Bayesian Model Choice

Hoff Chapter 9, Liang et al 2007, Hoeting et al (1999), Clyde & George (2004) Statistical Science

October 31, 2022

Posterior Distribution

With a Normal-Gamma Prior $\mathrm{NG}(\mathrm{b}_0, \Phi_0, \nu_0, \mathrm{SS}_0)$, the posterior is $\mathrm{NG}(\mathrm{b}_n, \Phi_n, \nu_n, \mathrm{SS}_n))$: with

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\nu_n &= n + \nu_0 \\
\mathrm{SS}_n &= \mathrm{SSE} + \mathrm{SS}_0 + \hat{\boldsymbol{\beta}}^T\mathrm{X}^T\mathrm{X}\hat{\boldsymbol{\beta}} + \mathrm{b}_0^T\Phi_0\mathrm{b}_0 - \mathrm{b}_n^T\Phi_n\mathrm{b}_n
\end{aligned}$$

Marginal Distribution from Normal–Gamma

Theorem

Let $\boldsymbol{\theta} \mid \phi \sim N(m, \frac{1}{\phi}\Sigma)$ *and* $\phi \sim \mathsf{G}(\nu/2, \nu\hat{\sigma}^2/2)$. *Then* $\boldsymbol{\theta}$ $(p \times 1)$ *has a* p *dimensional multivariate* t *distribution*

$$\boldsymbol{\theta} \sim t_\nu(m, \hat{\sigma}^2\Sigma)$$

with density

$$p(\boldsymbol{\theta}) \propto \left[1 + \frac{1}{\nu}\frac{(\boldsymbol{\theta} - m)^T\Sigma^{-1}(\boldsymbol{\theta} - m)}{\hat{\sigma}^2}\right]^{-\frac{p+\nu}{2}}$$

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Marginal Posterior Distribution of $\boldsymbol{\beta}$

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Any linear combination $\mathrm{x}^T\boldsymbol{\beta}$

$$\mathrm{x}^T\boldsymbol{\beta} \mid \mathrm{Y} \sim t_{\nu_n}(\mathrm{x}^T\mathrm{b}_n, \hat{\sigma}^2\mathrm{x}^T\Phi_n^{-1}\mathrm{x})$$

has a univariate t distribution with v_n degrees of freedom

Predictive Distribution

Suppose $\mathsf{Y}^* \mid \boldsymbol{\beta}, \phi \sim \mathsf{N}(\mathsf{X}^*\boldsymbol{\beta}, \mathsf{I}/\phi)$ and is conditionally independent of Y given $\boldsymbol{\beta}$ and ϕ

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\mathbf{Y}^* \mid \mathbf{Y} &\sim t_{\nu_n}(\mathbf{X}^*\mathbf{b}_n, \hat{\sigma}^2(\mathbf{I} + \mathbf{X}^*\Phi_n^{-1}\mathbf{X}^T))
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Conditional Distribution:

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Requires completing the square/quadratic!

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A class of prior distributions $\mathcal{P}$ for $\boldsymbol{\theta}$ is conjugate for a sampling model $p(y \mid \boldsymbol{\theta})$ if for every $p(\boldsymbol{\theta}) \in \mathcal{P}$, $p(\boldsymbol{\theta} \mid \mathrm{Y}) \in \mathcal{P}$.

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Choice of conjugate prior?

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$$\mathcal{I}(\theta) = -\mathsf{E}[\left[\frac{\partial^2 \log(\mathcal{L}(\boldsymbol{\theta}))}{\partial\theta_i \partial\theta_j}\right]]$$

Fisher Information Matrix

Log Likelihood

$$\log(\mathcal{L}(\boldsymbol{\beta}, \phi)) = \frac{n}{2}\log(\phi) - \frac{\phi}{2}\|(\mathsf{I} - \mathsf{P}_{\mathsf{x}})\mathsf{Y}\|^2 - \frac{\phi}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T(\mathsf{X}^T\mathsf{X})(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

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$$\mathrm{E}[\frac{\partial^2 \log\mathcal{L}}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}] = \begin{bmatrix} -\phi(\mathrm{X}^T\mathrm{X}) & 0_p \\ 0_p^T & -\frac{n}{2}\frac{1}{\phi^2} \end{bmatrix}$$

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$$\begin{aligned}
\frac{\partial^2 \log\mathcal{L}}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T} &= \begin{bmatrix} -\phi(\mathrm{X}^T\mathrm{X}) & -(\mathrm{X}^T\mathrm{X})(\boldsymbol{\beta}-\hat{\boldsymbol{\beta}}) \\ -(\boldsymbol{\beta}-\hat{\boldsymbol{\beta}})^T(\mathrm{X}^T\mathrm{X}) & -\frac{n}{2}\frac{1}{\phi^2} \end{bmatrix} \\
\mathrm{E}[\frac{\partial^2 \log\mathcal{L}}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}] &= \begin{bmatrix} -\phi(\mathrm{X}^T\mathrm{X}) & 0_p \\ 0_p^T & -\frac{n}{2}\frac{1}{\phi^2} \end{bmatrix} \\
\mathcal{I}((\boldsymbol{\beta},\phi)^T) &= \begin{bmatrix} \phi(\mathrm{X}^T\mathrm{X}) & 0_p \\ 0_p^T & \frac{n}{2}\frac{1}{\phi^2} \end{bmatrix}
\end{aligned}$$

Jeffreys Prior

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$$p_J(\boldsymbol{\beta}, \phi) \quad \propto \quad |\mathcal{I}((\boldsymbol{\beta}, \phi)^T)|^{1/2}$$

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Improper prior $\int\int p_J(\boldsymbol{\beta}, \phi)\, d\boldsymbol{\beta}\, d\phi$ not finite

Formal Bayes Posterior

$$p(\boldsymbol{\beta}, \phi \mid \mathrm{Y}) \propto p(\mathrm{Y} \mid \boldsymbol{\beta}, \phi)\phi^{p/2-1}$$

Formal Bayes Posterior

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if this is integrable, then renormalize to obtain formal posterior distribution

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Jeffreys did not recommend using this Posterior does not depend on dimension p

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- Treat β and ϕ separately (“orthogonal parameterization”)

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Bayesian Credible Sets $p(\boldsymbol{\beta} \in C_\alpha) = 1 - \alpha$ correspond to frequentist Confidence Regions

$$\frac{\boldsymbol{\lambda}^T\boldsymbol{\beta} - \boldsymbol{\lambda}\hat{\boldsymbol{\beta}}}{\sqrt{\hat{\sigma}^2\boldsymbol{\lambda}^T(\mathrm{X}^T\mathrm{X})^{-1}\boldsymbol{\lambda}}} \sim t_{n-p}$$

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Zellner's g-prior(s) $\boldsymbol{\beta} \mid \phi \sim \mathsf{N}(\mathsf{b}_0, g(\mathsf{X}^T\mathsf{X})^{-1}/\phi)$

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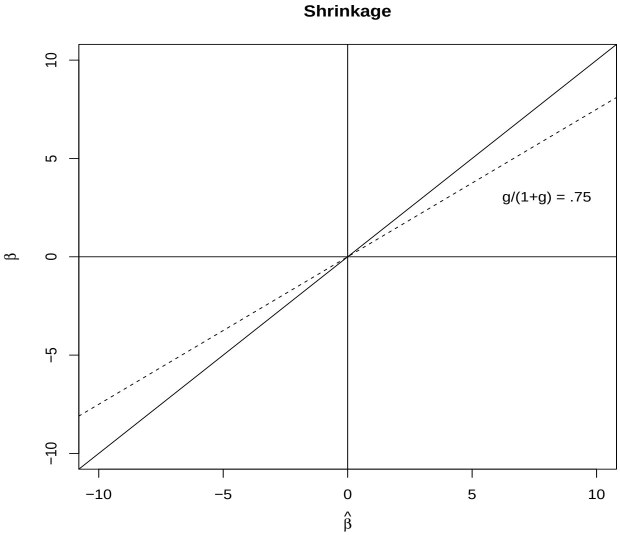
- Choice of g?
- $\frac{g}{1+g}$ weight given to the data
- Fixed g effect does not vanish as $n \to \infty$
- Use $g = n$ or place a prior diistribution on g

Shrinkage

Posterior mean under g-prior with $\mathrm{b}_0 = 0$ $\frac{g}{1+g}\hat{\beta}$



Ridge Regression

- If $X^T X$ is nearly singular, certain elements of $\boldsymbol{\beta}$ or (linear combinations of $\boldsymbol{\beta}$) may have huge variances under the g-prior (or flat prior) as the MLEs are highly unstable!
- **Ridge regression** protects against the explosion of variances and ill-conditioning with the conjugate prior:

$$\boldsymbol{\beta} \mid \phi \sim \mathrm{N}(0, \frac{1}{\phi\lambda} \mathrm{I}_p)$$

- Posterior for $\boldsymbol{\beta}$ (conjugate case)

$$\boldsymbol{\beta} \mid \phi, \lambda, Y \sim \mathrm{N}\left((\lambda \mathrm{I}_p + X^T X)^{-1} X^T Y, \frac{1}{\phi} (\lambda \mathrm{I}_p + X^T X)^{-1} \right)$$

- induces shrinkage as well!

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- Redundant variables lead to unstable estimates

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Model Choice ?

- Redundant variables lead to unstable estimates
- Some variables may not be relevant ($\beta_j = 0$)
- Can we infer a "good" model from the data?
- Expand model hierarchically to introduce another latent variable $\boldsymbol{\gamma}$ that encodes models $\mathcal{M}_\gamma$ $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots \gamma_p)^T$ where

$$
\begin{aligned}
\gamma_j = 0 &\Leftrightarrow \beta_j = 0 \\
\gamma_j = 1 &\Leftrightarrow \beta_j \neq 0
\end{aligned}
$$

- Find Bayes factors and posterior probabilities of models $\mathcal{M}_\gamma$
- 2^p models!

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Centered model:

$$Y = 1_n \alpha + X^c \beta + \epsilon$$

where X^c is the centered design matrix where all variables have had their mean subtracted

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- $\boldsymbol{\beta}_\gamma \mid \alpha, \phi, \boldsymbol{\gamma} \sim \mathsf{N}(0, g\phi^{-1}(\mathsf{X}_\gamma^{c\prime}\mathsf{X}_\gamma^c)^{-1})$

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which leads to marginal likelihood of $\boldsymbol{\gamma}$ that is proportional to

$$p(Y \mid \gamma) = C(1+g)^{\frac{n-p-1}{2}}(1 + g(1 - R_\gamma^2))^{-\frac{(n-1)}{2}}$$

where R^2 is the usual coefficient of determination for model $\mathcal{M}_\gamma$.

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where R^2 is the usual coefficient of determination for model $\mathcal{M}_\gamma$. Trade-off of model complexity versus goodness of fit

Lastly, assign distribution to space of models

Sketch

- Integrate out β_γ using sums of normals

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- Integrate out intercept (normal)
- Integrate out ϕ (gamma)
- algebra to simplify quadratic forms to R^2_γ

Or integrate α, $\boldsymbol{\beta}_\gamma$ and ϕ (complete the square!)

Priors on Model Space

$p(\mathcal{M}_\gamma) \Leftrightarrow p(\gamma)$

- $p(\gamma_j = 1) = .5 \Rightarrow P(\mathcal{M}_\gamma) = .5^p$ Uniform on space of models

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- $p(\gamma_j = 1) = .5 \Rightarrow P(\mathcal{M}_\gamma) = .5^p$ Uniform on space of models
  $p_\gamma \sim \text{Bin}(p, .5)$
- $\gamma_j \mid \pi \overset{\text{iid}}{\sim} \text{Ber}(\pi)$ and $\pi \sim \text{Beta}(a, b)$ then $p_\gamma \sim \text{BB}_p(a, b)$

$$p(p_\gamma \mid p, a, b) = \frac{\Gamma(p+1)\Gamma(p_\gamma + a)\Gamma(p - p_\gamma + b)\Gamma(a+b)}{\Gamma(p_\gamma + 1)\Gamma(p - p_\gamma + 1)\Gamma(p + a + b)\Gamma(a)\Gamma(b)}$$

- $p_\gamma \sim \text{BB}_p(1, 1) \sim \text{Unif}(0, p)$

Posterior Probabilities of Models

- Calculate analytically under enumeration

$$p(\mathcal{M}_\gamma \mid \mathsf{Y}) = \frac{p(\mathsf{Y} \mid \gamma)p(\gamma)}{\sum_{\gamma' \in \Gamma} p(\mathsf{Y} \mid \gamma')p(\gamma')}$$

  Express as a function of Bayes factors and prior odds!
- Use MCMC over Γ - Gibbs, Metropolis Hastings
- Do we need to run MCMC over γ, $\boldsymbol{\beta}_\gamma$, α, and ϕ?

Inference/Decisions ?