

# BAYESIAN LEARNING - LECTURE 5

Mattias Villani

**Division of Statistics and Machine Learning  
Department of Computer and Information Science  
Linköping University**

# LECTURE OVERVIEW

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

# NORMAL MODEL - NORMAL PRIOR

- ▶ Model

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

- ▶ Conjugate prior

$$\theta | \sigma^2 \sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right)$$

$$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$$

# NORMAL MODEL WITH NORMAL PRIOR

## ► Posterior

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

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

$$\theta \sim t_{\nu_n}(\mu_n, \sigma_n^2/\kappa_n)$$

# THE LINEAR REGRESSION MODEL

- ▶ The ordinary linear regression model:

$$y_i = \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} + \varepsilon_i$$
$$\varepsilon_i \stackrel{iid}{\sim} N(0, \sigma^2).$$

- ▶ Parameters  $\theta = (\beta_1, \beta_2, \dots, \beta_k, \sigma^2)$ .
- ▶ Assumptions:
  - ▶  $E(y_i) = \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik}$  (linear function)
  - ▶  $\text{Var}(y_i) = \sigma^2$  (homoscedasticity)
  - ▶  $\text{Corr}(y_i, y_j | X) = 0, i \neq j$ .
  - ▶ Normality of  $\varepsilon_i$ .

# LINEAR REGRESSION IN MATRIX FORM

- ▶ The linear regression model in matrix form

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

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_k \end{pmatrix}, \quad \varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$
$$\mathbf{X} = \begin{pmatrix} \mathbf{x}'_1 \\ \vdots \\ \mathbf{x}'_n \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nk} \end{pmatrix}$$

- ▶ Usually  $x_{i1} = 1$ , for all  $i$ .  $\beta_1$  is the intercept.
- ▶ Likelihood for the full sample

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

# LINEAR REGRESSION - UNIFORM PRIOR

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

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

- ▶ Joint posterior of  $\beta$  and  $\sigma^2$ :

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

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 iteratively simulating from
  - ▶  $p(\sigma^2 | \mathbf{y})$
  - ▶  $p(\beta | \sigma^2, \mathbf{y})$
- ▶ Marginal posterior of  $\beta$  :

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

# LINEAR REGRESSION - CONJUGATE PRIOR

- Joint prior for  $\beta$  and  $\sigma^2$

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

- Posterior

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

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



# POLYNOMIAL REGRESSION

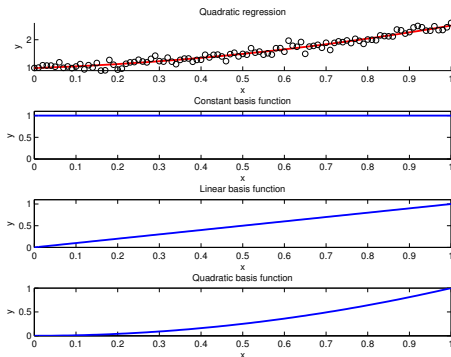
## ► Polynomial regression

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

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

where

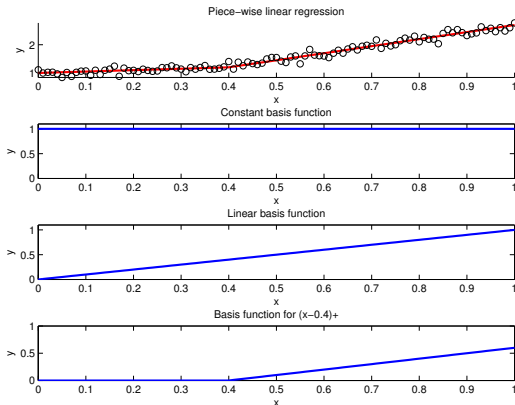
$$\mathbf{X}_P = (1, x, x^2, \dots, x^k).$$



# SPLINE REGRESSION

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

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



## SPLINES, CONT.

- ▶ Note: given the knots, the non-parametric spline regression model is a linear regression of  $y$  on the  $m$  'dummy variables'  $b_j$

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

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

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

- ▶ It is also common to include an intercept and the linear part of the model separately. In this case we have

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

# SMOOTHNESS PRIOR FOR SPLINES

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

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

- ▶ Larger  $\lambda$  gives smoother fit. Note: here we have  $\Omega_0 = \lambda I$ .
- ▶ Equivalent to a penalized likelihood:

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

- ▶ Posterior mean gives **ridge regression** estimator

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

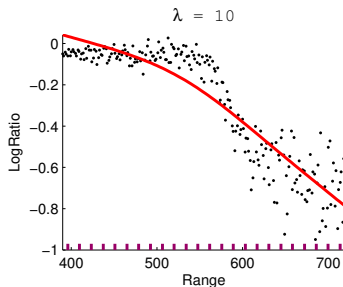
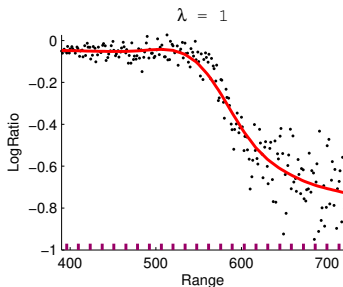
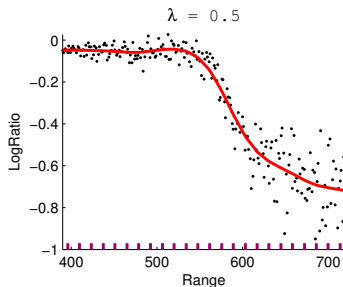
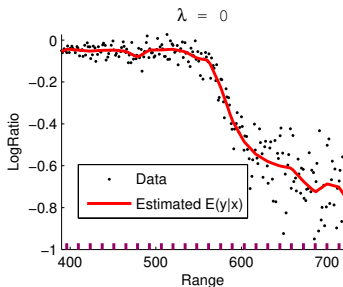
- ▶ **Shrinkage** toward zero

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

- ▶ When  $\mathbf{X}'\mathbf{X} = I$

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

# BAYESIAN SPLINE WITH SMOOTHNESS PRIOR



## SMOOTHNESS PRIOR FOR SPLINES, CONT.

- ▶ The famous **Lasso** variable selection method is equivalent to using the posterior mode estimate under the prior:

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

with density

$$p(\beta_i) = \frac{\lambda}{2\sigma^2} \exp \left( -\frac{\lambda |\beta_i|}{\sigma^2} \right)$$

- ▶ The Bayesian shrinkage prior is **interpretable**. **Not ad hoc**.
- ▶ Laplace distribution have heavy tails.
- ▶ Laplace: many  $\beta_i$  are close to zero, but some  $\beta_i$  may be very large.
- ▶ Normal distribution have light tails.
- ▶ Normal prior: most  $\beta_i$  are fairly equal in size, and no single  $\beta_i$  can be very much larger than the other ones.

# ESTIMATING THE SHRINKAGE

- ▶ How do we determine the degree of smoothness,  $\lambda$ ? Cross-validation is one possible approach.
- ▶ Bayesian:  $\lambda$  is unknown  $\Rightarrow$  use a prior for  $\lambda$ .
- ▶ One possibility:  $\lambda \sim \text{Inv} - \chi^2(\eta_0, \lambda_0)$ . The user specifies  $\eta_0$  and  $\lambda_0$ .
- ▶ Alternative approach: specify the prior on the *degrees of freedom*.
- ▶ Hierarchical setup:

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

# REGRESSION WITH ESTIMATED SHRINKAGE

- The joint posterior of  $\beta$ ,  $\sigma^2$  and  $\lambda$  is

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

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

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

where  $p(\lambda)$  is the prior for  $\lambda$ , and

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

$$\Omega_n = X'X + \Omega_0$$

$$v_n = v_0 + n$$

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



## MORE COMPLEXITY

- ▶ The **location of the knots** can be treated as unknown, and estimated from the data. Joint posterior

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

- ▶ The marginal posterior for  $\lambda, k_1, \dots, k_m$  is a nightmare.
- ▶ MCMC can be used to simulate from the joint posterior. Li and Villani (2013, SJS).
- ▶ 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 error term)
- ▶ MCMC can again be used to simulate from the joint posterior.