

Bayesian Statistics I

Lecture 6 - Bayesian regularization

Mattias Villani

Department of Statistics
Stockholm University

Department of Computer and Information Science
Linköping University



mattiasvillani.com



@matvil



[mattiasvillani](https://github.com/mattiasvillani)

Lecture overview

- Non-linear regression
- Regularization priors

Polynomial regression

Polynomial regression

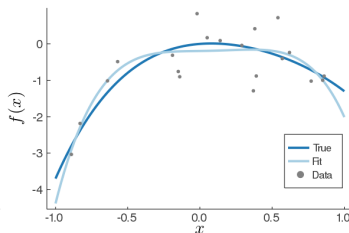
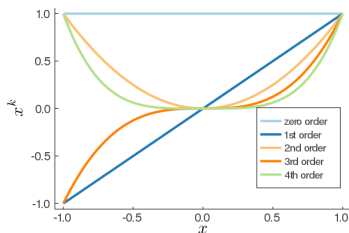
$$f(x_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \dots + \beta_k x_i^k, \quad \text{for } i = 1, \dots, n.$$

$$y = X\beta + \varepsilon,$$

where i th row of X is

$$(1, x_i, x_i^2, \dots, x_i^k).$$

- Still **linear in β** and $\hat{\beta} = (X^T X)^{-1} X^T y$. Bayes unchanged.



Spline regression

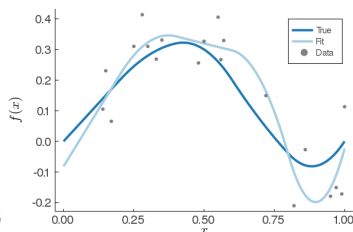
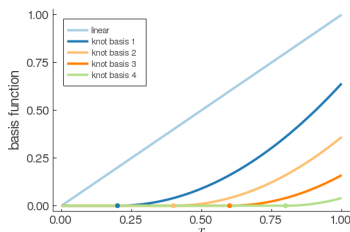
- Polynomials are too global. Need more local basis functions.
- Truncated quadratic splines** with **knot locations** $\kappa_1, \dots, \kappa_m$:

$$b_j(x) = \begin{cases} (x - \kappa_j)^2 & \text{if } x > \kappa_j \\ 0 & \text{otherwise} \end{cases}$$

$$y = X\beta + \varepsilon,$$

where i th row of X is

$$(1, x_i, b_1(x_i), \dots, b_m(x_i)).$$



Regularization prior - Ridge

- Too many knots leads to **over-fitting**.
- **Smoothness/shrinkage/regularization prior**

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

- Larger λ gives smoother fit. Note: $\mathbf{\Omega}_0 = \lambda I$ in conjugate prior.
- Equivalent to **penalized likelihood**:

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

- Posterior mean gives **ridge regression** estimator

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

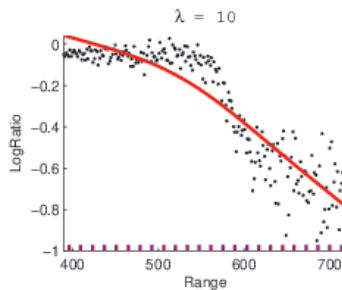
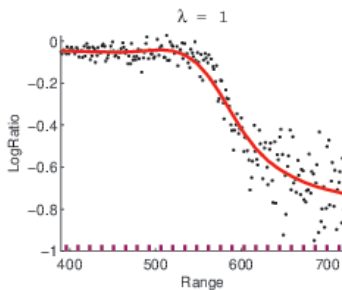
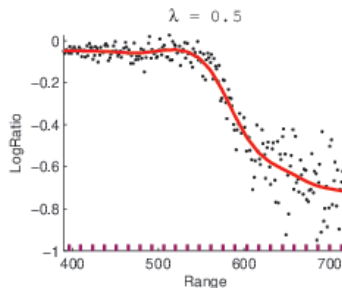
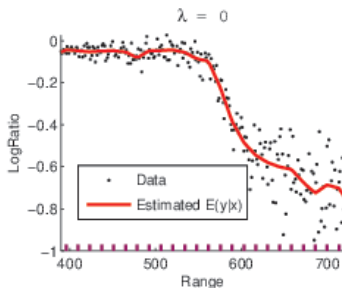
- **Shrinkage** toward zero

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

- When $X'X = I$

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

Bayesian spline with regularization prior



Regularization prior - Lasso

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

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

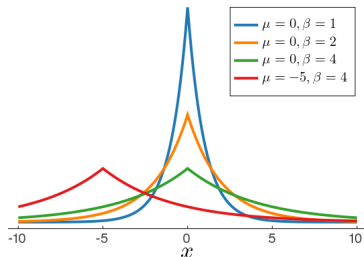
Laplace distribution

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

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

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

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



- The **Bayesian shrinkage** prior is **interpretable**. Not ad hoc.
- Laplace distribution have heavy tails.
- **Laplace prior**: many β_i close to zero, but some β_i very large.
- Normal distribution have light tails.

Learning the shrinkage

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

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

so $\Omega_0 = \lambda I_m$.

Regression with learned shrinkage

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

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

$$\sigma^2|\lambda, y \sim \text{Inv} - \chi^2(v_n, \sigma_n^2)$$

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

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

$$\mu_n = (X^T X + \Omega_0)^{-1} X^T y$$

$$\Omega_n = X^T X + \Omega_0$$

$$v_n = v_0 + n$$

$$v_n \sigma_n^2 = v_0 \sigma_0^2 + y^T y - \mu_n^T \Omega_n \mu_n$$

More complexity

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

$$p(\beta, \sigma^2, \lambda, \kappa_1, \dots, \kappa_m | y, X)$$

- The marginal posterior for $\kappa_1, \dots, \kappa_m$ 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)