

BAYESIAN LEARNING - LECTURE 5

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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)
 - ▶ $Var(y_i) = \sigma^2$ (homoscedasticity)
 - ▶ $Corr(y_i, y_j | X, \beta, \sigma^2) = 0, i \neq j$.
 - ▶ Normality of ε_i .
 - ▶ The x 's are assumed known (non-random).

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 . β_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 β and σ^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 β :

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

LINEAR REGRESSION - CONJUGATE PRIOR

- Joint prior for β and σ^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

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

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

POLYNOMIAL REGRESSION

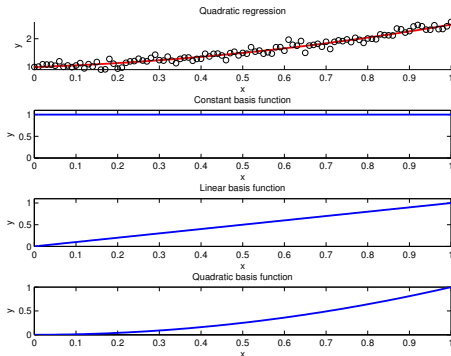
► Polynomial regression

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

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

where

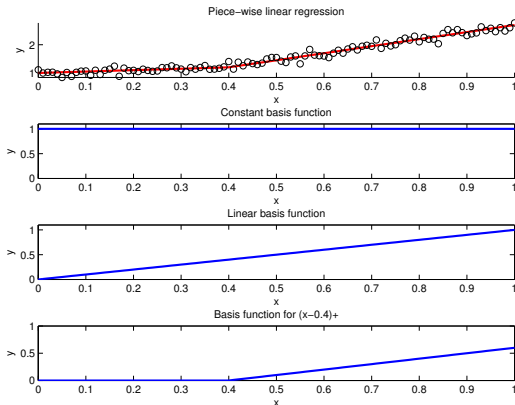
$$\mathbf{X}_P = (1, x, x^2, \dots, x^k).$$



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 λ 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

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

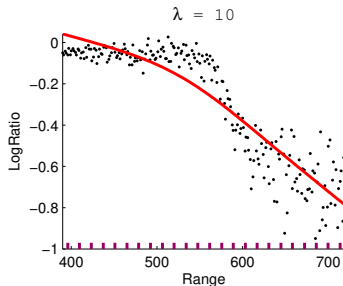
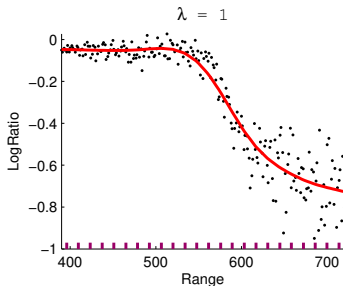
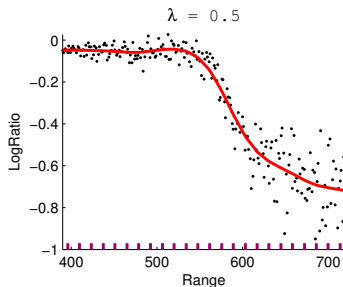
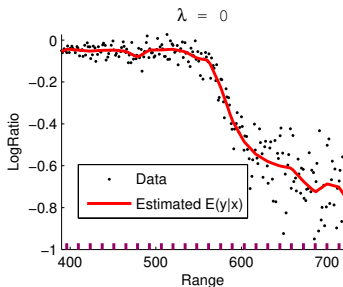
- ▶ **Shrinkage** toward zero

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

- ▶ 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 β_i are close to zero, but some β_i may be very large.
- ▶ Normal distribution have light tails.
- ▶ Normal prior: most β_i are fairly equal in size, and no single β_i can be very much larger than the other ones.

ESTIMATING THE SHRINKAGE

- ▶ How do we determine the degree of smoothness, λ ? Cross-validation is one possible approach.
- ▶ Bayesian: λ is unknown \Rightarrow use a prior for λ .
- ▶ One possibility: $\lambda \sim \text{Gamma}\left(\frac{\eta_0}{2}, \frac{\eta_0}{2\lambda_0}\right)$. The user specifies η_0 and λ_0 .
- ▶ Alternative approach: specify the prior on the *degrees of freedom*.
- ▶ Hierarchical setup:

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

so $\Omega_0 = \lambda I_m$ in the previous notation.

REGRESSION WITH ESTIMATED SHRINKAGE

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

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

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

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

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

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

$$\Omega_n = \mathbf{X}^T\mathbf{X} + \Omega_0$$

$$\nu_n = \nu_0 + n$$

$$\nu_n\sigma_n^2 = \nu_0\sigma_0^2 + \mathbf{y}^T\mathbf{y} - \mu_n^T\Omega_n\mu_n$$

MORE COMPLEXITY

- ▶ The **location of the knots** can be 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 λ, 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.