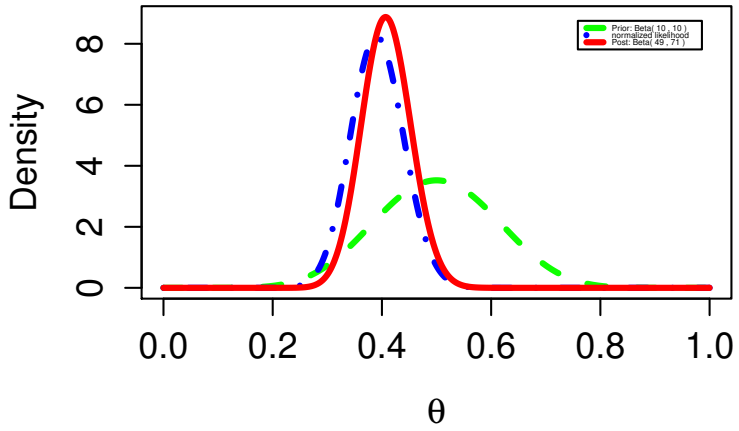


Spam data (n=100) - Prior is less influential

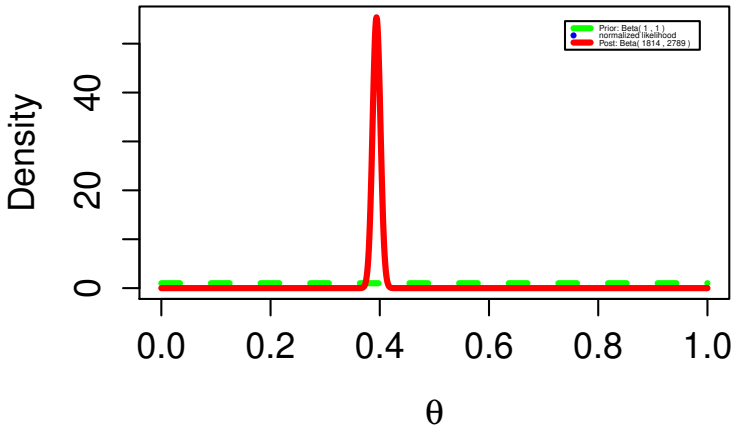


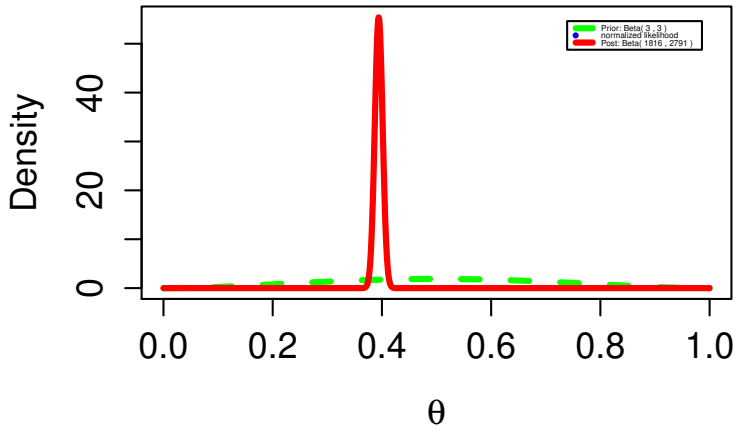


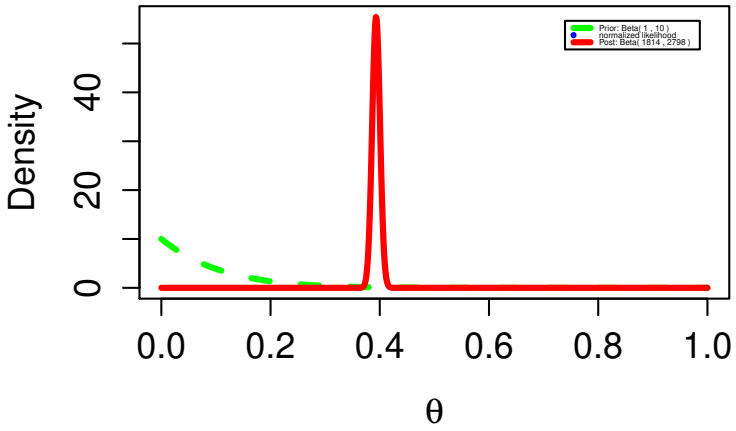


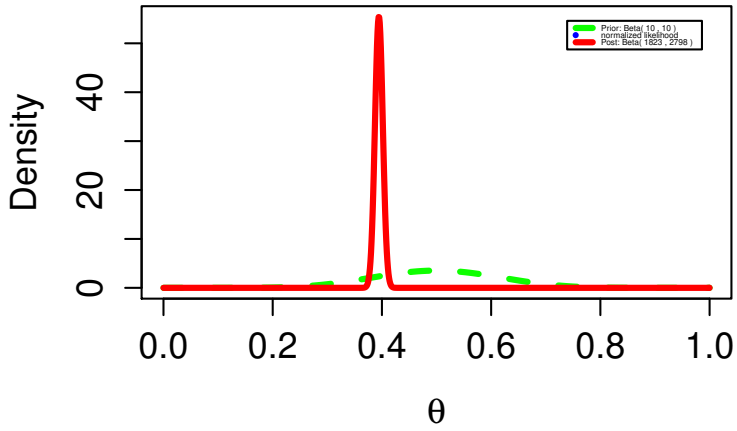


Spam data (n=4601) - Prior does not matter

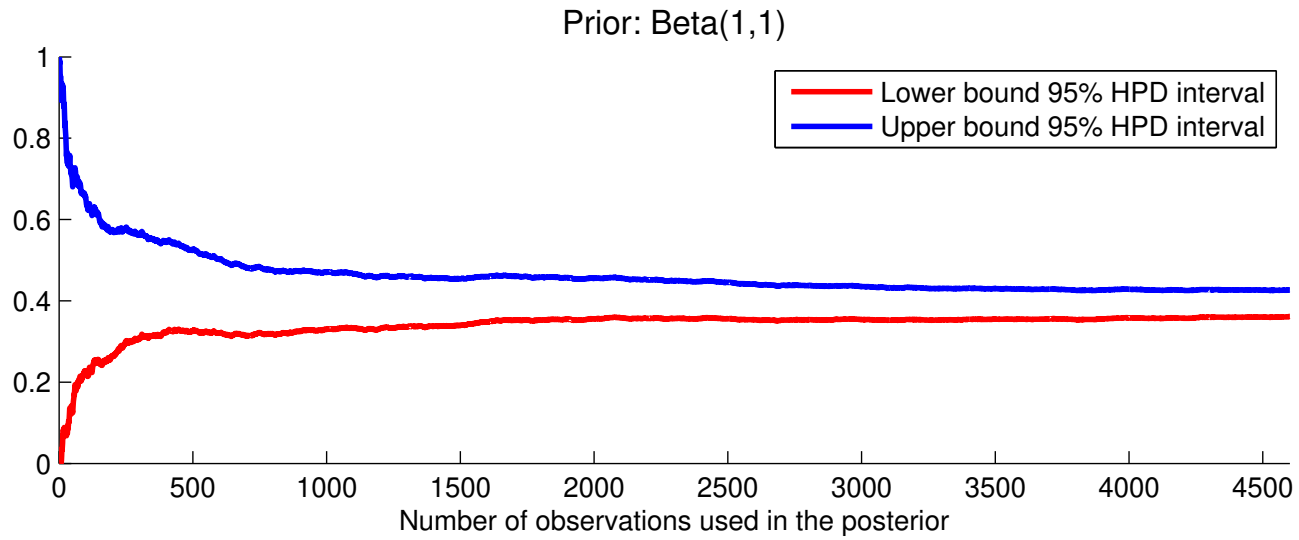


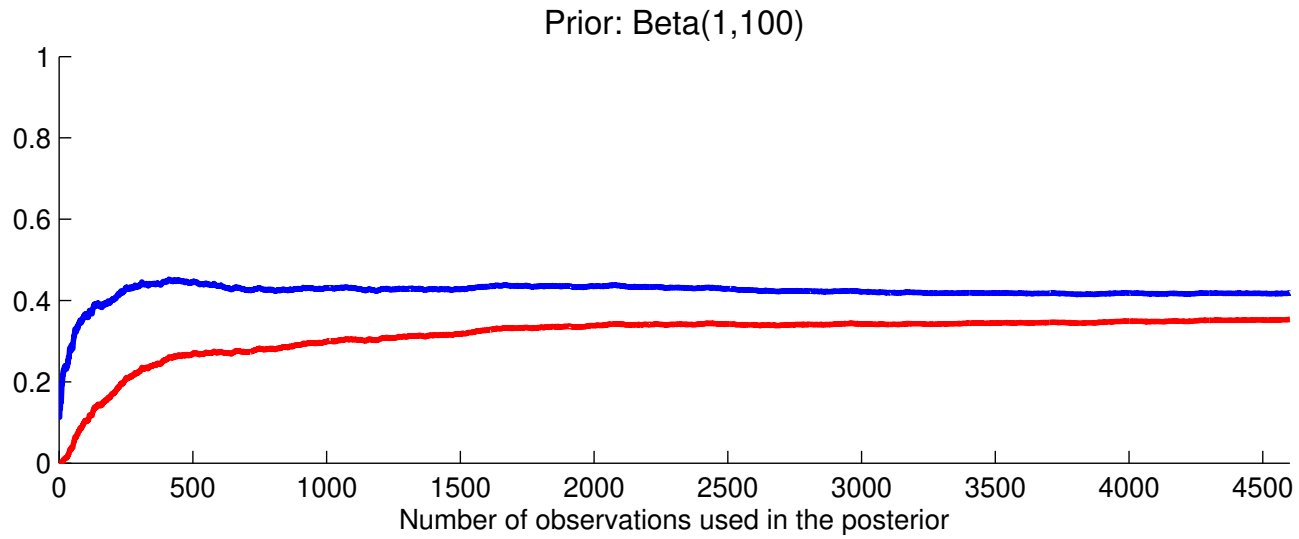






Spam data - posterior convergence





Bayes respects the Likelihood Principle

- **Bernoulli trials with order**:
  $x_1 = 1, x_2 = 0, ..., x_4 = 1, ..., x_n = 1$

$$p(\mathbf{x}|\theta) = \theta^s (1-\theta)^f$$

- **Bernoulli trials without order**. n fixed, s random.

$$p(s|\theta) = \binom{n}{s} \theta^s (1-\theta)^f$$

- **Negative binomial sampling**: sample until you get s successes. s fixed, n random.

$$p(n|\theta) = \binom{n-1}{s-1} \theta^s (1-\theta)^f$$

- The **posterior distribution is the same** in all three cases.
- Bayesian inference respects the **likelihood principle**.

Bayesian Learning

Lecture 2 - Normal and Poisson data. Prior elicitation.

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Lecture overview

- The **Normal model** with known variance
- The **Poisson model**
- **Conjugate priors**
- **Prior elicitation**
- **Jeffreys' prior**

Normal data, known variance - uniform prior

- **Model**

$$x_1, ..., x_n | \theta, \sigma^2 \overset{iid}{\sim} N(\theta, \sigma^2).$$

- **Prior**

$$p(\theta) \propto c \text{ (a constant)}$$

- **Likelihood**

$$\begin{aligned} p(x_1, ..., x_n | \theta, \sigma^2) &= \Pi_{i=1}^{n} (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{1}{2\sigma^2} (x_i - \theta)^2 \right] \\ &\propto \exp\left[-\frac{1}{2(\sigma^2/n)} (\theta - \bar{x})^2 \right]. \end{aligned}$$

- **Posterior**

$$\theta | x_1, ..., x_n \sim N(\bar{x}, \sigma^2/n)$$

Normal data, known variance - normal prior

- **Prior**

$$\theta \sim N(\mu_0, \tau_0^2)$$

- **Posterior**

$$\begin{aligned} p(\theta|x_1, ..., x_n) &\propto p(x_1, ..., x_n|\theta, \sigma^2)p(\theta) \\ &\propto N(\theta|\mu_n, \tau_n^2), \end{aligned}$$

where

$$\frac{1}{\tau_n^2} = \frac{n}{\sigma^2} + \frac{1}{\tau_0^2},$$

$$\mu_n = w\bar{x} + (1 - w)\mu_0,$$

and

$$w = \frac{\frac{n}{\sigma^2}}{\frac{n}{\sigma^2} + \frac{1}{\tau_0^2}}.$$

Normal data, known variance - normal prior

$$\theta \sim N(\mu_0, \tau_0^2) \overset{x_1,\ldots,x_n}{\Longrightarrow} \theta|x \sim N(\mu_n, \tau_n^2).$$

Posterior precision = Data precision + Prior precision

Posterior mean =

$$\frac{\text{Data precision}}{\text{Posterior precision}}(\text{Data mean}) + \frac{\text{Prior precision}}{\text{Posterior precision}}(\text{Prior mean})$$

Download speed

- **Data**: $\mathrm{x} = (22.42, 34.01, 35.04, 38.74, 25.15)$ Mbit/sec.
- **Model**: $X_1, ..., X_5 \sim N(\theta, \sigma^2)$.
- Assume $\sigma = 5$ (measurements can vary $\pm$10MBit with 95% probability)
- My **prior**: $\theta \sim N(50, 5^2)$.

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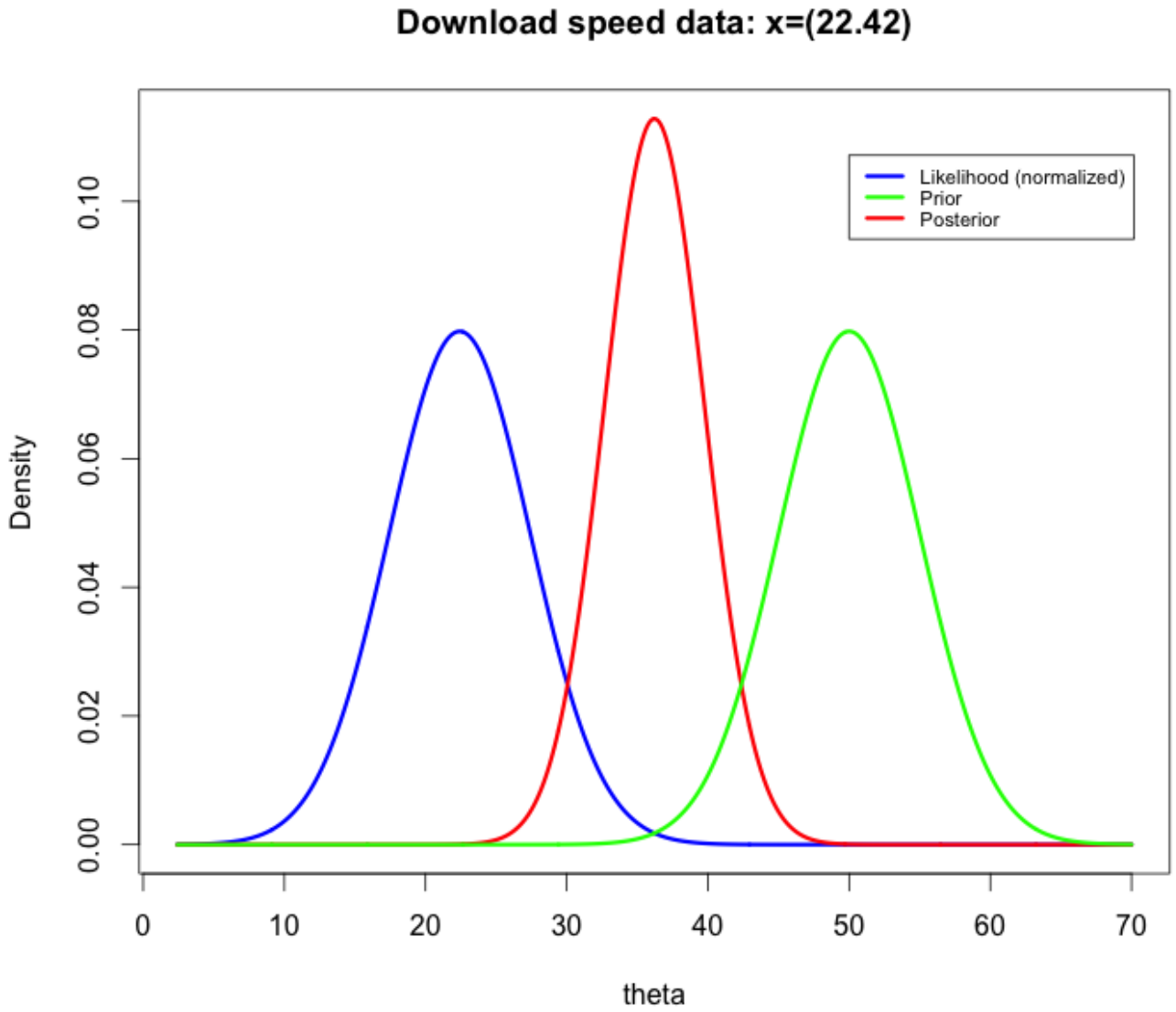

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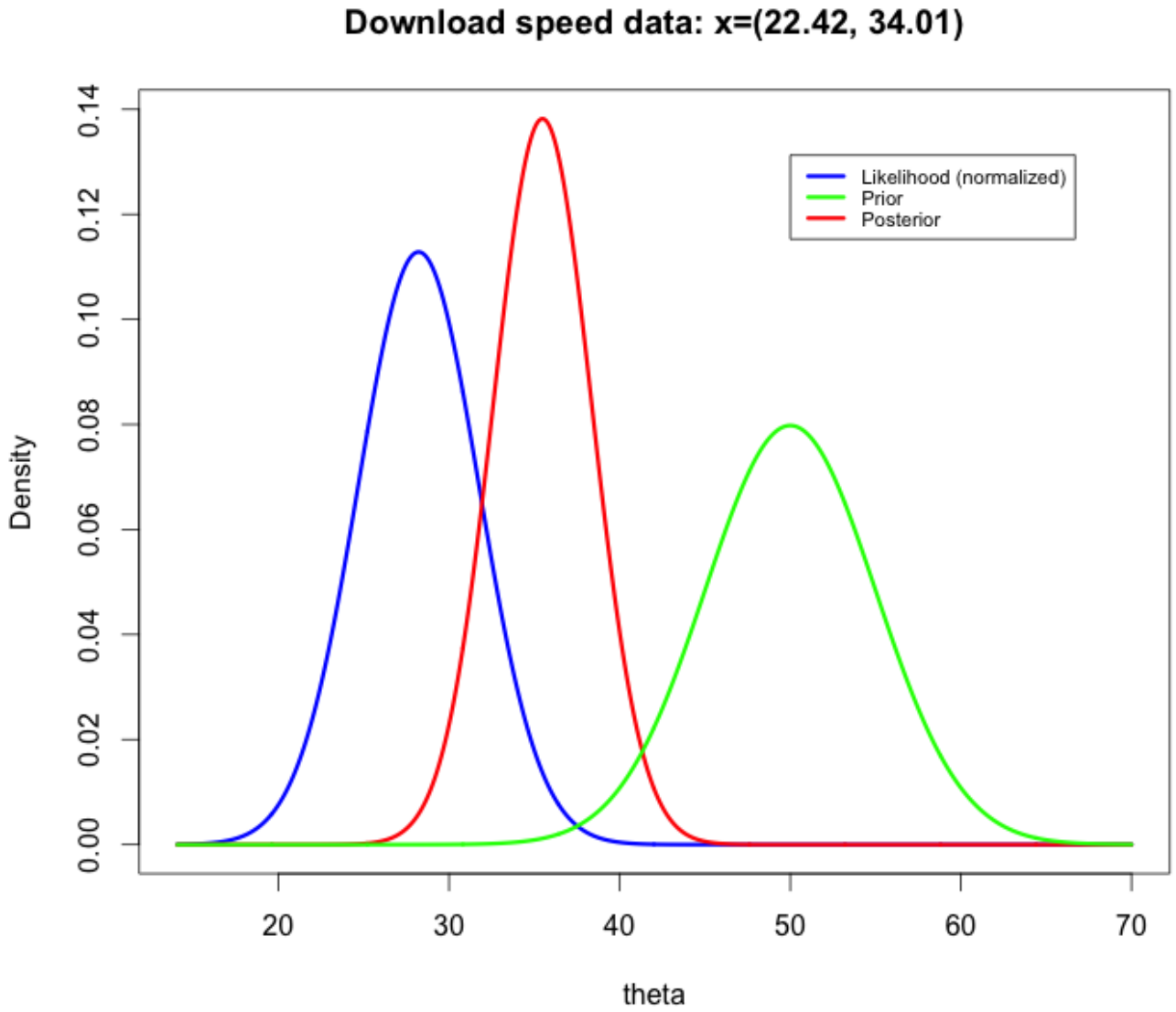

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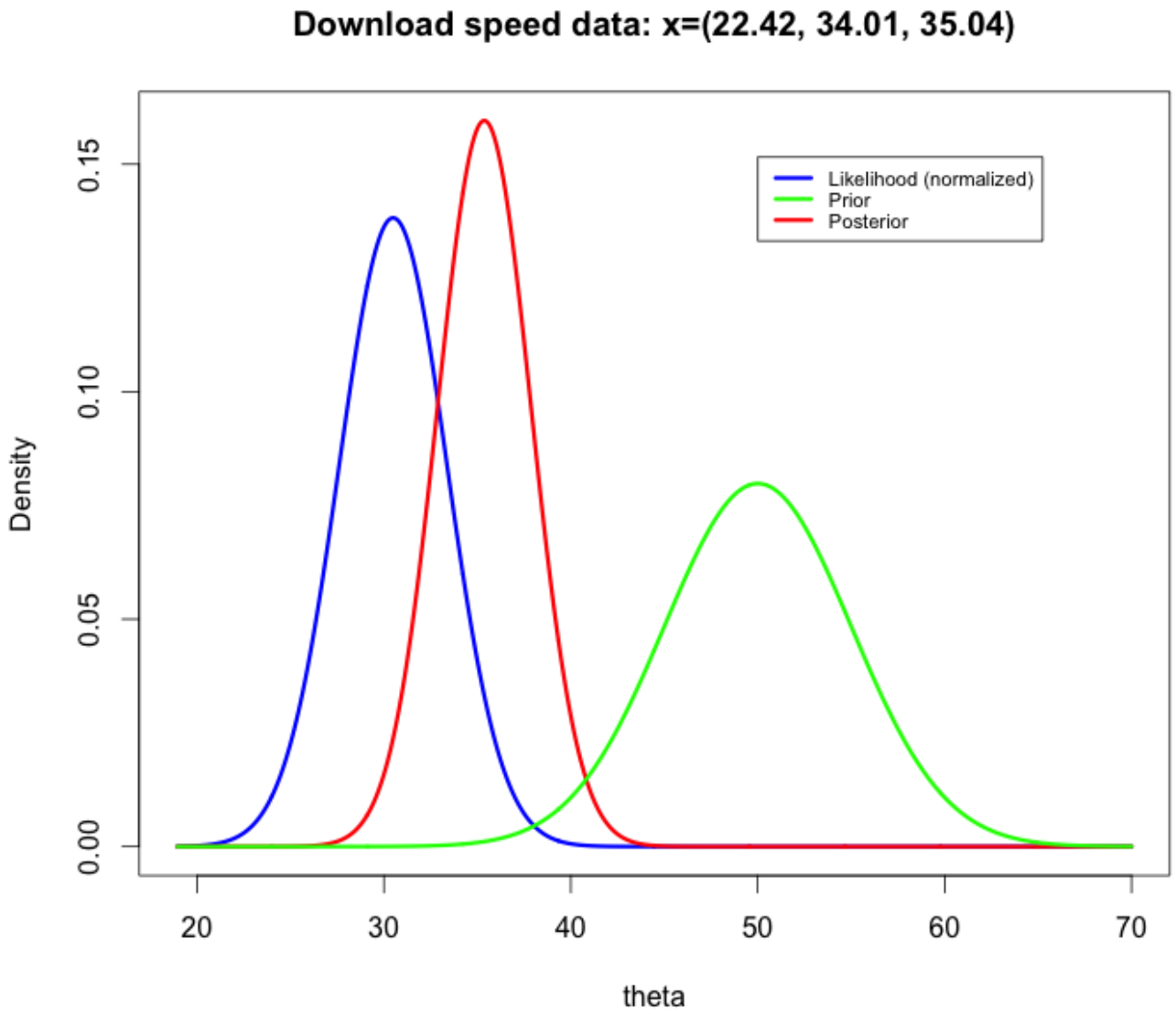

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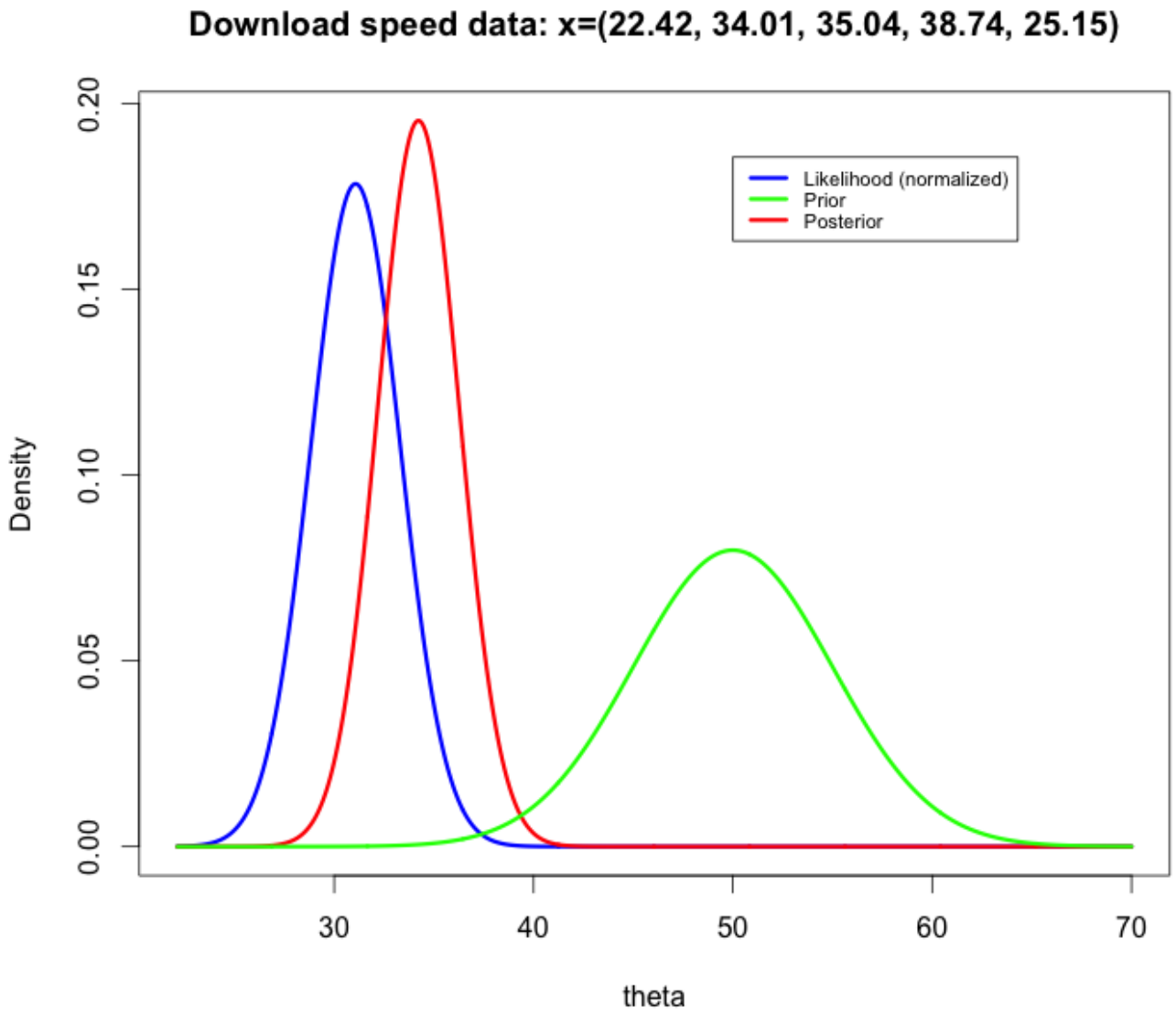
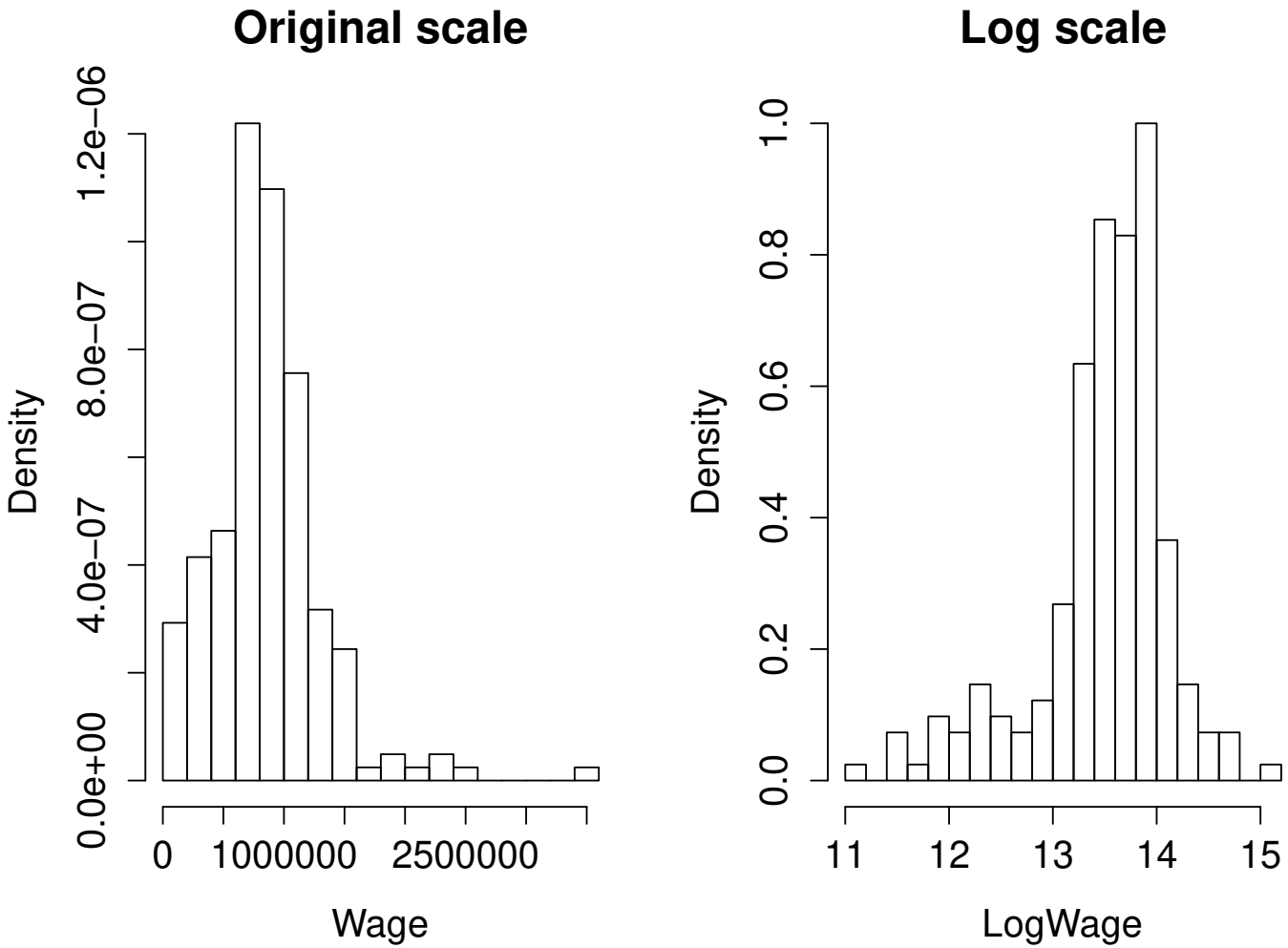


Canadian wages data

- Data on wages for 205 Canadian workers.



Canadian wages

- **Model**

$$X_1, ..., X_n|\theta \sim N(\theta, \sigma^2),\ \sigma^2 = 0.4$$

- **Prior**

$$\theta \sim N(\mu_0, \tau_0^2),\ \mu_0 = 12 \text{ and } \tau_0 = 10$$

- **Posterior**

$$\theta|x_1, ..., x_n \sim N\left(\mu_n, \tau_n^2\right),$$

where $\mu_n = w\bar{x} + (1-w)\mu_0$.

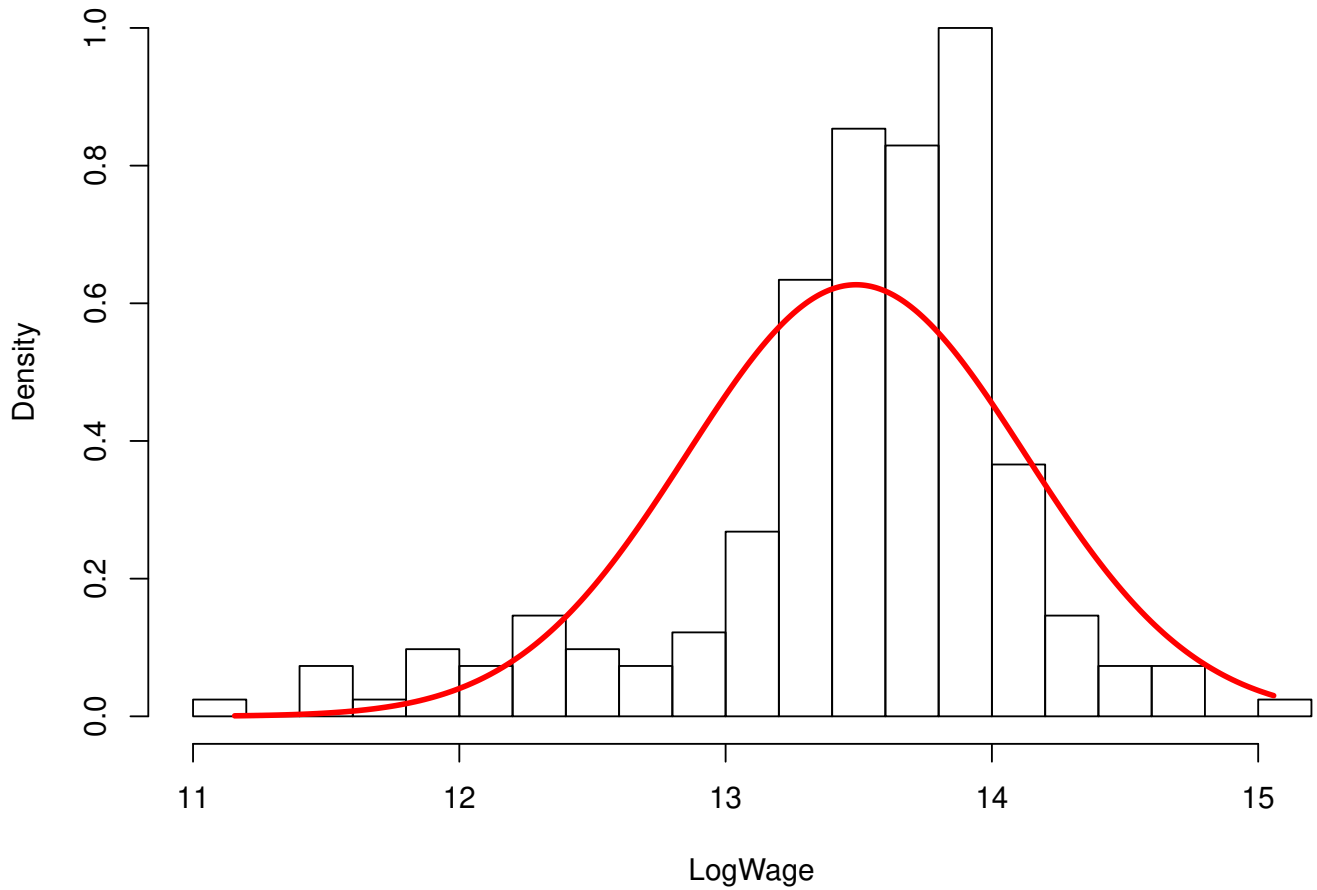
- For the Canadian wage data:

$$w = \frac{\sigma^{-2}n}{\sigma^{-2}n + \tau_0^{-2}} = \frac{2.5 \cdot 205}{2.5 \cdot 205 + 1/100} = 0.999.$$

$$\mu_n = w\bar{x} + (1-w)\mu_0 = 0.999 \cdot 13.489 + (1-0.999) \cdot 12 \approx 13.489$$

$$\tau_n^2 = (2.5 \cdot 205 + 1/100)^{-1} = 0.00195$$

Canadian wages data - model fit



Poisson model

- **Model**

$$y_1, ..., y_n | \theta \overset{iid}{\sim} Pois(\theta)$$

- **Poisson distribution**

$$p(y) = \frac{\theta^y e^{-\theta}}{y!}$$

- **Likelihood** from iid Poisson sample $y = (y_1, ..., y_n)$

$$p(y|\theta) = \left[\prod_{i=1}^n p(y_i|\theta)\right] \propto \theta^{(\sum_{i=1}^n y_i)} \exp(-\theta n),$$

- **Prior**

$$p(\theta) \propto \theta^{\alpha-1} \exp(-\theta\beta) \propto Gamma(\alpha, \beta)$$

which contains the info: $\alpha - 1$ counts in β observations.

Poisson model, cont.

Posterior

$$\begin{aligned} p(\theta|y_1,...,y_n) &\propto \left[\prod_{i=1}^n p(y_i|\theta)\right] p(\theta) \\ &\propto \theta^{\sum_{i=1}^n y_i} \exp(-\theta n)\theta^{\alpha-1}\exp(-\theta\beta) \\ &= \theta^{\alpha+\sum_{i=1}^n y_i-1}\exp[-\theta(\beta+n)], \end{aligned}$$

which is proportional to the $Gamma(\alpha+\sum_{i=1}^n y_i, \beta+n)$ distribution.

Prior-to-Posterior mapping

$$\begin{aligned} \text{Model:} \quad & y_1,...,y_n|\theta \overset{iid}{\sim} Pois(\theta) \\ \text{Prior:} \quad & \theta \sim Gamma(\alpha,\beta) \\ \text{Posterior:} \quad & \theta|y_1,...,y_n \sim Gamma(\alpha+\sum_{i=1}^n y_i, \beta+n). \end{aligned}$$

Example - Number of bids in eBay auctions

- **Data**:
  - Number of placed bids in $n = 1000$ eBay coin auctions.
  - Sum of counts: $\sum_{i=1}^{n} y_i = 3635$.
  - Average number bids per auction: $\bar{y} = 3635/1000 = 3.635$.
- **Prior**: $\alpha = 2$, $\beta = 1/2$.

$$E(\theta) = \frac{\alpha}{\beta} = 4$$

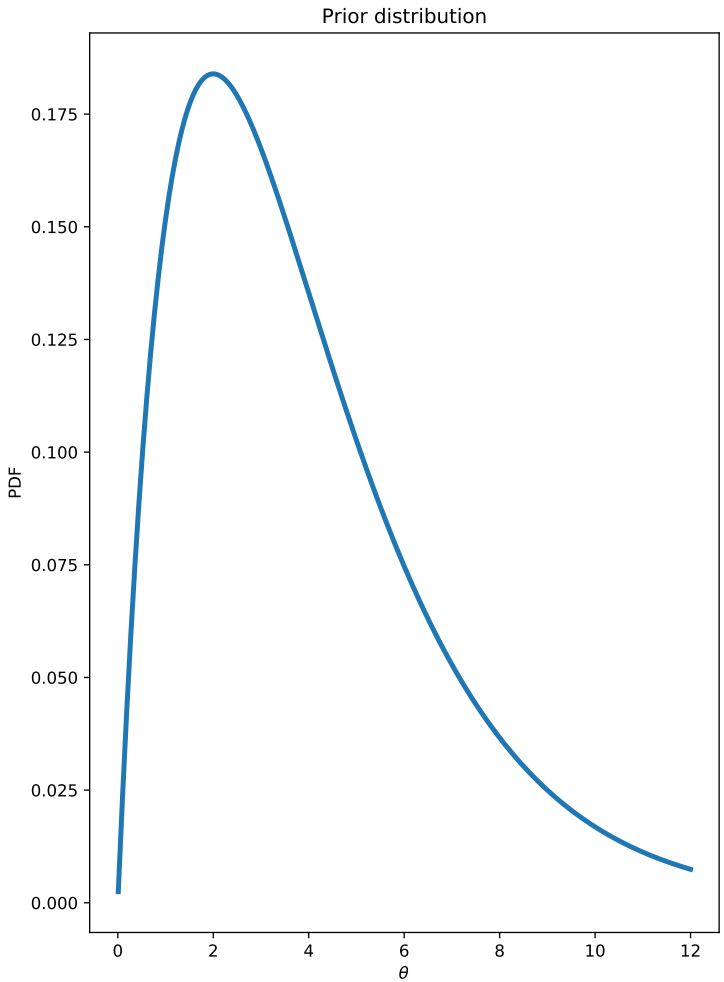
$$SD(\theta|\boldsymbol{y}) = \frac{\alpha}{\beta^2} = 2.823$$

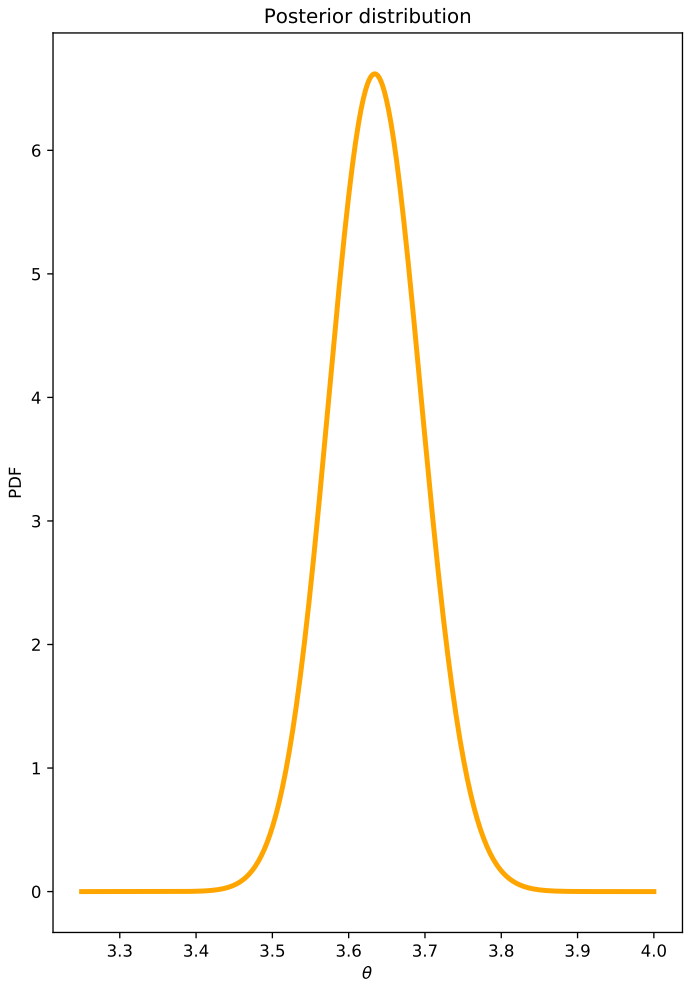
- **Posterior**

$$E(\theta|\boldsymbol{y}) = \frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n} = \frac{2 + 3635}{1/2 + 1000} \approx 3.635.$$

$$SD(\theta|\boldsymbol{y}) = \left(\frac{\alpha + \sum_{i=1}^{n} y_i}{(\beta + n)^2}\right)^{1/2} \approx 0.060.$$

eBay data - Posterior of θ





Posterior intervals

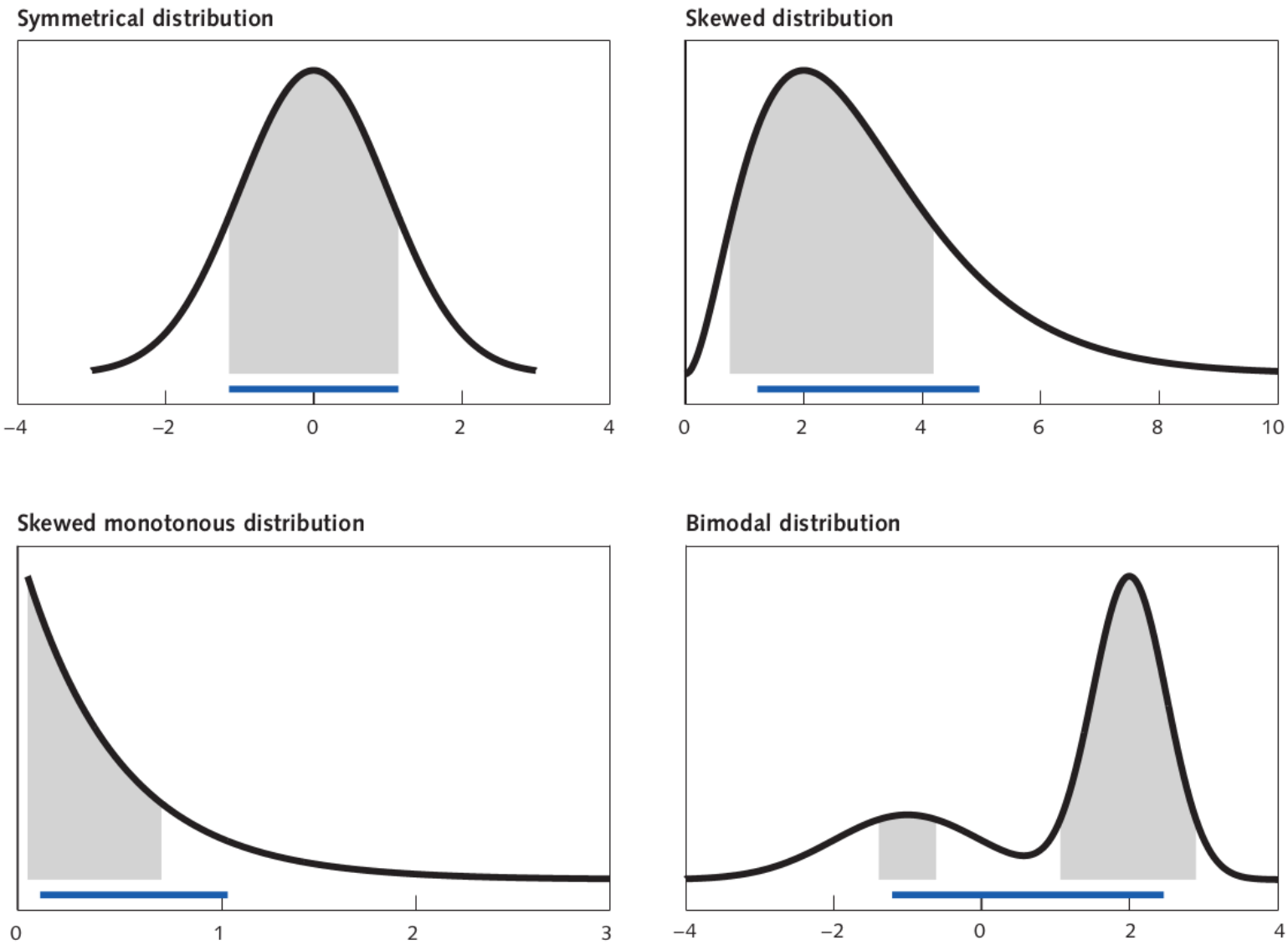
- **Bayesian 95% credible interval**: the probability that the unknown parameter θ lies in the interval is 0.95.
- Approximate 95% **credible interval** for θ

$$E(\theta|y) \pm 1.96 \cdot SD(\theta|y) = [3.517; 3.753]$$

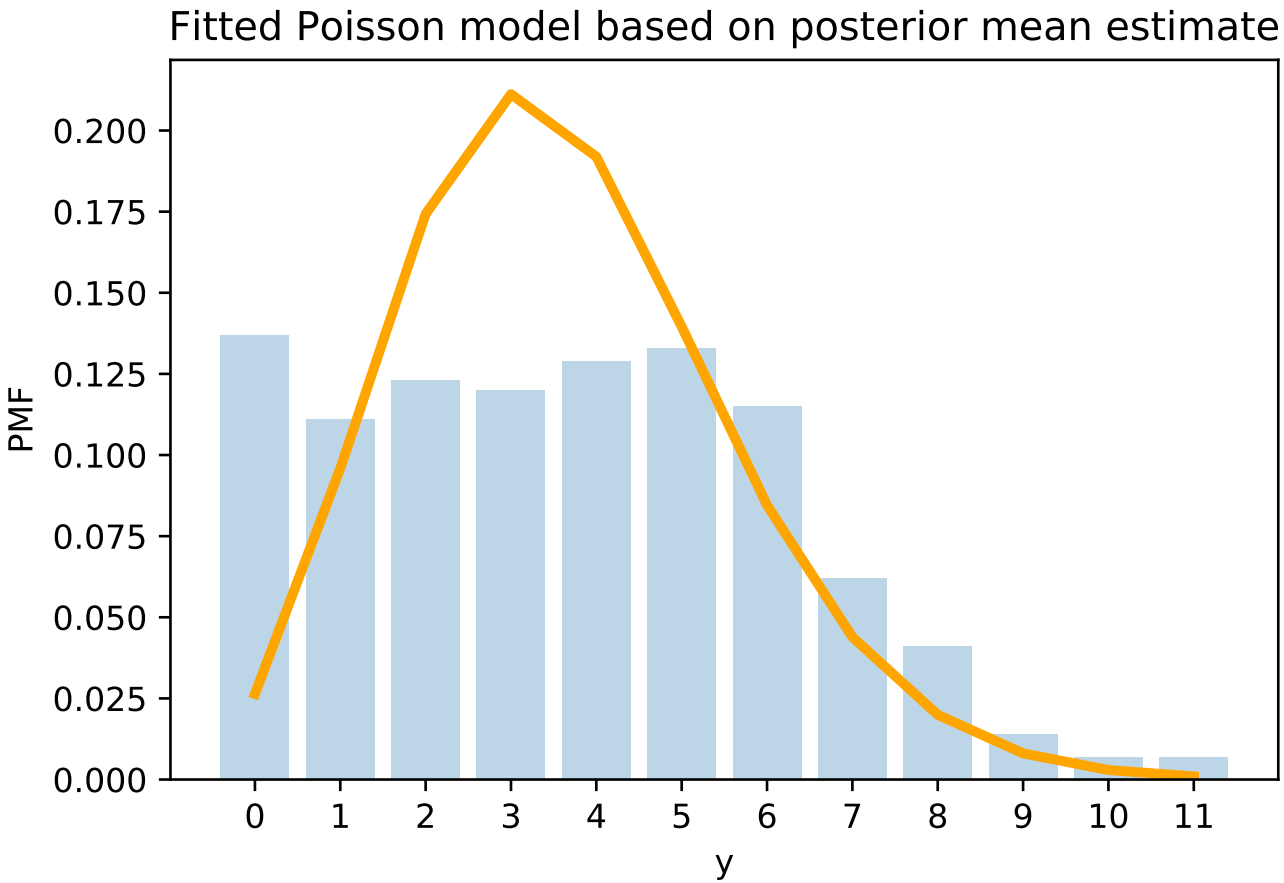
- An exact 95% **equal-tail interval** is $[3.518;\ 3.754]$
- **Highest Posterior Density** (**HPD**) interval contains the θ values with highest pdf.

$$[3.518; 3.752]$$

Illustration of different interval types



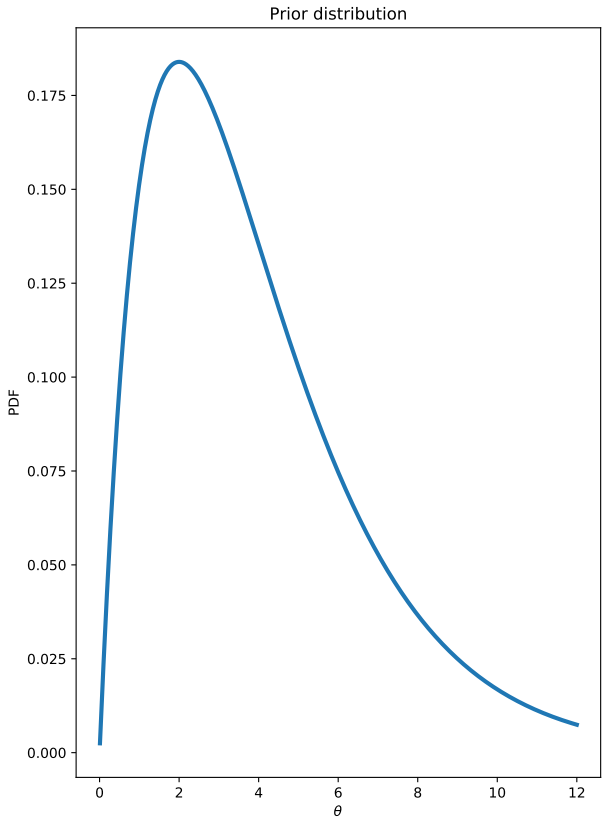
eBay dat - Fit

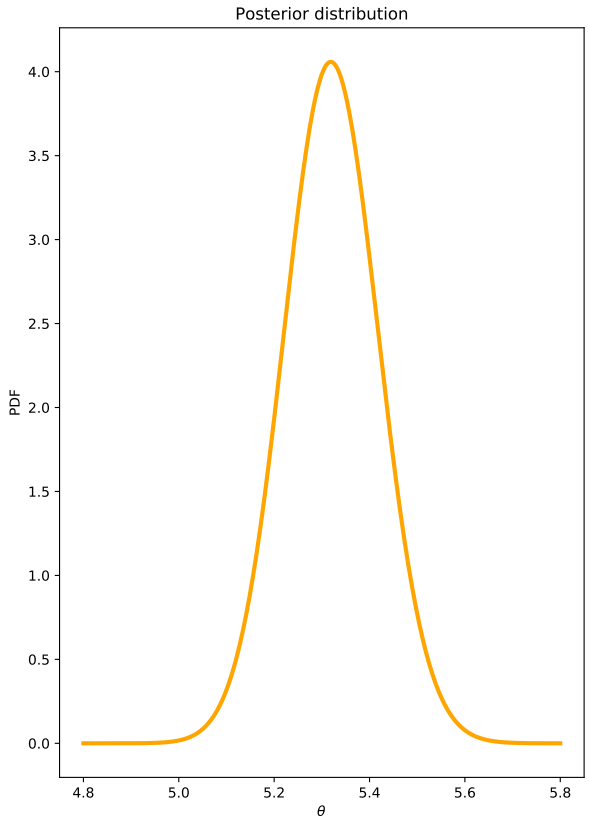

Fitted Poisson model based on posterior mean estimate
PMF
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
0
1
2
3
4
5
6
7
8
9
10
11
y

eBay - low/high seller's reservation price

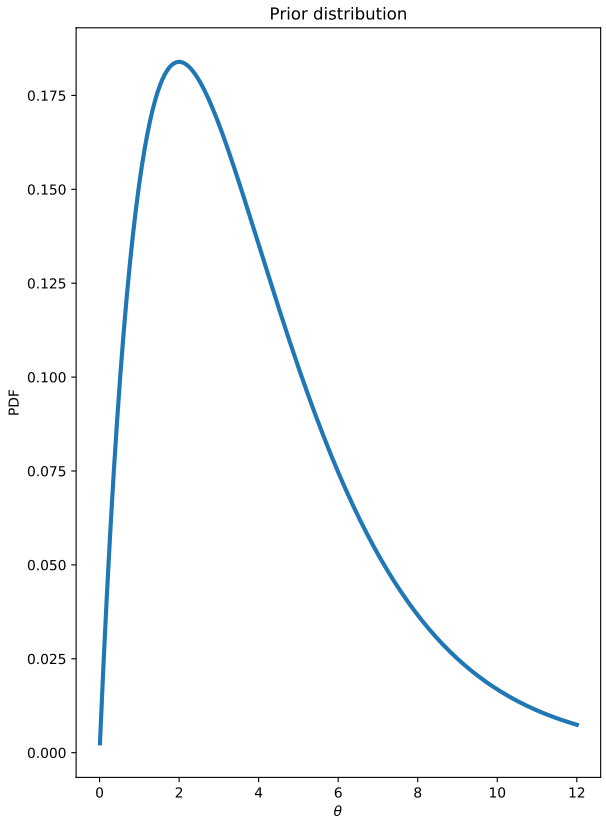
- The data is very heterogenous. Some auctions start with very high reservations prices (lowest price accepted by the seller).
- Split the data into auctions with low/high reservation prices.
- **Low reservation price auctions**:
  - $n = 550$ eBay coin auctions.
  - Posterior mean: 5.321 bids.
- **High reservation price auctions**:
  - $n = 450$ eBay coin auctions.
  - Posterior mean: 1.576 bids.

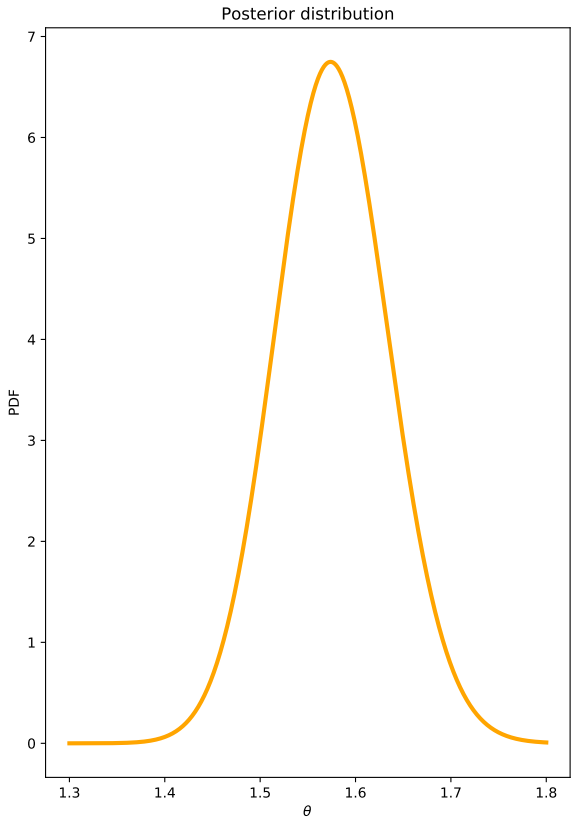
eBay - low seller's reservation price



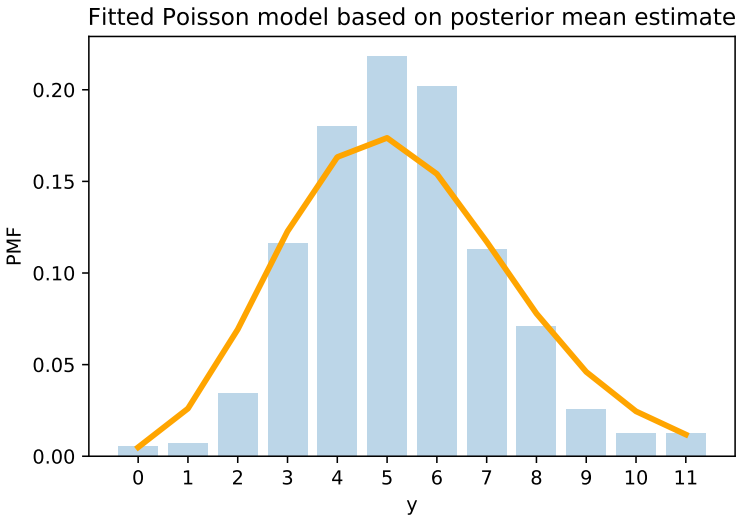


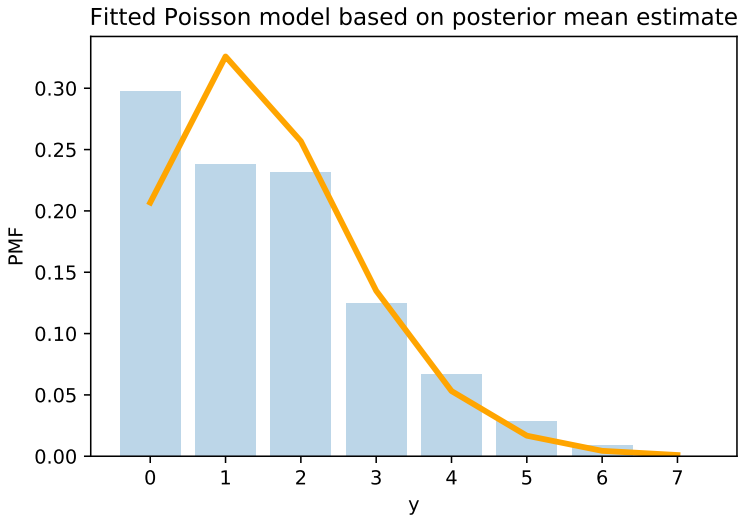
eBay - high seller's reservation price





eBay - fit low/high reservation prices





- Better fits, but still not good enough.
- Lab: Fit **Poisson regression** with reservation price as continuous covariate.

Conjugate priors

- Normal likelihood: Normal prior$\rightarrow$Normal posterior.
- Bernoulli likelihood: Beta prior$\rightarrow$Beta posterior.
- Poisson likelihood: Gamma prior$\rightarrow$Gamma posterior.
- **Conjugate priors**: A prior is conjugate to a model if the prior and posterior belong to the same distributional family.
- Formal definition: Let $\mathcal{F} = \{p(y|\theta), \theta \in \Theta\}$ be a class of sampling distributions. A family of distributions $\mathcal{P}$ is **conjugate** for $\mathcal{F}$ if

$$p(\theta) \in \mathcal{P} \Rightarrow p(\theta|x) \in \mathcal{P}$$

holds for all $p(y|\theta) \in \mathcal{F}$.

Prior elicitation

- The prior should be determined (elicited) by an **expert**. Typically, expert$\neq$statistician.
- Elicit the prior on a quantity that the expert knows well. Convert afterwards.
- Ask probabilistic questions to the expert:
  - $E(\theta) = ?$
  - $SD(\theta) = ?$
  - $Pr(\theta < c) = ?$
  - $Pr(y > c) = ?$
- Show some consequences of the elicitated prior to the expert.
- Beware of psychological effects, such as anchoring.

Prior elicitation - AR(p) example

- **Autoregressive process** or order p

$$y_t = \mu + \phi_1(y_{t-1} - \mu) + ... + \phi_p(y_{t-p} - \mu) + \varepsilon_t, \ \varepsilon_t \overset{iid}{\sim} N(0, \sigma^2)$$

- Informative prior on the unconditional mean: $\mu \sim N(\mu_0, \tau_0^2)$.
- "Noninformative" prior on σ^2: $p(\sigma^2) \propto 1/\sigma^2$
- Assume $\phi_i \sim N(\mu_i, \psi_i)$, $i = 1, ..., p$ are independent a priori.
- Prior on $\phi = (\phi_1, ..., \phi_p)$ centered on persistent AR(1) process: $\mu_1 = 0.8, \mu_2 = ... = \mu_p = 0$
- $Var(\phi_i) = \frac{c}{i^\lambda}$. "Longer" lags are more likely to be zero a priori.

Jeffreys' prior

- **Observed information**

$$J_{\theta,\mathbf{x}} = -\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta^2}\Big|_{\theta=\hat{\theta}}$$

- **Fisher information**

$$I_\theta = E_{\mathbf{x}|\theta}\left(J_{\theta,\mathbf{x}}\right)$$

- A common non-informative prior is **Jeffreys' prior**

$$p(\theta) = |I_\theta|^{1/2}.$$

- **Invariant** to 1:1 transformations of θ.
- Often non-conjugate.
- Often problematic in multiparameter settings.

Jeffreys' prior for Bernoulli sampling

$$x_1, ..., x_n|\theta \overset{iid}{\sim} Bern(\theta).$$

$$\ln p(\mathbf{x}|\theta) = s \ln \theta + f \ln(1-\theta)$$

$$\frac{d \ln p(\mathbf{x}|\theta)}{d\theta} = \frac{s}{\theta} - \frac{f}{(1-\theta)}$$

$$\frac{d^2 \ln p(\mathbf{x}|\theta)}{d\theta^2} = -\frac{s}{\theta^2} - \frac{f}{(1-\theta)^2}$$

$$I(\theta) = \frac{E_{\mathbf{x}|\theta}(s)}{\theta^2} + \frac{E_{\mathbf{x}|\theta}(f)}{(1-\theta)^2} = \frac{n\theta}{\theta^2} + \frac{n(1-\theta)}{(1-\theta)^2} = \frac{n}{\theta(1-\theta)}$$

Thus, the Jeffreys' prior is

$$p(\theta) = |I(\theta)|^{1/2} \propto \theta^{-1/2}(1-\theta)^{-1/2} \propto Beta(1/2, 1/2).$$

Jeffreys' prior for negative binomial sampling

- Jeffreys' prior:

$$n|\theta \overset{iid}{\sim} NegBin(s, \theta).$$

$$\ln p(\mathbf{x}|\theta) = \ln \binom{n-1}{s-1} + s \ln \theta + f \ln(1-\theta)$$

$$\frac{d^2 \ln p(\mathbf{x}|\theta)}{d\theta^2} = -\frac{s}{\theta^2} - \frac{f}{(1-\theta)^2}$$

$$I(\theta) = \frac{s}{\theta^2} + \frac{E_{n|\theta}(n-s)}{(1-\theta)^2} = \frac{s}{\theta^2} + \frac{s/\theta - s}{(1-\theta)^2} = \frac{s}{\theta^2(1-\theta)}$$

- Thus, the Jeffreys' prior is

$$p(\theta) = |I(\theta)|^{1/2} \propto \theta^{-1}(1-\theta)^{-1/2} \propto Beta(\theta|0, 1/2).$$

- Jeffreys' prior is **improper**, but the posterior is proper: $\theta|n \sim \text{Beta}(s, f + 1/2)$ which is proper since $s \geq 1$.
- Jeffreys' prior **violates the likelihood principle** because $I(\theta)$ is sampling-based.

Different types of prior information

- Real **expert information**. Combo of previous studies and experience.
- **Vague prior** information.
- **Reporting priors**. Easy to understand the information they contain.
- **Smoothness priors**. Regularization. Shrinkage. Big thing in modern statistics/machine learning.

Bayesian Learning

Lecture 3 - Multi-parameter models

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Lecture overview

- **Multiparameter** models
- **Marginalization**
- **Normal model with unknown variance**
- Bayesian analysis of **multinomial data**
- Bayesian analysis of **multivariate normal data**

Marginalization

- Models with **multiple parameters** $\theta_1, \theta_2, ...$
- Examples: $x_i \overset{iid}{\sim} N(\theta, \sigma^2)$; multiple regression ...
- **Joint posterior distribution**

$$p(\theta_1, \theta_2, ..., \theta_p|y) \propto p(y|\theta_1, \theta_2, ..., \theta_p)p(\theta_1, \theta_2, ..., \theta_p).$$

$$p(\theta|y) \propto p(y|\theta)p(\theta).$$

- **Marginalize** out parameter of no direct interest (**nuisance**).
- Example: $\theta = (\theta_1, \theta_2)'$. **Marginal posterior** of θ_1

$$p(\theta_1|y) = \int p(\theta_1, \theta_2|y)d\theta_2 = \int p(\theta_1|\theta_2, y)p(\theta_2|y)d\theta_2.$$

Normal model with unknown variance

- **Model**

$$x_1, \ldots, x_n \overset{iid}{\sim} N(\theta, \sigma^2)$$

- **Prior**

$$p(\theta, \sigma^2) \propto (\sigma^2)^{-1}$$

- **Posterior**

$$\theta|\sigma^2, \mathbf{x} \sim N\left(\bar{x}, \frac{\sigma^2}{n}\right)$$
$$\sigma^2|\mathbf{x} \sim \text{Inv} - \chi^2(n-1, s^2),$$

where

$$s^2 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}$$

is the usual sample variance.

Normal model with unknown variance

- **Simulating** from the posterior :
  1. Draw $X \sim \chi^2(n-1)$
  2. Compute $\sigma^2 = \frac{(n-1)s^2}{X}$ (this a draw from Inv-$\chi^2(n-1, s^2)$)
  3. Draw a θ from $N\left(\bar{x}, \frac{\sigma^2}{n}\right)$ conditional on the previous draw σ^2
  4. Repeat step 1-3 many times.
- The sampling is implemented in the R program `NormalNonInfoPrior.R`
- We may derive the **marginal posterior** analytically as

$$\theta|\mathbf{x} \sim t_{n-1}\left(\bar{x}, \frac{s^2}{n}\right).$$

Normal model - normal prior

- **Model**

$$y_1, ..., y_n | \theta, \sigma^2 \overset{iid}{\sim} N(\theta, \sigma^2)$$

- **Conjugate prior**

$$\theta | \sigma^2 \sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right)$$
$$\sigma^2 \sim Inv\text{-}\chi^2(\nu_0, \sigma_0^2)$$

Normal model with normal prior

Posterior

$$\theta|\mathbf{y}, \sigma^2 \sim N\left(\mu_n, \frac{\sigma^2}{\kappa_n}\right)$$
$$\sigma^2|\mathbf{y} \sim \mathit{Inv}\text{-}\chi^2(\nu_n, \sigma_n^2).$$

where

$$\begin{aligned}
\mu_n &= \frac{\kappa_0}{\kappa_0 + n}\mu_0 + \frac{n}{\kappa_0 + n}\bar{y} \\
\kappa_n &= \kappa_0 + n \\
\nu_n &= \nu_0 + n \\
\nu_n\sigma_n^2 &= \nu_0\sigma_0^2 + (n-1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n}(\bar{y} - \mu_0)^2.
\end{aligned}$$

Normal model with normal prior

Posterior

$$\theta|\mathbf{y}, \sigma^2 \sim N\left(\mu_n, \frac{\sigma^2}{\kappa_n}\right)$$
$$\sigma^2|\mathbf{y} \sim \mathit{Inv}\text{-}\chi^2(\nu_n, \sigma_n^2).$$

where

$$\begin{aligned}
\mu_n &= \frac{\kappa_0}{\kappa_0 + n}\mu_0 + \frac{n}{\kappa_0 + n}\bar{y} \\
\kappa_n &= \kappa_0 + n \\
\nu_n &= \nu_0 + n \\
\nu_n\sigma_n^2 &= \nu_0\sigma_0^2 + (n-1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n}(\bar{y} - \mu_0)^2.
\end{aligned}$$

Marginal posterior

$$\theta|\mathbf{y} \sim t_{\nu_n}\left(\mu_n, \sigma_n^2/\kappa_n\right)$$

Multinomial model with Dirichlet prior

- **Categorical counts**: $y = (y_1, ...y_K)$, where $\sum_{k=1}^{K} y_k = n$.
- y_k= number of observations in kth category. Brand choices.
- **Multinomial model**:

$$p(y|\theta) \propto \prod_{k=1}^{K} \theta_k^{y_k}, \text{ where } \sum_{k=1}^{K} \theta_k = 1.$$

- **Dirichlet prior**: $\text{Dirichlet}(\alpha_1, ..., \alpha_K)$

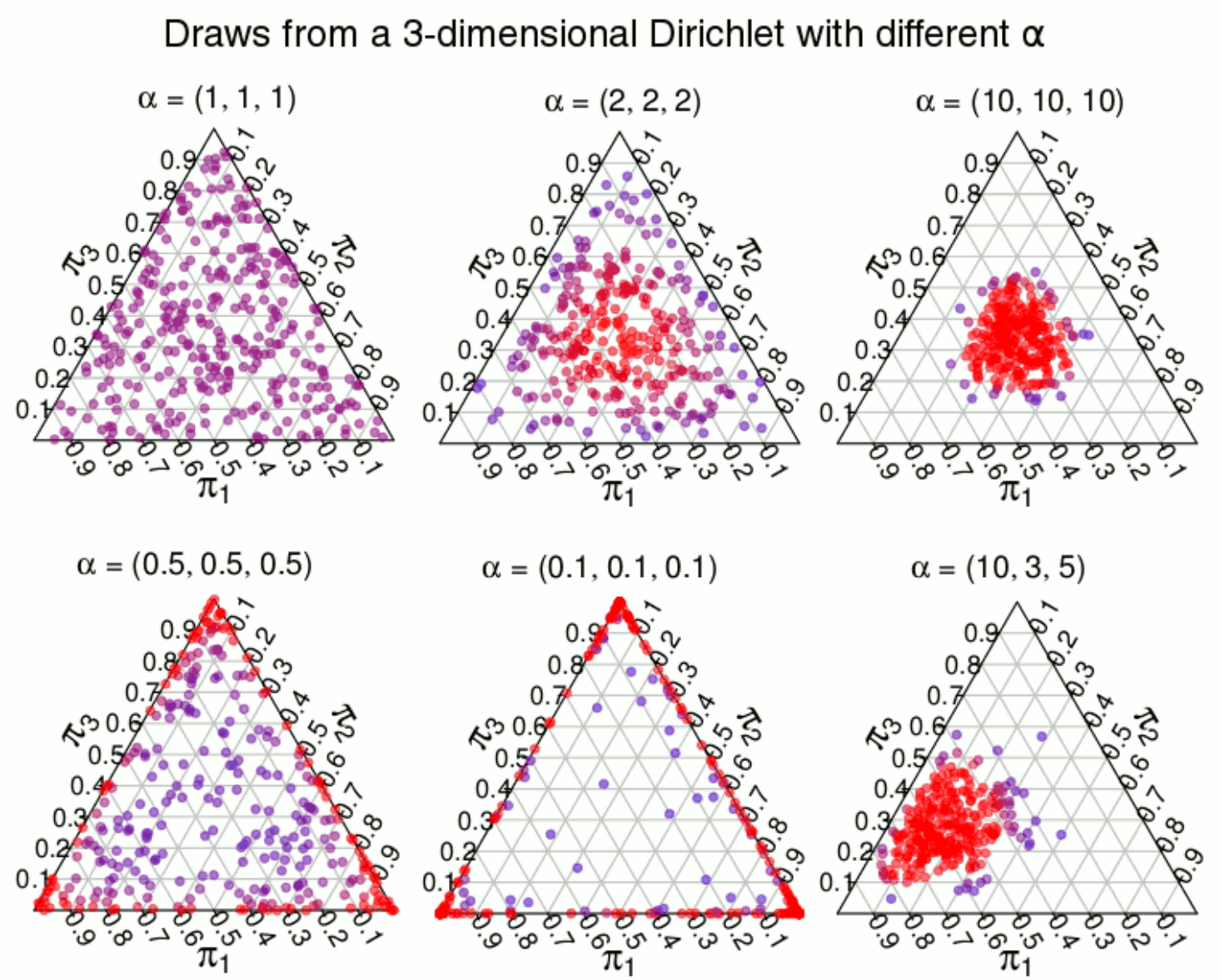
$$p(\theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}.$$

- **Mean and variance** for $(\theta_1, \ldots, \theta_K) \sim \textit{Dirichlet}(\alpha_1, ..., \alpha_K)$

$$\text{E}(\theta_k) = \frac{\alpha_k}{\sum_{j=1}^{K} \alpha_j}$$

$$\text{V}(\theta_k) = \frac{\text{E}(\theta_k)\left[1 - \text{E}(\theta_k)\right]}{1 + \sum_{j=1}^{K} \alpha_j}$$

Dirichlet distribution



Multinomial model with Dirichlet prior

- 'Non-informative': $\alpha_1 = ... = \alpha_K = 1$ (uniform and proper).

- **Simulating** from the Dirichlet distribution:
  - Generate $x_1 \sim Gamma(\alpha_1, 1), ..., x_K \sim Gamma(\alpha_K, 1)$.
  - Compute $z_k = x_k / (\sum_{j=1}^{K} x_j)$.
  - Then $z = (z_1, ..., z_K) \sim \text{Dirichlet}(\alpha_1, ..., \alpha_K)$.

- ***Prior-to-Posterior updating***:

$$
\begin{aligned}
\textit{Model}: \quad & y = (y_1, ...y_K) \sim \text{Multin}(n; \theta_1, ..., \theta_K) \\
\textit{Prior}: \quad & \theta = (\theta_1, ..., \theta_K) \sim \text{Dirichlet}(\alpha_1, ..., \alpha_K) \\
\textit{Posterior}: \quad & \theta | y \sim \text{Dirichlet}(\alpha_1 + y_1, ..., \alpha_K + y_K).
\end{aligned}
$$

Example: market shares

- Survey among 513 smartphones owners:
  - 180 used mainly an iPhone
  - 230 used mainly an Android phone
  - 62 used mainly a Windows phone
  - 41 used mainly some other mobile phone.
- Old survey: iPhone 30%, Android 30%, Windows 20%, Other 20%.
- **Pr(Android has largest share | Data)**
- Prior: $\alpha_1 = 15, \alpha_2 = 15, \alpha_3 = 10$ and $\alpha_4 = 10$ (prior info is equivalent to a survey with only 50 respondents)
- Posterior: $(\theta_1, \theta_2, \theta_3, \theta_4)|\mathbf{y} \sim \text{Dirichlet}(195, 245, 72, 51)$.
- `DirichletSurveyData` Rnotebook on web page.

Multivariate normal - known Σ

- **Model**

$$y_1, ..., y_n \overset{iid}{\sim} N_p(\mu, \Sigma)$$

where Σ is a known covariance matrix.

- Density

$$p(y|\mu, \Sigma) = |2\pi\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(y-\mu)'\Sigma^{-1}(y-\mu)\right)$$

- **Likelihood**

$$p(y_1, ..., y_n|\mu, \Sigma) \propto |\Sigma|^{-n/2} \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(y_i-\mu)'\Sigma^{-1}(y_i-\mu)\right)$$

$$= |\Sigma|^{-n/2} \exp\left(-\frac{1}{2} tr\Sigma^{-1}S_\mu\right)$$

where $S_\mu = \sum_{i=1}^{n}(y_i-\mu)(y_i-\mu)'$.

Multivariate normal - known Σ

- **Prior**

$$\mu \sim N_p(\mu_0, \Lambda_0)$$

- **Posterior**

$$\mu|y \sim N(\mu_n, \Lambda_n)$$

where

$$\mu_n = (\Lambda_0^{-1} + n\Sigma^{-1})^{-1}(\Lambda_0^{-1}\mu_0 + n\Sigma^{-1}\bar{y})$$
$$\Lambda_n^{-1} = \Lambda_0^{-1} + n\Sigma^{-1}$$

- Posterior mean is a weighted average of prior and data information.
- **Noninformative prior**: let the precision go to zero: $\Lambda_0^{-1} \to 0$.

Bayesian Learning

Lecture 4 - Predictions

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Lecture overview

- **Prediction**
  - Normal model
  - More complex examples
- **Decision theory**
  - The elements of a decision problem
  - The Bayesian way
  - Point estimation as a decision problem

Prediction/Forecasting

- **Posterior predictive density** for future $\tilde{y}$ given observed $\mathbf{y}$

$$p(\tilde{y}|\mathbf{y}) = \int_\theta p(\tilde{y}|\theta, \mathbf{y}) p(\theta|\mathbf{y}) d\theta$$

- If $p(\tilde{y}|\theta, \mathbf{y}) = p(\tilde{y}|\theta)$ [not true for time series], then

$$p(\tilde{y}|\mathbf{y}) = \int_\theta p(\tilde{y}|\theta) p(\theta|\mathbf{y}) d\theta$$

- **Parameter uncertainty** in $p(\tilde{y}|\mathbf{y})$ by **averaging over** $p(\theta|\mathbf{y})$.

Prediction - Normal data, known variance

- Under the uniform prior $p(\theta) \propto c$, then

$$p(\tilde{y}|\mathbf{y}) = \int_{\theta} p(\tilde{y}|\theta)p(\theta|\mathbf{y})d\theta$$
$$\theta|\mathbf{y} \sim N(\bar{y}, \sigma^2/n)$$
$$\tilde{y}|\theta \sim N(\theta, \sigma^2)$$

Prediction - Normal data, known variance

- Under the uniform prior $p(\theta) \propto c$, then

$$p(\tilde{y}|\mathbf{y}) = \int_{\theta} p(\tilde{y}|\theta)p(\theta|\mathbf{y})d\theta$$
$$\theta|\mathbf{y} \sim N(\bar{y}, \sigma^2/n)$$
$$\tilde{y}|\theta \sim N(\theta, \sigma^2)$$

Simulation algorithm:

1. Generate a **posterior draw** of θ ($\theta^{(1)}$) from $N(\bar{y}, \sigma^2/n)$
2. Generate a **predictive draw** of $\tilde{y}$ ($\tilde{y}^{(1)}$) from $N(\theta^{(1)}, \sigma^2)$
3. Repeat Steps 1 and 2 N times to output:
   - Sequence of posterior draws: $\theta^{(1)}, ..., \theta^{(N)}$
   - Sequence of predictive draws: $\tilde{y}^{(1)}, ..., \tilde{y}^{(N)}$.

Predictive distribution - Normal model

- $\theta^{(1)} = \bar{y} + \varepsilon^{(1)}$, where $\varepsilon^{(1)} \sim N(0, \sigma^2/n)$. (Step 1).
- $\tilde{y}^{(1)} = \theta^{(1)} + v^{(1)}$, where $v^{(1)} \sim N(0, \sigma^2)$. (Step 2).
- $\tilde{y}^{(1)} = \bar{y} + \varepsilon^{(1)} + v^{(1)}$.
- $\varepsilon^{(1)}$ and $v^{(1)}$ are independent.
- The sum of two normal random variables is normal so

$$\begin{aligned} E(\tilde{y}|\mathbf{y}) &= \bar{y} \\ V(\tilde{y}|\mathbf{y}) &= \frac{\sigma^2}{n} + \sigma^2 = \sigma^2\left(1 + \frac{1}{n}\right) \end{aligned}$$

$$\tilde{y}|\mathbf{y} \sim N\left[\bar{y}, \sigma^2\left(1 + \frac{1}{n}\right)\right]$$

Predictive distribution - Normal model and prior

- Easy to see that the predictive distribution is normal.
- The mean

$$E_{\tilde{y}|\theta}(\tilde{y}) = \theta$$

and then remove the conditioning on θ by averaging over θ

$$E(\tilde{y}|\mathbf{y}) = E_{\theta|\mathbf{y}}(\theta) = \mu_n \text{ (Posterior mean of } \theta).$$

- The predictive variance of $\tilde{y}$ (total variance formula):

$$\begin{aligned} V(\tilde{y}|\mathbf{y}) &= E_{\theta|\mathbf{y}}[V_{\tilde{y}|\theta}(\tilde{y})] + V_{\theta|\mathbf{y}}[E_{\tilde{y}|\theta}(\tilde{y})] \\ &= E_{\theta|\mathbf{y}}(\sigma^2) + V_{\theta|\mathbf{y}}(\theta) \\ &= \sigma^2 + \tau_n^2 \\ &= \text{(Population variance + Posterior variance of } \theta). \end{aligned}$$

- In summary:

$$\tilde{y}|\mathbf{y} \sim N(\mu_n, \sigma^2 + \tau_n^2).$$

Bayesian prediction for time series

Autoregressive process

$$y_t = \mu + \phi_1(y_{t-1} - \mu) + ... + \phi_p(y_{t-p} - \mu) + \varepsilon_t, \ \varepsilon_t \overset{iid}{\sim} N(0, \sigma^2)$$

Simulation algorithm. Repeat N times:

1. Generate a **posterior draw** of $\theta^{(1)} = (\phi_1^{(1)}, ..., \phi_p^{(1)}, \mu^{(1)}, \sigma^{(1)})$ from $p(\phi_1, ..., \phi_p, \mu, \sigma | \mathbf{y}_{1:T})$.
2. Generate a **predictive draw** of future time series by:
   1. $\tilde{y}_{T+1} \sim p(y_{T+1} | y_T, y_{T-1}, ..., y_{T-p}, \theta^{(1)})$
   2. $\tilde{y}_{T+2} \sim p(y_{T+2} | \tilde{y}_{T+1}, y_T, ..., y_{T-p}, \theta^{(1)})$
   3. $\tilde{y}_{T+3} \sim p(y_{T+3} | \tilde{y}_{T+2}, \tilde{y}_{T+1}, y_T, ..., y_{T-p}, \theta^{(1)})$
   4. ...

Predicting auction prices on eBay

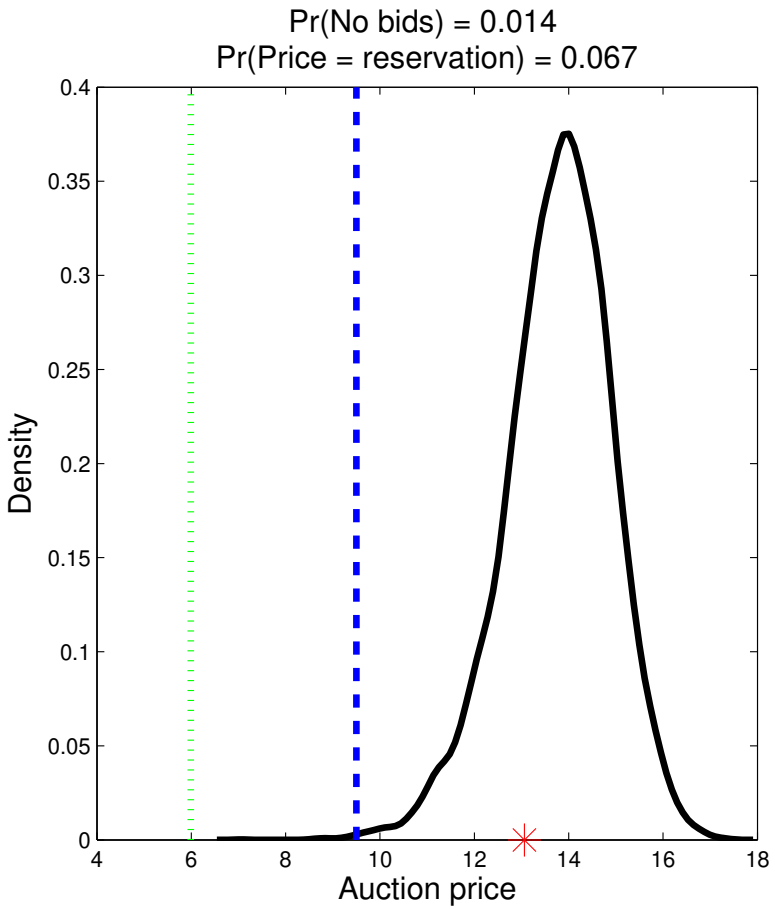
- Problem: **Predicting the auctioned price** in eBay coin auctions.
- **Data**: Bid from 1000 auctions on eBay.
  - The highest bid is not observed.
  - The lowest bids are also not observed because of the seller's reservation price.
- **Covariates**: auction-specific, e.g. Book value from catalog, seller's reservation price, quality of sold object, rating of seller, powerseller, verified seller ID etc
- Buyers are **strategic**. Their bids does not fully reflect their valuation. **Game theory**. Very complicated likelihood.

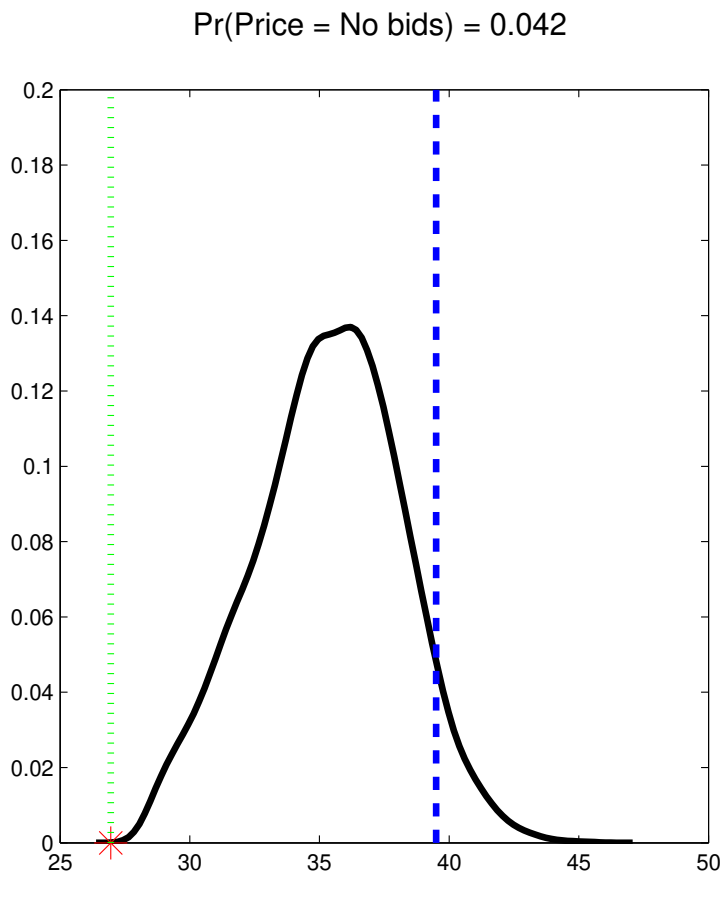
Simulating auction prices on eBay

- Simulate from **posterior predictive distibution** of the **price** in a new auction:

1. Simulate a draw $\theta^{(i)}$ from the posterior $p(\theta|\text{historical bids})$
2. Simulate the number of bidders conditional on $\theta^{(i)}$ (Poisson)
3. Simulate the bidders' valuations, $\mathbf{v}^{(i)}$
4. Simulate all bids, $\mathbf{b}^{(i)}$, conditional on the valuations
5. For $\mathbf{b}^{(i)}$, return the next to largest bid (proxy bidding).

Predicting auction prices on eBay





Decision Theory

- Let θ be an **unknown quantity**. **State of nature**. Examples: Future inflation, Global temperature, Disease.
- Let $a \in \mathcal{A}$ be an **action**. Ex: Interest rate, Energy tax, Surgery.
- Choosing action a when state of nature is θ gives **utility**

$$U(a, \theta)$$

- Alternatively **loss** $L(a, \theta) = -U(a, \theta)$.
- Loss table:

	θ_1	θ_2
a_1	$L(a_1, \theta_1)$	$L(a_1, \theta_2)$
a_2	$L(a_2, \theta_1)$	$L(a_2, \theta_2)$

- Example:

	Rainy	Sunny
Umbrella	20	10
No umbrella	50	0

Decision Theory, cont.

- Example **loss functions** when both a and θ are continuous:
  - **Linear**: $L(a, \theta) = |a - \theta|$
  - **Quadratic**: $L(a, \theta) = (a - \theta)^2$
  - **Lin-Lin**:

$$L(a, \theta) = \begin{cases} c_1 \cdot |a - \theta| & \text{if } a \leq \theta \\ c_2 \cdot |a - \theta| & \text{if } a > \theta \end{cases}$$

- Example:
  - θ is the number of items demanded of a product
  - a is the number of items in stock
  - Utility

$$U(a, \theta) = \begin{cases} p \cdot \theta - c_1(a - \theta) & \text{if } a > \theta \text{ [too much stock]} \\ p \cdot a - c_2(\theta - a)^2 & \text{if } a \leq \theta \text{ [too little stock]} \end{cases}$$

Optimal decision

- Ad hoc decision rules: *Minimax*. *Minimax-regret* ...
- **Bayesian theory**: maximize the **posterior expected utility**:

$$a_{bayes} = \text{argmax}_{a \in \mathcal{A}} \; E_{p(\theta|y)}[U(a, \theta)],$$

where $E_{p(\theta|y)}$ denotes the posterior expectation.

- Using simulated draws $\theta^{(1)}, \theta^{(2)}, ..., \theta^{(N)}$ from $p(\theta|y)$:

$$E_{p(\theta|y)}[U(a, \theta)] \approx N^{-1} \sum_{i=1}^{N} U(a, \theta^{(i)})$$

- **Separation principle**:

1. First do inference, $p(\theta|y)$
2. then form utility $U(a, \theta)$ and finally
3. choose action a that maximes $E_{p(\theta|y)}[U(a, \theta)]$.

Choosing a point estimate is a decision

- Choosing a **point estimator** is a decision problem.
- Which to choose: posterior median, mean or mode?
- It depends on your loss function:
  - **Linear loss** $\rightarrow$ Posterior median
  - **Quadratic loss** $\rightarrow$ Posterior mean
  - **Zero-one loss** $\rightarrow$ Posterior mode
  - **Lin-Lin loss** $\rightarrow$ $c_2/(c_1+c_2)$ quantile of the posterior

Bayesian Learning

Lecture 5 - Regression and Regularization

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Lecture overview

- **Normal model** with conjugate prior
- The **linear regression** model
- **Non-linear regression**
- **Regularization priors**

Linear regression

- The linear regression model in **matrix form**

$$\underset{(n\times 1)}{\mathbf{y}} = \underset{(n\times k)(k\times 1)}{\mathbf{X}\beta} + \underset{(n\times 1)}{\varepsilon}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \ \beta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_k \end{pmatrix}, \ \varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1' \\ \vdots \\ \mathbf{x}_n' \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nk} \end{pmatrix}$$

- Usually $x_{i1} = 1$, for all i. β_1 is the intercept.
- **Likelihood**

$$\mathbf{y}|\beta, \sigma^2, \mathbf{X} \sim N(\mathbf{X}\beta, \sigma^2 I_n)$$

Linear regression - uniform prior

- Standard **non-informative prior**: uniform on $(\beta, \log \sigma^2)$

$$p(\beta, \sigma^2) \propto \sigma^{-2}$$

- **Joint posterior** of β and σ^2:

$$\begin{aligned} \beta|\sigma^2, \mathbf{y} &\sim N\left[\hat{\beta}, \sigma^2(\mathbf{X}'\mathbf{X})^{-1}\right] \\ \sigma^2|\mathbf{y} &\sim \textit{Inv-}\chi^2(n-k, s^2) \end{aligned}$$

  where $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ and $s^2 = \frac{1}{n-k}(\mathbf{y} - \mathbf{X}\hat{\beta})'(\mathbf{y} - \mathbf{X}\hat{\beta})$.

- **Simulate** from the joint posterior by simulating from
  - $p(\sigma^2|\mathbf{y})$
  - $p(\beta|\sigma^2, \mathbf{y})$
- **Marginal posterior** of β :

$$\beta|\mathbf{y} \sim t_{n-k}\left[\hat{\beta}, s^2(X'X)^{-1}\right]$$

Linear regression - conjugate prior

- **Joint prior** for β and σ^2

$$\begin{aligned}\beta|\sigma^2 &\sim N\left(\mu_0, \sigma^2\Omega_0^{-1}\right)\\ \sigma^2 &\sim Inv-\chi^2\left(\nu_0, \sigma_0^2\right)\end{aligned}$$

- **Posterior**

$$\begin{aligned}\beta|\sigma^2, \mathbf{y} &\sim N\left[\mu_n, \sigma^2\Omega_n^{-1}\right]\\ \sigma^2|\mathbf{y} &\sim Inv-\chi^2\left(\nu_n, \sigma_n^2\right)\end{aligned}$$

$$\begin{aligned}\mu_n &= \left(\mathbf{X}'\mathbf{X}+\Omega_0\right)^{-1}\left(\mathbf{X}'\mathbf{X}\hat{\beta}+\Omega_0\mu_0\right)\\ \Omega_n &= \mathbf{X}'\mathbf{X}+\Omega_0\\ \nu_n &= \nu_0+n\\ \nu_n\sigma_n^2 &= \nu_0\sigma_0^2+\left(\mathbf{y}'\mathbf{y}+\mu_0'\Omega_0\mu_0-\mu_n'\Omega_n\mu_n\right)\end{aligned}$$

Polynomial regression

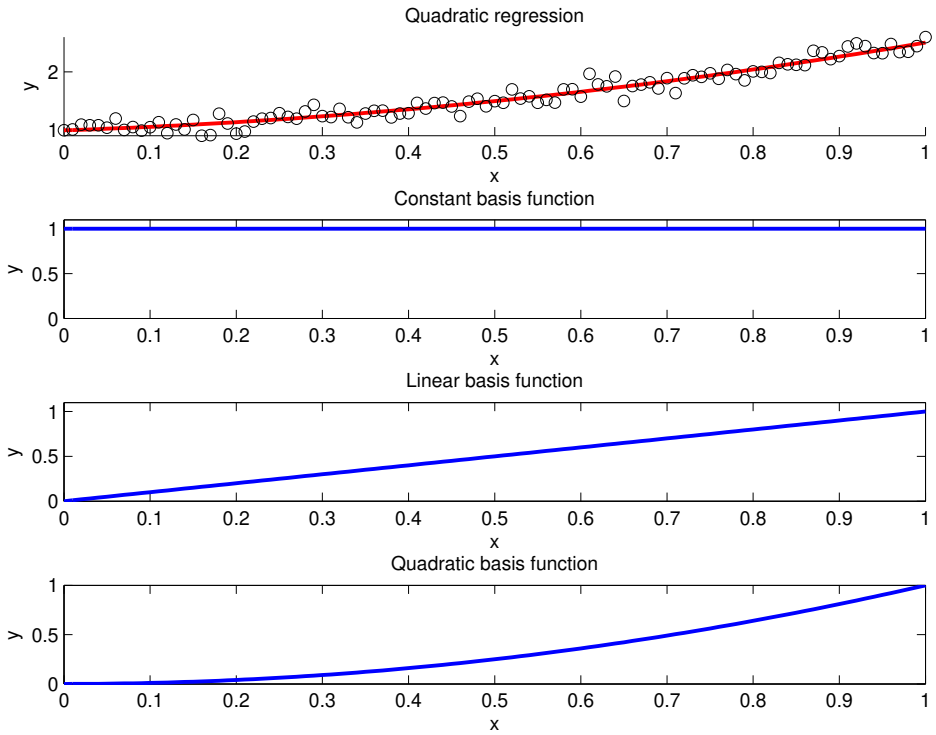
Polynomial regression

$$f(x_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + ... + \beta_k x_i^k.$$

$$\mathbf{y} = \mathbf{X}_P \beta + \varepsilon,$$

where

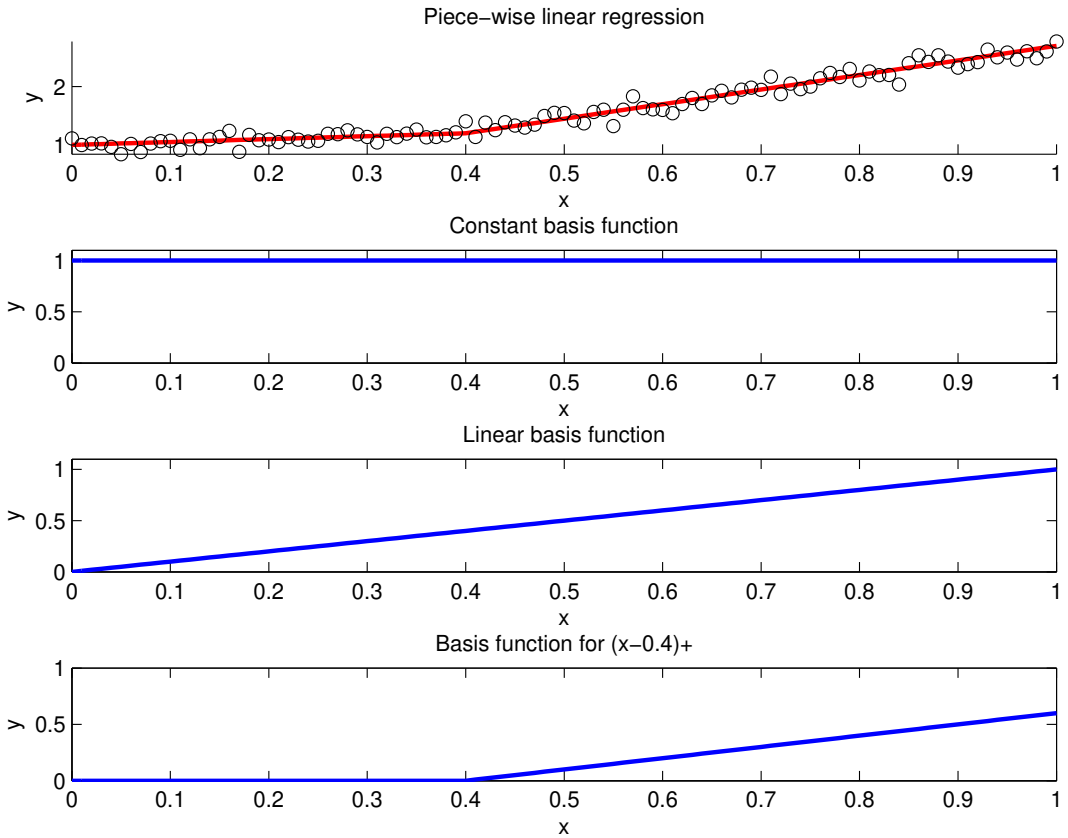
$$\mathbf{X}_P = (1, x, x^2, ..., x^k).$$



Spline regression

- Polynomials are too global. Need more local basis functions.
- **Truncated power splines** given **knot locations** $k_1, \ldots, k_m$

$$b_{ij} = \begin{cases} (x_i - k_j) & \text{if } x_i > k_j \\ 0 & \text{otherwise} \end{cases}$$



Splines

- **Spline regression is linear** in the m 'knot variables' b_j

$$\mathbf{y} = \mathbf{X}_b \beta + \varepsilon,$$

where $\mathbf{X}_b$ is the **basis matrix**

$$\mathbf{X}_b = (b_1, ..., b_m).$$

- Adding intercept and linear term

$$\mathbf{X}_b = (1, x, b_1, ..., b_m).$$

Smoothness prior for splines

- Problem: too many knots leads to **over-fitting**.
- **Smoothness/shrinkage/regularization prior**

$$\beta_i|\sigma^2 \overset{iid}{\sim} N\left(0, \frac{\sigma^2}{\lambda}\right)$$

- Larger λ gives smoother fit. More **shrinkage**. Note: $\Omega_0 = \lambda I$.
- Equivalent to **penalized likelihood**:

$$-2 \cdot \log p(\beta|\sigma^2, \mathbf{y}, \mathbf{X}) \propto (\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) + \lambda\beta'\beta$$

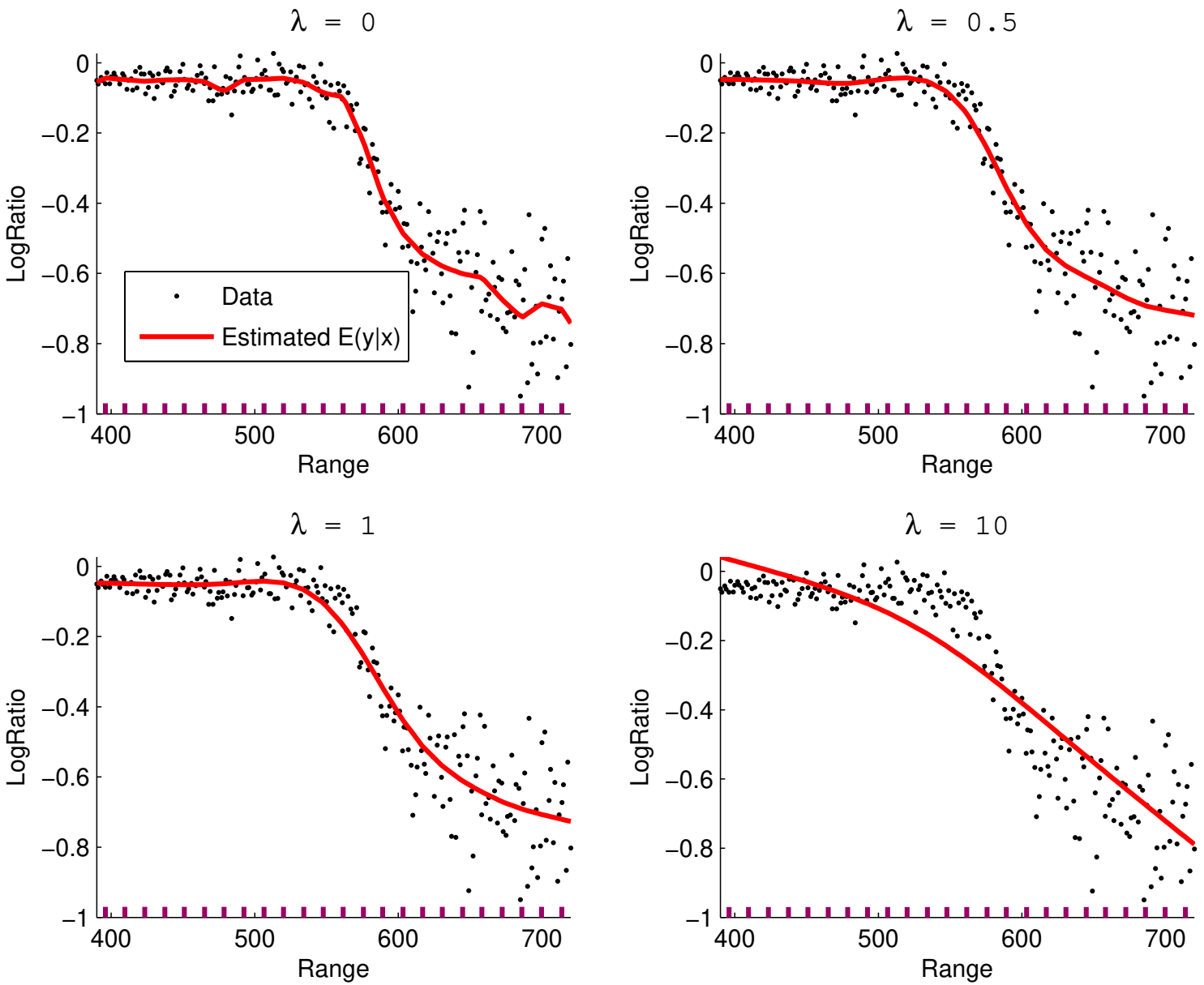
- Posterior mean/mode gives **ridge regression** estimator

$$\tilde{\beta} = \left(\mathbf{X}'\mathbf{X} + \lambda I\right)^{-1}\mathbf{X}'\mathbf{y}$$

- When $\mathbf{X}'\mathbf{X} = I$ (orthogonal, "uncorrelated" features)

$$\tilde{\beta} = \frac{1}{1+\lambda}\hat{\beta}$$

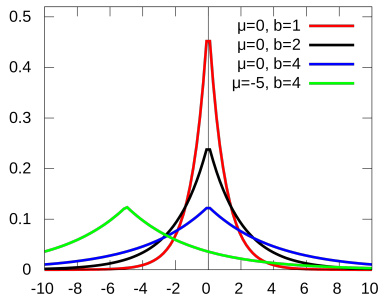
Bayesian spline with smoothness prior



Smoothness prior for splines

- **Lasso** is equivalent to posterior mode under Laplace prior

$$\beta_i|\sigma^2 \overset{iid}{\sim} \text{Laplace}\left(0, \frac{\sigma^2}{\lambda}\right)$$



- The **Bayesian shrinkage** prior is **interpretable**. **Not ad hoc**.
- **Laplace prior**:
  - tails in distribution die off slowly
  - many β_i close to zero, but some β_i very large.
- **Normal prior**:
  - tails in distribution die off rapidly
  - all β_i's are similar in magnitude.

Estimating the shrinkage

- Cross-validation: determine λ by performance on test data.
- Bayesian: λ is **unknown** $\Rightarrow$ **use a prior** for λ.
- $\lambda \sim Inv - \chi^2(\eta_0, \lambda_0)$.
- Hierarchical setup:

$$\begin{aligned} \mathbf{y}|\beta, \mathbf{X} &\sim N(\mathbf{X}\beta, \sigma^2 I_n) \\ \beta|\sigma^2, \lambda &\sim N\left(0, \sigma^2 \lambda^{-1} I_m\right) \\ \sigma^2 &\sim Inv - \chi^2(\nu_0, \sigma_0^2) \\ \lambda &\sim Inv - \chi^2(\eta_0, \lambda_0) \end{aligned}$$

so $\Omega_0 = \lambda I_m$.

Regression with estimated shrinkage

- The **joint posterior** of β, σ^2 and λ is

$$\begin{aligned}
\beta|\sigma^2, \lambda, \mathbf{y} &\sim N\left(\mu_n, \Omega_n^{-1}\right) \\
\sigma^2|\lambda, \mathbf{y} &\sim Inv-\chi^2\left(\nu_n, \sigma_n^2\right) \\
p(\lambda|\mathbf{y}) &\propto \sqrt{\frac{|\Omega_0|}{|\mathbf{X}^T\mathbf{X}+\Omega_0|}}\left(\frac{\nu_n\sigma_n^2}{2}\right)^{-\nu_n/2} \cdot p(\lambda)
\end{aligned}$$

where $\Omega_0 = \lambda I_m$, and $p(\lambda)$ is the prior for λ, and

$$\begin{aligned}
\mu_n &= \left(\mathbf{X}^T\mathbf{X}+\Omega_0\right)^{-1}\mathbf{X}^T\mathbf{y} \\
\Omega_n &= \mathbf{X}^T\mathbf{X}+\Omega_0 \\
\nu_n &= \nu_0 + n \\
\nu_n\sigma_n^2 &= \nu_0\sigma_0^2 + \mathbf{y}^T\mathbf{y} - \mu_n^T\Omega_n\mu_n
\end{aligned}$$

More complexity

- The **location of the knots** can be unknown. Joint posterior:

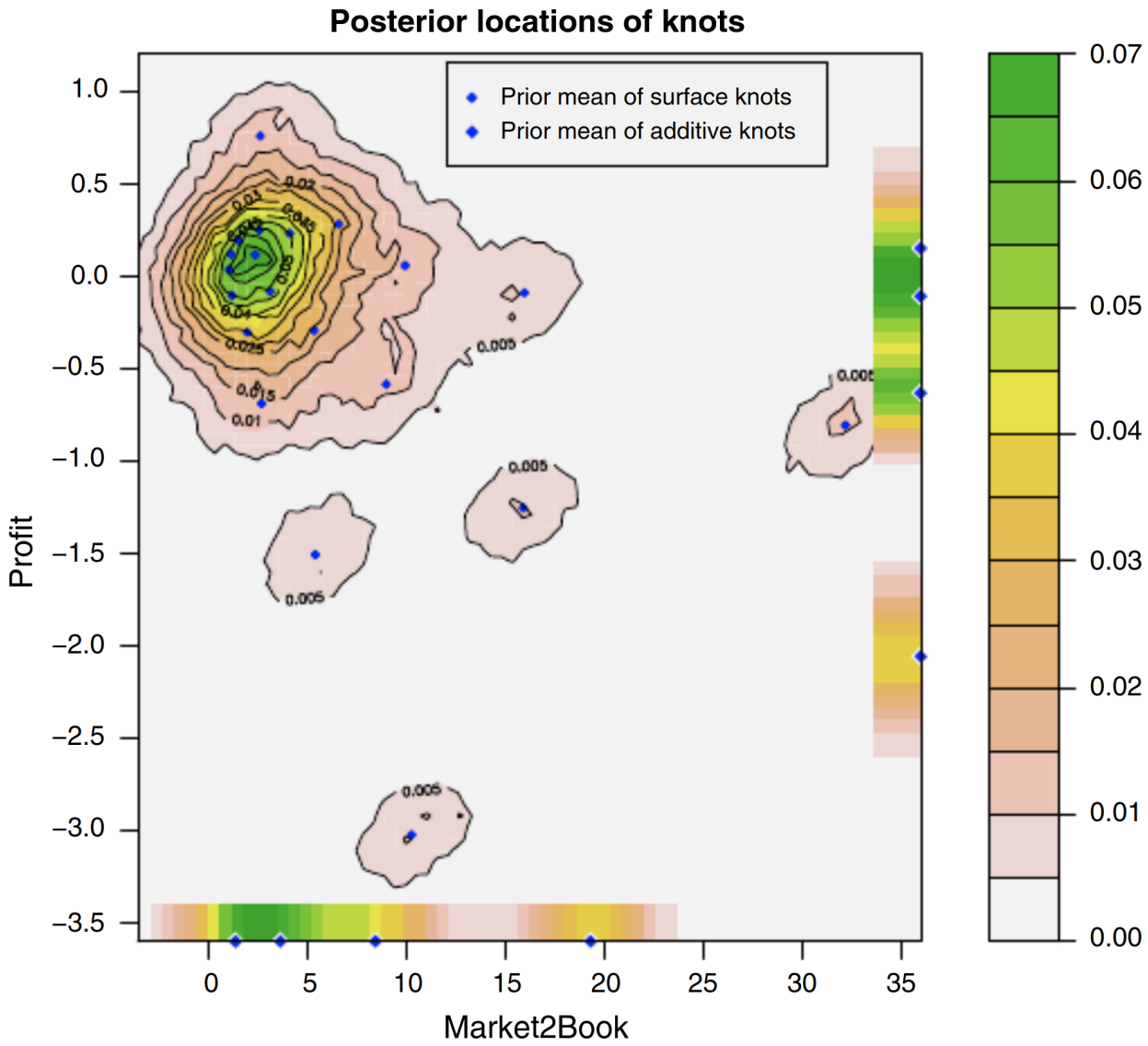
$$p(\beta, \sigma^2, \lambda, k_1, ..., k_m | \mathbf{y}, \mathbf{X})$$

- The marginal posterior for $\lambda, k_1, ..., k_m$ is a nightmare.

- Simulate from joint posterior by MCMC. Li and Villani (2013).

- The basic spline model can be extended with:
  - **Heteroscedastic errors** (also modelled with a spline)
  - **Non-normal errors** (student-t or mixture distributions)
  - **Autocorrelated/dependent errors** (AR process for the errors)

Moving the knots



Bayesian Learning

Lecture 6 - Large sample approximations. Classification.

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Lecture overview

- **Classification**
- **Naive Bayes**
- **Normal approximation** of posterior
- **Logistic regression** - demo in R

Bayesian classification

- **Classification: output is a discrete label.**
  - Binary (0-1). Spam/Ham.
  - Multi-class. ($c = 1, 2, ..., C$). Brand choice.
- **Bayesian classification**

$$\underset{c \in \mathcal{C}}{\operatorname{argmax}}\, p(c|\mathbf{x})$$

  where $\mathbf{x} = (x_1, ..., x_p)$ is a covariate/feature vector.
- **Discriminative models** - model $p(c|\mathbf{x})$ directly.
  - Examples: logistic regression, support vector machines.
- **Generative models** - Use Bayes' theorem

$$p(c|\mathbf{x}) \propto p(\mathbf{x}|c)p(c)$$

  with class-conditional distribution $p(\mathbf{x}|c)$ and prior $p(c)$.
  - Examples: discriminant analysis, naive Bayes.

Naive Bayes

- By Bayes' theorem

$$p(c|\mathbf{x}) \propto p(\mathbf{x}|c)p(c)$$

- $p(c)$ can be estimated by Multinomial-Dirichlet analysis.
- $p(\mathbf{x}|c)$ can be $N(\theta_c, \Sigma_c)$
- $p(\mathbf{x}|c)$ can be very high-dimensional and hard to estimate.
- Even with binary features, the outcome space of $p(\mathbf{x}|c)$ can be huge.
- **Naive Bayes**: features are assumed **independent**

$$p(\mathbf{x}|c) = \prod_{j=1}^{n} p(x_j|c)$$

Classification with logistic regression

- Response is assumed to be **binary** ($y = 0$ or 1).
- Example: Spam/Ham. Covariates: \$-symbols, etc.
- **Logistic regression**

$$\Pr(y_i = 1 \mid x_i) = \frac{\exp(x_i'\beta)}{1 + \exp(x_i'\beta)}.$$

- **Likelihood**

$$p(\mathbf{y}|\mathbf{X}, \beta) = \prod_{i=1}^{n} \frac{[\exp(x_i'\beta)]^{y_i}}{1 + \exp(x_i'\beta)}.$$

- Prior $\beta \sim N(0, \tau^2 I)$. Posterior is non-standard (demo later).
- Alternative: **Probit regression**

$$Pr(y_i = 1|x_i) = \Phi(x_i'\beta)$$

- **Multi-class** ($c = 1, 2, ..., C$) logistic regression

$$\Pr(y_i = c \mid x_i) = \frac{\exp(x_i'\beta_c)}{\sum_{k=1}^{C} \exp(x_i'\beta_k)}$$

Large sample approximate posterior

- **Taylor expansion of log-posterior** around mode $\theta = \tilde{\theta}$:

$$\ln p(\theta|\mathbf{y}) = \ln p(\tilde{\theta}|\mathbf{y}) + \frac{\partial \ln p(\theta|\mathbf{y})}{\partial \theta}|_{\theta=\tilde{\theta}}(\theta - \tilde{\theta}) + \frac{1}{2!}\frac{\partial^2 \ln p(\theta|\mathbf{y})}{\partial \theta^2}|_{\theta=\tilde{\theta}}(\theta - \tilde{\theta})^2 + ...$$

- From the definition of the posterior mode:

$$\frac{\partial \ln p(\theta|\mathbf{y})}{\partial \theta}|_{\theta=\tilde{\theta}} = 0$$

- So, in **large samples** (higher order terms negligible):

$$p(\theta|\mathbf{y}) \approx p(\tilde{\theta}|\mathbf{y}) \exp\left(-\frac{1}{2}J_{\mathbf{y}}(\tilde{\theta})(\theta - \tilde{\theta})^2\right)$$

where $J_{\mathbf{y}}(\tilde{\theta}) = -\frac{\partial^2 \ln p(\theta|\mathbf{y})}{\partial \theta^2}|_{\theta=\tilde{\theta}}$ is the **observed information**.

- **Approximate normal posterior** in large samples.

$$\theta|\mathbf{y} \overset{approx}{\sim} N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$$

Example: gamma posterior

- **Poisson model**: $\theta|y_1, ..., y_n \sim Gamma(\alpha + \sum_{i=1}^n y_i, \beta + n)$

$$\log p(\theta|y_1, ..., y_n) \propto (\alpha + \sum_{i=1}^n y_i - 1) \log \theta - \theta(\beta + n)$$

- First derivative of log density

$$\frac{\partial \ln p(\theta|\mathbf{y})}{\partial \theta} = \frac{\alpha + \sum_{i=1}^n y_i - 1}{\theta} - (\beta + n)$$

$$\tilde{\theta} = \frac{\alpha + \sum_{i=1}^n y_i - 1}{\beta + n}$$

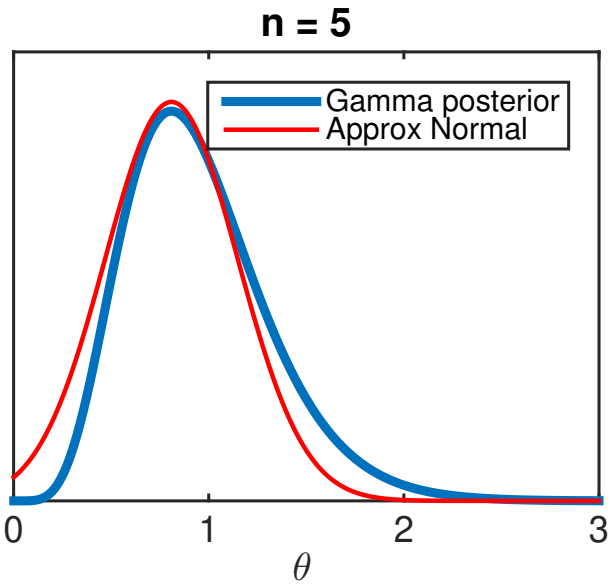
- Second derivative at mode $\tilde{\theta}$

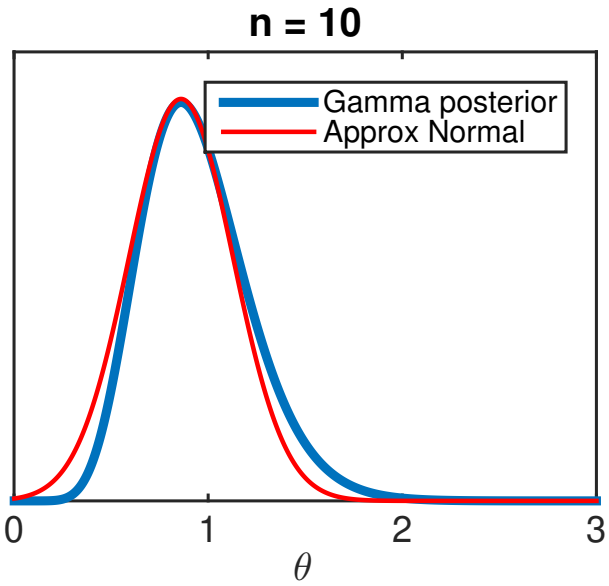
$$\frac{\partial^2 \ln p(\theta|\mathbf{y})}{\partial \theta^2}|_{\theta=\tilde{\theta}} = -\frac{\alpha + \sum_{i=1}^n y_i - 1}{\left(\frac{\alpha + \sum_{i=1}^n y_i - 1}{\beta + n}\right)^2} = -\frac{(\beta + n)^2}{\alpha + \sum_{i=1}^n y_i - 1}$$

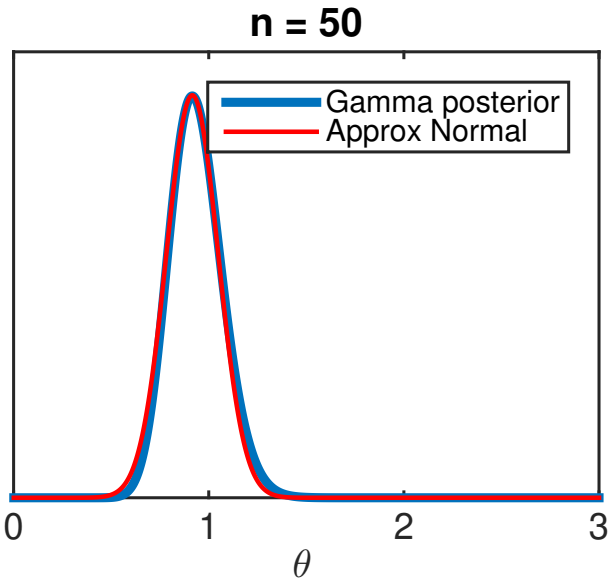
- **Normal approximation**

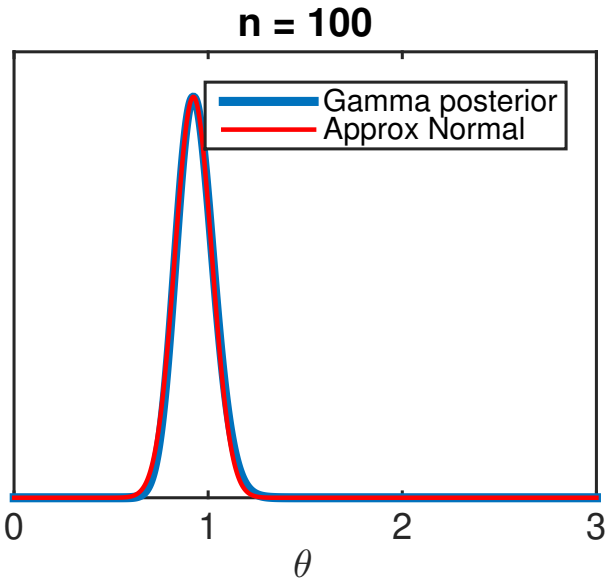
$$N\left[\frac{\alpha + \sum_{i=1}^n y_i - 1}{\beta + n}, \frac{\alpha + \sum_{i=1}^n y_i - 1}{(\beta + n)^2}\right]$$

Example: gamma posterior









Normal approximation of posterior

- $\theta|\mathbf{y} \overset{approx}{\sim} N\left[\tilde{\theta}, J_y^{-1}(\tilde{\theta})\right]$ works also when θ is a vector.
- How to compute $\tilde{\theta}$ and $J_{\mathbf{y}}(\tilde{\theta})$?
- Standard **optimization routines** may be used. (`optim.r`).
  - **Input**: expression proportional to $\log p(\theta|\mathbf{y})$. Initial values.
  - **Output**: $\log p(\tilde{\theta}|\mathbf{y})$, $\tilde{\theta}$ and Hessian matrix $(-J_{\mathbf{y}}(\tilde{\theta}))$.
- **Automatic differentiation** (autodiff in Python, ForwardDiff in Julia, R?)
- **Re-parametrization** may improve normal approximation. [Don't forget the **Jacobian**!]
  - If $\theta \geq 0$ use $\phi = \log(\theta)$.
  - If $0 \leq \theta \leq 1$, use $\phi = \ln[\theta/(1-\theta)]$.
- **Heavy tailed approximation**: $\theta|\mathbf{y} \overset{approx}{\sim} t_v\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$ for suitable degrees of freedom v.

Reparametrization - Gamma posterior

- Poisson model. Reparameterize to $\phi = \log(\theta)$.
- Change-of-variables formula from a basic probability course

$$\log p(\phi|y_1, ..., y_n) \propto (\alpha + \sum_{i=1}^{n} y_i - 1)\phi - \exp(\phi)(\beta + n) + \phi$$

- Taking first and second derivatives and evaluating at $\tilde{\phi}$ gives

$$\tilde{\phi} = \log\left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n}\right) \text{ and } \frac{\partial^2 \ln p(\phi|y)}{\partial \phi^2}|_{\phi=\tilde{\phi}} = \alpha + \sum_{i=1}^{n} y_i$$

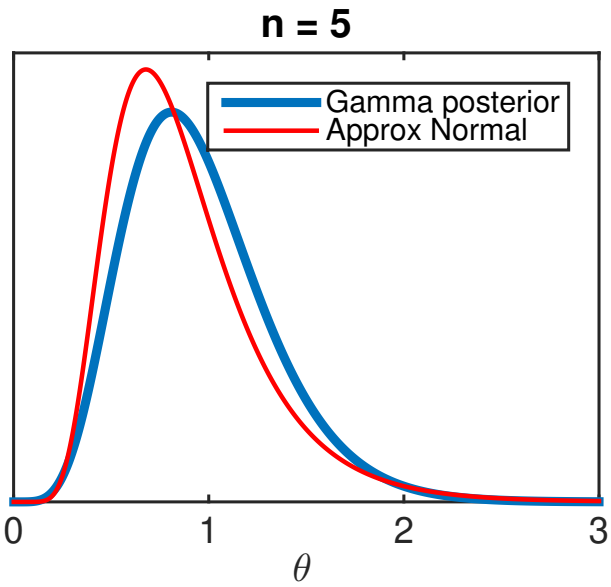
- So, the normal approximation for $p(\phi|y_1, ...y_n)$ is

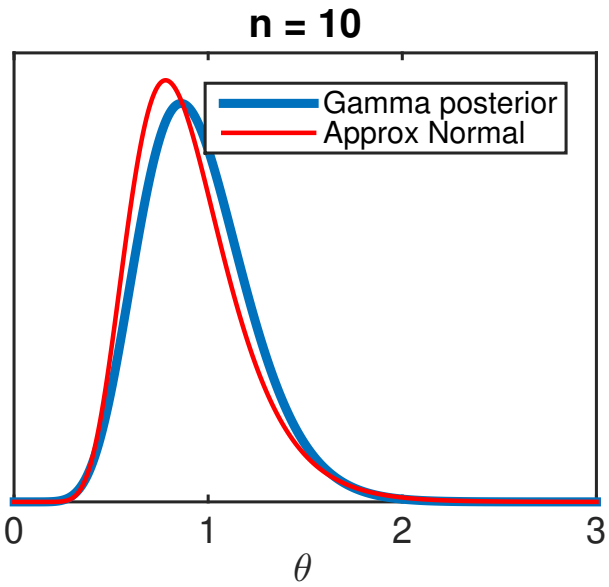
$$\phi = \log(\theta) \sim N\left[\log\left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n}\right), \frac{1}{\alpha + \sum_{i=1}^{n} y_i}\right]$$

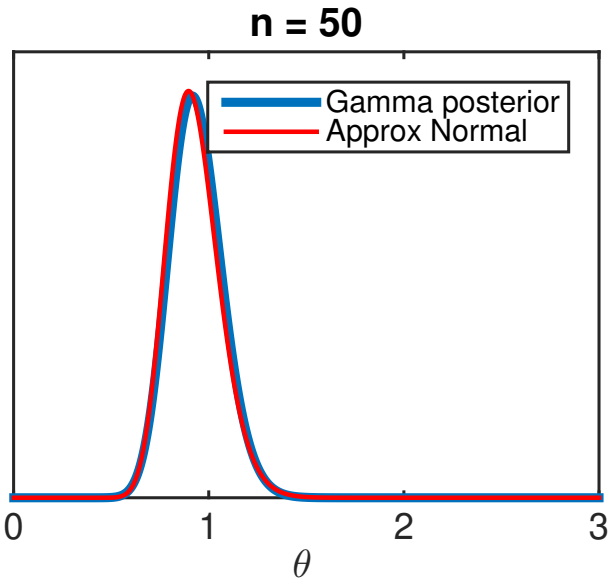
which means that $p(\theta|y_1, ...y_n)$ is log-normal:

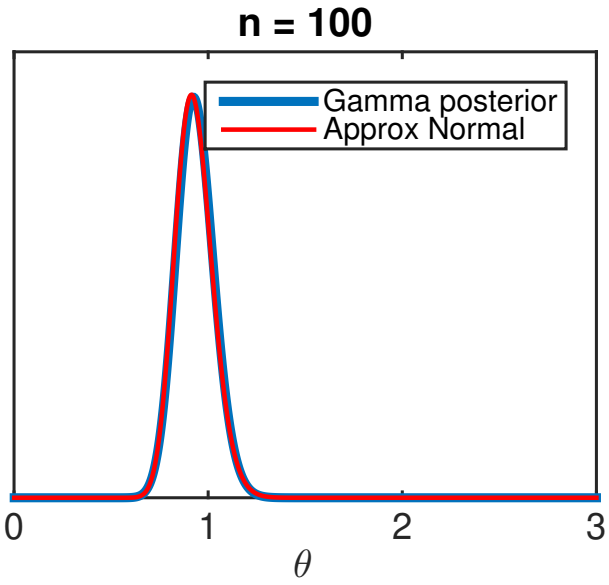
$$\theta|\mathbf{y} \sim LN\left[\log\left(\frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n}\right), \frac{1}{\alpha + \sum_{i=1}^{n} y_i}\right]$$

Reparametrization - Gamma posterior









Normal approximation of posterior

- Even if the posterior of θ is approx normal, **interesting functions** of $g(\theta)$ may not be (e.g. predictions).
- But approximate posterior of $g(\theta)$ can be obtained by **simulating** from $N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
- Posterior of **Gini coefficient**
  - Model: $x_1, ..., x_n | \mu, \sigma^2 \sim LN(\mu, \sigma^2)$.
  - Let $\phi = \log(\sigma^2)$. And $\theta = (\mu, \phi)$.
  - Joint posterior $p(\mu, \phi)$ may be approximately normal: $\theta|\mathbf{y} \overset{approx}{\sim} N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
  - Simulate $\theta^{(1)}, ..., \theta^{(N)}$ from $N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
  - Compute $\sigma^{(1)}, ..., \sigma^{(N)}$.
  - Compute $G^{(i)} = 2\Phi\left(\sigma^{(i)}/\sqrt{2}\right)$ for $i = 1, ..., N$.

Bayesian Learning

Lecture 7 - Monte Carlo and Gibbs sampling

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Lecture overview

- Monte Carlo simulation
- Gibbs sampling
- Data augmentation
  - Mixture models
  - Probit regression
- Regularized regression

Monte Carlo sampling

- If $\theta^{(1)}, ..., \theta^{(N)}$ is an **iid sequence** from $p(\theta)$, then

$$\bar{\theta} = \frac{1}{N}\sum_{t=1}^{N}\theta^{(t)} \quad \rightarrow \quad E(\theta)$$

$$\bar{g}(\theta) = \frac{1}{N}\sum_{t=1}^{N} g(\theta^{(t)}) \quad \rightarrow \quad E[g(\theta)]$$

  for some function $g(\theta)$ of interest.
- $\mathbb{V}(\bar{g}(\theta)) = \frac{c}{N}$ for some constant c.
- Easy to compute **tail probabilities** $\Pr(\theta \leq c)$ by letting

$$g(\theta) = I(\theta \leq c)$$

  and

$$\frac{1}{N}\sum_{t=1}^{N} g(\theta^{(t)}) = \frac{\#\ \theta\text{-draws smaller than } c}{N}.$$

Direct sampling by the inverse CDF method

- Let $F(x)$ be the CDF of X. **Inverse CDF method**:
  1. Generate u from the uniform distribution on $[0, 1]$.
  2. Compute $x = F^{-1}(u)$.

- **Exponential distribution**:

$$u = F(x) = 1 - \exp(-\lambda x)$$

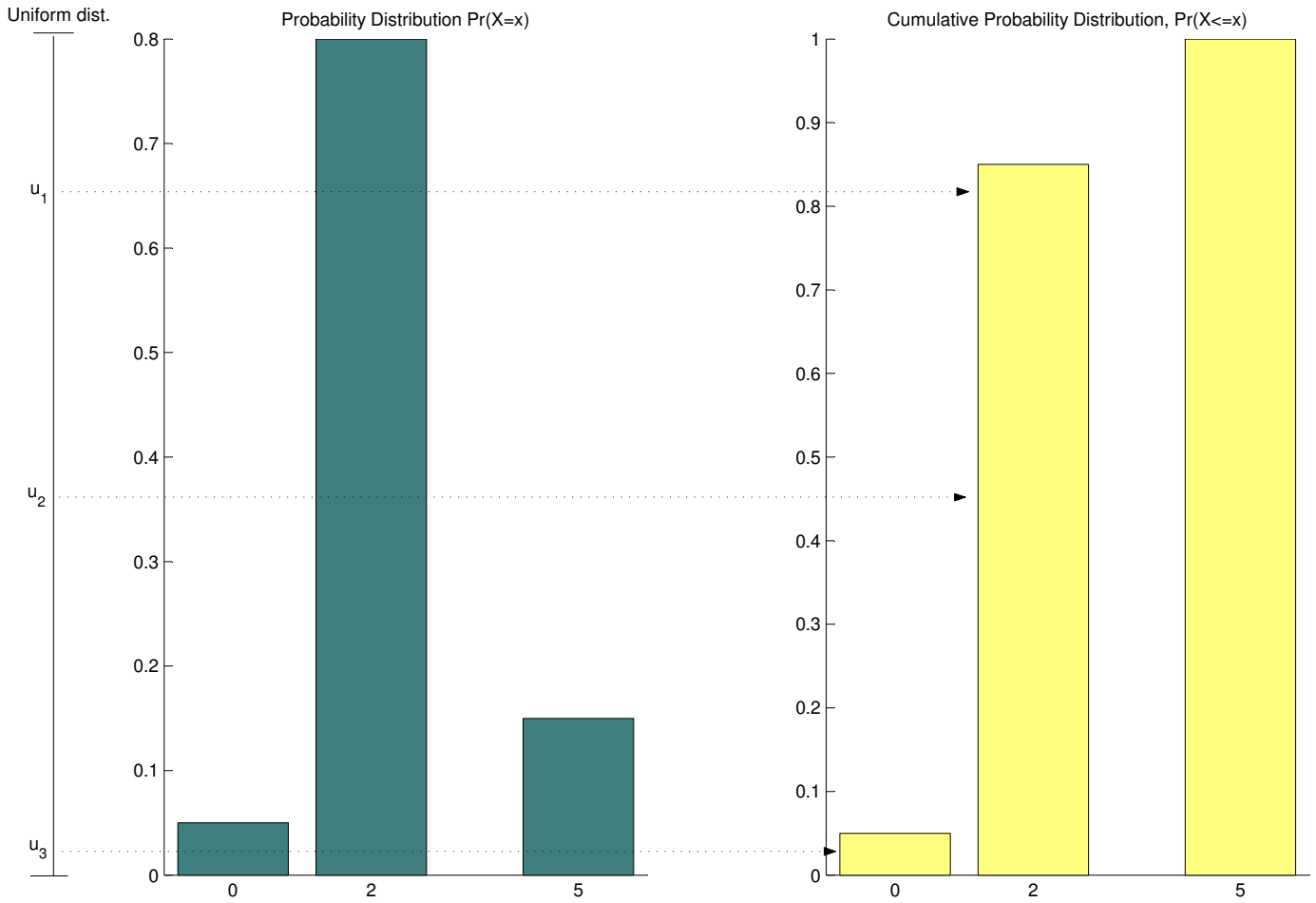
  Inverting gives

$$x = -\ln(1 - u)/\lambda$$

- So, if $u \sim U(0, 1)$ then

$$x = -\ln(1 - u)/\lambda \sim Expon(\lambda)$$

Inverse CDF method, discrete case



Direct sampling by the inverse CDF method

- **Cauchy distribution**:

$$\begin{aligned} f(x) &= \frac{1}{\pi}\frac{1}{1+x^2} \\ u &= F(x) = \frac{1}{2} + \frac{1}{\pi}\arctan(x) \end{aligned}$$

  Inverting ...

$$x = \tan[\pi(u - 1/2)].$$

- Can also use **relations**:

$$y, z \text{ are indep } N(0,1) \Rightarrow \frac{y}{z} \sim \text{Cauchy}(0,1)$$

- **Chi-square**. If $x_1, ..., x_\nu \overset{iid}{\sim} N(0,1)$, then $\sum_{i=1}^{\nu} x_i^2 \sim \chi^2_\nu$.

Gibbs sampling

- Easily implemented methods for **sampling from multivariate distributions**, $p(\theta_1, ..., \theta_k)$.
- Requirements: Easily sampled **full conditional distributions**:
  - $p(\theta_1|\theta_2, \theta_3..., \theta_k)$
  - $p(\theta_2|\theta_1, \theta_3, ..., \theta_k)$
  - $\vdots$
  - $p(\theta_k|\theta_1, \theta_2, ..., \theta_{k-1})$
- Gibbs sampling is a special case of **Metropolis-Hastings** (see Lecture 8).
- Metropolis-Hastings is a **Markov Chain Monte Carlo** (**MCMC**) algorithm.

The Gibbs sampling algorithm

- Choose initial values $\theta_2^{(0)}, \theta_3^{(0)}, ..., \theta_k^{(0)}$.
- Repeat for $j = 1, ..., N$:
  - Draw $\theta_1^{(j)}$ from $p(\theta_1 | \theta_2^{(j-1)}, \theta_3^{(j-1)}, ..., \theta_k^{(j-1)})$
  - Draw $\theta_2^{(j)}$ from $p(\theta_2 | \theta_1^{(j)}, \theta_3^{(j-1)}, ..., \theta_k^{(j-1)})$
  - $\vdots$
  - Draw $\theta_k^{(j)}$ from $p(\theta_k | \theta_1^{(j)}, \theta_2^{(j)}, ..., \theta_{k-1}^{(j)})$
- Return draws: $\theta^{(1)}, ..., \theta^{(N)}$, where $\theta^{(j)} = (\theta_1^{(j)}, ..., \theta_k^{(j)})$.

Gibbs sampling, cont.

- Gibbs draws $\theta^{(1)}, ..., \theta^{(N)}$ are **dependent**, but

$$\bar{\theta} = \frac{1}{N} \sum_{t=1}^{N} \theta_j^{(t)} \quad \rightarrow \quad E(\theta_j)$$

$$\bar{g}(\theta) = \frac{1}{N} \sum_{t=1}^{N} g(\theta^{(t)}) \quad \rightarrow \quad E[g(\theta)]$$

- $\theta^{(1)}, ..., \theta^{(N)}$ **converges in distribution** to the target $p(\theta)$.
- $\theta_j^{(1)}, ..., \theta_j^{(N)}$ converges to the marginal distribution of θ_j.
- **Dependent draws** $\rightarrow$ **less efficient** than iid sampling.
- **IID samples**: $\theta^{(1)}, ..., \theta^{(N)}$: $\mathrm{Var}(\bar{\theta}) = \frac{\sigma^2}{N}$.
- **Autocorrelated samples**: $\mathrm{Var}(\bar{\theta}) = \frac{\sigma^2}{N}\left(1 + 2\sum_{k=1}^{\infty} \rho_k\right)$, where ρ_k is the autocorrelation at lag k.
- **Inefficiency factor**: $1 + 2\sum_{k=1}^{\infty} \rho_k$.

Gibbs sampling bivariate normal

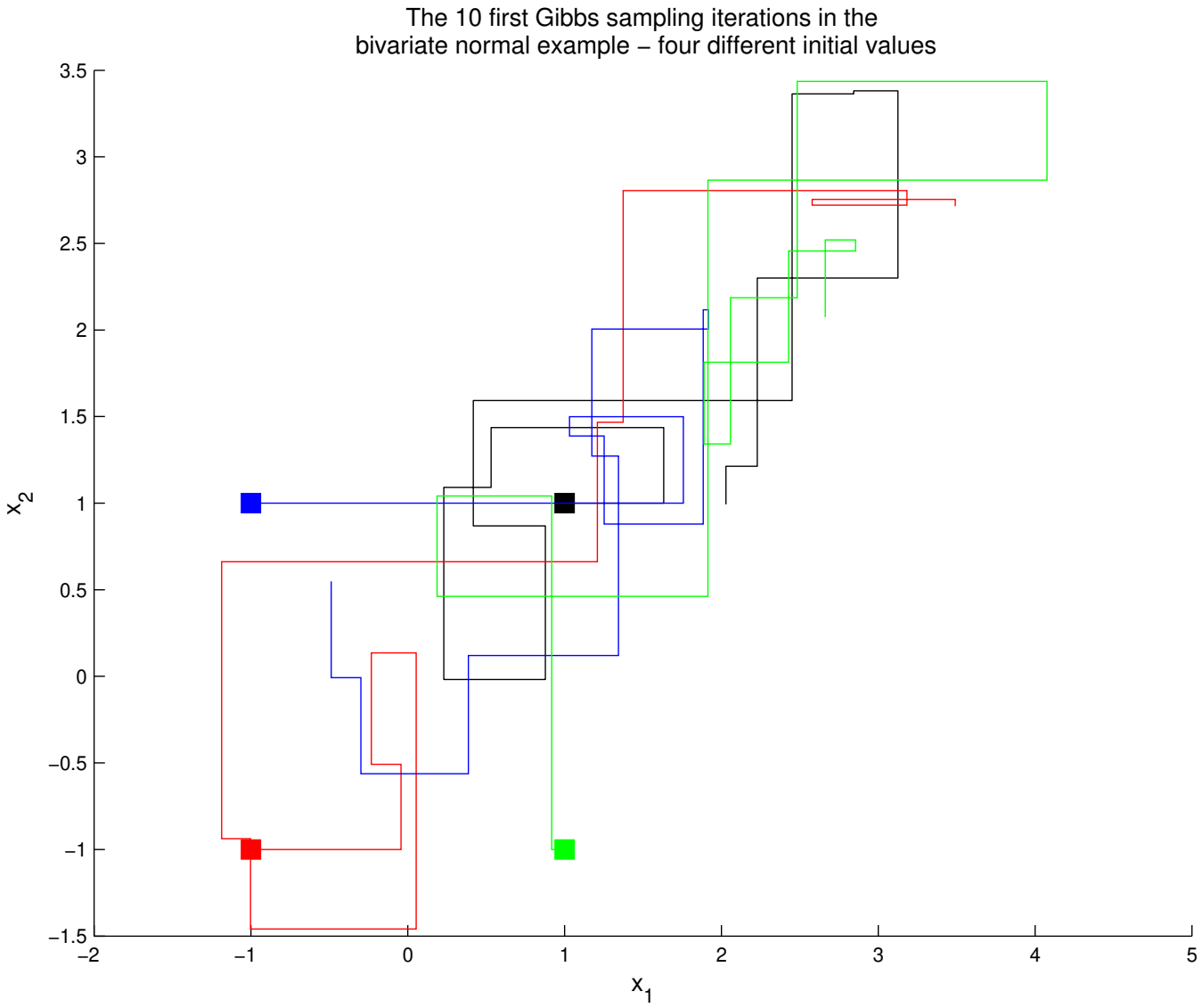
- **Joint distribution**

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim N_2 \left[\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right]$$

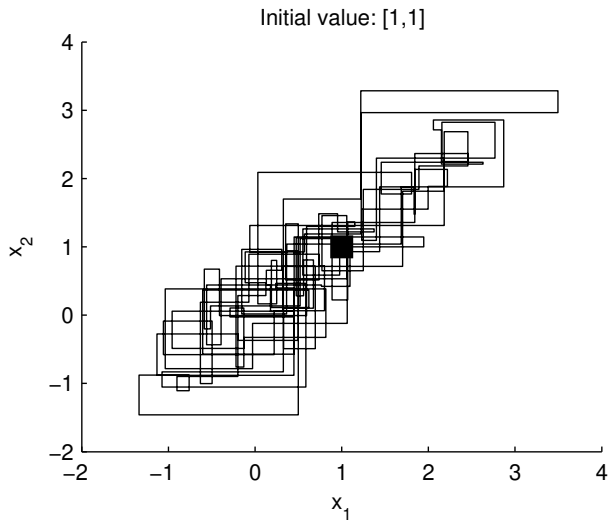
- **Full conditional posteriors**

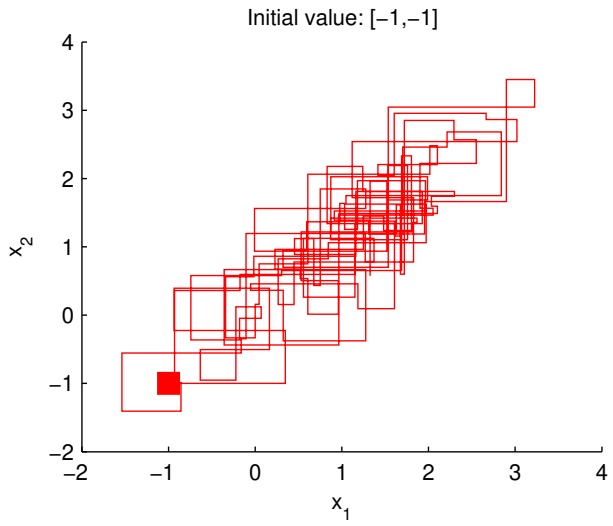
$$\begin{aligned} \theta_1|\theta_2 &\sim N[\mu_1 + \rho(\theta_2 - \mu_2), 1 - \rho^2] \\ \theta_2|\theta_1 &\sim N[\mu_2 + \rho(\theta_1 - \mu_1), 1 - \rho^2] \end{aligned}$$

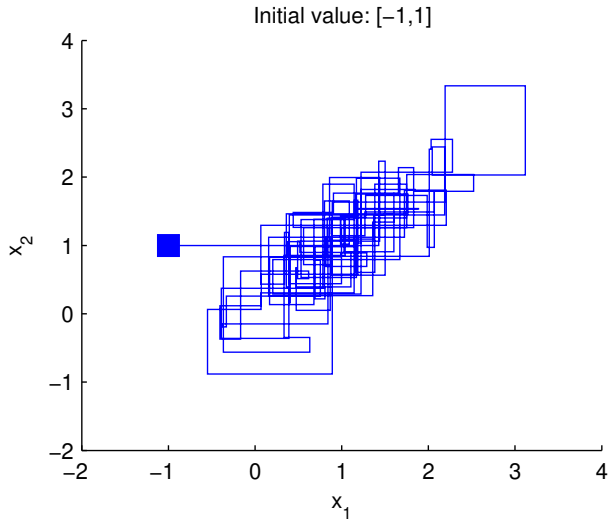
Gibbs sampling - Bivariate normal

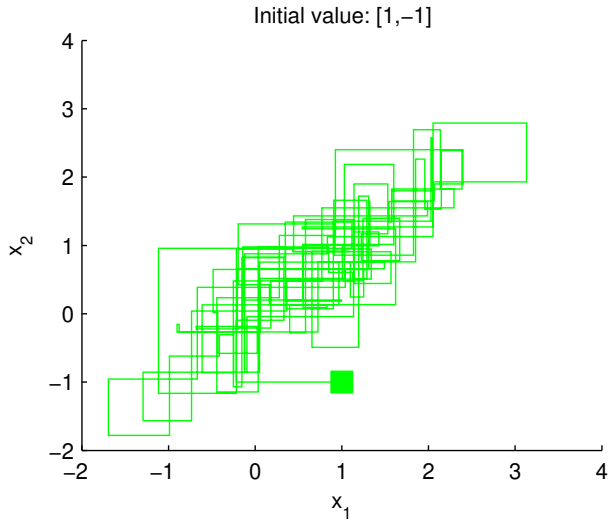


Gibbs sampling - Bivariate normal

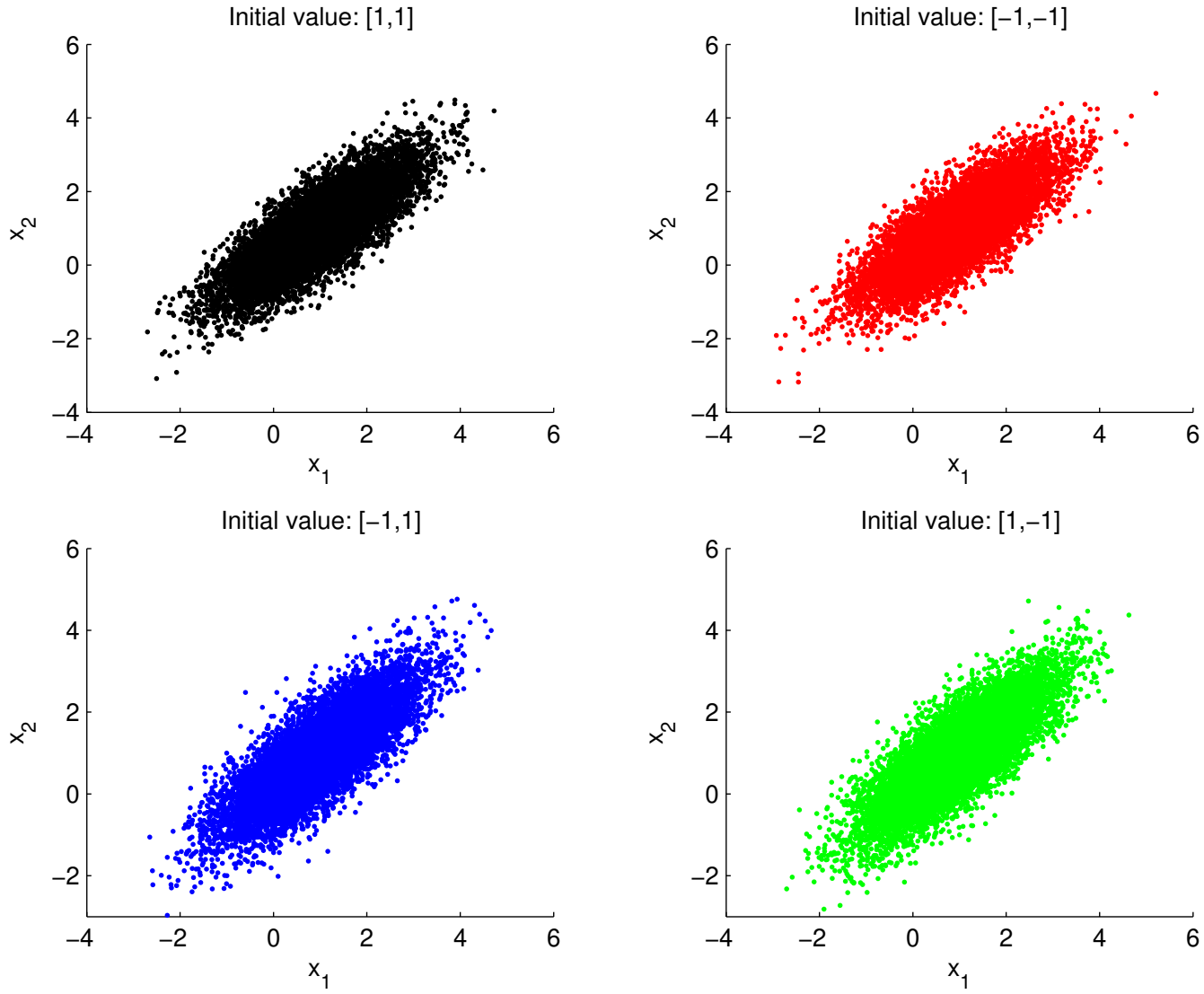




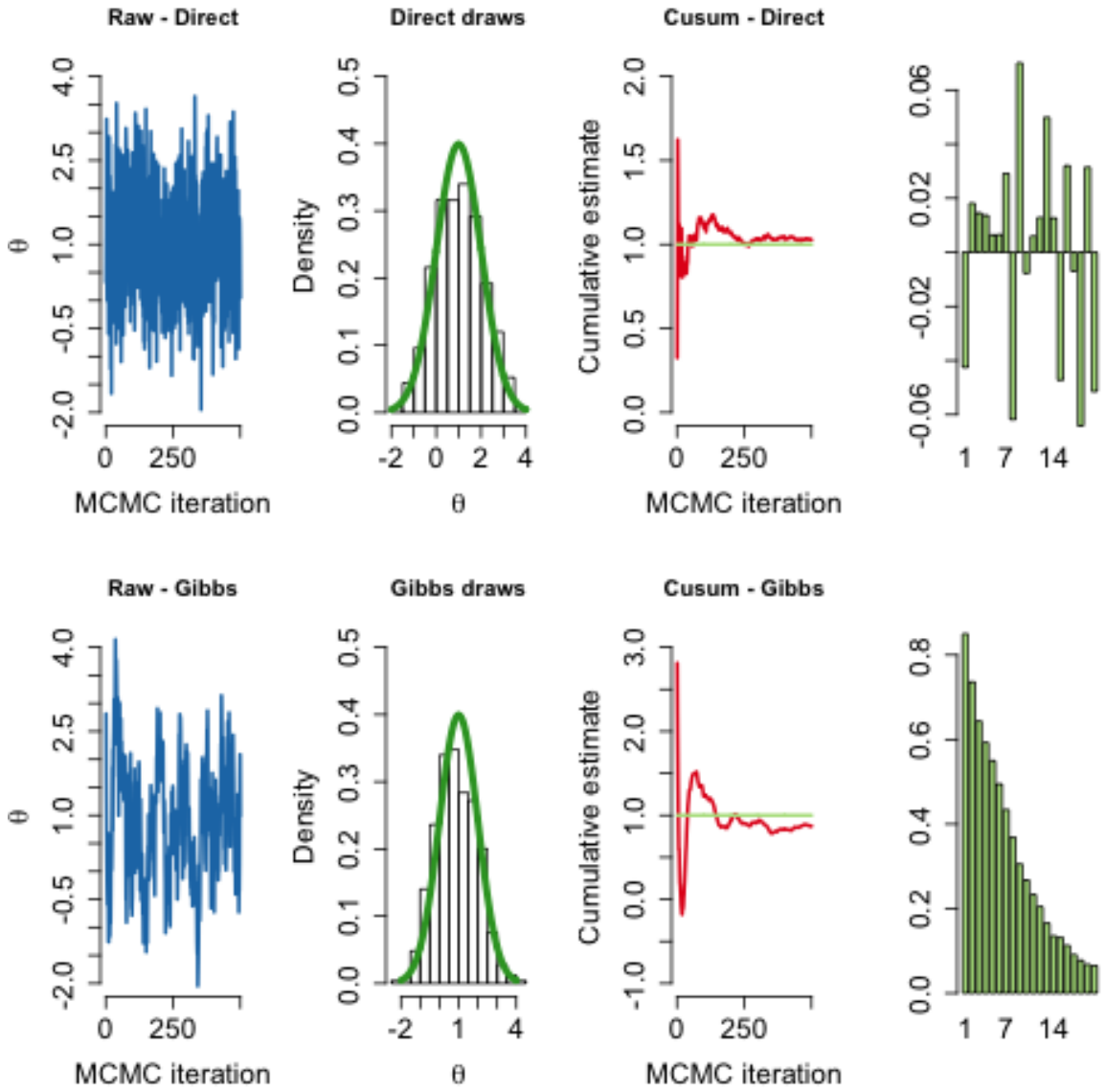




Gibbs sampling - Bivariate normal



Direct sampling vs Gibbs sampling

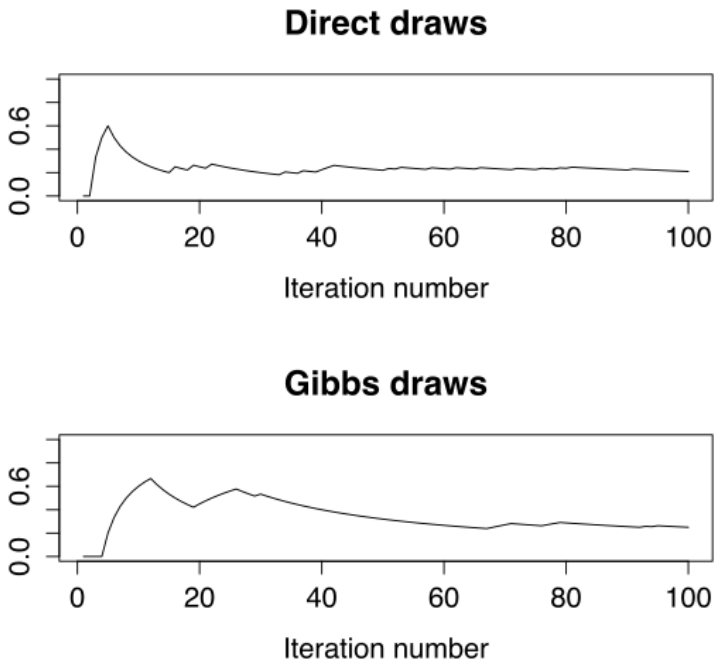


Estimating $Pr(\theta_1 > 0, \theta_2 > 0)$

- Joint probability by counting:

$$Pr(\theta_1 > 0, \theta_2 > 0) \approx N^{-1} \sum_{i=1}^{N} 1(\theta_1^{(i)} > 0, \theta_2^{i)} > 0)$$

.



Normal model with conditionally conjugate prior

- **Normal model** with **conditionally conjugate prior**

$$\mu \sim N(\mu_0, \tau_o^2)$$
$$\sigma^2 \sim Inv - \chi^2(\nu_0, \sigma_0^2)$$

- **Full conditional posteriors**

$$\mu|\sigma^2, x \sim N\left(\mu_n, \tau_n^2\right)$$
$$\sigma^2|\mu, x \sim Inv - \chi^2\left(\nu_n, \frac{\nu_0\sigma_0^2 + \sum_{i=1}^{n}\left(x_i - \mu\right)^2}{n + \nu_0}\right)$$

with μ_n and τ_n^2 defined the same as when σ^2 is known.

Gibbs sampling for AR processes

- **AR(p) process**

$$x_t = \mu + \phi_1(x_{t-1} - \mu) + ... + \phi_p(x_{t-p} - \mu) + \varepsilon_t, \quad \varepsilon_t \overset{iid}{\sim} N(0, \sigma^2).$$

- Let $\phi = (\phi_1, ..., \phi_p)'$.
- **Prior**:
  - $\mu \sim$Normal
  - $\phi \sim$Multivariate Normal
  - $\sigma^2 \sim$Scaled Inverse χ^2.
- The **posterior** can be simulated by **Gibbs sampling**[1]:
  - $\mu|\phi, \sigma^2, x \sim$ Normal
  - $\phi|\mu, \sigma^2, x \sim$ Multivariate Normal
  - $\sigma^2|\mu, \phi, x \sim$ Scaled Inverse χ^2

[1] Villani (2009). Steady State Priors for Vector Autoregressions. *Journal of Applied Econometrics*.

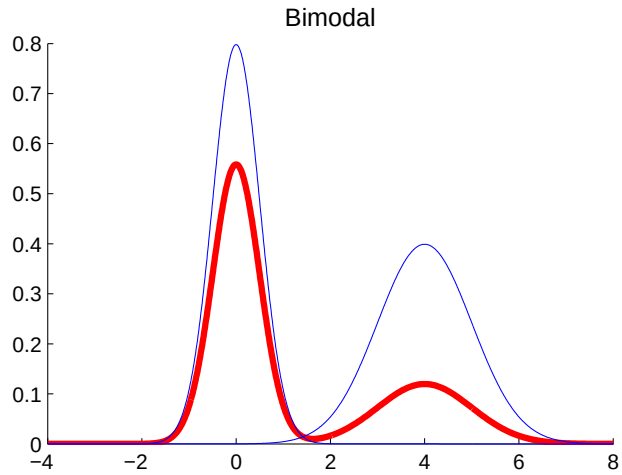
Data augmentation - Mixture distributions

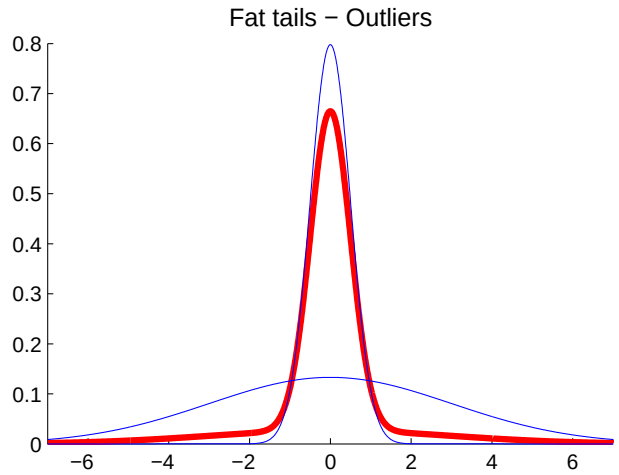
- Let $\phi(x|\mu, \sigma^2)$ denote the **PDF** of $x \sim N(\mu, \sigma^2)$.
- Two-component **mixture of normals** [MN(2)]

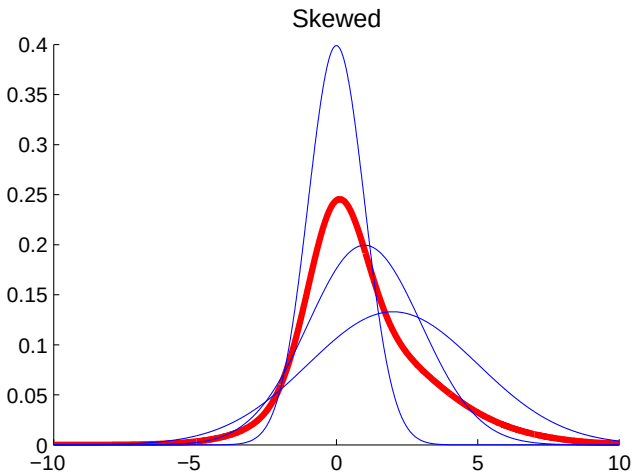
$$p(x) = \pi \cdot \phi(x|\mu_1, \sigma_1^2) + (1 - \pi) \cdot \phi(x|\mu_2, \sigma_2^2)$$

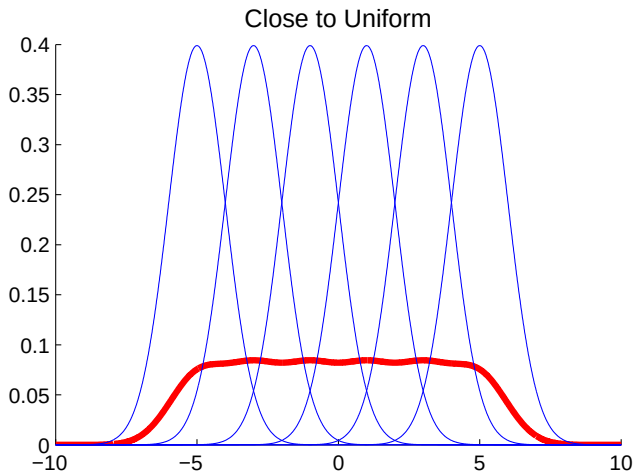
- **Simulate** from a MN(2):
  - Simulate a **membership indicator** $I \in \{1, 2\}$: $I \sim Bern(\pi)$.
  - If $I = 1$, simulate x from $N(\mu_1, \sigma_1^2)$
  - If $I = 2$, simulate x from $N(\mu_2, \sigma_2^2)$.

Illustration of mixture distributions









Mixture distributions, cont.

- The **likelihood** is a product of sums. **Messy** to work with.
- **Assume** that we know where each observation comes from

$$I_i = \begin{cases} 1 \text{ if } x_i \text{ came from Density 1} \\ 2 \text{ if } x_i \text{ came from Density 2} \end{cases}.$$

- Given $I_1, ..., I_n$ it is easy to estimate π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$ by separating the sample according to the I's.
- But we do **not** know $I_1, ..., I_n$!
- **Data augmentation**: add $I_1, ..., I_n$ as unknown parameters.
- **Gibbs sampling**:
  - Sample π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$ **given** $I_1, ..., I_n$
  - Sample $I_1, ..., I_n$ **given** π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$

Gibbs sampling for mixture distributions

- Prior: $\pi \sim Beta(\alpha_1, \alpha_2)$. Conjugate prior for (μ_j, σ_j^2), see L5.
- Define: $n_1 = \sum_{i=1}^{n} (I_i = 1)$ and $n_2 = n - n_1$.
- **Gibbs sampling**:
  - $\pi \mid \mathbf{I}, \mathbf{x} \sim Beta(\alpha_1 + n_1, \alpha_2 + n_2)$
  - $\sigma_1^2 \mid \mathbf{I}, \mu_1, \mathbf{x} \sim Inv\text{-}\chi^2(\nu_{n_1}, \sigma_{n_1}^2)$ and $\mu_1 | \mathbf{I}, \sigma_1^2, \mathbf{x} \sim N\left(\mu_{n_1}, \tau_{n_1}^2\right)$
  - $\sigma_2^2 \mid \mathbf{I}, \mu_2, \mathbf{x} \sim Inv\text{-}\chi^2(\nu_{n_2}, \sigma_{n_2}^2)$ and $\mu_2 | \mathbf{I}, \sigma_2^2, \mathbf{x} \sim N\left(\mu_{n_2}, \tau_{n_2}^2\right)$
  - $I_i \mid \pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2, \mathbf{x} \sim Bern(\theta_i),\ i = 1, ..., n,$

$$\theta_i = \frac{(1-\pi)\phi(x_i; \mu_2, \sigma_2^2)}{\pi\phi(x_i; \mu_1, \sigma_1^2) + (1-\pi)\phi(x_i; \mu_2, \sigma_2^2)}.$$

Gibbs sampling for mixture distributions

- K-component mixture of normals

$$p(x) = \sum_{k=1}^{K} \pi_k \phi(x; \mu_k, \sigma_k^2)$$

- Multi-class indicators: $I_i = k$ if x_i comes from component k.
- Gibbs sampling
  - $(\pi_1, ..., \pi_K) \mid \mathbf{I}, \mathbf{x} \sim \textit{Dirichlet}(\alpha_1 + n_1, \alpha_2 + n_2, ..., \alpha_K + n_K)$
  - $\sigma_k^2 \mid \mathbf{I}, \mathbf{x} \sim \textit{Inv-}\chi^2$ and $\mu_k | \mathbf{I}, \sigma_k^2, \mathbf{x} \sim \textit{Normal}, \quad \textit{for } k = 1, ..., K,$
  - $I_i \mid \pi, \mu, \sigma^2, \mathbf{x} \sim \textit{Categorical}(\theta_{i1}, ..., \theta_{iK}),$ *for* $i = 1, ..., n,$

$$\theta_{ij} = \frac{\pi_j \phi(x_i; \mu_j, \sigma_j^2)}{\sum_{r=1}^{k} \pi_r \phi(x_i; \mu_r, \sigma_r^2)}.$$

- Gibbs sampling is very powerful for missing data problems.
- Semi-supervised learning.

Data augmentation - Probit regression

- **Probit regression**:

$$\Pr(y_i = 1 \mid x_i) = \Phi(x_i^T \beta)$$

- **Random utility formulation**:

$$\begin{aligned} u_i &\sim N(x_i^T \beta, 1) \\ y_i &= \begin{cases} 1 & \text{if } u_i > 0 \\ 0 & \text{if } u_i \leq 0 \end{cases}. \end{aligned}$$

- Check: $\Pr(y_i = 1 \mid x_i) = \Pr(u_i > 0) = 1 - \Pr(u_i \leq 0) = 1 - \Pr(u_i - x_i^T \beta < -x_i^T \beta) = 1 - \Phi(-x_i^T \beta) = \Phi(x_i^T \beta)$.
- Given $u = (u_1, ..., u_n)$, β can be analyzed by linear regression.
- u is **not observed**. Gibbs sampling to the rescue![2]

[2] Albert and Chib (1993). Bayesian Analysis of Binary and Polychotomous Response Data. *JASA*.

Gibbs sampling for the Probit regression

- Simulate from **joint posterior** $p(u, \beta|y)$ by iterating between
  - $p(\beta|u, y)$ is multivariate normal (linear regression)
  - $p(u_i|\beta, y),\ i = 1, ..., n.$
- The **full conditional** posterior distribution of u_i

$$p(u_i|\beta, y) \propto p(y_i|\beta, u_i)p(u_i|\beta)$$

$$= \begin{cases} N(u_i|x_i'\beta, 1) & \text{truncated to } u_i \in (-\infty, 0] \text{ if } y_i = 0 \\ N(u_i|x_i'\beta, 1) & \text{truncated to } u_i \in (0, \infty) \text{ if } y_i = 1 \end{cases}$$

- Histogram of β-draws approximates the marginal posterior of β

$$p(\beta|y) = \int p(u, \beta|y)du$$

Gibbs sampling for Regularized regression

- Recap: The joint posterior of β, σ^2 and λ is

$$\beta|\sigma^2, \lambda, \mathbf{y}, \mathbf{X} \sim N\left(\mu_n, \Omega_n^{-1}\right)$$
$$\sigma^2|\lambda, \mathbf{y}, \mathbf{X} \sim Inv-\chi^2\left(\nu_n, \sigma_n^2\right)$$
$$p(\lambda|\mathbf{y}, \mathbf{X}) \propto \sqrt{\frac{|\Omega_0|}{|X'X+\Omega_0|}}\left(\frac{\nu_n\sigma_n^2}{2}\right)^{-\nu_n/2} \cdot p(\lambda)$$

- This is the **conditional-marginal decomposition**

$$p(\beta, \sigma^2, \lambda|\mathbf{y}, \mathbf{X}) = p(\beta|\sigma^2, \lambda, \mathbf{y}, \mathbf{X})p(\sigma^2|\lambda, \mathbf{y}, \mathbf{X})p(\lambda|\mathbf{y}, \mathbf{X})$$

- **Gibbs sampling** can instead be used:
  - Sample $\beta|\sigma^2, \lambda, \mathbf{y}, \mathbf{X}$ from Normal
  - Sample $\sigma^2|\beta, \lambda, \mathbf{y}, \mathbf{X}$ from Inv-χ^2
  - Sample $\lambda|\beta, \sigma^2, \mathbf{y}, \mathbf{X}$ from Gamma
- λ is **easy** to simulate **conditional on** β and σ^2.

Gibbs sampling for Regularized regression

- Assume a Gamma prior for λ (same as $\lambda^{-1} \sim \text{Inv} - \chi^2$)

$$\lambda \sim \text{Gamma}\left(\frac{\eta_0}{2}, \frac{\eta_0}{2\lambda_0}\right).$$

- $\mathbb{E}(\lambda) = \frac{\eta_0/2}{\eta_0/(2\lambda_0)} = \lambda_0$ and $\mathbb{V}(\lambda) = \frac{\eta_0/2}{(\eta_0/(2\lambda_0))^2} = \frac{1}{2\eta_0\lambda_0^2}$.
- Using Bayes' theorem twice:

$$\begin{aligned} p\left(\lambda|\beta,\sigma^2,\mathbf{y}\right) &\propto p\left(\mathbf{y}|\beta,\sigma^2,\lambda\right) p\left(\lambda|\beta,\sigma^2\right) \\ &\propto p\left(\beta|\sigma^2,\lambda\right) p\left(\lambda|\sigma^2\right) \\ &\propto p\left(\beta|\sigma^2,\lambda\right) p\left(\lambda\right) \end{aligned}$$

- Note:
  - likelihood $p\left(\mathbf{y}|\beta,\sigma^2,\lambda\right)$ does not depend on λ.
  - prior $p\left(\lambda|\sigma^2\right)$ is assumed to not depend on σ^2.

Gibbs sampling for Regularized regression

- Full conditional posterior

$$
\begin{aligned}
p\left(\lambda|\beta,\sigma^2,\mathbf{y}\right) &\propto p\left(\beta|\sigma^2,\lambda\right)p\left(\lambda\right)\\
&\propto \prod_{i=1}^{m}\frac{1}{\sqrt{2\pi\sigma^2/\lambda}}\exp\left(-\frac{\beta_i^2}{2\sigma^2/\lambda}\right)\cdot\lambda^{\eta_0/2-1}\exp\left(-\lambda\frac{\eta_0}{2\lambda_0}\right)\\
&\propto \lambda^{m/2}\exp\left(-\frac{\lambda}{2\sigma^2}\sum_{i=1}^{m}\beta_i^2\right)\cdot\lambda^{\eta_0/2-1}\exp\left(-\lambda\frac{\eta_0}{2\lambda_0}\right)\\
&\propto \lambda^{(m+\eta_0)/2-1}\exp\left(-\lambda\left(\frac{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}{2}\right)\right)
\end{aligned}
$$

- This shows that

$$
\lambda|\beta,\sigma^2,\mathbf{y}\sim\text{Gamma}\left(\frac{m+\eta_0}{2},\frac{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}{2}\right).
$$

- $\mathbb{E}(\lambda|\beta,\sigma^2,\mathbf{y})=\frac{m+\eta_0}{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}$, so λ is learned from variability of the β_i. Large m helps!

Improving the efficiency of the Gibbs sampler

- **Efficient blocking**. Correlated parameters should ideally be included in the same updating block.

- **Reparametrization**. Convergence can improve dramatically in alternative parametrizations.

- **Data augmentation**.
  - Augment with latent variables to make **full conditional posteriors more easily sampled** (Probit, Mixture models).
  - But typically **increases the autocorrelation** between draws.

Bayesian Learning

Lecture 8 - Markov Chain Monte Carlo and Metropolis-Hastings

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Lecture overview

- Markov Chain Monte Carlo
- Metropolis-Hastings
- MCMC - efficiency, burn-in and convergence

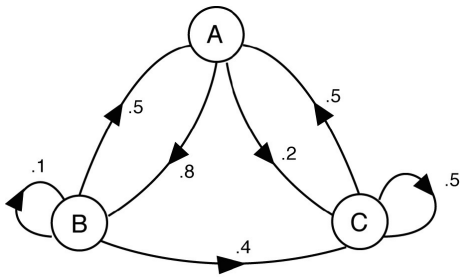
Markov chains

- Let $\mathcal{S} = \{s_1, s_2, ..., s_k)$ be a finite set of **states**.
  - Weather: $\mathcal{S} = \{\text{sunny}, \text{ rain}\}$.
  - School grades: $\mathcal{S} = \{A, B, C, D, E, F\}$
- **Markov chain** is a stochastic process $\{X_t\}_{t=1}^{T}$ with **state transitions**

$$p_{ij} = \Pr(X_{t+1} = s_j | X_t = s_i)$$

- School grades: $X_1 = C, X_2 = C, X_3 = B, X_4 = A, X_5 = B$.
- **Transition matrix** for weather example

$$P = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} 0.9 & 0.1 \\ 0.7 & 0.3 \end{pmatrix}$$



Stationary distribution

- *h*-step transition probabilities

$$P_{ij}^{(h)} = \Pr(X_{t+h} = s_j | X_t = s_i)$$

- *h*-step transition matrix by matrix power

$$P^{(h)} = P^h$$

- **Unique** equilbrium distribution $\pi = (\pi_1, ..., \pi_k)$ if chain is
  - **irreducible** (possible to get to any state from any state)
  - **aperiodic** (does not get stuck in predictable cycles)
  - **positive recurrent** (expected time of returning is finite)
- Limiting long-run distribution

$$P^t \to \begin{pmatrix} \pi \\ \pi \\ \vdots \\ \pi \end{pmatrix} = \begin{pmatrix} \pi_1 & \pi_2 & \cdots & \pi_k \\ \pi_1 & \pi_2 & \cdots & \pi_k \\ \vdots & \vdots & & \vdots \\ \pi_1 & \pi_2 & \cdots & \pi_k \end{pmatrix} \text{ as } t \to \infty$$

Stationary distribution, cont.

- Limiting long-run distribution

$$P^t \to \begin{pmatrix} \pi \\ \pi \\ \vdots \\ \pi \end{pmatrix} = \begin{pmatrix} \pi_1 & \pi_2 & \cdots & \pi_k \\ \pi_1 & \pi_2 & \cdots & \pi_k \\ \vdots & \vdots & & \vdots \\ \pi_1 & \pi_2 & \cdots & \pi_k \end{pmatrix} \text{ as } t \to \infty$$

- **Stationary distribution**

$$\pi = \pi P$$

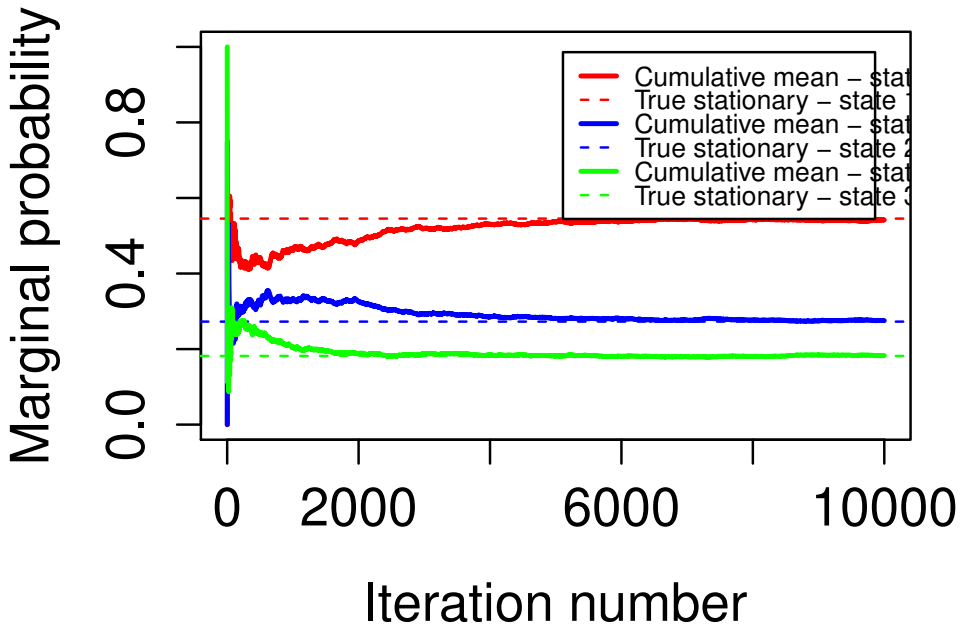
- Example:

$$P = \begin{pmatrix} 0.8 & 0.1 & 0.1 \\ 0.2 & 0.6 & 0.2 \\ 0.3 & 0.3 & 0.4 \end{pmatrix}$$

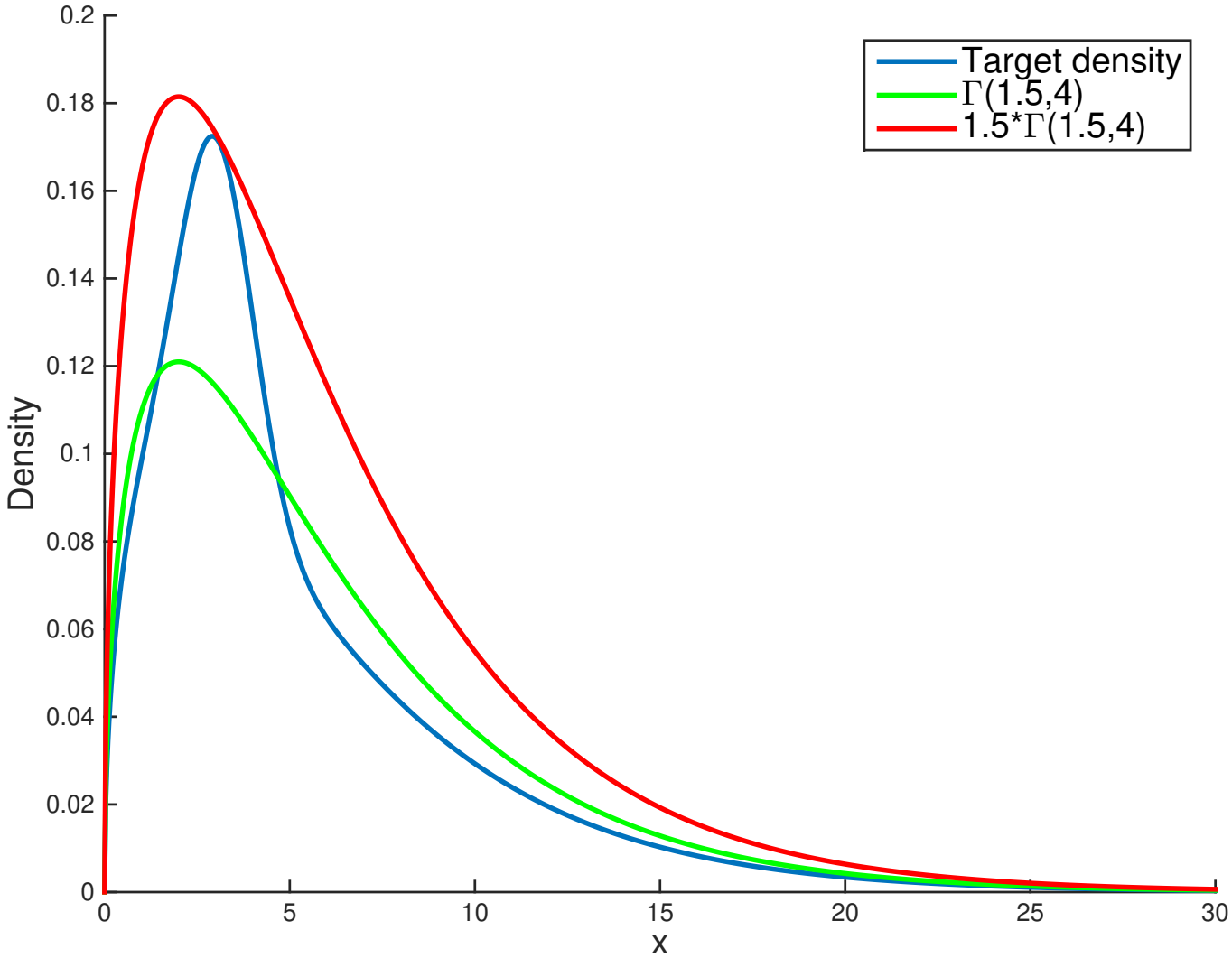
$$\pi = (0.545, 0.272, 0.181)$$

The basic MCMC idea

- Simulate from discrete distribution $p(x)$ when $x \in \{s_1, .., s_k\}$.
- MCMC: simulate a Markov Chain with a stationary distribution that is exactly $p(x)$.
- How to set up the transition matrix P? Metropolis-Hastings!



Rejection sampling



Random walk Metropolis algorithm

- **Initialize** $\theta^{(0)}$ and iterate for $i = 1, 2, \ldots$

  1. **Sample proposal**: $\theta_p | \theta^{(i-1)} \sim N\left(\theta^{(i-1)}, c \cdot \Sigma\right)$
  2. Compute the **acceptance probability**

$$\alpha = \min\left(1, \frac{p(\theta_p|\mathbf{y})}{p(\theta^{(i-1)}|\mathbf{y})}\right)$$

  3. With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

Random walk Metropolis, cont.

- Assumption: we can compute $p(\theta_p|\mathbf{y})$ for any θ.
- Proportionality constants in posterior cancel out in

$$\alpha = \min\left(1, \frac{p(\theta_p|\mathbf{y})}{p(\theta^{(i-1)}|\mathbf{y})}\right).$$

- In particular:

$$\frac{p(\theta_p|\mathbf{y})}{p(\theta^{(i-1)}|\mathbf{y})} = \frac{p(\mathbf{y}|\theta_p)p(\theta_p)/p(y)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})/p(y)} = \frac{p(\mathbf{y}|\theta_p)p(\theta_p)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})}$$

- **Proportional form of posterior is enough!**

$$\alpha = \min\left(1, \frac{p\left(\mathbf{y}|\theta_p\right)p\left(\theta_p\right)}{p\left(\mathbf{y}|\theta^{(i-1)}\right)p\left(\theta^{(i-1)}\right)}\right)$$

Random walk Metropolis, cont.

- Common choices of Σ in proposal $N\left(\theta^{(i-1)}, c \cdot \Sigma\right)$:
  - $\Sigma = I$ (proposes 'off the cigar')
  - $\Sigma = J^{-1}_{\hat{\theta},\mathbf{y}}$ (propose 'along the cigar')
  - **Adaptive**. Start with $\Sigma = I$. Update Σ from initial run.
- Set c so average acceptance probability is 25-30%.
- **Good proposal**:
  - **Easy to sample**
  - **Easy to compute** α
  - Proposals should take reasonably **large steps** in θ-space
  - Proposals should **not be reject too often**.

The Metropolis-Hastings algorithm

- Generalization when the proposal density is not symmetric.

- Initialize $\theta^{(0)}$ and iterate for $i = 1, 2, \ldots$

  1. **Sample proposal**: $\theta_p \sim q\left(\cdot|\theta^{(i-1)}\right)$
  2. Compute the **acceptance probability**

$$\alpha = \min\left(1, \frac{p(\mathbf{y}|\theta_p)p(\theta_p)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})} \frac{q\left(\theta^{(i-1)}|\theta_p\right)}{q\left(\theta_p|\theta^{(i-1)}\right)}\right)$$

  3. With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

The independence sampler

- **Independence sampler**: $q\left(\theta_p|\theta^{(i-1)}\right) = q\left(\theta_p\right)$.
- **Proposal** is **independent of previous draw**.
- Example:

$$\theta_p \sim t_v\left(\hat{\theta}, J^{-1}_{\hat{\theta},\mathbf{y}}\right),$$

  where $\hat{\theta}$ and , $J_{\hat{\theta},\mathbf{y}}$ are computed by numerical optimization.
- Can be very **efficient**, but has a tendency to **get stuck**.
- Make sure that $q\left(\theta_p\right)$ has **heavier tails** than $p(\theta|\mathbf{y})$.

Metropolis-Hastings within Gibbs

- **Gibbs sampling** from $p(\theta_1, \theta_2, \theta_3|\mathbf{y})$
  - Sample $p(\theta_1|\theta_2, \theta_3, \mathbf{y})$
  - Sample $p(\theta_2|\theta_1, \theta_3, \mathbf{y})$
  - Sample $p(\theta_3|\theta_1, \theta_2, \mathbf{y})$
- When a **full conditional is not easily sampled** we can simulate from it using **MH**.
- Example: at ith iteration, propose θ_2 from $q(\theta_2|\theta_1, \theta_3, \theta_2^{(i-1)}, \mathbf{y})$. Accept/reject.
- **Gibbs sampling is a special case of MH** when $q(\theta_2|\theta_1, \theta_3, \theta_2^{(i-1)}, \mathbf{y}) = p(\theta_2|\theta_1, \theta_3, \mathbf{y})$, which gives $\alpha = 1$. Always accept.

The efficiency of MCMC

- **How efficient** is MCMC compared to iid sampling?
- If $\theta^{(1)}, \theta^{(2)}, ..., \theta^{(N)}$ are **iid** with variance σ^2, then

$$\text{Var}(\bar{\theta}) = \frac{\sigma^2}{N}.$$

- Autocorrelated $\theta^{(1)}, \theta^{(2)}, ..., \theta^{(N)}$ generated by **MCMC**

$$\text{Var}(\bar{\theta}) = \frac{\sigma^2}{N}\left(1 + 2\sum_{k=1}^{\infty}\rho_k\right)$$

where $\rho_k = Corr(\theta^{(i)}, \theta^{(i+k)})$ is the autocorrelation at lag k.

- **Inefficiency factor**

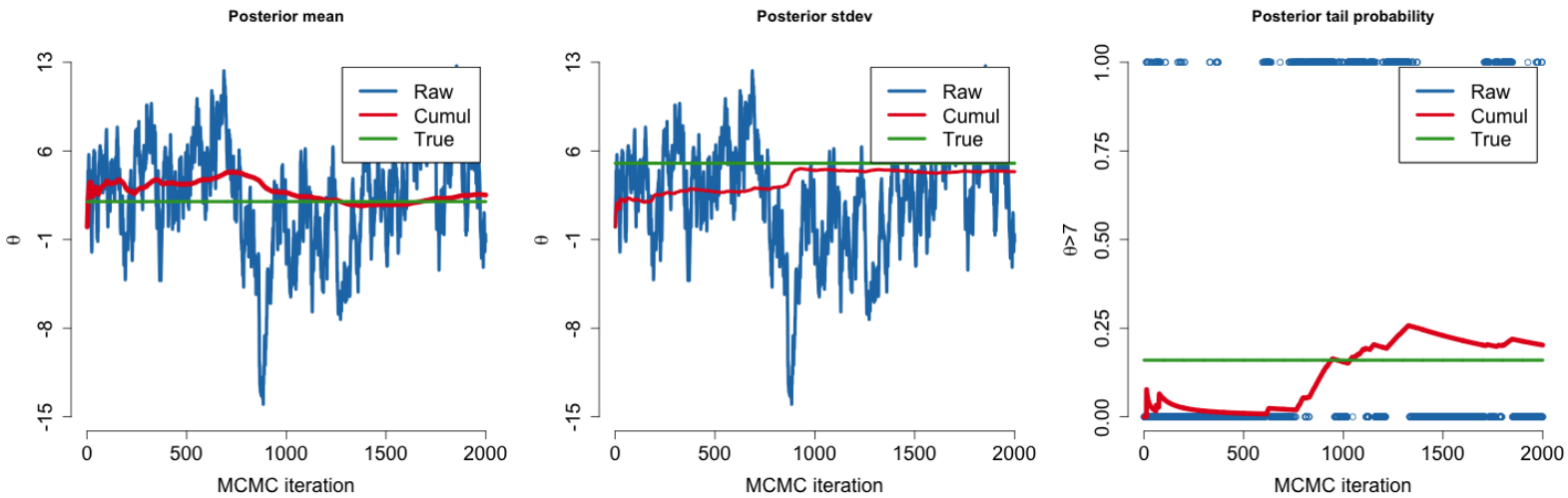
$$\text{IF} = 1 + 2\sum_{k=1}^{\infty}\rho_k$$

- **Effective sample size** from MCMC

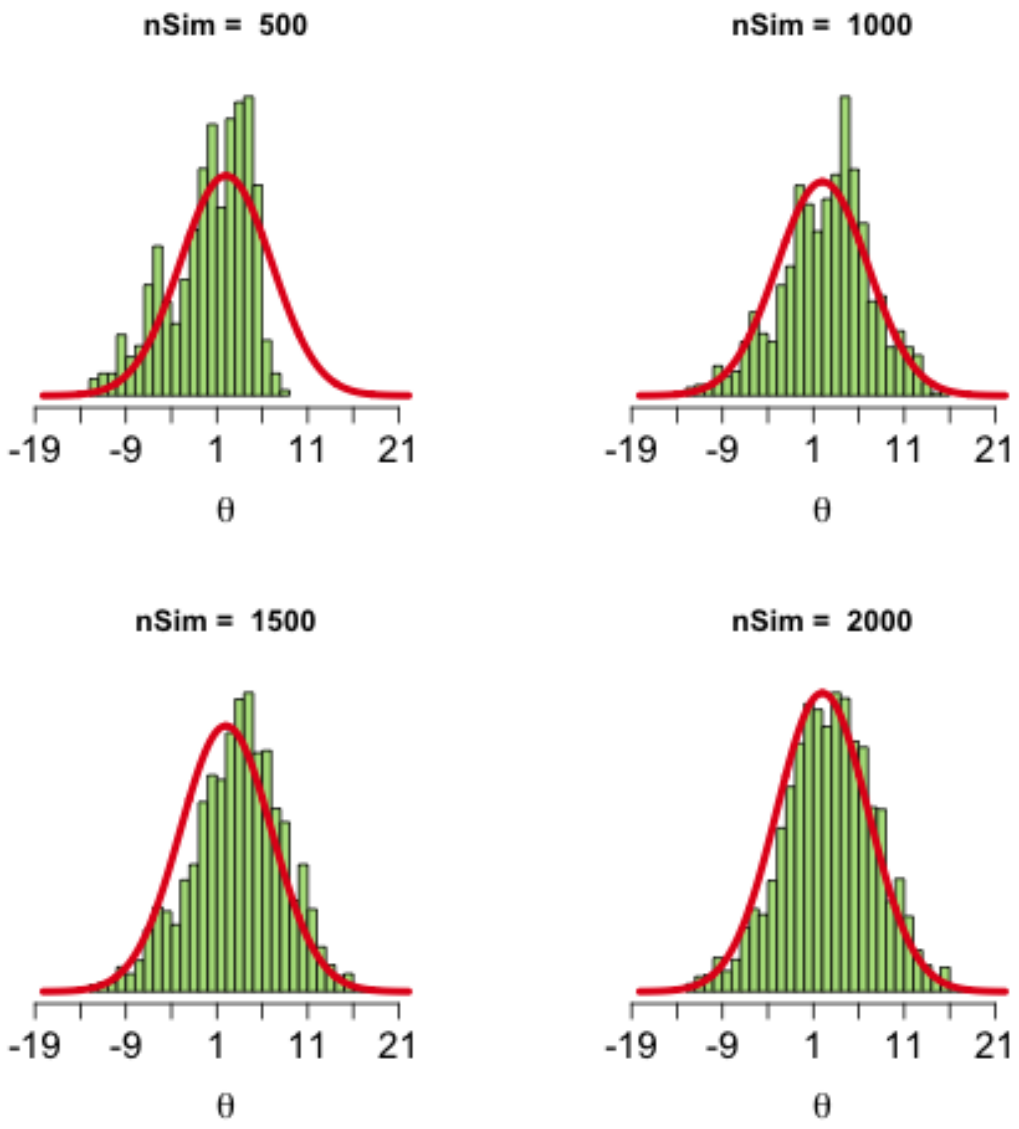
$$\text{ESS} = N/\text{IF}$$

Burn-in and convergence

- How long **burn-in**?
- **How long to sample** after burn-in?
- **Thinning**? Keeping every h draw reduces autocorrelation.
- **Convergence diagnostics**
  - Raw plots of simulated sequences (trajectories)
  - CUSUM plots
  - Potential scale reduction factor, R.



Burn-in and convergence



Bayesian Learning

Lecture 9 - HMC, Stan and Variational Inference

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Lecture overview

- Hamiltonian Monte Carlo
- Stan
- Variational Inference

Hamiltonian Monte Carlo

- When $\theta = (\theta_1, \ldots, \theta_p)$ is **high-dimensional**, $p(\theta|\mathbf{y})$ usually located in some subregion of $\mathbb{R}^p$ with complicated geometry.
- MH: hard to find good proposal distribution $q\left(\cdot|\theta^{(i-1)}\right)$.
- MH: use very small step sizes otherwise too many rejections.
- **Hamiltonian Monte Carlo** (**HMC**):
  - distant proposals **and**
  - high acceptance probabilities.
- HMC: add extra **momentum** parameters $\phi = (\phi_1, \ldots, \phi_p)$ and sample from

$$p(\theta, \phi|\mathbf{y}) = p(\theta|\mathbf{y})\, p(\phi)$$

.

Hamiltonian Monte Carlo

- Physics: **Hamiltonian** system $H(\theta, \phi) = U(\theta) + K(\phi)$, where U is the **potential energy** and K is the **kinetic energy**.
- **Hamiltonian Dynamics**

$$\frac{d\theta_i}{dt} = \frac{\partial H}{\partial \phi_i} = \frac{\partial K}{\partial \phi_i},$$
$$\frac{d\phi_i}{dt} = -\frac{\partial H}{\partial \theta_i} = -\frac{\partial U}{\partial \theta_i}$$

- Hockey puck sliding over a friction-less surface: illustration.
- Use $U(\theta) = -\log[p(\theta)\, p(\mathbf{y}|\theta)]$.
- Use $\phi \sim N(0, \mathbf{M})$ where $\mathbf{M}$ is the mass matrix and

$$K(\phi) = -\log[p(\phi)] = \frac{1}{2}\phi^T \mathbf{M}^{-1}\phi + \text{const}$$

- If we could propose θ in continuous time (spoiler: we can't), the acceptance probability would be one.

Hamiltonian Monte Carlo

Hamiltonian Dynamics

$$\frac{d\theta_i}{dt} = \left[\mathbf{M}^{-1}\phi\right]_i,$$
$$\frac{d\phi_i}{dt} = \frac{\partial \log p\left(\theta|\mathbf{y}\right)}{\partial \theta_i}$$

which can be simulated using the **leapfrog algorithm**

$$\phi_i\left(t+\frac{\varepsilon}{2}\right) = \phi_i\left(t\right) + \frac{\varepsilon}{2}\frac{\partial \log p\left(\theta(t)|\mathbf{y}\right)}{\partial \theta_i},$$
$$\theta\left(t+\varepsilon\right) = \theta\left(t\right) + \varepsilon\mathbf{M}^{-1}\phi(t),$$
$$\phi_i\left(t+\varepsilon\right) = \phi_i\left(t+\frac{\varepsilon}{2}\right) + \frac{\varepsilon}{2}\frac{\partial \log p\left(\theta(t)|\mathbf{y}\right)}{\partial \theta_i},$$

where ε is the step size.

- **Discretization** $\Rightarrow$ acceptance probability drops with ε.

The Hamiltonian Monte Carlo algorithm

- Initialize $\theta^{(0)}$ and iterate for $i = 1, 2, \ldots$

  1. Sample the starting **momentum** $\phi_s \sim N(0, \mathbf{M})$
  2. Simulate new values for (θ_p, ϕ_p) by iterating the **leapfrog algorithm** L times, starting in $\left(\theta^{(i-1)}, \phi_s\right)$.
  3. Compute the **acceptance probability**

$$\alpha = \min\left(1, \frac{p(\mathbf{y}|\theta_p)p(\theta_p)}{p(\mathbf{y}|\theta^{(i-1)})p(\theta^{(i-1)})}\frac{p(\phi_p)}{p(\phi_s)}\right)$$

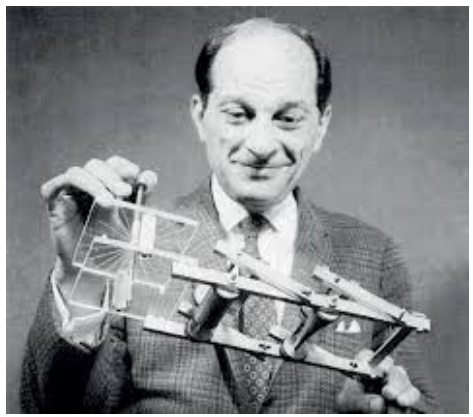
  4. With probability α set $\theta^{(i)} = \theta_p$ and $\theta^{(i)} = \theta^{(i-1)}$ otherwise.

- Tuning parameters: 1. **stepsize** ε, 2. **number of leapfrog** iterations L and 3. **mass matrix** M. No U-turn.

Stan

- **Stan** is a probabilistic programming language based on HMC.
- Allows for Bayesian inference in many models with automatic implementation of the MCMC sampler.
- Named after Stanislaw Ulam (1909-1984), co-inventor of the Monte Carlo algorithm.
- Written in C++ but can be run from R using the package `rstan`

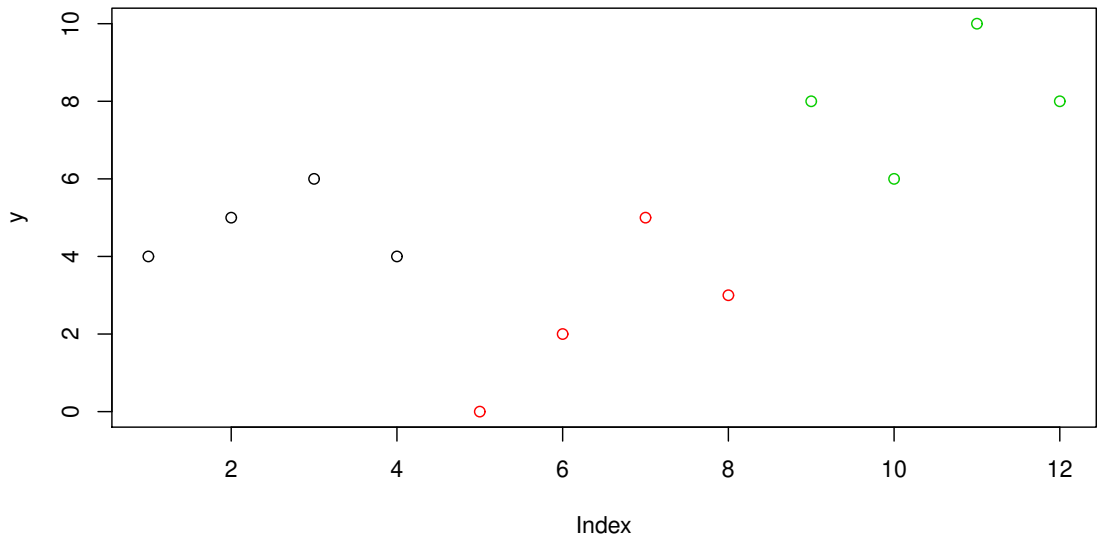
Stan logo



Stanislaw Ulam

Stan - toy example: three plants

- Three plants were observed for four months, measuring the number of flowers



Stan Model 1: iid normal

$$y_i \overset{iid}{\sim} N\left(\mu, \sigma^2\right)$$

```
library(rstan)
y = c(4,5,6,4,0,2,5,3,8,6,10,8)
N = length(y)

StanModel = '
data {
  int<lower=0> N; // Number of observations
  int<lower=0> y[N]; // Number of flowers
}
parameters {
  real mu;
  real<lower=0> sigma2;
}
model {
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2
  for(i in 1:N)
    y[i] ~ normal(mu,sqrt(sigma2));
}'
```

Stan Model 2: multilevel normal

$$y_{i,p} \sim N\left(\mu_p, \sigma_p^2\right), \quad \mu_p \sim N\left(\mu, \sigma^2\right)$$

```
StanModel = '
data {
  int<lower=0> N; // Number of observations
  int<lower=0> y[N]; // Number of flowers
  int<lower=0> P; // Number of plants
}
transformed data {
  int<lower=0> M; // Number of months
  M = N / P;
}
parameters {
  real mu;
  real<lower=0> sigma2;
  real mup[P];
  real sigmap2[P];
}
model {
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2
  for(p in 1:P){
    mup[p] ~ normal(mu,sqrt(sigma2));
    for(m in 1:M)
      y[M*(p-1)+m] ~ normal(mup[p],sqrt(sigmap2[p]));
  }
}'
```

Stan Model 3: multilevel Poisson

$$y_{i,p} \sim Poisson\left(\mu_p\right), \quad \mu_p \sim logN\left(\mu, \sigma^2\right)$$

```
StanModel = '
data {
  int<lower=0> N; // Number of observations
  int<lower=0> y[N]; // Number of flowers
  int<lower=0> P; // Number of plants
}
transformed data {
  int<lower=0> M; // Number of months
  M = N / P;
}
parameters {
  real mu;
  real<lower=0> sigma2;
  real mup[P];
}
model {
  mu ~ normal(0,100); // Normal with mean 0, st.dev. 100
  sigma2 ~ scaled_inv_chi_square(1,2); // Scaled-inv-chi2 with nu 1, sigma 2
  for(p in 1:P){
    mup[p] ~ lognormal(mu,sqrt(sigma2)); // Log-normal
    for(m in 1:M)
      y[M*(p-1)+m] ~ poisson(mup[p]); // Poisson
  }
}'
```

Stan: fit model and analyze output

```
data = list(N=N, y=y, P=P)
burnin = 1000
niter = 2000
fit = stan(model_code=StanModel,data=data,
           warmup=burnin,iter=niter,chains=4)

# Print the fitted model
print(fit,digits_summary=3)

# Extract posterior samples
postDraws <- extract(fit)

# Do traceplots of the first chain
par(mfrow = c(1,1))
plot(postDraws$mu[1:(niter-burnin)],type="l",ylab="mu",main="Traceplot")

# Do automatic traceplots of all chains
traceplot(fit)

# Bivariate posterior plots
pairs(fit)
```

Stan - useful links

- Getting started with RStan
- RStan vignette
- Stan Modeling Language User's Guide and Reference Manual
- Stan Case Studies

Variational Inference

- Let $\theta = (\theta_1, ..., \theta_p)$. Approximate the posterior $p(\theta|y)$ with a (simpler) distribution $q(\theta)$.
- Before: **Normal approximation** from optimization: $q(\theta) = N\left[\tilde{\theta}, J_{\mathbf{y}}^{-1}(\tilde{\theta})\right]$.
- **Mean field Variational Inference (VI)**: $q(\theta) = \prod_{i=1}^{p} q_i(\theta_i)$
- **Parametric VI**: Parametric family $q_\lambda(\theta)$ with parameters λ
- Find the $q(\theta)$ that **minimizes the Kullback-Leibler distance** between the true posterior p and the approximation q:

$$KL(q, p) = \int q(\theta) \ln \frac{q(\theta)}{p(\theta|y)} d\theta = E_q \left[\ln \frac{q(\theta)}{p(\theta|y)} \right].$$

Mean field approximation

- **Mean field VI** is based on factorized approximation:

$$q(\theta) = \prod_{i=1}^{p} q_i(\theta_i)$$

- **No specific functional forms** are assumed for the $q_i(\theta)$.

- **Optimal densities** can be shown to satisfy:

$$q_j(\theta) \propto \exp\left(E_{-\theta_j} \ln p(\mathbf{y}, \theta)\right)$$

  where $E_{-\theta_j}(\cdot)$ is the expectation with respect to $\prod_{k \neq j} q_k(\theta_k)$.

- **Structured mean field approximation**. Group subset of parameters in tractable blocks. Similar to Gibbs sampling.

Mean field approximation - algorithm

- Initialize: $q_2^*(\theta_2), ..., q_M^*(\theta_p)$
- Repeat until convergence:
  - $q_1^*(\theta_1) \leftarrow \frac{\exp\left[E_{-\theta_1} \ln p(\mathbf{y},\theta)\right]}{\int \exp\left[E_{-\theta_1} \ln p(\mathbf{y},\theta)\right] d\theta_1}$
  - $\vdots$
  - $q_p^*(\theta_p) \leftarrow \frac{\exp\left[E_{-\theta_p} \ln p(\mathbf{y},\theta)\right]}{\int \exp\left[E_{-\theta_p} \ln p(\mathbf{y},\theta)\right] d\theta_p}$
- Note: no assumptions about parametric form of the $q_i(\theta)$.
- Optimal $q_i(\theta)$ often **turn out** to be parametric (normal etc).
- Just update hyperparameters in the optimal densities.

Mean field approximation - Normal model

- **Model**: $X_i|\theta, \sigma^2 \overset{iid}{\sim} N(\theta, \sigma^2)$.
- **Prior**: $\theta \sim N(\mu_0, \tau_0^2)$ **independent** of $\sigma^2 \sim Inv - \chi^2(\nu_0, \sigma_0^2)$.
- **Mean-field approximation**: $q(\theta, \sigma^2) = q_\theta(\theta) \cdot q_{\sigma^2}(\sigma^2)$.
- Optimal densities

$$q_\theta^*(\theta) \propto \exp\left[E_{q(\sigma^2)} \ln p(\theta, \sigma^2, \mathbf{x})\right]$$
$$q_{\sigma^2}^*(\sigma^2) \propto \exp\left[E_{q(\theta)} \ln p(\theta, \sigma^2, \mathbf{x})\right]$$

Normal model - VB algorithm

- **Variational density for σ^2**

$$\sigma^2 \sim Inv - \chi^2\left(\tilde{\nu}_n, \tilde{\sigma}_n^2\right)$$

where $\tilde{\nu}_n = \nu_0 + n$ and $\tilde{\sigma}_n = \frac{\nu_0\sigma_0^2 + \sum_{i=1}^{n}(x_i - \tilde{\mu}_n)^2 + n\cdot\tilde{\tau}_n^2}{\nu_0 + n}$

- **Variational density for θ**

$$\theta \sim N\left(\tilde{\mu}_n, \tilde{\tau}_n^2\right)$$

where

$$\tilde{\tau}_n^2 = \frac{1}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

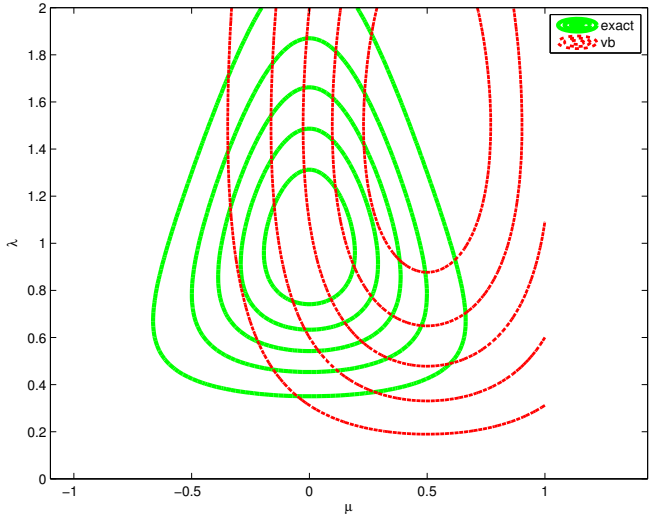
$$\tilde{\mu}_n = \tilde{w}\bar{x} + (1 - \tilde{w})\mu_0,$$

where

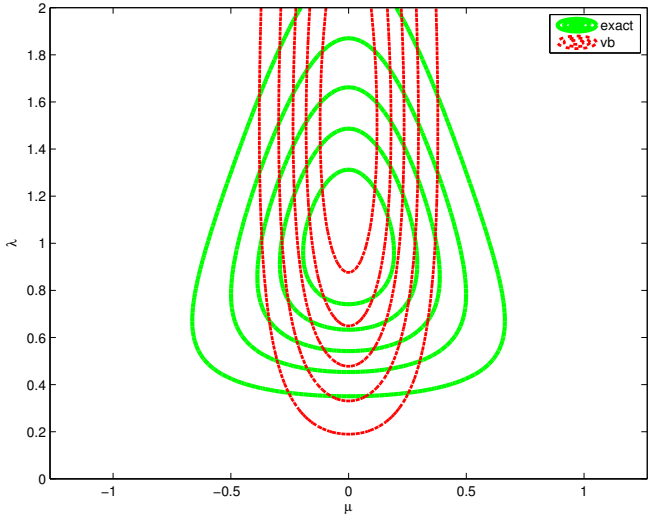
$$\tilde{w} = \frac{\frac{n}{\tilde{\sigma}_n^2}}{\frac{n}{\tilde{\sigma}_n^2} + \frac{1}{\tau_0^2}}$$

Normal example from Murphy ($\lambda = 1/\sigma^2$)

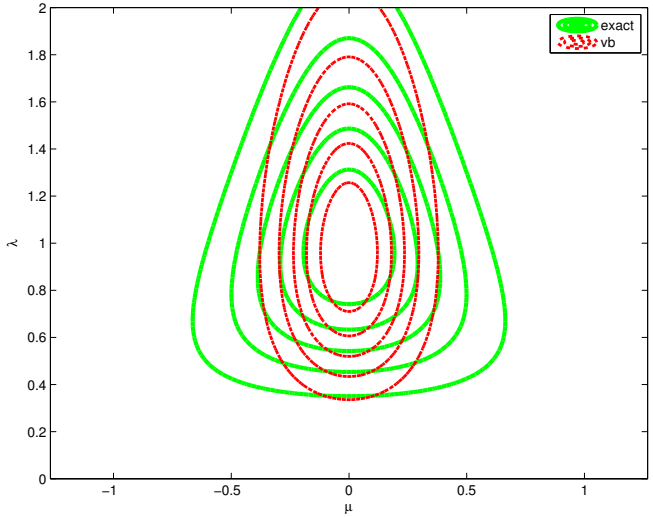
Initial values



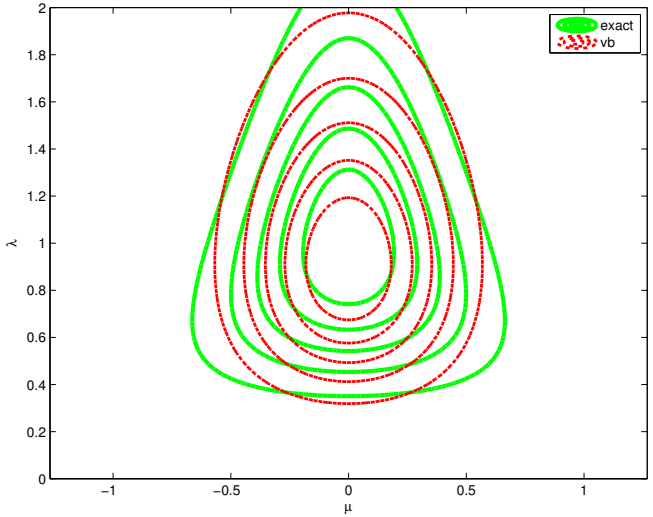
After updating q_μ



After updating q_{σ^2}



At convergence



Probit regression

- **Model**:

$$\Pr(y_i = 1|\mathbf{x}_i) = \Phi(\mathbf{x}_i^T \beta)$$

- **Prior**: $\beta \sim N(0, \Sigma_\beta)$. For example: $\Sigma_\beta = \tau^2 I$.
- **Latent variable formulation** with $u = (u_1, ..., u_n)'$

$$\mathbf{u}|\beta \sim N(\mathbf{X}\beta, 1)$$

and

$$y_i = \begin{cases} 0 & \text{if } u_i \leq 0 \\ 1 & \text{if } u_i > 0 \end{cases}$$

- Factorized **variational approximation**

$$q(\mathbf{u}, \beta) = q_{\mathbf{u}}(\mathbf{u}) q_\beta(\beta)$$

VI for probit regression

VI posterior

$$\beta \sim N\left(\tilde{\mu}_\beta, \left(\mathbf{X}^T\mathbf{X} + \Sigma_\beta^{-1}\right)^{-1}\right)$$

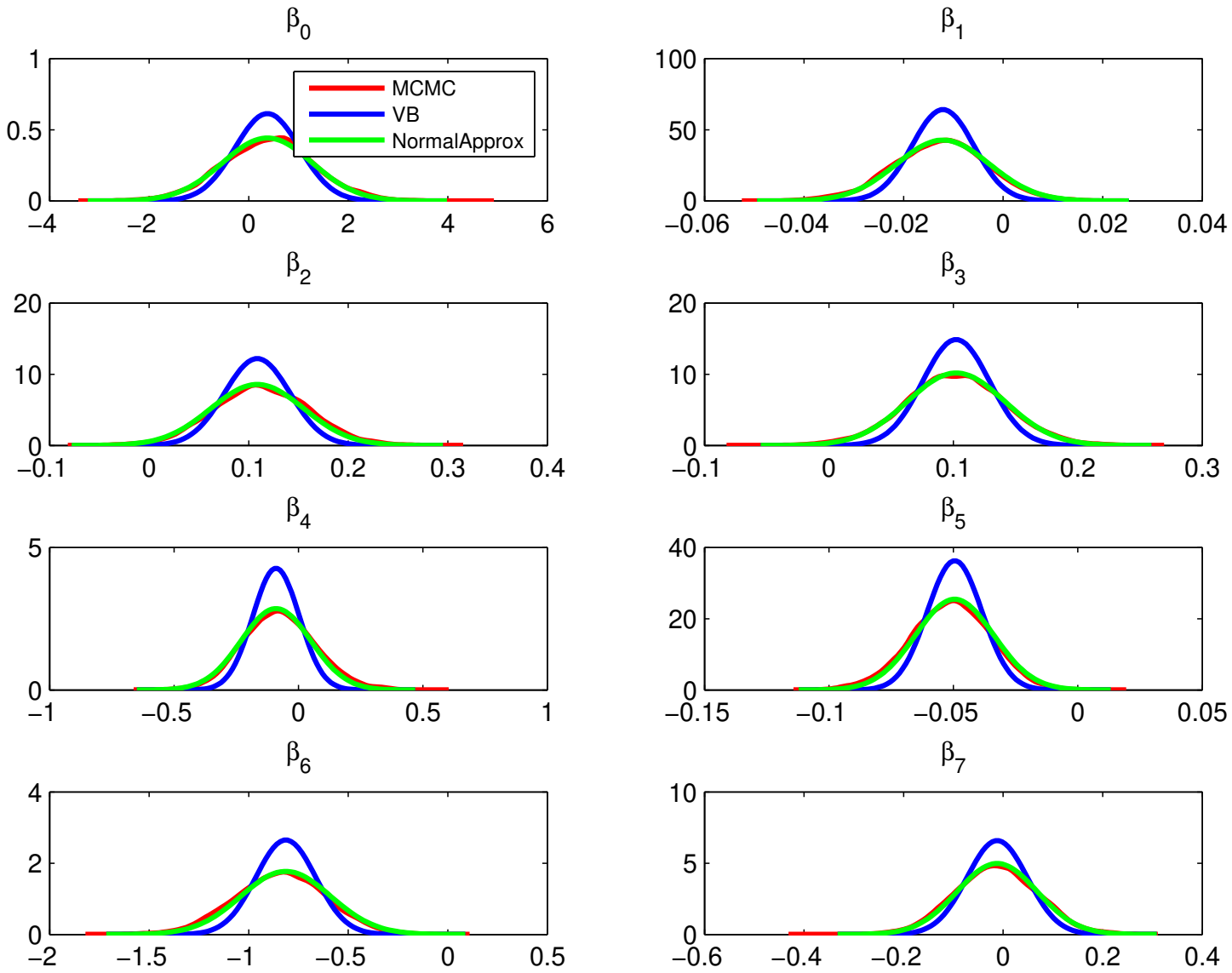
where

$$\tilde{\mu}_\beta = \left(\mathbf{X}^T\mathbf{X} + \Sigma_\beta^{-1}\right)^{-1}\mathbf{X}^T\tilde{\mu}_\mathbf{u}$$

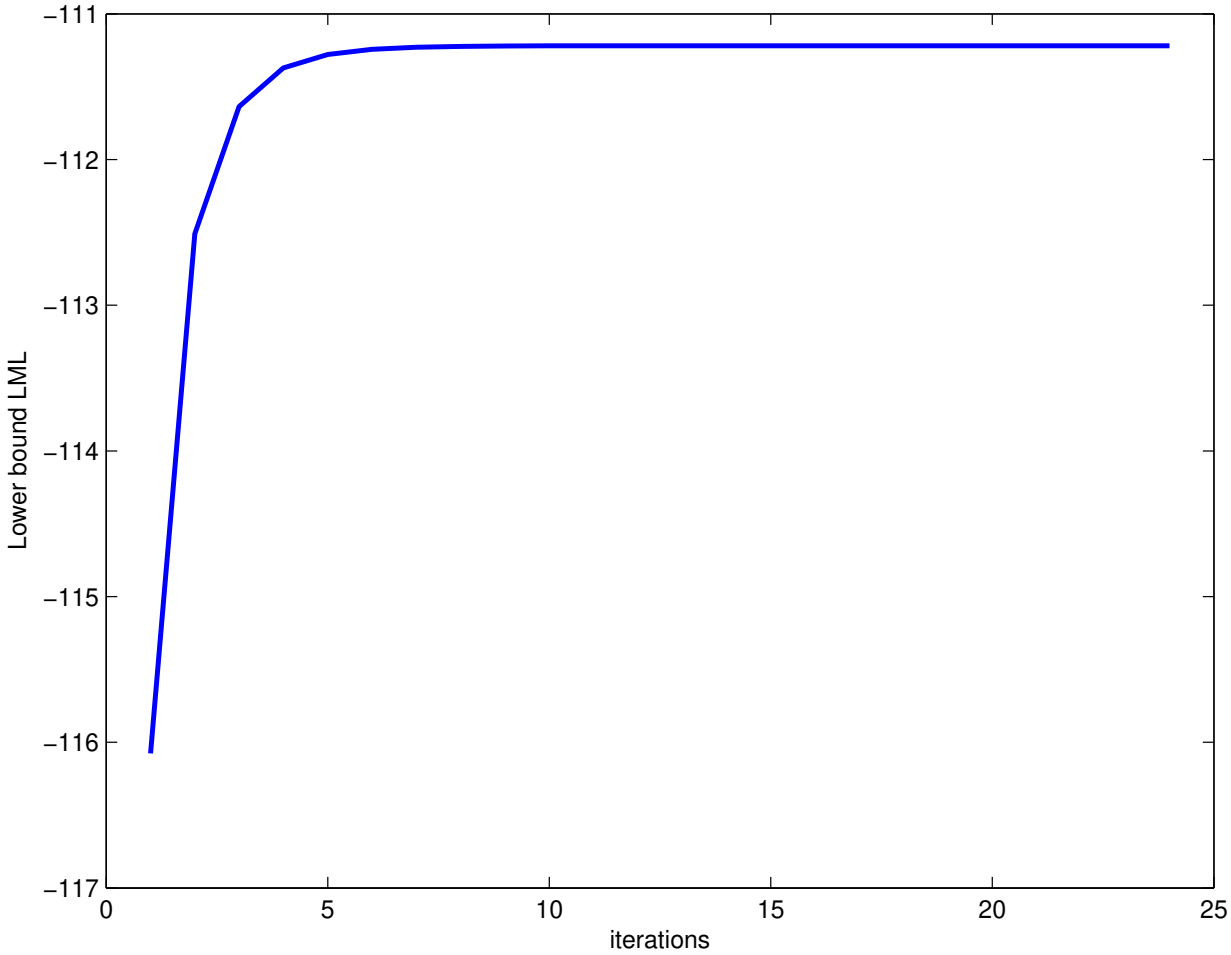
and

$$\tilde{\mu}_\mathbf{u} = \mathbf{X}\tilde{\mu}_\beta + \frac{\phi\left(\mathbf{X}\tilde{\mu}_\beta\right)}{\Phi\left(\mathbf{X}\tilde{\mu}_\beta\right)^\mathbf{y}\left[\Phi\left(\mathbf{X}\tilde{\mu}_\beta\right) - \mathbf{1}_n\right]^{\mathbf{1}_n - \mathbf{y}}}.$$

Probit example (n=200 observations)



Probit example



Bayesian Learning

Lecture 10 - Bayesian Model Comparison

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Overview

- Bayesian model comparison
- Marginal likelihood
- Log Predictive Score

Using likelihood for model comparison

- Consider two models for the data $\mathbf{y} = (y_1, ..., y_n)$: M_1 and M_2.
- Let $p_i(\mathbf{y}|\theta_i)$ denote the data density under model M_i.
- If we know θ_1 and θ_2, the **likelihood ratio** is useful

$$\frac{p_1(\mathbf{y}|\theta_1)}{p_2(\mathbf{y}|\theta_2)}.$$

- The **likelihood ratio** with **ML estimates** plugged in:

$$\frac{p_1(\mathbf{y}|\hat{\theta}_1)}{p_2(\mathbf{y}|\hat{\theta}_2)}.$$

- Bigger models always win in estimated likelihood ratio.
- **Hypothesis tests** are problematic for non-nested models. End results are not very useful for analysis.

Bayesian model comparison

- Just use your priors $p_1(\theta_1)$ och $p_2(\theta_2)$.
- The **marginal likelihood** for model M_k with parameters θ_k

$$p_k(y) = \int p_k(y|\theta_k)p_k(\theta_k)d\theta_k.$$

- θ_k is 'removed' by the averaging wrt prior. **Priors matter!**
- The **Bayes factor**

$$B_{12}(y) = \frac{p_1(y)}{p_2(y)}.$$

- **Posterior model probabilities**

$$\underbrace{\Pr(M_k|\mathbf{y})}_{\text{posterior model prob.}} \propto \underbrace{p(\mathbf{y}|M_k)}_{\text{marginal likelihood}} \cdot \underbrace{\Pr(M_k)}_{\text{prior model prob.}}$$

Bayesian hypothesis testing - Bernoulli

- **Hypothesis testing** is just a special case of model selection:

$$M_0 : x_1, ..., x_n \overset{iid}{\sim} Bernoulli(\theta_0)$$

$$M_1 : x_1, ..., x_n \overset{iid}{\sim} Bernoulli(\theta), \theta \sim Beta(\alpha, \beta)$$

$$p(x_1, ..., x_n | M_0) = \theta_0^s (1-\theta_0)^f,$$

$$\begin{aligned} p(x_1, ..., x_n | M_1) &= \int_0^1 \theta^s (1-\theta)^f B(\alpha, \beta)^{-1} \theta^{\alpha-1} (1-\theta)^{\beta-1} d\theta \\ &= B(\alpha + s, \beta + f) / B(\alpha, \beta), \end{aligned}$$

where $B(\cdot, \cdot)$ is the Beta function.

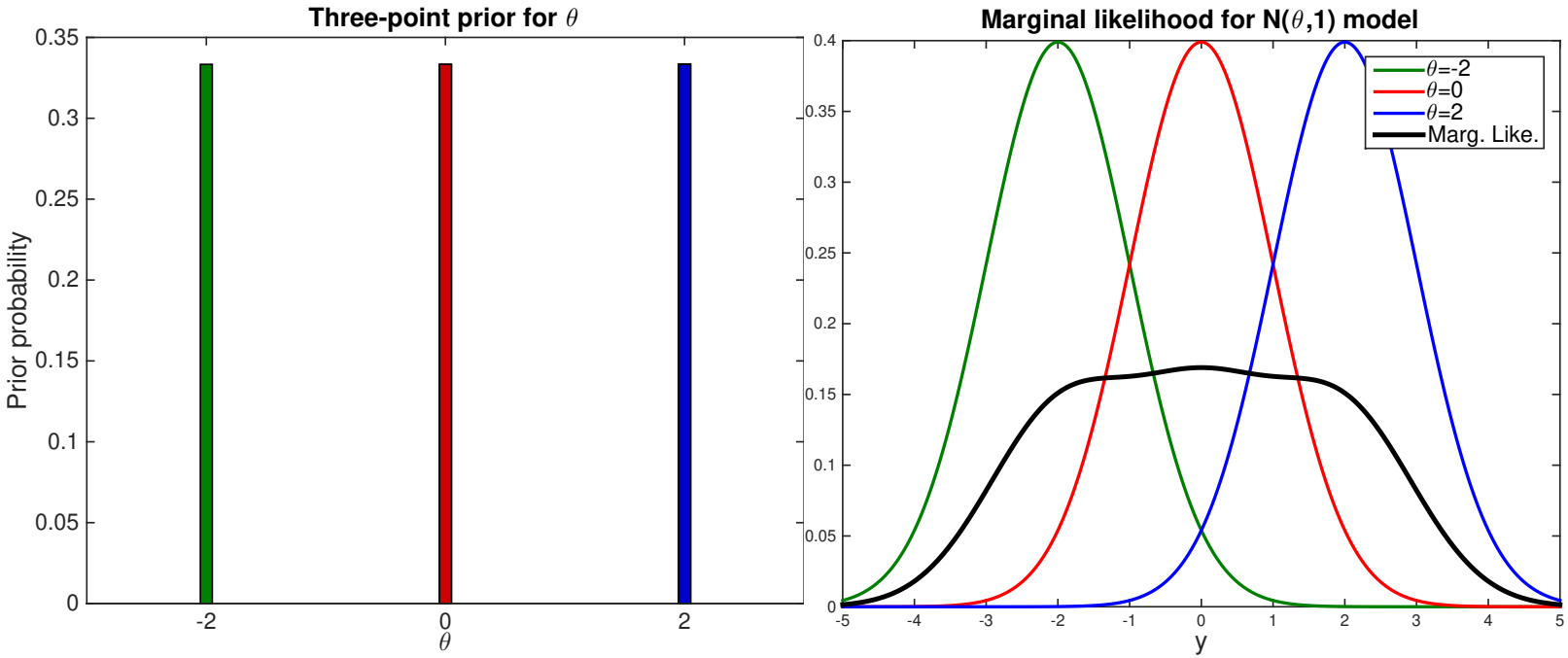
- **Posterior model probabilities**

$$Pr(M_k | x_1, ..., x_n) \propto p(x_1, ..., x_n | M_k) Pr(M_k), \text{ for } k = 0, 1.$$

- The **Bayes factor**

$$BF(M_0; M_1) = \frac{p(x_1, ..., x_n | H_0)}{p(x_1, ..., x_n | H_1)} = \frac{\theta_0^s (1-\theta_0)^f B(\alpha, \beta)}{B(\alpha + s, \beta + f)}.$$

Priors matter



Example: Geometric vs Poisson

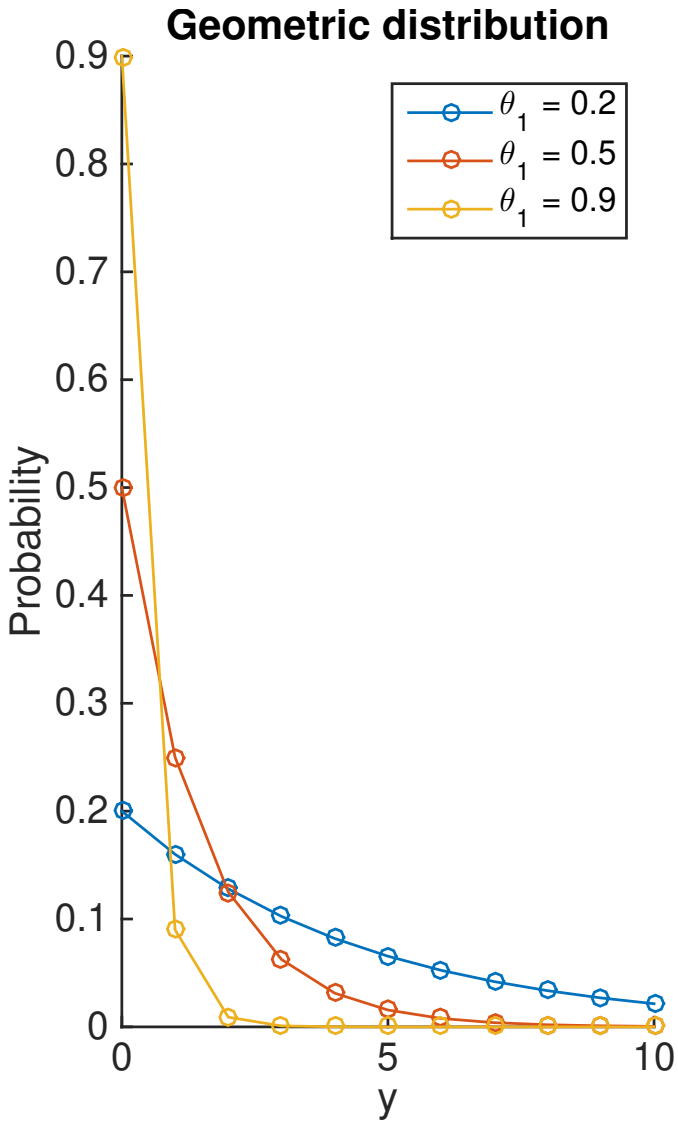
- Model 1 - **Geometric** with Beta prior:
  - $y_1, ..., y_n|\theta_1 \sim Geo(\theta_1)$
  - $\theta_1 \sim Beta(\alpha_1, \beta_1)$
- Model 2 - **Poisson** with Gamma prior:
  - $y_1, ..., y_n|\theta_2 \sim Poisson(\theta_2)$
  - $\theta_2 \sim Gamma(\alpha_2, \beta_2)$
- **Marginal likelihood** for M_1

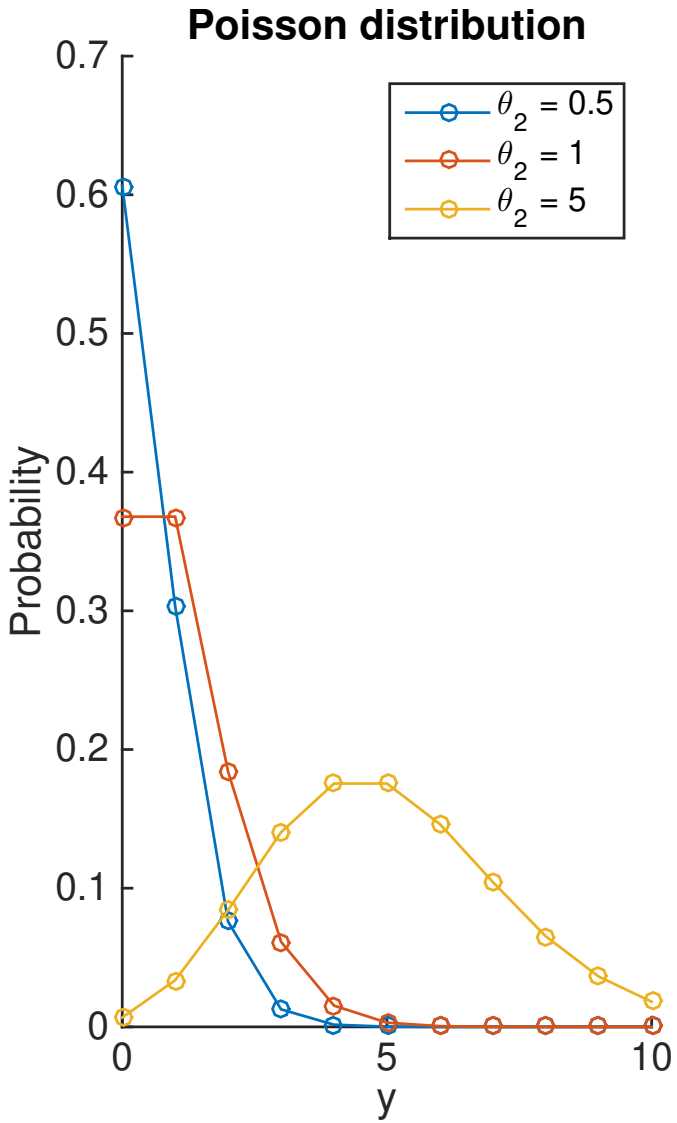
$$p_1(y_1, ..., y_n) = \int p_1(y_1, ..., y_n|\theta_1)p(\theta_1)d\theta_1$$
$$= \frac{\Gamma(\alpha_1 + \beta_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)} \frac{\Gamma(n + \alpha_1)\Gamma(n\bar{y} + \beta_1)}{\Gamma(n + n\bar{y} + \alpha_1 + \beta_1)}$$

- **Marginal likelihood** for M_2

$$p_2(y_1, ..., y_n) = \frac{\Gamma(n\bar{y} + \alpha_2)\beta_2^{\alpha_2}}{\Gamma(\alpha_2)(n + \beta_2)^{n\bar{y}+\alpha_2}} \frac{1}{\prod_{i=1}^n y_i!}$$

Geometric and Poisson





Geometric vs Poisson

- Priors match prior predictive means:

$$E(y_i|M_1) = E(y_i|M_2) \iff \alpha_1\alpha_2 = \beta_1\beta_2$$

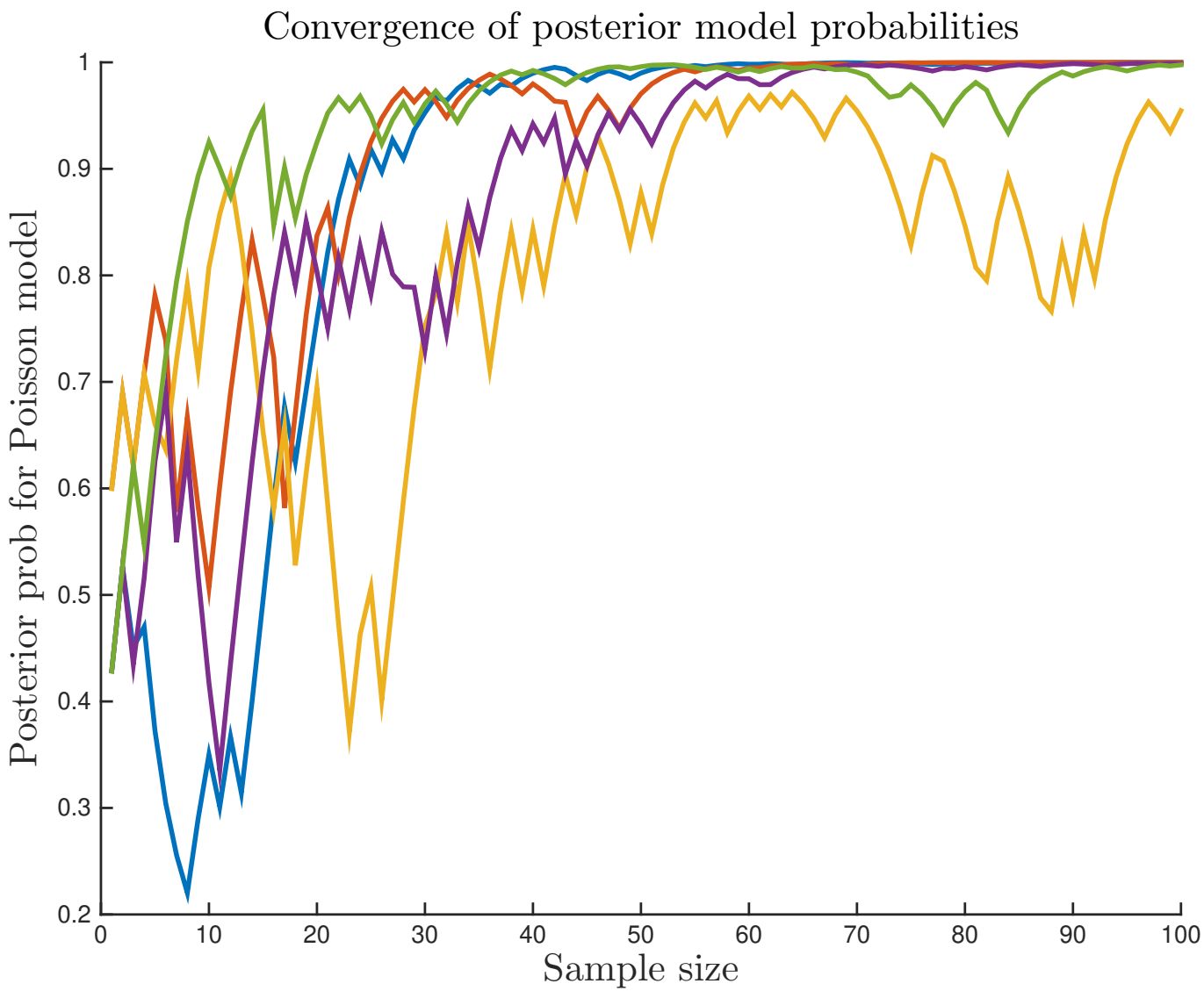
- **Data**: $y_1 = 0,\ y_2 = 0.$

	$\alpha_1 = 1, \beta_1 = 2$ $\alpha_2 = 2, \beta_2 = 1$	$\alpha_1 = 10, \beta_1 = 20$ $\alpha_2 = 20, \beta_2 = 10$	$\alpha_1 = 100, \beta_1 = 200$ $\alpha_2 = 200, \beta_2 = 100$
BF_{12}	1.5	4.54	5.87
$\Pr(M_1\|\mathbf{y})$	0.6	0.82	0.85
$\Pr(M_2\|\mathbf{y})$	0.4	0.18	0.15

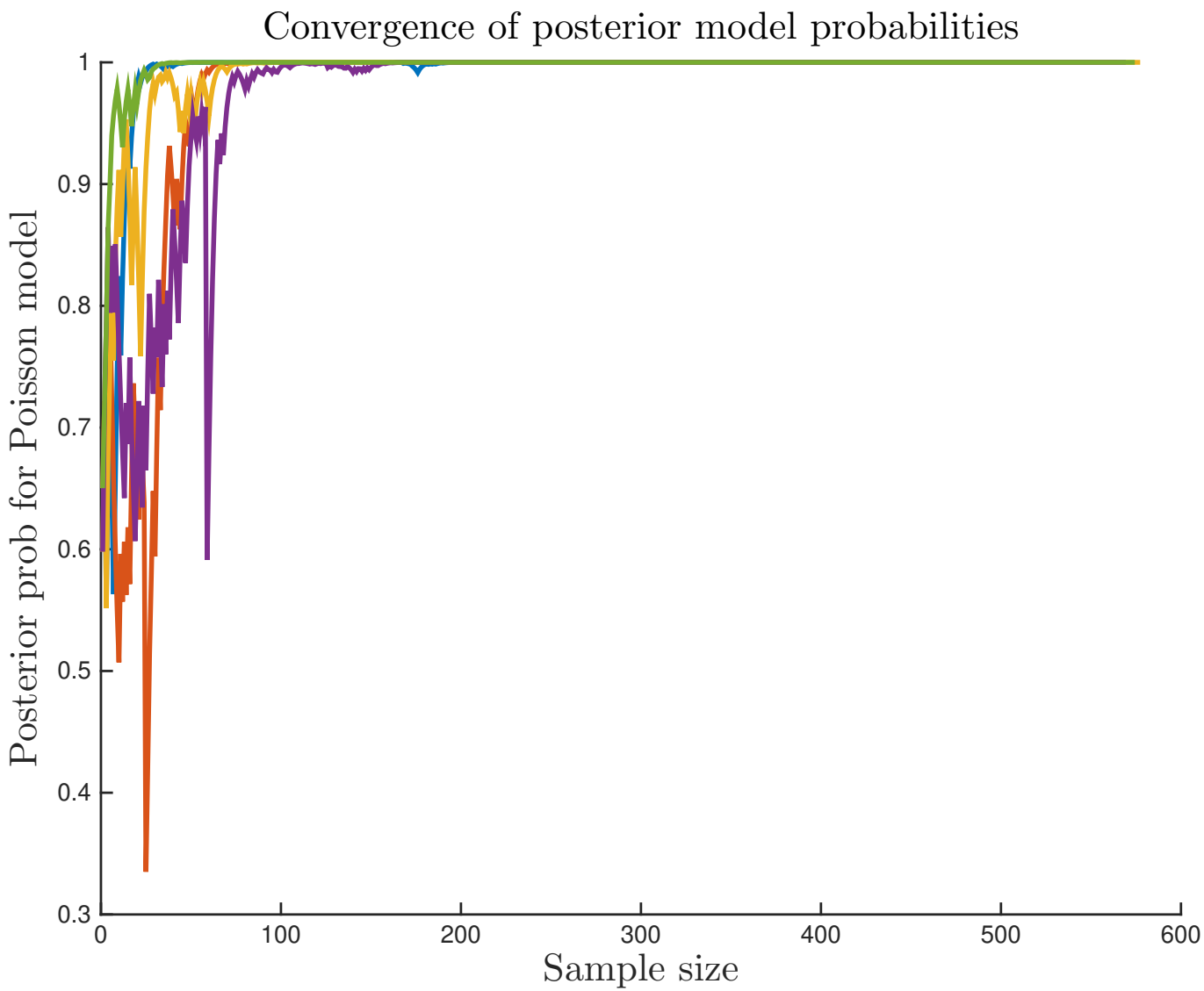
- **Data**: $y_1 = 3,\ y_2 = 3.$

	$\alpha_1 = 1, \beta_1 = 2$ $\alpha_2 = 2, \beta_2 = 1$	$\alpha_1 = 10, \beta_1 = 20$ $\alpha_2 = 20, \beta_2 = 10$	$\alpha_1 = 100, \beta_1 = 200$ $\alpha_2 = 200, \beta_2 = 100$
BF_{12}	0.26	0.29	0.30
$\Pr(M_1\|\mathbf{y})$	0.21	0.22	0.23
$\Pr(M_2\|\mathbf{y})$	0.79	0.78	0.77

Geometric vs Poisson for Pois(1) data



Geometric vs Poisson for Pois(1) data



Model choice in multivariate time series[1]

- **Multivariate time series**

$$\mathbf{x}_t = \alpha\beta'\mathbf{z}_t + \Phi_1\mathbf{x}_{t-1} + ...\Phi_k\mathbf{x}_{t-k} + \Psi_1 + \Psi_2 t + \Psi_3 t^2 + \varepsilon_t$$

- Need to choose:
  - **Lag length**, $(k = 1, 2.., 4)$
  - **Trend model** $(s = 1, 2, ..., 5)$
  - **Long-run (cointegration) relations** $(r = 0, 1, 2, 3, 4)$.

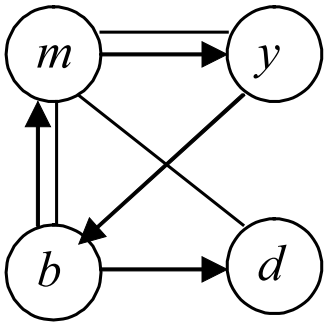
THE MOST PROBABLE (k, r, s) COMBINATIONS IN THE DANISH MONETARY DATA.

k	1	1	1	1	1	1	1	1	0	1
r	3	3	2	4	2	1	2	3	4	3
s	3	2	2	2	3	3	4	4	4	5
$p(k, r, s\|y, x, z)$	.106	.093	.091	.060	.059	.055	.054	.049	.040	.038

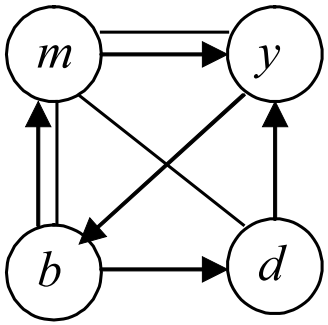
[1] Corander and Villani (2004). Statistica Neerlandica.

Graphical models for multivariate time series[2]

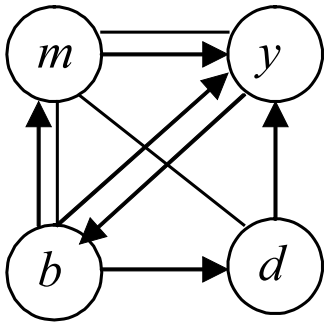
- **Graphical models** for multivariate time series.
- Zero-restrictions on the effect from time series i on time series j, for all lags. (**Granger Causality**).
- Zero-restrictions on inverse covariance matrix of the errors. Contemporaneous conditional independence.



$p(G|\mathbf{X}) = 0.0033$



$p(G|\mathbf{X}) = 0.0028$



$p(G|\mathbf{X}) = 0.0025$

[2] Corander and Villani (2004). Journal of Time Series Analysis.

Properties of Bayesian model comparison

- Coherence of pair-wise comparisons

$$B_{12} = B_{13} \cdot B_{32}$$

- **Consistency** when true model is in $\mathcal{M} = \{M_1, ..., M_K\}$

$$\Pr(M = M_{TRUE}|\mathbf{y}) \to 1 \quad \text{as} \quad n \to \infty$$

- "KL-consistency" when $M_{TRUE} \notin \mathcal{M}$

$$\Pr(M = M^*|\mathbf{y}) \to 1 \quad \text{as} \quad n \to \infty,$$

  M^* minimizes **KL divergence** between $p_M(\mathbf{y})$ and $p_{TRUE}(\mathbf{y})$.

- Smaller models always win when priors are very vague.

- **Improper priors** cannot be used for model comparison. 

$\Pr(M_k|y)$ can be overfident - macroeconomics[3]

Table: Posterior model probabilities - Smets-Wouters DSGE model

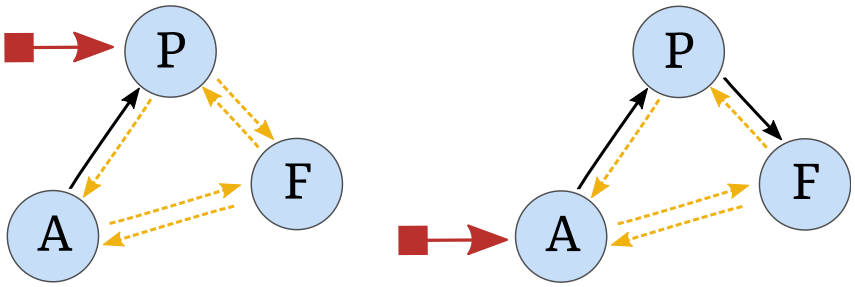
Base	M1	M2	M3	M4	M5	M6	M7	M8
0.01	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00

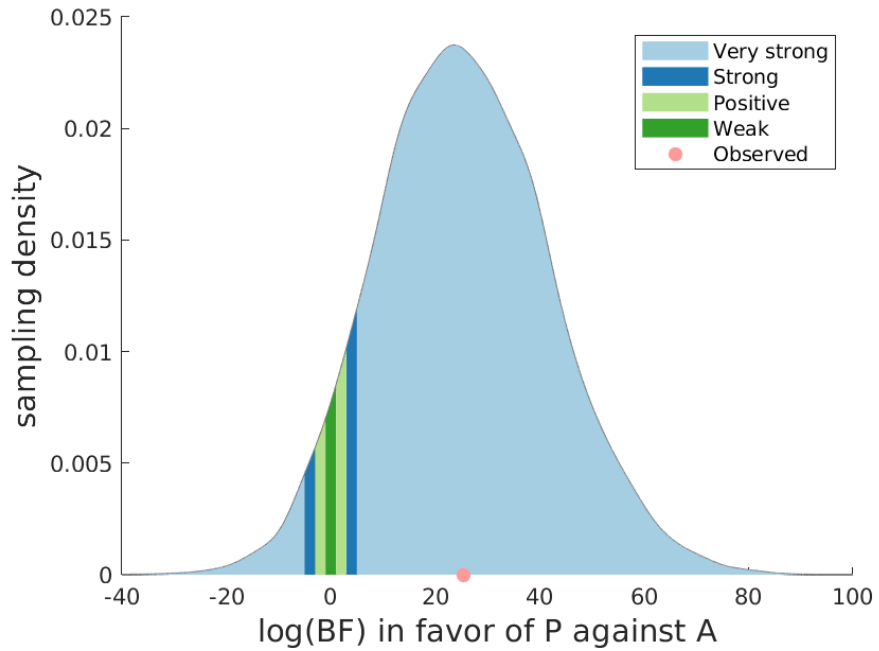
[3]Oelrich et al (2020). When are Bayesian model probabilities overconfident?

$\Pr(M_k|y)$ can be overfident - neuroscience[4]

Table: Posterior model probabilities - Dynamic Causal Models

A	F	P	AF	PA	PF	PAF
0.00	0.00	1.00	0.00	0.00	0.00	0.00





[4]Oelrich et al (2020). When are Bayesian model probabilities overconfident?

Marginal likelihood measures out-of-sample predictive performance

- The **marginal likelihood** can be **decomposed** as

$$p(y_1, ..., y_n) = p(y_1)p(y_2|y_1) \cdots p(y_n|y_1, y_2, ..., y_{n-1})$$

- Assume that y_i is independent of $y_1, ..., y_{i-1}$ conditional on θ:

$$p(y_i|y_1, ..., y_{i-1}) = \int p(y_i|\theta)p(\theta|y_1, ..., y_{i-1})d\theta$$

- **Prediction of y_1** is based on the prior of θ. Sensitive to prior.
- **Prediction of y_n** uses almost all the data to infer θ. Not sensitive to prior when n is not small.

Normal example

- **Model**: $y_1, ..., y_n|\theta \sim N(\theta, \sigma^2)$ with σ^2 known.
- **Prior**: $\theta \sim N(0, \kappa^2\sigma^2)$.
- **Intermediate posterior** at time $i-1$

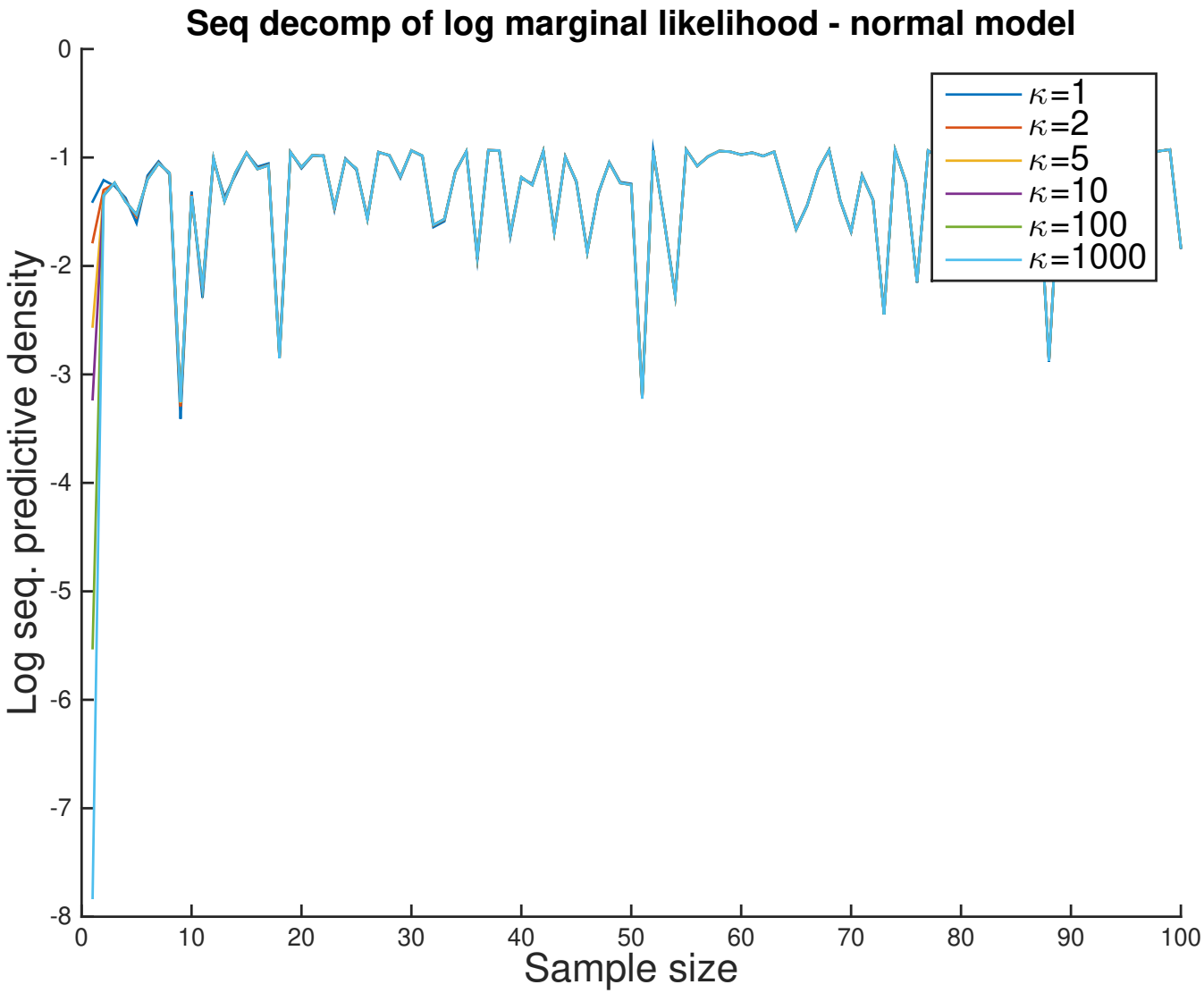
$$\theta|y_1, ..., y_{i-1} \sim N\left[w_i(\kappa) \cdot \bar{y}_{i-1}, \frac{\sigma^2}{i-1+\kappa^{-2}}\right]$$

  where $w_i(\kappa) = \frac{i-1}{i-1+\kappa^{-2}}$.
- **Intermediate predictive density** at time $i-1$

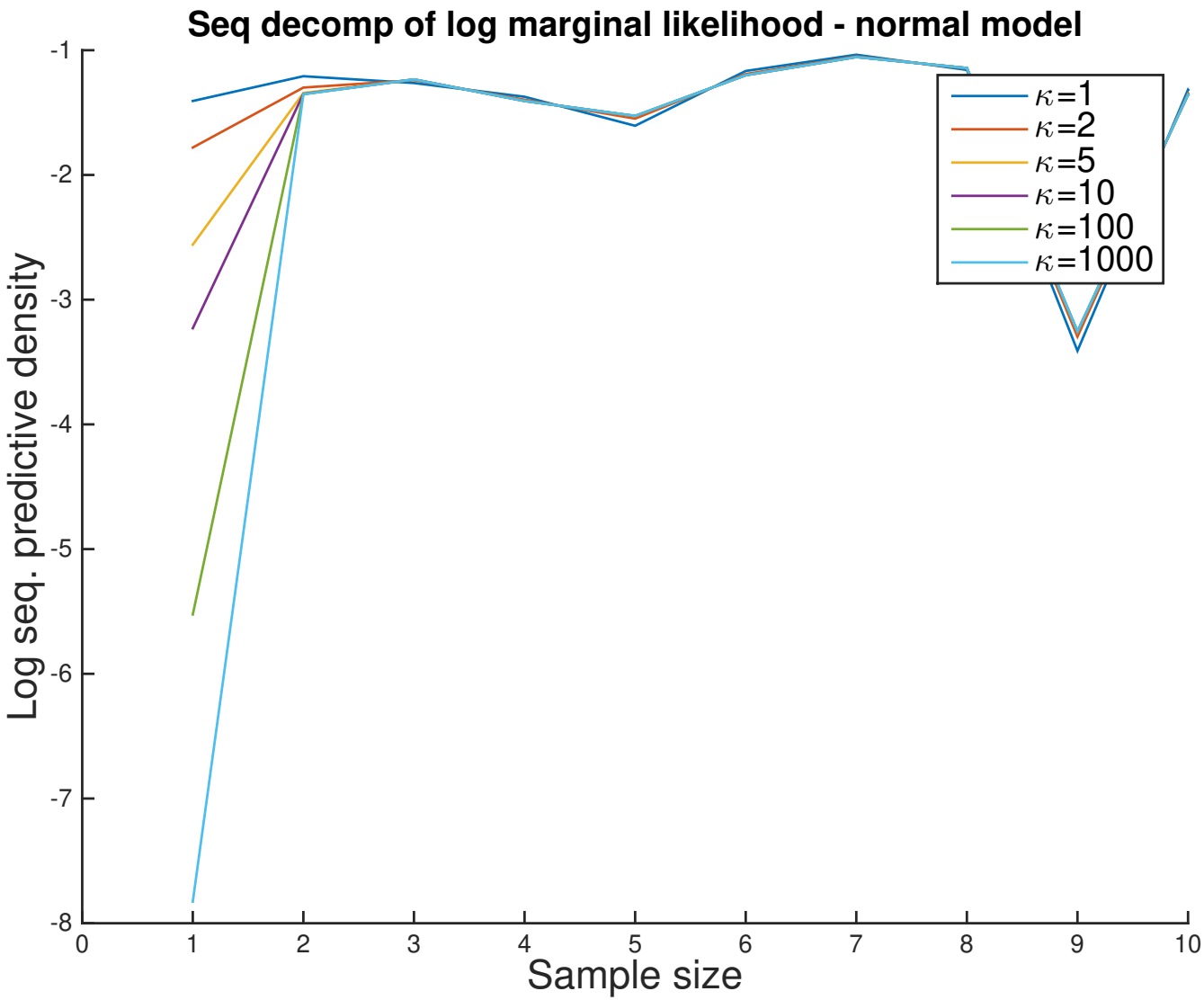
$$y_i|y_1, ..., y_{i-1} \sim N\left[w_i(\kappa) \cdot \bar{y}_{i-1}, \sigma^2\left(1 + \frac{1}{i-1+\kappa^{-2}}\right)\right]$$

- For $i = 1$, $y_1 \sim N\left[0, \sigma^2\left(1 + \frac{1}{\kappa^{-2}}\right)\right]$ can be very sensitive to κ.
- For large i: $y_i|y_1, ..., y_{i-1} \overset{approx}{\sim} N\left(\bar{y}_{i-1}, \sigma^2\right)$, not sensitive to κ.

First observation is sensitive to κ



First observation is sensitive to κ - zoomed



Log Predictive Score - LPS

- Reduce sensitivity to the prior: sacrifice n^* observations to train the prior into a posterior.
- **Predictive (Density) Score (PS)**. Decompose $p(y_1, ..., y_n)$ as

$$\underbrace{p(y_1)p(y_2|y_1)\cdots p(y_{n^*}|y_{1:(n^*-1)})}_{\textit{training}} \underbrace{p(y_{n^*+1}|y_{1:n^*})\cdots p(y_n|y_{1:(n-1)})}_{\textit{test}}$$

- Usually report on log scale: **Log Predictive Score (LPS)**.
- Time-series: obvious which data are used for training.
- Cross-sectional data: training-test split by **cross-validation**:

Fold 1	Fold 2	Fold 3	Fold 4	**Fold 5**
Fold 1	Fold 2	Fold 3	**Fold 4**	Fold 5
Fold 1	Fold 2	**Fold 3**	Fold 4	Fold 5
Fold 1	**Fold 2**	Fold 3	Fold 4	Fold 5
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

And hey! ... let's be careful out there

- Be especially **careful** with Bayesian model comparison when
  - The **compared models** are
    - very different in structure
    - severly misspecified
    - very complicated (black boxes).
  - The **priors** for the parameters in the models are
    - not carefully elicited
    - only weakly informative
    - not matched across models.
  - The **data**
    - has outliers (in all models)
    - has a multivariate response.

Bayesian Learning

Lecture 11 - Computations. Variable selection.

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Overview

- Computing the marginal likelihood
- Bayesian variable selection
- Model averaging

Marginal likelihood in conjugate models

- **Marginal likelihood**: $\int p(\mathbf{y}|\theta)p(\theta)d\theta$. Integration!
- Short cut for **conjugate models**:

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

- Bernoulli model example

$$p(\theta) = \frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$
$$p(y|\theta) = \theta^{s}(1-\theta)^{f}$$
$$p(\theta|y) = \frac{1}{B(\alpha+s,\beta+f)}\theta^{\alpha+s-1}(1-\theta)^{\beta+f-1}$$

- Marginal likelihood

$$p(y) = \frac{\theta^{s}(1-\theta)^{f}\frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\frac{1}{B(\alpha+s,\beta+f)}\theta^{\alpha+s-1}(1-\theta)^{\beta+f-1}} = \frac{B(\alpha+s,\beta+f)}{B(\alpha,\beta)}$$

Computing the marginal likelihood

- Usually difficult to evaluate the integral

$$p(\mathbf{y}) = \int p(\mathbf{y}|\theta)p(\theta)d\theta = E_{p(\theta)}[p(\mathbf{y}|\theta)].$$

- **Monte Carlo estimate**. Draw from the prior $\theta^{(1)}, ..., \theta^{(N)}$ and

$$\hat{p}(\mathbf{y}) = \frac{1}{N}\sum_{i=1}^{N} p(\mathbf{y}|\theta^{(i)}).$$

  Unstable when posterior is different from prior.
- **Importance sampling**. Let $\theta^{(1)}, ..., \theta^{(N)}$ be draws from $g(\theta)$.

$$\int p(\mathbf{y}|\theta)p(\theta)d\theta = \int \frac{p(\mathbf{y}|\theta)p(\theta)}{g(\theta)}g(\theta)d\theta \approx N^{-1}\sum_{i=1}^{N} \frac{p(\mathbf{y}|\theta^{(i)})p(\theta^{(i)})}{g(\theta^{(i)})}$$

- **Modified Harmonic mean**: $g(\theta) = N(\tilde{\theta}, \tilde{\Sigma}) \cdot I_c(\theta)$, where $\tilde{\theta}$ and $\tilde{\Sigma}$ is the posterior mean and covariance matrix estimated from MCMC, and $I_c(\theta) = 1$ if $(\theta - \tilde{\theta})'\tilde{\Sigma}^{-1}(\theta - \tilde{\theta}) \leq c$.

Computing the marginal likelihood, cont.

- To use $p(\mathbf{y}) = p(\mathbf{y}|\theta)p(\theta)/p(\theta|\mathbf{y})$ we need $p(\theta|\mathbf{y})$.
- But we only need to know $p(\theta|\mathbf{y})$ in a single point θ_0.
- **Kernel density estimator** to approximate $p(\theta_0|\mathbf{y})$. Unstable.
- **Chib's method** (1995, JASA). Great, but only **Gibbs sampling**.
- **Chib-Jeliazkov** (2001, JASA) generalizes to **MH algorithm** (good for IndepMH, terrible for RWM).
- **Reversible Jump MCMC** (RJMCMC) for model inference.
  - MCMC methods that moves in model space.
  - Proportion of iterations spent in model k estimates $\Pr(M_k|\mathbf{y})$.
  - Usually hard to find efficient proposals. Sloooow convergence.
- **Bayesian nonparametrics** (e.g. Dirichlet process priors).

Laplace approximation

- Taylor approximation of the log likelihood

$$\ln p(\mathbf{y}|\theta) \approx \ln p(\mathbf{y}|\hat{\theta}) - \frac{1}{2} J_{\hat{\theta},\mathbf{y}} (\theta - \hat{\theta})^2,$$

so

$$\begin{aligned} p(\mathbf{y}|\theta)p(\theta) &\approx p(\mathbf{y}|\hat{\theta}) \exp\left[-\frac{1}{2} J_{\hat{\theta},\mathbf{y}} (\theta - \hat{\theta})^2\right] p(\hat{\theta}) \\ &= p(\mathbf{y}|\hat{\theta}) p(\hat{\theta}) (2\pi)^{p/2} \left|J_{\hat{\theta},\mathbf{y}}^{-1}\right|^{1/2} \\ &= \underbrace{\times (2\pi)^{-p/2} \left|J_{\hat{\theta},\mathbf{y}}^{-1}\right|^{-1/2} \exp\left[-\frac{1}{2} J_{\hat{\theta},\mathbf{y}} (\theta - \hat{\theta})^2\right]}_{\text{multivariate normal density}} \end{aligned}$$

- **The Laplace approximation**:

$$\ln \hat{p}(\mathbf{y}) = \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) + \frac{1}{2} \ln \left|J_{\hat{\theta},\mathbf{y}}^{-1}\right| + \frac{p}{2} \ln(2\pi),$$

where p is the number of unrestricted parameters.

BIC

- **The Laplace approximation**:

$$\ln \hat{p}(\mathbf{y}) = \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) + \frac{1}{2} \ln \left| J^{-1}_{\hat{\theta},\mathbf{y}} \right| + \frac{p}{2} \ln(2\pi).$$

- $\hat{\theta}$ and $J_{\hat{\theta},\mathbf{y}}$ can be obtained with **optimization**/**autodiff**.

- The **BIC approximation** assumes that $J_{\hat{\theta},\mathbf{y}}$ behaves like $n \cdot I_p$ in large samples and the small term $\frac{p}{2} \ln(2\pi)$ is ignored

$$\ln \hat{p}(\mathbf{y}) = \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) - \frac{p}{2} \ln n.$$

Bayesian variable selection

- Linear regression:

$$y = \beta_0 + \beta_1 x_1 + ... + \beta_p x_p + \varepsilon.$$

- Which variables have **non-zero** coefficient?

$$\begin{aligned} H_0 &: \beta_0 = \beta_1 = ... = \beta_p = 0 \\ H_1 &: \beta_1 = 0 \\ H_2 &: \beta_1 = \beta_2 = 0 \end{aligned}$$

- Introduce variable selection indicators $\mathcal{I} = (I_1, ..., I_p)$.
- Example: $\mathcal{I} = (1, 1, 0)$ means that $\beta_1 \neq 0$ and $\beta_2 \neq 0$, but $\beta_3 = 0$, so x_3 drops out of the model.

Bayesian variable selection

- Model inference, just crank the Bayesian machine:

$$p(\mathcal{I}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathcal{I}) \cdot p(\mathcal{I})$$

- The prior $p(\mathcal{I})$ is typically taken to be

$$I_1, ..., I_p|\theta \overset{iid}{\sim} Bernoulli(\theta)$$

- θ is the **prior inclusion probability**.
- Challenge: Computing the **marginal likelihood** for each model $(\mathcal{I})$

$$p(\mathbf{y}|\mathbf{X}, \mathcal{I}) = \int p(\mathbf{y}|\mathbf{X}, \mathcal{I}, \beta) p(\beta|\mathbf{X}, \mathcal{I}) d\beta$$

Bayesian variable selection

- Let $\beta_{\mathcal{I}}$ denote the **non-zero** coefficients under $\mathcal{I}$.
- Prior:

$$\beta_{\mathcal{I}}|\sigma^2 \sim N\left(0, \sigma^2 \Omega_{\mathcal{I},0}^{-1}\right)$$
$$\sigma^2 \sim Inv - \chi^2\left(\nu_0, \sigma_0^2\right)$$

- **Marginal likelihood**

$$p(\mathbf{y}|\mathbf{X}, \mathcal{I}) \propto \left|\mathbf{X}_{\mathcal{I}}'\mathbf{X}_{\mathcal{I}} + \Omega_{\mathcal{I},0}^{-1}\right|^{-1/2} \left|\Omega_{\mathcal{I},0}\right|^{1/2} \left(\nu_0\sigma_0^2 + RSS_{\mathcal{I}}\right)^{-(\nu_0+n-1)/2}$$

where $\mathbf{X}_{\mathcal{I}}$ is the covariate matrix for the subset selected by $\mathcal{I}$.

- $RSS_{\mathcal{I}}$ is (almost) the residual sum of squares for model with $\mathcal{I}$

$$RSS_{\mathcal{I}} = \mathbf{y}'\mathbf{y} - \mathbf{y}'\mathbf{X}_{\mathcal{I}}\left(\mathbf{X}_{\mathcal{I}}'\mathbf{X}_{\mathcal{I}} + \Omega_{\mathcal{I},0}\right)^{-1}\mathbf{X}_{\mathcal{I}}'\mathbf{y}$$

Bayesian variable selection via Gibbs sampling

- But there are 2^p model combinations to go through! *Ouch*!
- ... but most have essentially zero posterior probability. *Phew*!
- **Simulate** from the joint posterior distribution:

$$p(\beta, \sigma^2, \mathcal{I}|\mathbf{y},\mathbf{X}) = p(\beta, \sigma^2|\mathcal{I}, \mathbf{y},\mathbf{X})p(\mathcal{I}|\mathbf{y}, \mathbf{X}).$$

- Simulate from $p(\mathcal{I}|\mathbf{y}, \mathbf{X})$ using **Gibbs sampling**:
  - Draw $I_1|\mathcal{I}_{-1}, \mathbf{y}, \mathbf{X}$
  - Draw $I_2|\mathcal{I}_{-2}, \mathbf{y}, \mathbf{X}$
  - ...
  - Draw $I_p|\mathcal{I}_{-p}, \mathbf{y}, \mathbf{X}$
- Note that: $Pr(I_i = 0|\mathcal{I}_{-i}, \mathbf{y}, \mathbf{X}) \propto Pr(I_i = 0, \mathcal{I}_{-i}|\mathbf{y}, \mathbf{X})$.
- Compute $p(\mathcal{I}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathcal{I}) \cdot p(\mathcal{I})$ for $I_i = 0$ and for $I_i = 1$.
- **Model averaging** in a single simulation run.
- If needed, simulate from $p(\beta, \sigma^2|\mathcal{I}, \mathbf{y},\mathbf{X})$ for each draw of $\mathcal{I}$.

Simple general Bayesian variable selection

- The previous algorithm only works when we can compute

$$p(\mathcal{I}|\mathbf{y},\mathbf{X}) = \int p(\beta,\sigma^2,\mathcal{I}|\mathbf{y},\mathbf{X})d\beta d\sigma$$

- MH - **propose** β and $\mathcal{I}$ jointly from the proposal distribution

$$q(\beta_p|\beta_c,\mathcal{I}_p)q(\mathcal{I}_p|\mathcal{I}_c)$$

- Main difficulty: how to propose the non-zero elements in β_p?
- Simple approach:
  - Approximate posterior with **all** variables in the model:

$$\beta|\mathbf{y},\mathbf{X} \overset{approx}{\sim} N\left[\hat{\beta}, J_{\mathbf{y}}^{-1}(\hat{\beta})\right]$$

  - Propose β_p from $N\left[\hat{\beta}, J_{\mathbf{y}}^{-1}(\hat{\beta})\right]$, conditional on the zero restrictions implied by $\mathcal{I}_p$. Formulas are available.

Variable selection in more complex models

Posterior summary of the one-component split-t model.[a]

Parameters	Mean	Stdev	Post.Incl.
Location μ			
Const	0.084	0.019	–
Scale ϕ			
Const	0.402	0.035	–
LastDay	−0.190	0.120	0.036
LastWeek	**−0.738**	**0.193**	**0.985**
LastMonth	**−0.444**	**0.086**	**0.999**
CloseAbs95	0.194	0.233	0.035
CloseSqr95	0.107	0.226	0.023
MaxMin95	**1.124**	**0.086**	**1.000**
CloseAbs80	0.097	0.153	0.013
CloseSqr80	0.143	0.143	0.021
MaxMin80	−0.022	0.200	0.017
Degrees of freedom v			
Const	2.482	0.238	–
LastDay	0.504	0.997	0.112
LastWeek	**−2.158**	**0.926**	**0.638**
LastMonth	0.307	0.833	0.089
CloseAbs95	0.718	1.437	0.229
CloseSqr95	1.350	1.280	0.279
MaxMin95	1.130	1.488	0.222
CloseAbs80	0.035	1.205	0.101
CloseSqr80	0.363	1.211	0.112
MaxMin80	−1.672	1.172	0.254
Skewness λ			
Const	−0.104	0.033	–
LastDay	−0.159	0.140	0.027
LastWeek	−0.341	0.170	0.135
LastMonth	−0.076	0.112	0.016
CloseAbs95	−0.021	0.096	0.008
CloseSqr95	−0.003	0.108	0.006
MaxMin95	0.016	0.075	0.008
CloseAbs80	0.060	0.115	0.009
CloseSqr80	0.059	0.111	0.010
MaxMin80	0.093	0.096	0.013

Model averaging

- Let γ be a quantity with the same interpretation in the two models.
- Example: Prediction $\gamma = (y_{T+1}, ..., y_{T+h})'$.
- The marginal posterior distribution of γ reads

$$p(\gamma|\mathbf{y}) = p(M_1|\mathbf{y})p_1(\gamma|\mathbf{y}) + p(M_2|\mathbf{y})p_2(\gamma|\mathbf{y}),$$

  $p_k(\gamma|\mathbf{y})$ is the marginal posterior of γ conditional on M_k.

- Predictive distribution includes **three sources of uncertainty**:
  - **Future errors**/disturbances (e.g. the ε's in a regression)
  - **Parameter uncertainty** (the predictive distribution has the parameters integrated out by their posteriors)
  - **Model uncertainty** (by model averaging)

Bayesian Learning

Lecture 12 - Model evaluation.

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Overview

- Model evaluation - Posterior predictive analysis

Models - why?

- We now know how to **compare** models.
- But how do we know if any given model is 'any good'?
- George Box: '**All models are false, but some are useful**'.

What is your model for really?

- **Prediction**.
  - Interpretation not a concern
  - Black-box approach may be ok.
  - Extrapolation?
  - Model averaging may be a good idea.
- Abstraction to **aid in thinking** about a phenomena.
  - Prediction accuracy of less concern.
  - Model averaging may be a bad idea.
- Model as a **compact description of a complex phenomena**.
  - Computational cost of model evaluation may be a concern.
  - Online/real-time analysis.

Posterior predictive analysis

- If $p(y|\theta)$ is a 'good' model, then the data actually observed should not differ 'too much' from simulated data from $p(y|\theta)$.
- Bayesian: simulate data from the **posterior predictive distribution**:

$$p(y^{rep}|y) = \int p(y^{rep}|\theta)p(\theta|y)d\theta.$$

- Difficult to compare y and y^{rep} because of dimensionality.
- Solution: compare **low-dimensional statistic** $T(y, \theta)$ to $T(y^{rep}, \theta)$.
- Evaluates the full probability model consisting of both the likelihood *and* prior distribution.

Posterior predictive analysis

- **Algorithm** for simulating from the posterior predictive density $p[T(y^{rep})|y]$:

1. Draw a $\theta^{(1)}$ from the posterior $p(\theta|y)$.
2. Simulate a data-replicate $y^{(1)}$ from $p(y^{rep}|\theta^{(1)})$.
3. Compute $T(y^{(1)})$.
4. Repeat steps 1-3 a large number of times to obtain a sample from $T(y^{rep})$.

- We may now compare the observed statistic $T(y)$ with the distribution of $T(y^{rep})$.
- **Posterior predictive p-value**: $\Pr[T(y^{rep}) \geq T(y)]$
- Informal graphical analysis.

Posterior predictive analysis - Examples

- Ex. 1. Model: $y_1, ..., y_n \overset{iid}{\sim} N(\mu, \sigma^2)$. $T(y) = \max_i |y_i|$.
- Ex. 2. Assumption of no reciprocity in networks. $y_{ij}|\theta \overset{iid}{\sim} Bernoulli(\theta)$. $T(y) =$proportion of reciprocated node pairs.
- Ex. 3. ARIMA-process. $T(y)$ may be the autocorrelation function.
- Ex. 4. Poisson regression. $T(y)$ frequency distribution of the response counts. Proportions of zero counts.

Posterior predictive analysis - Normal model, max statistic