Winter Conference in Statistics Bayesian Machine Learning

Bayesics

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- **Bayesian inference**
- The **normal model** with known variance
- The **linear regression** model
- **Regularization priors**

Slides and code:
https://github.com/mattiasvillani/WinterConfHemavan2019

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

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

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

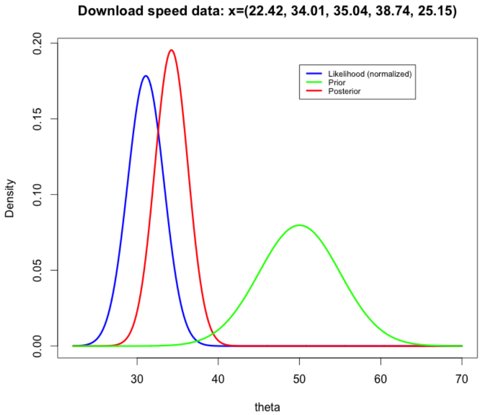
$$p(x_1, ..., x_n|\theta) \propto \exp\left(-\frac{1}{2(\sigma^2/n)}(\theta - \bar{x})^2\right)$$

- **Maximum likelihood**: $\hat{\theta} = \bar{x}$ maximizes $p(x_1, ..., x_n|\theta)$.

- **Likelihood function**: $p(x_1, ..., x_n|\theta)$ as a function of θ.

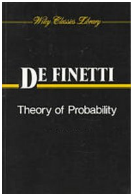
Example: Am I really getting my 50Mbit/sec?

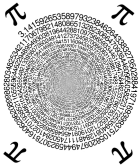
- My broadband provider promises me at least 50Mbit/sec.
- **Data**: $x = (22.42, 34.01, 35.04, 38.74, 25.15)$ Mbit/sec.
- **Measurement errors**: $\sigma = 5$ ($\pm$10Mbit with 95% probability)
- The likelihood function is proportional to $\mathrm{N}(\bar{x}, \sigma^2/n)$ density.



Uncertainty and subjective probability

- $\Pr(\theta \geq 50|\text{data})$ 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 $\Pr(\text{10th decimal of } \pi = 9) = 0.1$ makes sense.





- **Bayesian learning** about a model parameter θ:
  - **prior** knowledge as a probability distribution $p(\theta)$.
  - collect data and form the **likelihood** $p(Data|\theta)$.
  - **combine prior** and **data** information.
- **How to combine** the **data** and **prior** information?
- **Bayes' theorem**

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

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

Posterior $\propto$ Likelihood $\cdot$ 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

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

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

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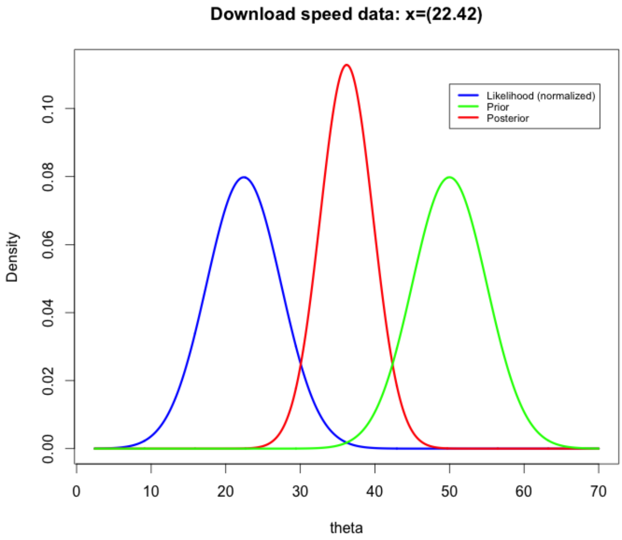

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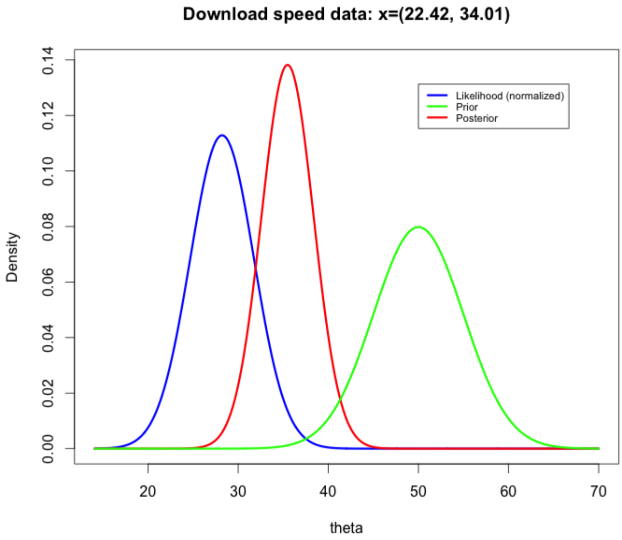

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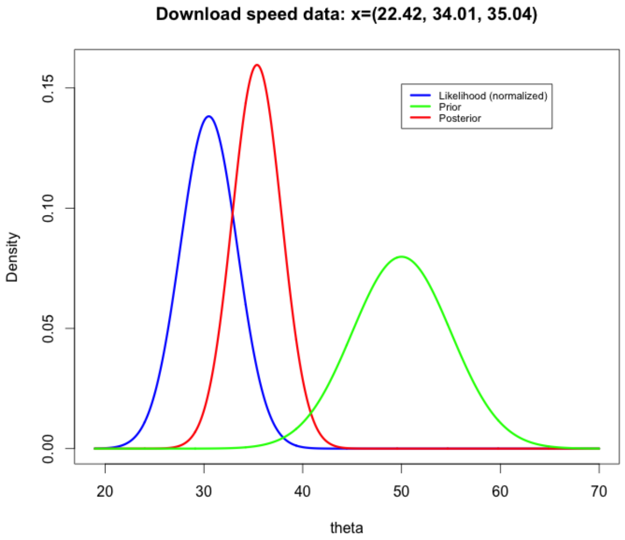

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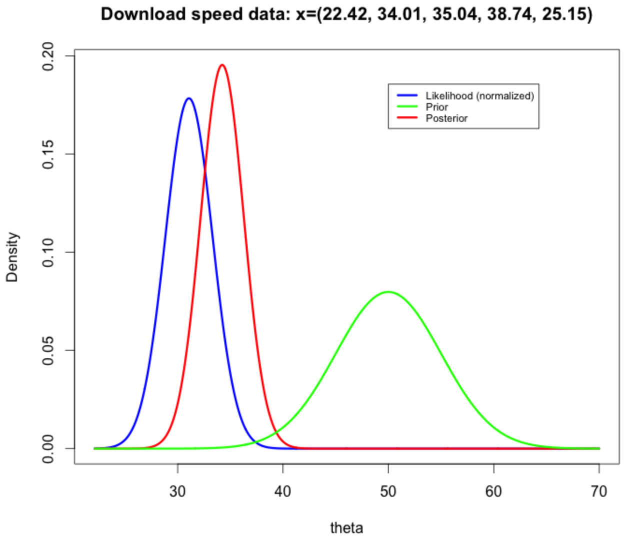


- **Prediction**

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

- **Decision making**

$$\mathrm{argmax}_{a\in\mathcal{A}}\ E_{p(\theta|\mathbf{y})}[U(a,\theta)]$$

- **Model inference**

$\Pr(M_i|\mathbf{y})$ for models M_i in a collection of models $\mathcal{M}$

- **Smoothness priors** - Use extremely flexible nonlinear models and encode smoothness via the prior.

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

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

- Usually first column of $\mathbf{X}$ 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**

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

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

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

- **Joint posterior** of β and σ^2:

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

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 :

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

- **Joint prior** for β and σ^2

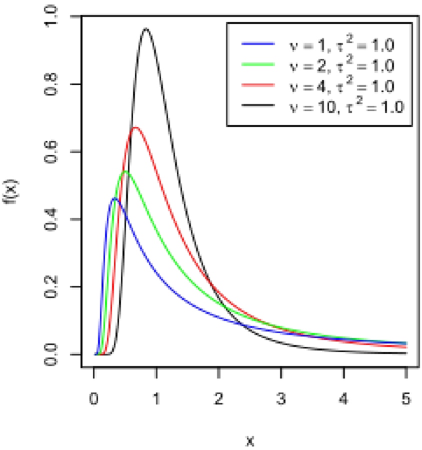
$$
\begin{aligned}
\beta|\sigma^2 &\sim N\left(\mu_0, \sigma^2\Omega_0^{-1}\right)\\
\sigma^2 &\sim Inv-\chi^2\left(\nu_0, \sigma_0^2\right)
\end{aligned}
$$

- **Posterior**

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

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

- **Scaled inverse χ^2 distribution**



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

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

- Equivalent to **penalized likelihood**:

$$-2 \cdot \log p(\beta|\sigma^2, \mathbf{y}, \mathbf{X}) \propto (y - X\beta)^T (y - X\beta) + \lambda\beta'\beta$$

- Posterior mean gives **ridge regression** estimator

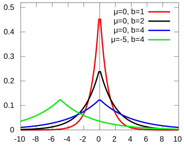
$$\tilde{\beta} = \left(\mathbf{X}'\mathbf{X} + \lambda I\right)^{-1} \mathbf{X}'\mathbf{y}$$

- When $\mathbf{X}'\mathbf{X} = I$. **Shrinkage**

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

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

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



- **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.

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

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

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

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

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

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

- **Polynomial regression**

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

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

where

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

- 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**?

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

.

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

Finding the time for maximum