Bayesian Linear Regression

Guest lecture at KTH 2021

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Lecture overview

- Bayesian inference
- The normal model with known variance
- Linear regression
- Regularization priors
- Outlook: Bayes in complex problems

Slides at: https://mattiasvillani.com/news

Rough draft book at: https://github.com/mattiasvillani/BayesianLearningBook

Likelihood function - normal data regression

- **Normal data** with **known variance**:

$$X_1, ..., X_n|\theta \overset{iid}{\sim} \mathrm{N}(\theta, \sigma^2).$$

- **Likelihood** from independent observations: $x_1, ..., x_n$

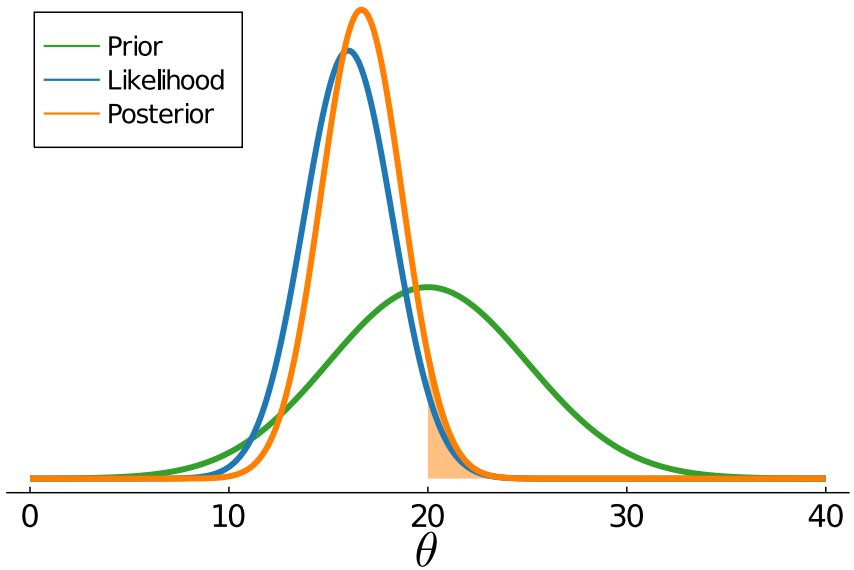
$$p(x_1, ..., x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\theta)^2\right)$$
$$\propto \exp\left(-\frac{1}{2(\sigma^2/n)}(\theta-\bar{x})^2\right)$$

- **Maximum likelihood**: $\hat{\theta} = \bar{x}$ 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.

Am I really getting my 20Mbit/sec?

- I have a 50Mbit/sec internet connection.
- ISP promises at least 20Mbit/sec on average.
- **Data**: $\mathrm{x} = (15.77, 20.5, 8.26, 14.37, 21.09)$ Mbit/sec.
- **Measurement errors**: $\sigma = 5$ ($\pm$10Mbit with 95% probability)
- The likelihood function is proportional to $\mathrm{N}(\bar{x}, \sigma^2/n)$ density.



The likelihood function

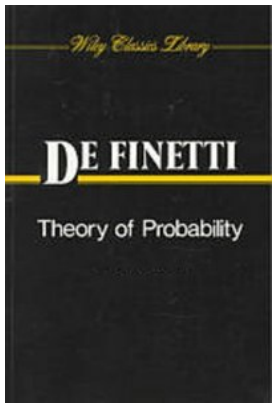
- The mantra:

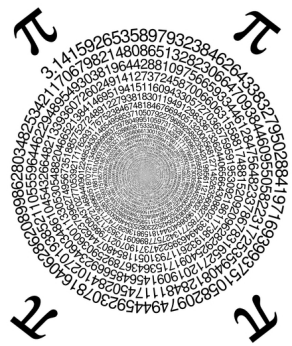
  The likelihood function is
  the probability of the observed data
  considered as a function of the parameter.

- Likelihood function is **NOT** a probability distribution for θ.
- Statements like $\Pr(\theta \geq 20|\text{data})$ makes no sense.
- Unless ...

Uncertainty and subjective probability

- $\Pr(\theta \geq 20|\text{data})$ 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.



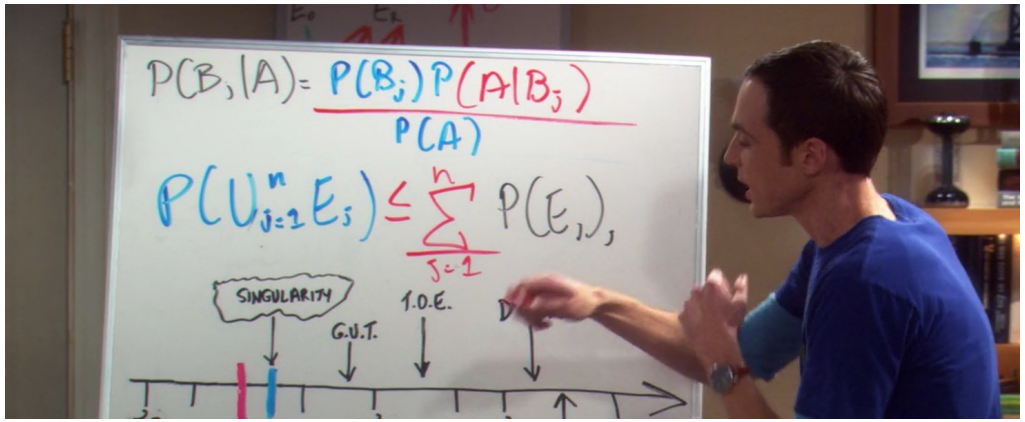


Bayesian learning

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

- **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

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

- It is the prior $p(\theta)$ that takes us from $p(\text{Data}|\theta)$ to $p(\theta|\text{Data})$.
- A probability distribution for θ is extremely useful:
  - **Predictions**
  - **Decision making**
  - **Regularization**

Great theorems make great tattoos

- Bayes theorem

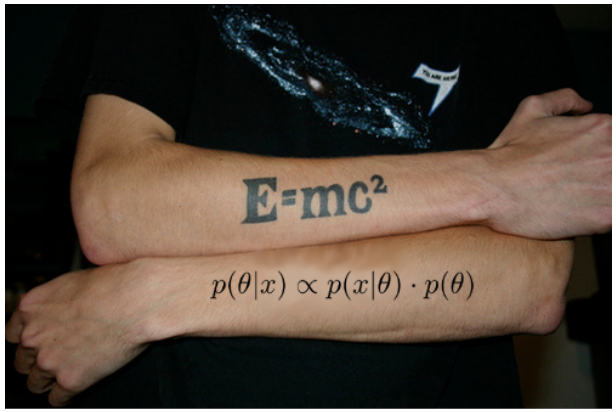
$$p(\theta|\text{Data}) = \frac{p(\text{Data}|\theta)p(\theta)}{p(\text{Data})}$$

- All you need to know:

$$p(\theta|\text{Data}) \propto p(\text{Data}|\theta)p(\theta)$$

or

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



Normal data, known variance - uniform prior

- **Model**

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

- **Prior**

$$p(\theta) \propto 1 \text{ (improper prior)}$$

- **Likelihood**

$$p(x_1, ..., x_n | \theta, \sigma^2) \propto \exp\left[-\frac{1}{2(\sigma^2/n)}(\theta - \bar{x})^2\right]$$

- **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

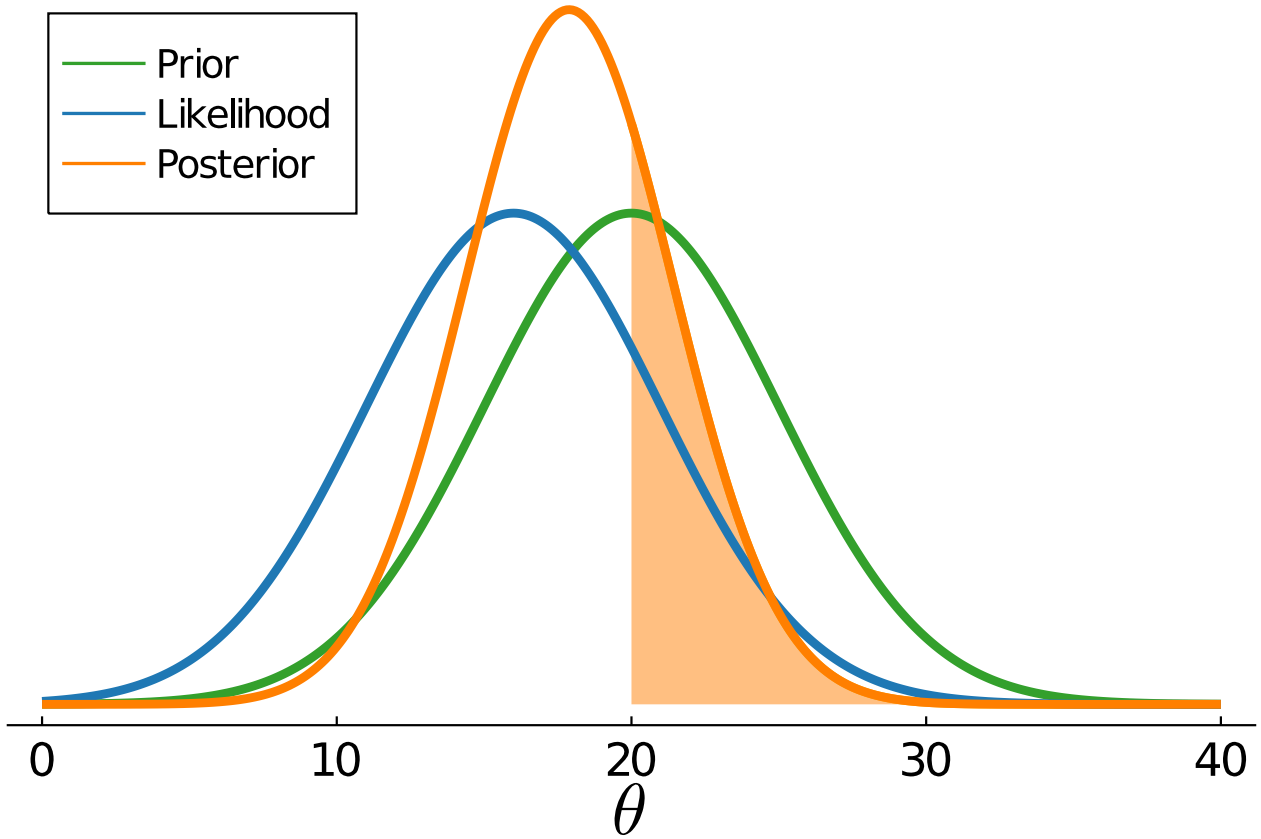
$$w = \frac{\frac{n}{\sigma^2}}{\frac{n}{\sigma^2} + \frac{1}{\tau_0^2}}.$$

- Proof: complete the squares in the exponential.

Download speed

- **Data**: $\mathrm{x} = (15.77, 20.5, 8.26, 14.37, 21.09)$ 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**: $\theta \sim N(20, 5^2)$.

Download speed n=1



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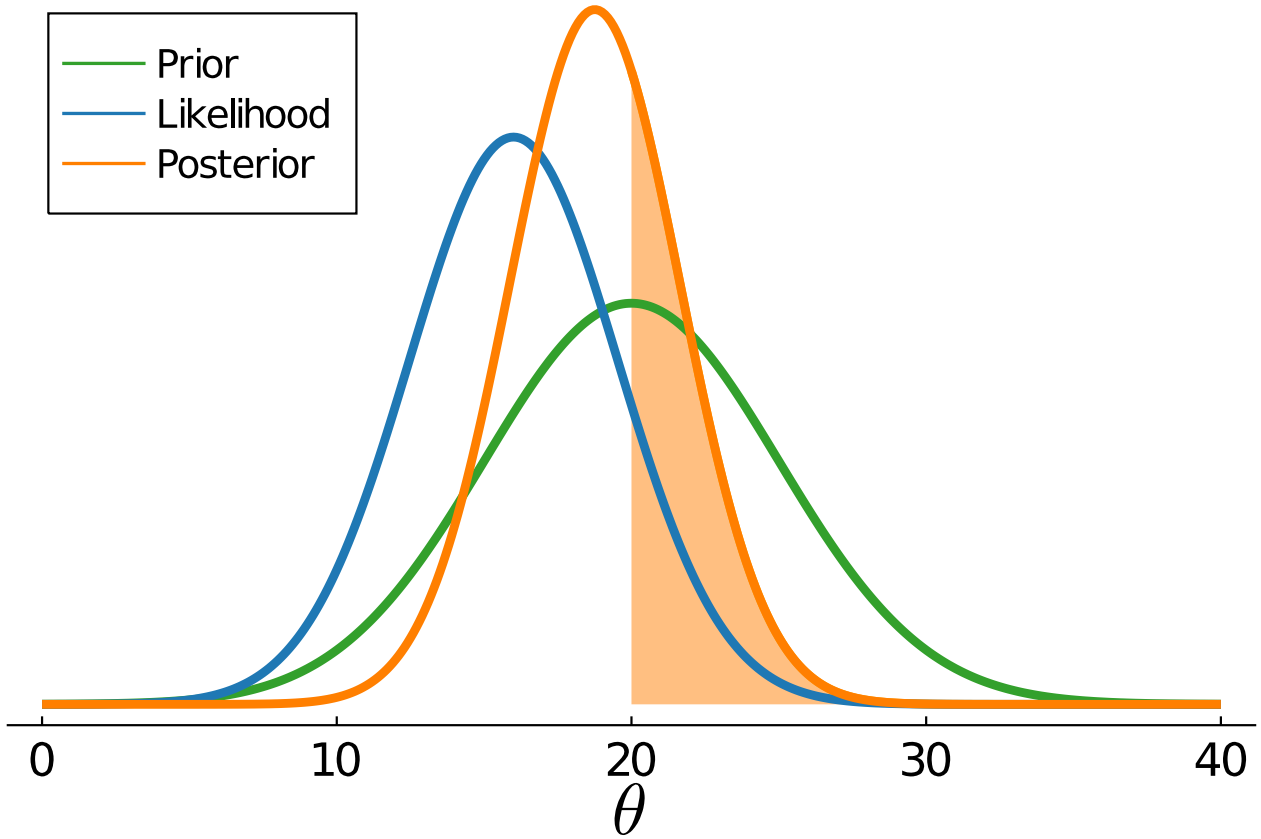

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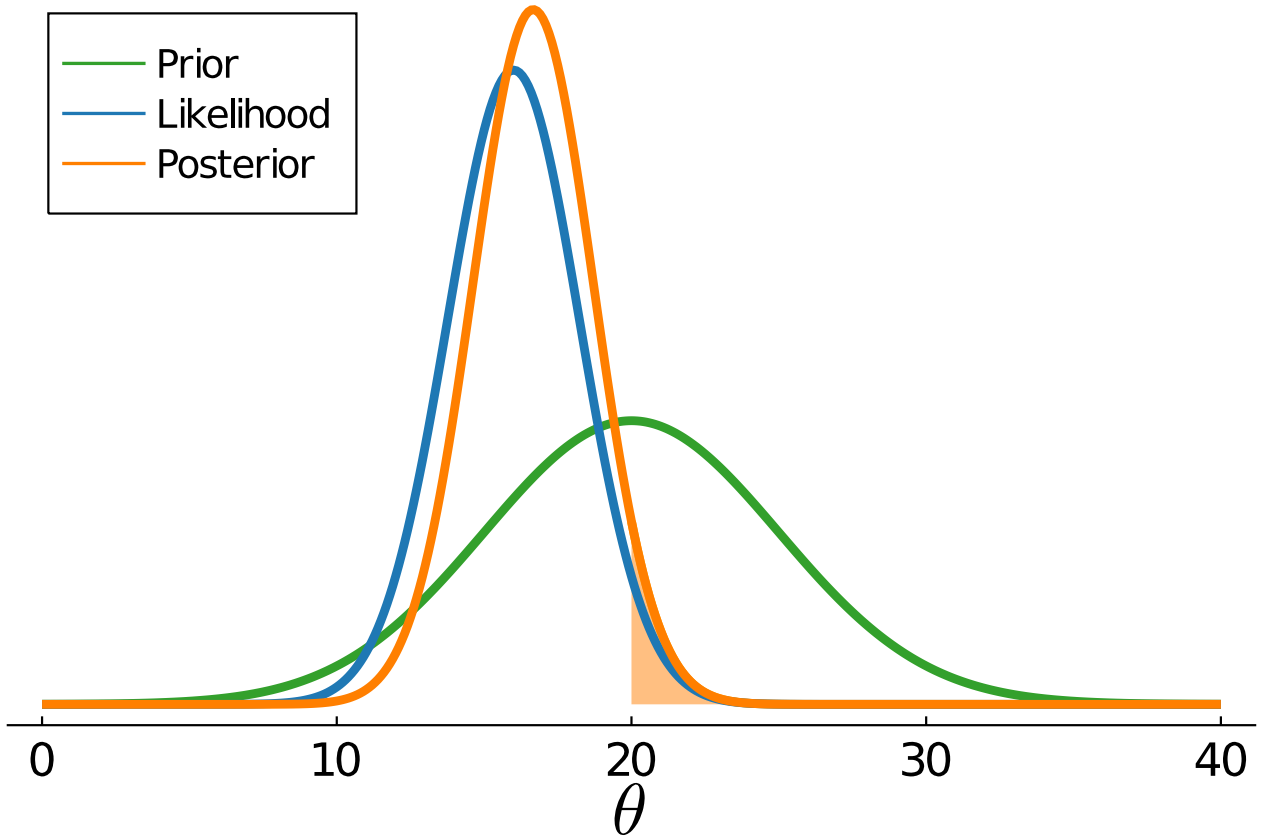
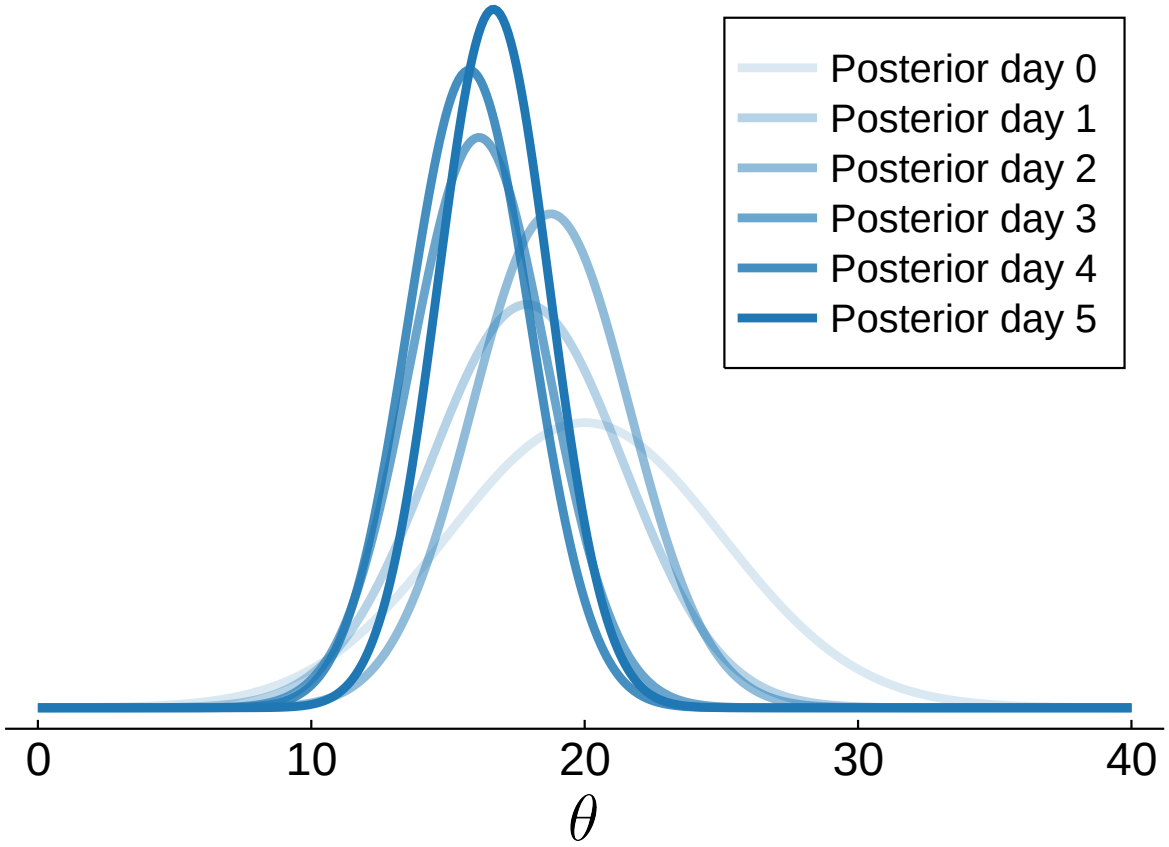


Bayesian Online learning

- Yesterday's posterior is today's prior.



Bayesian Prediction

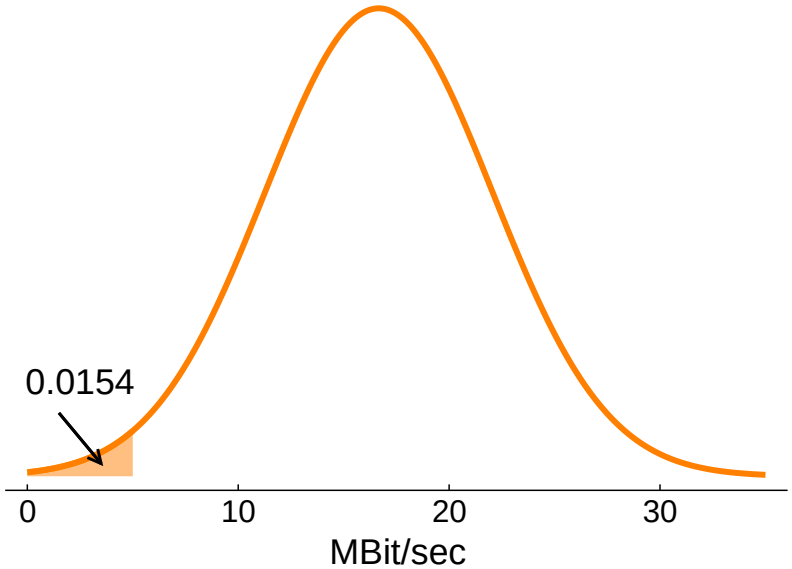
- **Predictive distribution** averages over the unknown parameter

$$\underbrace{p(x_{n+1}|x_{1:n})}_{\text{predictive dist}} = \int \underbrace{p(x_{n+1}|\theta)}_{\text{model}} \underbrace{p(\theta|x_n)}_{\text{posterior}} d\theta$$

- Normal data, normal prior:

$$x_{n+1}|x_{1:n} \sim N(\mu_n, \sigma^2 + \tau_n^2)$$

- My streaming buffers whenever $x < 5$ MBit/Sec. 



Linear regression

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

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

- First column of X is the unit vector and β_1 is the intercept.
- Normal errors: $\varepsilon_i \overset{iid}{\sim} N(0, \sigma^2)$, so $\varepsilon \sim N(0, \sigma^2 I_n)$.
- **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:

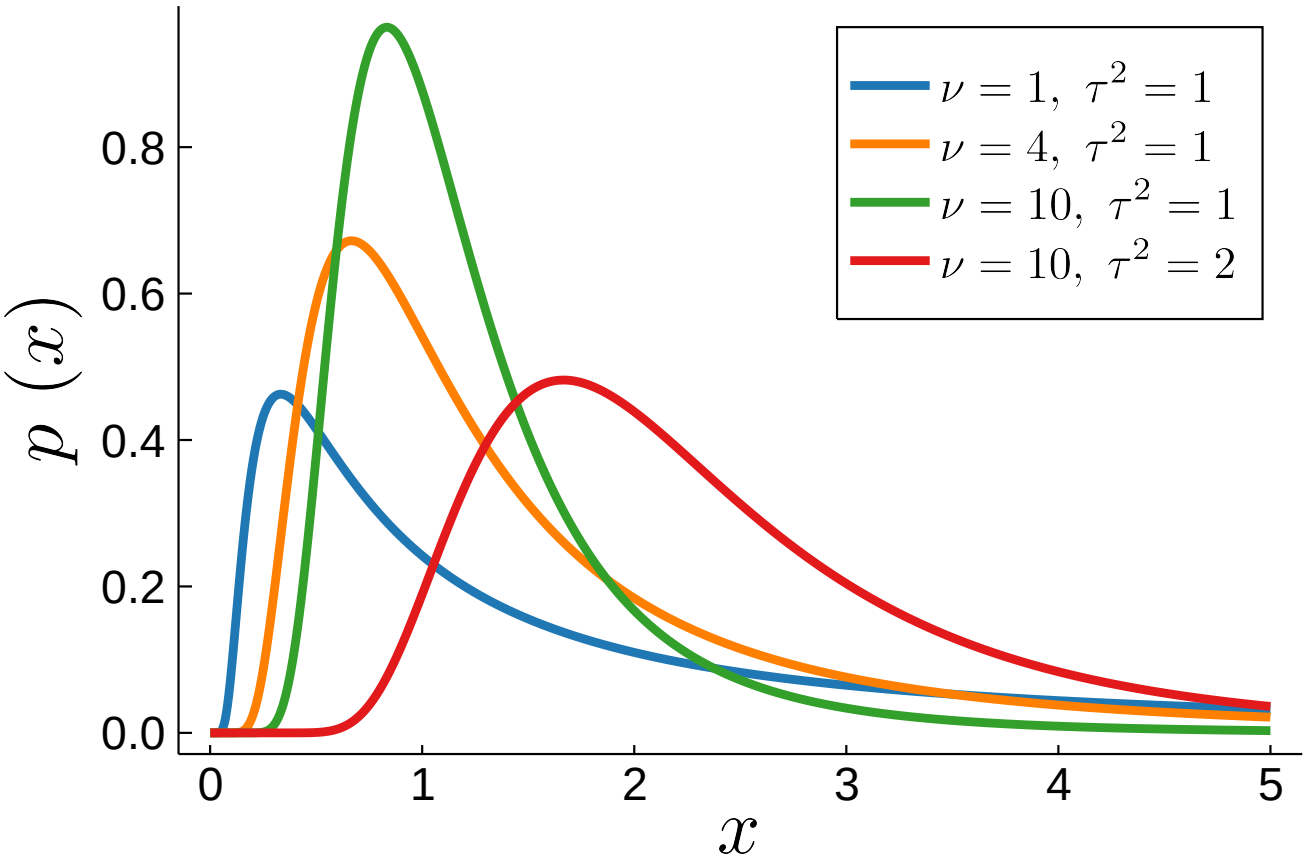
$$\begin{aligned} \beta|\sigma^2, \mathrm{y} &\sim N\left[\hat{\beta}, \sigma^2(\mathrm{X}^\top \mathrm{X})^{-1}\right] \\ \sigma^2|\mathrm{y} &\sim \text{Inv-}\chi^2(n-k, s^2) \end{aligned}$$

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

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

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

Scaled inverse χ^2 distribution



- **Inverse gamma** distribution.

Linear regression - conjugate prior

- **Joint prior** for β and σ^2

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

- **Posterior**

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

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

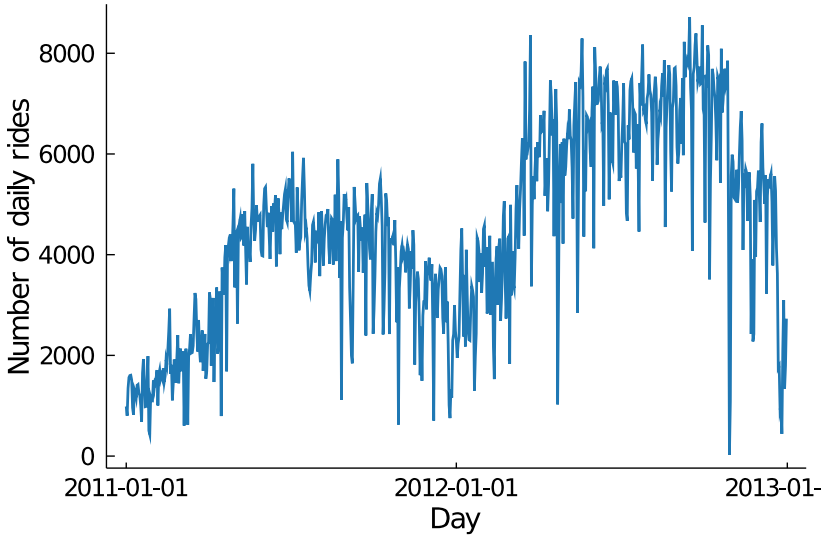
Bike share data

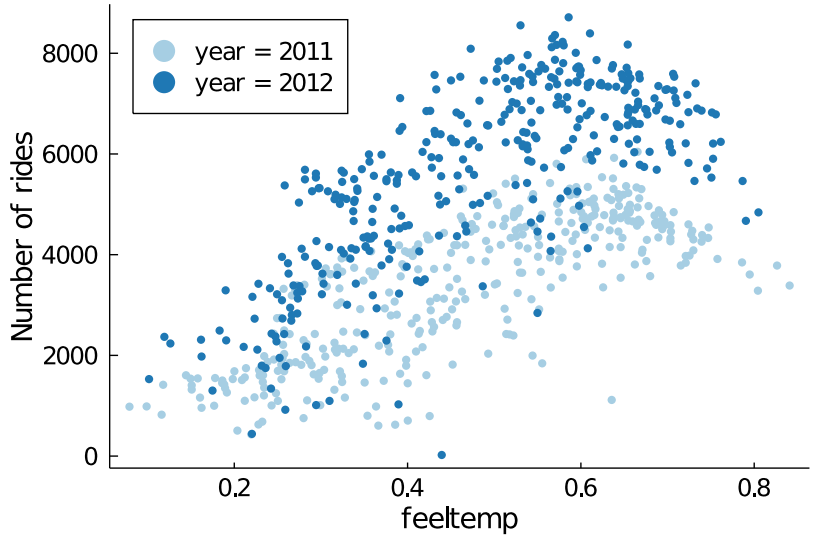
- **Bike share data**. Predict the number of bike rides.
- Response variable: number of rides on 731 days.

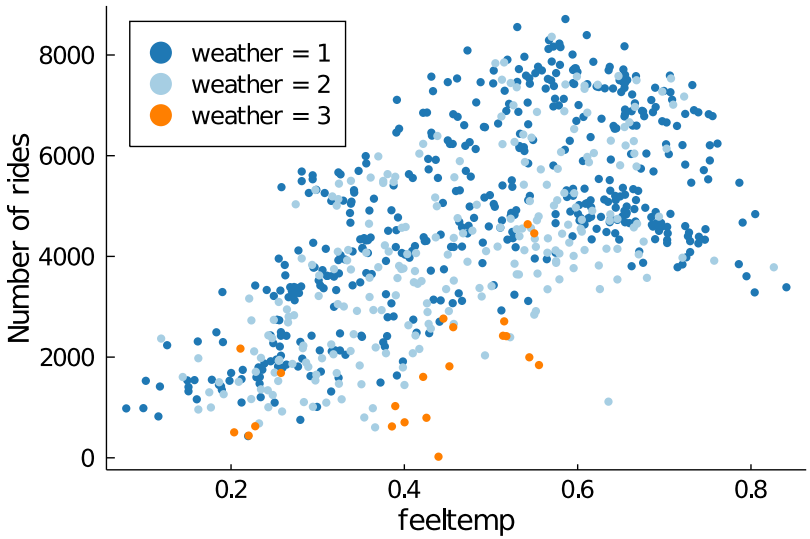
variable	description	data type	values	comment
`nrides`	number of rides	counts	$\{0, 1, ...\}$	min$=22$, max$=8714$
`feeltemp`	perceived temp	continuous	$[0, 1]$	min$=0.07$, max$=0.85$
`hum`	humidity	continuous	$[0, 1]$	min$=0.00$, max$=0.98$
`wind`	wind speed	continuous	$[0, 1]$	min$=0.02$, max$=0.51$
`year`	year	binary	$\{0, 1\}$	year 2011 $= 0$
`season`	season	categorical	$\{1, 2, 3, 4\}$	winter $\rightarrow$ fall
`weather`	weather	ordinal	$\{1, 2, 3\}$	clear $\rightarrow$ rain/snow
`weekday`	day of week	categorical	$\{0, 1, ..., 6\}$	sunday $\rightarrow$ saturday
`holiday`	holiday	binary	$\{0, 1\}$	holiday $= 1$

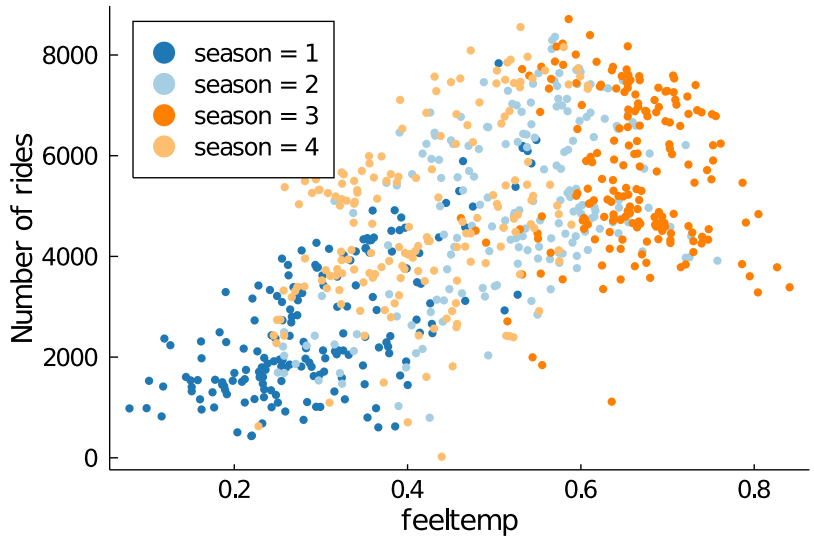
- Prior:
  - $\mu_0 = (1000, 0, \ldots, 0)^\top$
  - $\Omega_0 = \frac{1}{n} X^\top X$
  - $\sigma_0^2 = 1000^2$ and $\nu_0 = 5$.

Bike share data

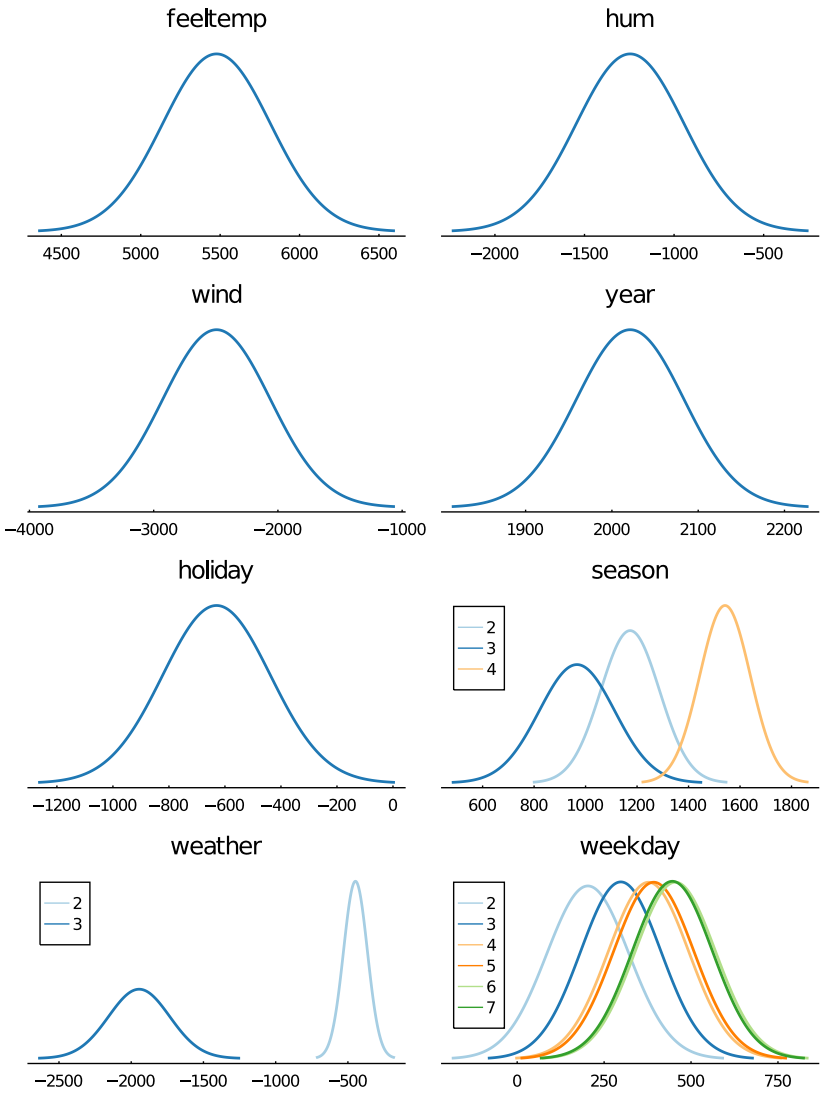




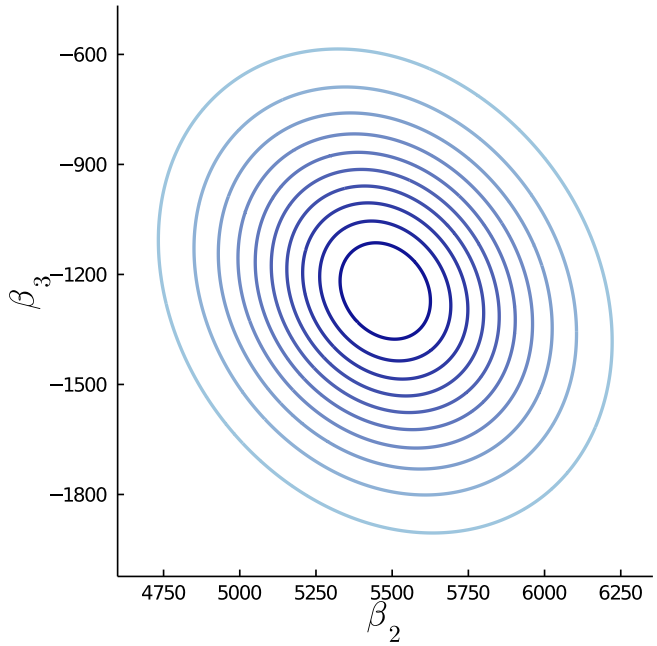


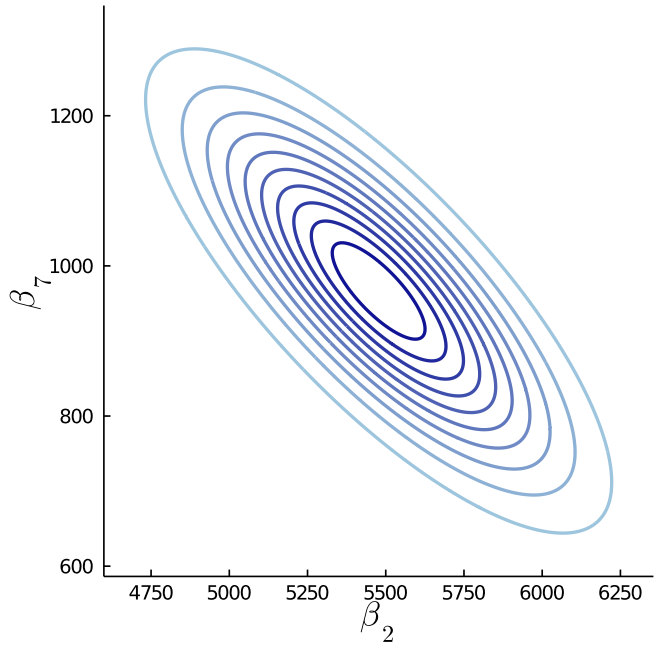


Bike share data - marginal posteriors of β



Bike share data - joint posteriors of β





Ridge regression = normal prior

- **Smoothness/shrinkage/regularization prior**

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

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

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

- Posterior mean gives **ridge regression** estimator

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

- **Shrinkage** toward zero

$$\text{As } \lambda \to \infty,\ \tilde{\beta} \to 0$$

- When $\mathrm{X}^\top\mathrm{X} = I$

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

Lasso regression = Laplace prior

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

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

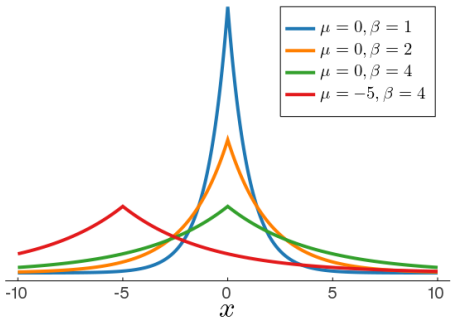
Laplace distribution

$X \sim \text{Laplace}(\mu, \beta)$ for $X \in \mathbb{R}$.

$$p(x) = \frac{1}{2\beta}\exp\left(-\frac{|x-\mu|}{\beta}\right)$$

$$\mathbb{E}(X) = \mu$$

$$\mathbb{V}(X) = 2\beta^2$$



- **Laplace prior**:
  - heavy tails
  - many β_i close to zero, but some β_i can be very large.
- **Normal prior**:
  - light tails
  - all β_i's are similar in magnitude and no β_i very large.

Estimating the shrinkage

- Cross-validation is often used to determine the degree of smoothness, λ.
- Bayesian: λ is **unknown** $\Rightarrow$ **use a prior** for λ.
- $\lambda \sim \text{Inv-}\chi^2(\eta_0, \lambda_0)$. The user specifies η_0 and λ_0.
- Hierarchical setup:

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

Regression with estimated shrinkage

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

$$\beta|\sigma^2, \lambda, \mathrm{y} \sim \mathrm{N}\left(\mu_n, \Omega_n^{-1}\right)$$

$$\sigma^2|\lambda, \mathrm{y} \sim \mathrm{Inv}{-}\chi^2\left(\nu_n, \sigma_n^2\right)$$

$$p(\lambda|\mathrm{y}) \propto \sqrt{\frac{|\Omega_0(\lambda)|}{|\mathrm{X}^T\mathrm{X} + \Omega_0(\lambda)|}} \left(\frac{\nu_n \sigma_n^2(\lambda)}{2}\right)^{-\nu_n/2} \cdot p(\lambda)$$

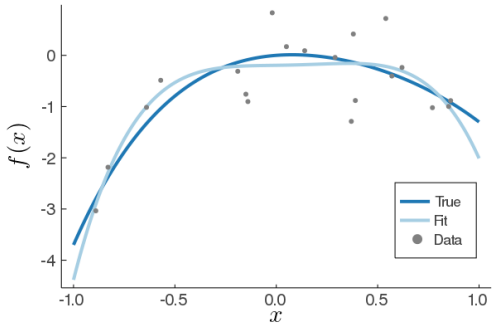
$\Omega_0(\lambda) = \lambda I_m$, and $p(\lambda)$ is the prior for λ.

Polynomial regression

- **Polynomial regression** is linear in β:

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

$$\mathrm{y} = \mathrm{X}\beta + \varepsilon, \text{ where } \mathrm{X}=(1,\mathrm{x},x^2,...,x^k).$$



- Problem: higher order polynomials can **overfit** the data.
- Solution: **shrink** higher order coefficients harder:

$$\beta|\sigma^2 \sim N\left[0, \begin{pmatrix} 100 & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda} & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{2\lambda} & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & 0 & \cdots & \frac{1}{k\lambda} \end{pmatrix}\right]$$

Finding the time for maximum

- Quadratic relationship between pain relief (y) and time (x)

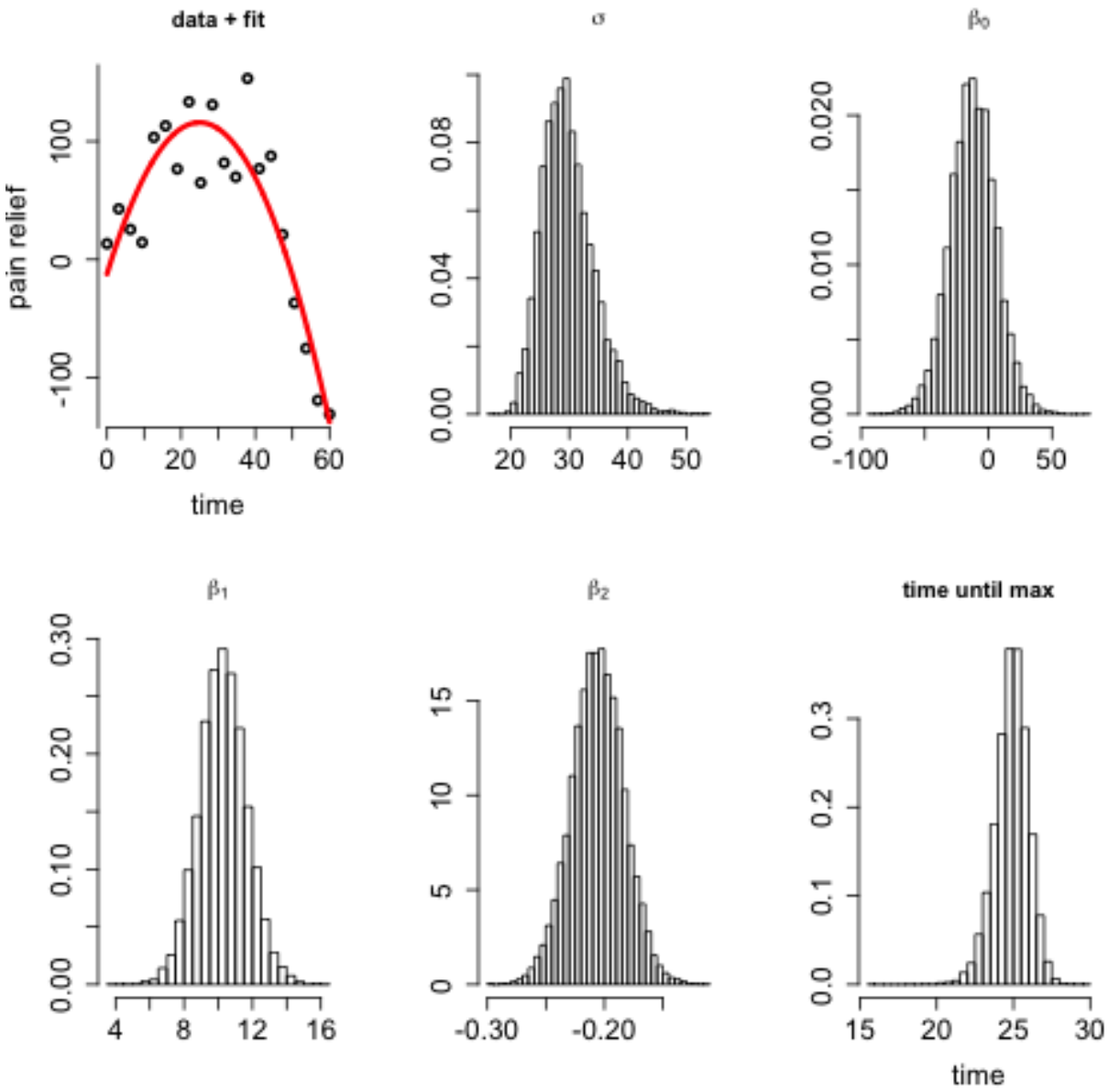
$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon.$$

- At what time $x_{\max}$ is there **maximal pain relief**?

$$x_{\max} = -\beta_1 / 2\beta_2$$

- Easy to obtain marginal posterior $p(x_{max}|\mathrm{y}, \mathrm{X})$ by **simulation**:
  - Simulate N coefficient vectors from the posterior $\beta, \sigma^2|\mathrm{y}, \mathrm{X}$
  - For each simulated β, compute $x_{\max} = -\beta_1 / 2\beta_2$.
  - Plot a histogram. Converges to $p(x_{max}|\mathrm{y}, \mathrm{X})$ as $N \to \infty$.

Finding the time for maximum



Bayes is easy to use

- Substantially more complex models can be analyzed by
  - **Markov Chain Monte Carlo** (MCMC) simulation
  - **Hamiltonian Monte Carlo** (HMC) simulation
  - **Variational inference** optimization

- **Deep Learning**. Bayes quantifies uncertainty $\Rightarrow$ Probabilistic predictions $\Rightarrow$ Decisions under uncertainty.

- Ongoing research on making Bayes more scalable to large data. My own contributions: **https://mattiasvillani.com/research**

- Probabilistic programming languages makes Bayes easy:
  - **Stan**
  - **Turing.jl**

- Bayesian Learning course at SU (March-April): **https://github.com/mattiasvillani/BayesLearnCourse**

Poisson regression in Turing.jl (Julia)

- Poisson regression:

$$y_i|\theta_i \sim \text{Pois}\left(\exp(\theta_i)\right)$$
$$\theta_i = \mathrm{x}_i^\top \boldsymbol{\beta}$$
$$\boldsymbol{\beta} \sim N(0, \tau_0^2 I)$$

```
# Bayesian poisson regression model in Turing.jl
@model poisson_reg(x, y, τ₀) = begin
    n = length(y)
    β₀ ~ Normal(0, τ₀^2)
    β₁ ~ Normal(0, τ₀^2)
    β₂ ~ Normal(0, τ₀^2)
    β₃  ~ Normal(0, τ₀^2)
    for i = 1:n
        θ = β₀ + β₁*X[i, 1] + β₂*X[i,2] + β₃*X[i,3]
        y[i] ~ Poisson(exp(θ))
    end
end

# Simulate from the posterior using HMC with NUTS tuning
sample(poisson_reg(X, y, 10), NUTS(200, 0.65), 2500)
```

- Deep Neural Net in Turing.jl: https://turing.ml/dev/tutorials/3-bayesnn/.