Bayesian Statistics I

Lecture 5 - Regression and Regularization

Mattias Villani

Department of Statistics
Stockholm University

Department of Computer and Information Science
Linköping University

LINKÖPING UNIVERSITY

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

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

- **Posterior**

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

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

Polynomial regression

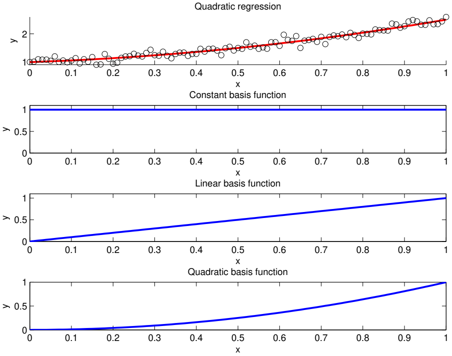
Polynomial regression

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

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

where

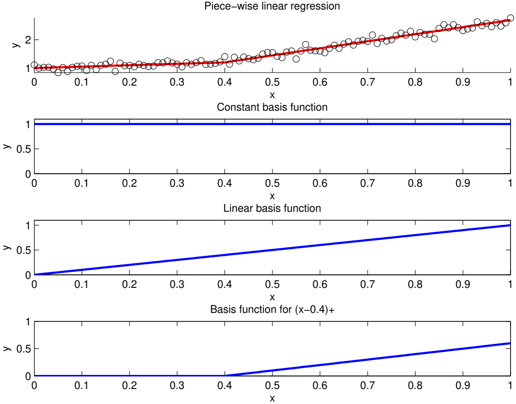
$$\mathbf{X}_P = (1, x, x^2, \ldots, x^k).$$



Spline regression

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

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



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:

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

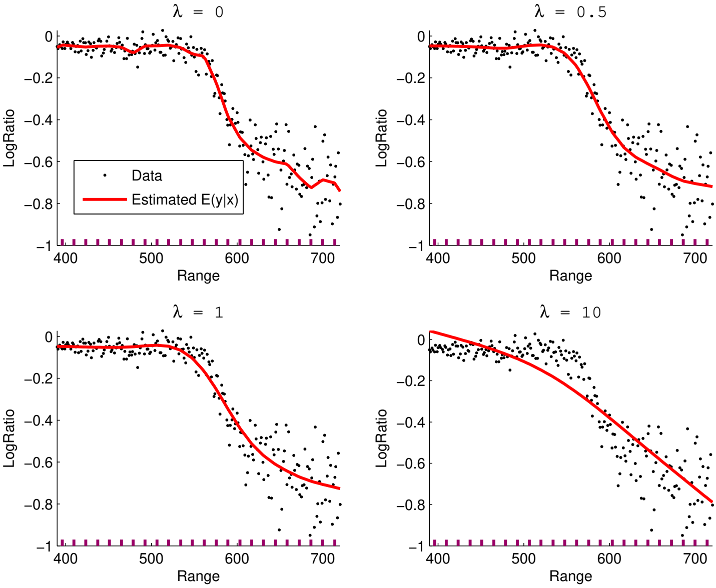
- Posterior mean/mode gives ridge regression estimator

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

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

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

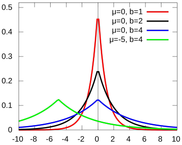
Bayesian spline with smoothness prior



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

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

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

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

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