

$$p(\Theta|D) = \frac{p(D|\Theta)p(\Theta)}{p(D|\Theta)p(\Theta) + p(D|\neg\Theta)p(\neg\Theta)}$$

Bayesian Learning 732A46: Lecture 5

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- ▶ The normal model with a conjugate prior for both θ, σ^2 .
- ▶ Bayesian treatment of the standard linear regression model.
- ▶ 'non-informative' prior + Conjugate prior for the linear model.
- ▶ Shrinkage (regularization/smoothing) through prior distributions. Connection to the frequentist approach.
- ▶ Prediction in the Bayesian linear regression model.

Normal model - conjugate prior for both θ and σ^2

► Model

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

► Conjugate prior

$$\begin{aligned}\theta | \sigma^2 &\sim N\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right) \\ \sigma^2 &\sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)\end{aligned}$$

- Possible to derive $p(\theta, \sigma^2 | y)$ by
 1. Using invaluable techniques #1-#3 from **Lecture 3**.
 2. **Ignoring** normalizing constants!
 3. Having **A LOT** of patience.

Normal model - conjugate prior for both θ and σ^2 , cont.

► Posterior

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

where

$$\begin{aligned}\mu_n &= \frac{\kappa_0}{\kappa_0 + n} \mu_0 + \frac{n}{\kappa_0 + n} \bar{y} \\ \kappa_n &= \kappa_0 + n \\ \nu_n &= \nu_0 + n \\ \nu_n \sigma_n^2 &= \nu_0 \sigma_0^2 + (n - 1) s^2 + \frac{\kappa_0 n}{\kappa_0 + n} (\bar{y} - \mu_0)^2.\end{aligned}$$

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► Marginal posterior

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

► ... or just simulate (marginalization by simulation).

The standard linear regression model

- ▶ The model is

$$\begin{aligned}y_i &= \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \varepsilon_i \\ \varepsilon_i &\sim \mathcal{N}(0, \sigma^2),\end{aligned}$$

where $i = 1, \dots, n$. Usually $x_{i1} = 1$ for all i [β_1 is the intercept].

- ▶ **Parameters** $\theta = (\beta_1, \dots, \beta_k, \sigma^2)'$. **Covariates** $x_i = (1, x_{i2}, \dots, x_{ik})'$

- ▶ **Assumptions**

1. $E[y_i | x_i, \theta] = \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik}$ [linear].
2. $V[y_i | x_i, \theta] = \sigma^2$ [homoscedasticity].
3. $y_i | x_i, \theta$ conditionally independent for $i = 1, \dots, n$.
4. ε_i are Normal.

- ▶ **The notation of**, the posterior distribution

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

omits explicit conditioning.

- ▶ **We are implicitly conditioning** on the x 's (covariates) since they are **non-random**.

The standard linear regression model in matrix form

- The model in **matrix form**

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

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

$$X = \begin{bmatrix} x'_1 \\ \vdots \\ x'_n \end{bmatrix} = \begin{bmatrix} 1 & x_{12} & \dots & x_{1k} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n2} & \dots & x_{nk} \end{bmatrix}$$

- **The likelihood:** $\left[\Sigma = \sigma^2 \underset{(n \times n)}{I} \right]$

$$p(y|\beta, \sigma^2) \propto |\Sigma|^{-1/2} \exp \left(-\frac{1}{2} (y - X\beta)' \Sigma^{-1} (y - X\beta) \right)$$

- $|\Sigma|^{-1/2} = (\sigma^{2n})^{-1/2} = \sigma^{-n}$ and $\Sigma^{-1} = \frac{1}{\sigma^2} I$

- ▶ The **standard 'non-informative'** prior $p(\beta, \log(\sigma^2)) \propto c$.
- ▶ **Equivalently:** $p(\beta, \sigma^2) \propto \frac{1}{\sigma^2}$.
- ▶ **Summary:** The posterior is \mathcal{N} -Inv- $\chi^2(\beta_n, \Sigma_n; \nu_n, s_n^2)$

$$\begin{aligned}\beta_n &= (X'X)^{-1}X'y & \nu_n &= n - k \\ \Sigma_n &= \sigma^2(X'X)^{-1} & s_n^2 &= \frac{1}{n-k} (y - X\beta_n)'(y - X\beta_n)\end{aligned}$$

- ▶ **Simulate** from the joint posterior $p(\beta, \sigma^2|y)$:
 1. $\sigma^2|y \sim \text{Inv-}\chi^2(\nu_n, s_n^2)$
 2. $\beta|\sigma^2, y \sim \mathcal{N}(\beta_n, \Sigma_n)$.

► Some remarks

1. β_n is the **MLE** of β in classical statistic [and s_n^2 the **MLE** of σ^2].
2. We can show that

$$p(\beta|y) = \int p(\beta|\sigma^2, y)p(\sigma^2|y)d\sigma^2 = t_{n-k}(\beta_n, s_n^2(X'X)^{-1})$$

$s_n^2(X'X)^{-1}$ - **standard errors for the MLE** of β .

- A Bayesian analysis with a '*non-informative prior*' gives the same **point estimates** as a Frequentist analysis...
- ... but the Bayesian is **richer** - **knows the whole probability distribution**.
- I have added slides with the derivation. But I will spare you the pain here.

If you dare, do it at home. Nothing but invaluable techniques #1-#3 (and patience!)

- **Factorize** the posterior (#1)

$$p(\beta, \sigma^2 | y) = p(\beta | \sigma^2, y) p(\sigma^2 | y)$$

- **Determine first** $p(\beta | \sigma^2, y)$ (#2). Use Bayes' theorem and **treat everything but β as proportionality constants**.
- $p(\beta | \sigma^2, y) = \frac{p(\beta, \sigma^2, y)}{p(\sigma^2, y)} \propto p(y | \beta, \sigma^2) \propto \exp\left(-\frac{1}{2\sigma^2} (y - X\beta)' (y - X\beta)\right)$
- A **quadratic form** in β . Thus $\beta | \sigma^2, y \sim \mathcal{N}(\beta_n = ?, \Sigma_n = ?)$

$$\begin{aligned} p(\beta | \sigma^2, y) &\propto \exp\left(-\frac{1}{2}(\beta - \beta_n)' \Sigma_n^{-1} (\beta - \beta_n)\right) \\ &= \exp\left(-\frac{1}{2}\left(\beta' \Sigma_n^{-1} \beta - 2\beta' \Sigma_n^{-1} \beta_n + \beta_n' \Sigma_n^{-1} \beta_n\right)\right) \\ &\propto \exp\left(-\frac{1}{2}\left(\beta' \Sigma_n^{-1} \beta - 2\beta' \Sigma_n^{-1} \beta_n\right)\right) \end{aligned}$$

- **Expand** $\exp\left(-\frac{1}{2\sigma^2} (y - X\beta)' (y - X\beta)\right)$ and **match terms**.

► **Expanding**

$$\begin{aligned}\exp\left(-\frac{1}{2\sigma^2}(y - X\beta)'(y - X\beta)\right) &= \exp\left(-\frac{1}{2\sigma^2}(y'y - 2\beta'X'y + \beta'X'X\beta)\right) \\ &\propto \exp\left(-\frac{1}{2\sigma^2}(\beta'X'X\beta - 2\beta'X'y)\right)\end{aligned}$$

► **Match** Σ_n :

$$\beta'X'X\beta/\sigma^2 = \beta'\Sigma_n^{-1}\beta \implies \Sigma_n^{-1} = \frac{1}{\sigma^2}X'X \implies \Sigma_n = \sigma^2(X'X)^{-1}$$

► For β_n , first rewrite

$$2\beta'X'y/\sigma^2 = 2\beta'\underbrace{\Sigma_n^{-1}\Sigma_n}_{I}X'y/\sigma^2$$

► **Match** β_n :

$$2\beta'\Sigma_n^{-1}\Sigma_nX'y/\sigma^2 = 2\beta'\Sigma_n^{-1}\beta_n \implies \beta_n = (X'X)^{-1}X'y$$

- **We conclude** that $p(\beta|\sigma^2, y) = \mathcal{N}(\beta_n, \Sigma_n)$

$$\begin{aligned}\beta_n &= (X'X)^{-1}X'y \\ \Sigma_n &= \sigma^2(X'X)^{-1}.\end{aligned}$$

- Derive $p(\sigma^2|y)$ (#3)

$$p(\sigma^2|y) = \frac{p(\beta, \sigma^2|y)}{p(\beta|\sigma^2, y)} \propto \frac{p(y|\beta, \sigma^2)p(\sigma^2)}{p(\beta|\sigma^2, y)}$$

- **Standard trick:** LHS does not depend on β (β cancels on RHS).
- Evaluate RHS using $\beta = \beta_n$ (simplifies the denominator)

$$\begin{aligned}\frac{p(y|\beta_n, \sigma^2)p(\sigma^2)}{p(\beta_n|\sigma^2, y)} &\propto \frac{\sigma^{-n} \exp\left(-\frac{1}{2\sigma^2} (y - X\beta_n)' (y - X\beta_n)\right) \sigma^{-2}}{|\Sigma_n|^{-1/2} \exp\left(-\frac{1}{2} (\beta_n - \beta_n)' \Sigma_n^{-1} (\beta_n - \beta_n)\right)} \\ &= \frac{\sigma^{-n} \exp\left(-\frac{1}{2\sigma^2} (y - X\beta_n)' (y - X\beta_n)\right) \sigma^{-2}}{|\Sigma_n|^{-1/2}}\end{aligned}$$

Derivations, cont.

- ▶ $|\Sigma_n| = |\sigma^2(X'X)^{-1}| = |\sigma^2 I (X'X)^{-1}| = \overbrace{|\sigma^2 I|}^{=\sigma^{2k}} |(X'X)^{-1}|.$
- ▶ Thus $|\Sigma_n|^{-1/2} = (\sigma^{2k})^{-1/2} (|(X'X)^{-1}|)^{-1/2} \propto \sigma^{-k},$ and

$$p(\sigma^2|y) \propto \sigma^{-n+k-2} \exp\left(-\frac{1}{2\sigma^2} (y - X\beta_n)' (y - X\beta_n)\right).$$

- ▶ $p(\sigma^2|y) = \text{Inv-}\chi^2(\nu_n, s_n^2)$ if it is **proportional to**

$$\sigma^{-2(\nu_n/2+1)} \exp\left(-\frac{\nu_n s_n^2}{2\sigma^2}\right).$$

- ▶ Rewrite and **match terms**

$$p(\sigma^2|y) \propto \sigma^{-2(\overbrace{(n-k)}^{\nu_n})/2+1)} \exp\left(-\frac{\overbrace{n-k}^{\nu_n}}{2\sigma^2} \underbrace{\frac{1}{(n-k)} (y - X\beta_n)' (y - X\beta_n)}_{s_n^2}\right)$$

- **We have proven** that the posterior is $\mathcal{N}\text{-Inv-}\chi^2(\beta_n, \Sigma_n; \nu_n, s_n^2)$

$$\begin{aligned}\beta_n &= (X'X)^{-1}X'y & \nu_n &= n - k \\ \Sigma_n &= \sigma^2(X'X)^{-1} & s_n^2 &= \frac{1}{n-k} (y - X\beta_n)'(y - X\beta_n)\end{aligned}$$

Normal regression - Conjugate prior for β, σ^2

- ▶ An informative prior is helpful for **model regularization**.
- ▶ **Conjugate prior** $p(\beta, \sigma^2) = \mathcal{N}\text{-Inv-}\chi^2(\beta_0, \sigma^2 \Omega_0^{-1}; \nu_0, s_0^2)$,

$$\begin{aligned} p(\beta | \sigma^2) &= \mathcal{N}(\beta_0, \sigma^2 \Omega_0^{-1}) \\ p(\sigma^2) &= \text{Inv-}\chi^2(\nu_0, s_0^2) \end{aligned}$$

- ▶ The role of the **hyperparameters** in the prior.
 - (1) β_0 - the mean. $\beta_0 = 0$ common choice.
 - (2) Ω_0 - the "precision". Common choice $\Omega_0 = \lambda I$ [$\Omega_0^{-1} = \frac{1}{\lambda} I$].
Larger $\lambda \implies$ prior concentrates more around β_0 . We can even have

$$\Omega_0 = \text{diag}(\lambda_1, \dots, \lambda_k).$$

- (3) ν_0 - prior degrees of freedom.
 - (4) s_0^2 - prior average sum of squares.
- ▶ With $\beta_0 = 0$, (2) is an example of **model regularization through the prior**. Tackles **over-fitting problems** that occur in models with many parameters.

The posterior with the conjugate prior for β, σ^2

- ▶ **Tedious** algebra with 'non-informative' prior.
- ▶ A **nightmare** here - **but still only** invaluable techniques #1-#3.
- ▶ **It's form:** a matrix version of the normal model with a conjugate on θ, σ^2 .
- ▶ Let $\hat{\beta} = (X'X)^{-1}X'y$ ['Non-informative' case, **MLE**].
- ▶ **The posterior** $p(\beta, \sigma^2|y) = p(\beta|\sigma^2, y)p(\sigma^2|y)$

$$\begin{aligned}p(\beta|\sigma^2, y) &= \mathcal{N}(\beta_n, \sigma^2\Omega_n^{-1}) \\p(\sigma^2|y) &= \text{Inv-}\chi^2(\nu_n, s_n^2)\end{aligned}$$

$$\begin{aligned}\beta_n &= (X'X + \Omega_0)^{-1}(X'X\hat{\beta} + \Omega_0\beta_0) & \Omega_n &= X'X + \Omega_0 \\ \nu_n &= \nu_0 + n & \nu_n s_n^2 &= \nu_0 s_0^2 + y'y + \beta_0'\Omega_0\beta_0 - \beta_n'\Omega_n\beta_n\end{aligned}$$

- ▶ **Note:** the posterior mean is a weighted average of data and prior information.

Shrinkage illustration with the conjugate prior for β, σ^2

► Shrinkage illustration:

With $X'X = I$ and $p(\beta|\sigma^2) = \mathcal{N}(\beta_0, \sigma^2/\lambda I)$ [$\Omega_0 = \lambda I$]

$$\beta_n = (I + \lambda I)^{-1}(I\hat{\beta} + \lambda I\beta_0) = \underbrace{\frac{1}{1+\lambda}}_{0 < w_1 < 1} \hat{\beta} + \underbrace{\frac{\lambda}{1+\lambda}}_{0 < w_2 < 1} \beta_0 \quad [w_1 + w_2 = 1].$$

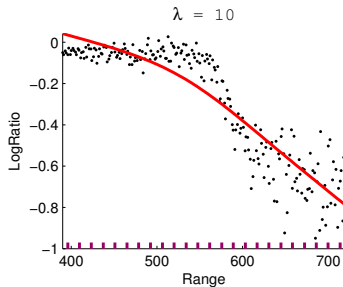
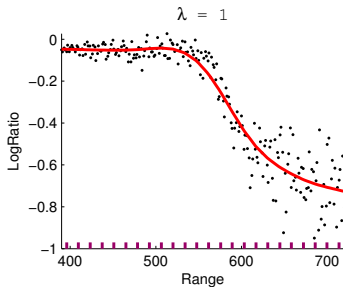
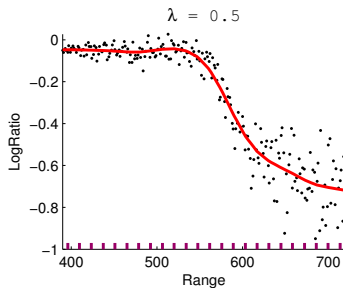
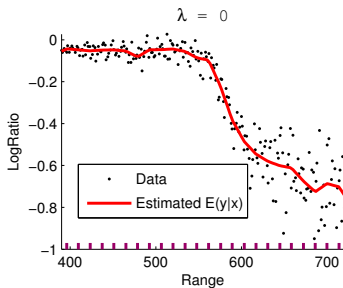
► Note that

1. $\lambda \rightarrow 0 \implies \beta_n \rightarrow \hat{\beta}$.
2. $\lambda \rightarrow \infty \implies \beta_n \rightarrow \beta_0$.

► 'Non-informative' priors [$\lambda = 0$] **do not shrink!**...

► ... Neither does **Frequentist OLS** nor **MLE** estimates!

Example: Bayesian spline with shrinkage prior



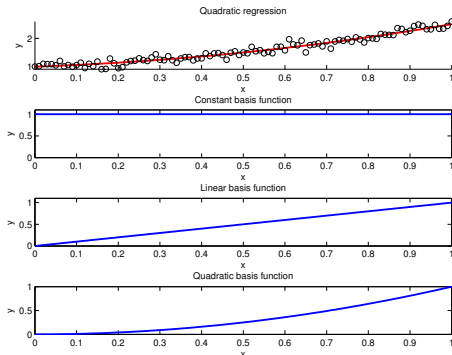
Polynomial regression as a simple linear regression

- ▶ Consider only a **single covariate** for simplicity.
- ▶ A general regression model with **additive noise**

$$y_i = f(x_i; \beta) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2).$$

- ▶ **Polynomial regression**

- ▶ $f(x_i; \beta) = \beta_0 + \beta_1 x_i$ - linear regression
- ▶ $f(x_i; \beta) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$ - quadratic regression
- ▶ $f(x_i; \beta) = \beta_0 + \beta_1 x_i + \dots + \beta_p x_i^p$ - polynomial order p .



Polynomial regression as a simple linear regression, cont.

- Can be written

$$y = X_p \beta + \varepsilon, \quad X_p = (1, x, x^2, \dots, x^p) \in n \times (p+1).$$

- x is **basis expanded** $X_p = (h_0(x), h_1(x), h_2(x), \dots, h_p(x))$ where

$$h_j(x) = x^j, \quad j = 1, \dots, p, \text{ are the basis functions.}$$

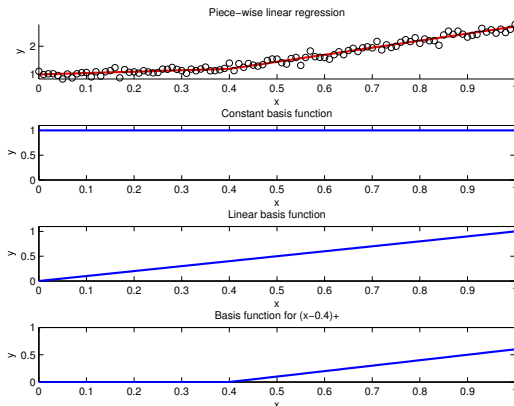
- **Note:** The model is **Non-linear** in data but **still linear in parameter**
- Estimation as before but with X_p in place of X .
- **Problem:** Polynomials are **too global** - fit becomes unstable.

Shrinkage in a spline regression model

- **Splines** to the rescue! Like polynomials but **more local**.
- **Example:** Truncated *power splines*. Basis functions

$$h_j(x) = \begin{cases} (x - \xi_j)^a & \text{if } x > \xi_j \\ 0 & \text{otherwise.} \end{cases},$$

where ξ_j ($j = 1, \dots, p$) are the **knots** which are given.



Shrinkage in a spline regression model

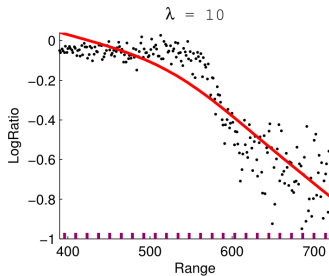
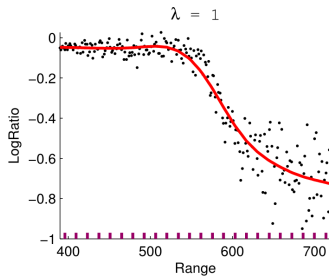
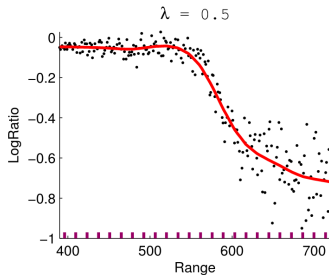
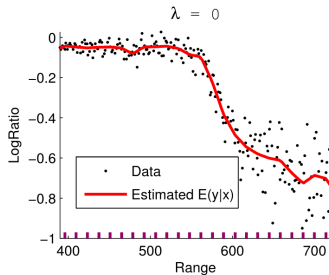
- **Note:** given the knots, the **spline regression model** is a linear regression of y on the basis expanded matrix

$$X_p = (1, x, h_1(x), \dots, h_p(x))$$

(common to include **an intercept** + **a linear basis** function).

- Estimation as in the linear regression. Just change X for X_p .
- Typically many knots. **Regularization** required for a smooth fit.
- **Let's see the figure again!**

Shrinkage in Bayesian spline (note the **knots**!)



Shrinkage: Frequentist vs Bayesian

- ▶ Frequentists instead shrink by minimizing a **penalized** RSS.
- ▶ Residual Sum of Squares (RSS):

$$\text{RSS}(\beta) = (y - f(X; \beta))'(y - f(X; \beta)).$$

- ▶ Example **ridge regression**:

$$\hat{\beta}_{\text{ridge}} = \arg \min_{\beta} \text{RSS}(\beta) + \lambda \beta' \beta \longrightarrow \hat{\beta}_{\text{ridge}} = (X'X + \lambda I)^{-1} X'y$$

- ▶ The same as the **Bayesian posterior mean** β_n we have derived with $\beta_0 = 0$ and $\Omega_0 = \lambda I \dots$

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- ▶ The same as the **Bayesian posterior mean** β_n we have derived with $\beta_0 = 0$ and $\Omega_0 = \lambda I \dots$
- ▶ ... the frequentists are indeed using "prior information" ... **but they are hiding it!**
- ▶ The Bayesian shrinkage prior is **interpretable**. Nothing ad hoc.

Other Shrinkage priors

- ▶ Other shrinkage priors can be used but they are **not conjugate**.
- ▶ MCMC methods can be used for estimation.
- ▶ The famous frequentist **Lasso variable selection** method is equivalent to **the posterior mode** using the prior

$$p(\beta_k | \sigma^2) = \frac{\lambda}{2\sigma^2} \exp\left(-\lambda \frac{|\beta_k|}{\sigma^2}\right) \quad \left[\text{Laplace}\left(0, \frac{\sigma^2}{\lambda}\right) \right].$$

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

Estimating the shrinkage parameter λ from the data

- ▶ So far implicitly assumed that λ **is known**.
- ▶ Crossvalidation is one possibility. But this **is not** a Bayesian solution.
- ▶ **Question**: What would a Bayesian solution be?

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Estimating the shrinkage parameter λ from the data

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- ▶ Crossvalidation is one possibility. But this **is not** a Bayesian solution.
- ▶ **Question**: What would a Bayesian solution be?
- ▶ **Clue**: Bayesians treat *any unknown quantity* as...
- ▶ ... a **random variable**!
- ▶ Treat λ as a r.v. Inference through $p(\beta, \sigma^2, \lambda|y)$
- ▶ Assign a prior $p(\lambda)$ and derive $p(\lambda|y)$.

Estimating the shrinkage parameter λ from the data, cont.

- The **joint posterior** factorizes (#1)

$$p(\beta, \sigma^2, \lambda | y) = p(\beta | \sigma^2, \lambda, y) p(\sigma^2 | \lambda, y) p(\lambda | y),$$

where (#1-#2 to derive)

Prior

→

Posterior

$$\beta | \sigma^2, \lambda \sim \mathcal{N}(0, \sigma^2 \Omega_0^{-1}) \quad \rightarrow \quad \beta | \sigma^2, \lambda, y \sim \mathcal{N}(\beta_n, \sigma^2 \Omega_n^{-1})$$

$$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, s_0^2) \quad \rightarrow \quad \sigma^2 | \lambda, y \sim \text{Inv-}\chi^2(\nu_n, s_n^2)$$

$$\lambda \sim p(\lambda) \quad \rightarrow \quad \lambda | y \sim \sqrt{\frac{|\Omega_0|}{|\Omega_n|}} \left(\frac{\nu_n s_n^2}{2} \right)^{-\nu_n/2} p(\lambda)$$

and

$$\begin{aligned} \beta_n &= (X'X + \Omega_0)^{-1} X'y & \Omega_n &= X'X + \Omega_0 \\ \nu_n &= \nu_0 + n & \nu_n s_n^2 &= \nu_0 s_0^2 + y'y - \beta_n' \Omega_n \beta_n \end{aligned}$$

- ▶ **Predict the outcome** \tilde{y} for a set of observations with covariates \tilde{X}
- ▶ **Posterior predictive density** [implicitly conditioning on X and \tilde{X}]

$$\begin{aligned}p(\tilde{y}|y) &= \int_{\sigma^2} \int_{\beta} p(\tilde{y}|y, \beta, \sigma^2) p(\beta, \sigma^2|y) d\beta d\sigma^2 \\ &= \int \int p(\tilde{y}|\beta, \sigma^2) p(\beta, \sigma^2|y) d\beta d\sigma^2\end{aligned}$$

if \tilde{y} and y are conditionally independent (given β, σ^2).

- ▶ **We can simulate** from $p(\tilde{y}|y)$ by
 1. $\beta, \sigma^2 \sim p(\beta, \sigma^2|y)$
 2. $\tilde{y}|\beta, \sigma^2 \sim p(\tilde{y}|\beta, \sigma^2) = \mathcal{N}(\tilde{X}\beta, \sigma^2 I)$.
- ▶ **Step 1.:** First σ^2 and then $\beta|\sigma^2$ [$p(\beta, \sigma^2|y) = p(\beta|\sigma^2, y)p(\sigma^2|y)$].
- ▶ If the **shrinkage** λ **is estimated** use $p(\beta, \sigma^2, \lambda|y)$ instead.