

Bayesian Learning 732A46: Lecture 5

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Lecture overview

- ▶ 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

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

► Conjugate prior θ , $\sigma^2 \sim \mathcal{N}$ -Inv- $\chi^2(\mu_0, \sigma^2/\kappa_0; \nu_0, \sigma_0^2)$

$$heta | \sigma^2 \sim \mathcal{N}\left(\mu_0, \frac{\sigma^2}{\kappa_0}\right)$$
 $\sigma^2 \sim \mathit{Inv-}\chi^2(\nu_0, \sigma_0^2)$

- ▶ 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 θ , $\sigma^2 | y \sim \mathcal{N}$ -Inv- $\chi^2(\mu_n, \sigma^2/\kappa_n; \nu_n, \sigma_n^2)$

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

where

$$\mu_{n} = \frac{\kappa_{0}}{\kappa_{0} + n} \mu_{0} + \frac{n}{\kappa_{0} + n} \bar{y}$$

$$\kappa_{n} = \kappa_{0} + n$$

$$\nu_{n} = \nu_{0} + n$$

$$\nu_{n}\sigma_{n}^{2} = \nu_{0}\sigma_{0}^{2} + (n - 1)s^{2} + \frac{\kappa_{0}n}{\kappa_{0} + n} (\bar{y} - \mu_{0})^{2}.$$

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

▶ Posterior θ , $\sigma^2 | y \sim \mathcal{N}$ -Inv- $\chi^2(\mu_n, \sigma^2/\kappa_n; \nu_n, \sigma_n^2)$

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where

$$\mu_{n} = \frac{\kappa_{0}}{\kappa_{0} + n} \mu_{0} + \frac{n}{\kappa_{0} + n} \bar{y}$$

$$\kappa_{n} = \kappa_{0} + n$$

$$\nu_{n} = \nu_{0} + n$$

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Marginal posterior

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

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

The standard linear regression model

▶ The model is

$$y_i = \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} + \varepsilon_i$$

$$\varepsilon_i \sim \mathcal{N}(0, \sigma^2),$$

where i = 1, ..., n. Usually $x_{i1} = 1$ for all $i [\beta_1]$ is the intercept].

- ▶ Parameters $\theta = (\beta_1, \dots, \beta_k, \sigma^2)'$. Covariates $x_i = (1, x_{i2}, \dots, x_{ik})'$
- Assumptions
 - 1. $E[y_i|x_i, \theta] = \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik}$ [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

$$y = X\beta + \varepsilon \atop (n \times k)(k \times 1) + (n \times 1)$$

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

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

► The likelihood: $\left[\Sigma = \sigma^2 \prod_{(n \times n)}\right]$

$$p(y|eta,\sigma^2) \propto |\Sigma|^{-1/2} \exp\left(-rac{1}{2} \left(y-Xeta
ight)' \Sigma^{-1} \left(y-Xeta
ight)
ight)$$

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

Normal regression - 'non-informative' prior

- ▶ 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- $\chi^2(\beta_n, \Sigma_n; \nu_n, s_n^2)$

$$eta_n = (X'X)^{-1}X'y$$
 $u_n = n - k$
 $\sum_n = \sigma^2(X'X)^{-1}$ $s_n^2 = \frac{1}{n-k} (y - X\beta_n)' (y - X\beta_n)$

- ▶ **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. $\beta | \sigma^2, y \sim \mathcal{N}(\beta_n, \Sigma_n)$.

Normal regression - 'non-informative' prior, cont.

► Some remarks

- 1. β_n is the MLE of β in classical statistic [and s_n^2 the MLE of σ^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.
- ▶ A quadratic form in β . Thus $\beta | \sigma^2, y \sim \mathcal{N}(\beta_n =?, \Sigma_n =?)$

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

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

Derivations, cont.

Expanding

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

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

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

▶ Match β_n :

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

Derivations, cont.

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

$$\beta_n = (X'X)^{-1}X'y$$

$$\Sigma_n = \sigma^2(X'X)^{-1}.$$

▶ 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)

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

$$= \frac{\sigma^{-n} \exp\left(-\frac{1}{2\sigma^2} (y - X\beta_n)' (y - X\beta_n)\right) \sigma^{-2}}{|\Sigma_n|^{-1/2}}$$

Derivations, cont.

$$\blacktriangleright \ |\Sigma_n| = \left|\sigma^2(X'X)^{-1}\right| = \left|\sigma^2I(X'X)^{-1}\right| = \widehat{\left|\sigma^2I\right|}\left|(X'X)^{-1}\right|.$$

► 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

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

Derivations, final slide!

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

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

Normal regression - Conjugate prior for β, σ^2

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

$$p(\beta|\sigma^2) = \mathcal{N}(\beta_0, \sigma^2 \Omega_0^{-1})$$

$$p(\sigma^2) = \text{Inv-}\chi^2(\nu_0, s_0^2)$$

- ▶ 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 $\Omega_0 = \lambda I \left[\Omega_0^{-1} = \frac{1}{\lambda}I\right]$. **Larger** $\lambda \Longrightarrow$ **prior concentrates more around** β_0 . We can even have

$$\Omega_0 = \operatorname{diag}(\lambda_1, \ldots, \lambda_k).$$

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

$$p(\beta|\sigma^2, y) = \mathcal{N}(\beta_n, \sigma^2 \Omega_n^{-1})$$

$$p(\sigma^2|y) = \text{Inv-}\chi^2(\nu_n, s_n^2)$$

$$\beta_{n} = (X'X + \Omega_{0})^{-1}(X'X\hat{\beta} + \Omega_{0}\beta_{0}) \qquad \Omega_{n} = X'X + \Omega_{0} \nu_{n} = \nu_{0} + n \qquad \qquad \nu_{n}s_{n}^{2} = \nu_{0}s_{0}^{2} + y'y + \beta_{0}'\Omega_{0}\beta_{0} - \beta_{n}'\Omega_{n}\beta_{n}$$

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

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

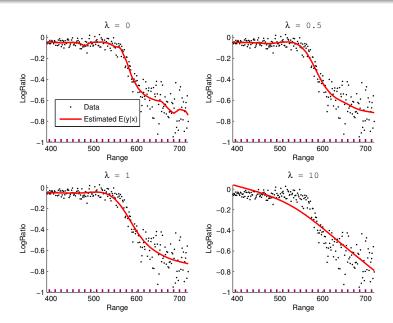
► Shrinkage illustration:

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

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

- ▶ Note that
 - 1. $\lambda \to 0 \implies \beta_n \to \hat{\beta}$.
 - 2. $\lambda \to \infty \implies \beta_n \to \beta_0$.
- ▶ 'Non-informative' priors $[\lambda = 0]$ do not shrink!...
- ▶ ... Neither does Frequentist OLS nor MLE estimates!

Example: Bayesian spline with shrinkage prior

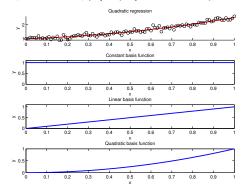


Polynomial regression as a simple linear regression

- 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

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

▶ x is **basis expanded** $X_p = (h_0(x), h_1(x), h_2(x), \dots h_p(x))$ where $h_j(x) = x^j, \quad j = 1, \dots, p$, are the basis functions.

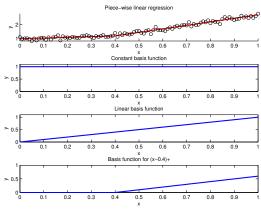
- ▶ Note: The model is Non-linear in data but still linear in parameter
- ▶ Estimation as before but with X_p in place of X.
- ▶ **Problem:** Polynomials are too global fit becomes unstable.

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, ..., p) are the **knots** which are given.



Shrinkage in a spline regression model

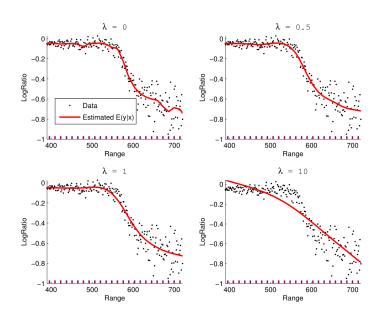
Note: given the knots, the spline regression model is a linear regression of y on the basis expanded matrix

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

(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):

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

► Example ridge regression:

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

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

Shrinkage: Frequentist vs Bayesian

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Example ridge regression:

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- ► The same as the Bayesian posterior mean β_n we have derived with $\beta_0 = 0$ and $\Omega_0 = \lambda I...$
- ► ... 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)

$$\begin{array}{cccc} \mathsf{Prior} & \to & \mathsf{Posterior} \\ \beta | \sigma^2, \lambda \sim \mathcal{N}(0, \sigma^2 \Omega_0^{-1}) & \to & \beta | \sigma^2, \lambda, y \sim \mathcal{N}(\beta_n, \sigma^2 \Omega_n^{-1}) \\ \\ \sigma^2 \sim \mathsf{Inv-} \chi^2(\nu_0, s_0^2) & \to & \sigma^2 | \lambda, y \sim \mathsf{Inv-} \chi^2(\nu_n, s_n^2) \\ \\ \lambda \sim p(\lambda) & \to & \lambda | y \sim \sqrt{\frac{|\Omega_0|}{|\Omega_n|}} \left(\frac{\nu_n s_n^2}{2}\right)^{-\nu_n/2} p(\lambda) \end{array}$$

and

$$\beta_n = (X'X + \Omega_0)^{-1}X'y \qquad \Omega_n = X'X + \Omega_0$$

$$\nu_n = \nu_0 + n \qquad \qquad \nu_n s_n^2 = \nu_0 s_0^2 + y'y - \beta_n'\Omega_n\beta_n$$

Prediction in linear regression

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

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

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.