Bayesian Variable Selection & Bayesian Model Averaging

Hoff Chapter 9, Liang et al 2008, Hoeting et al (1999), Clyde & George (2004)

October 31, 2022

Zellner's g-prior

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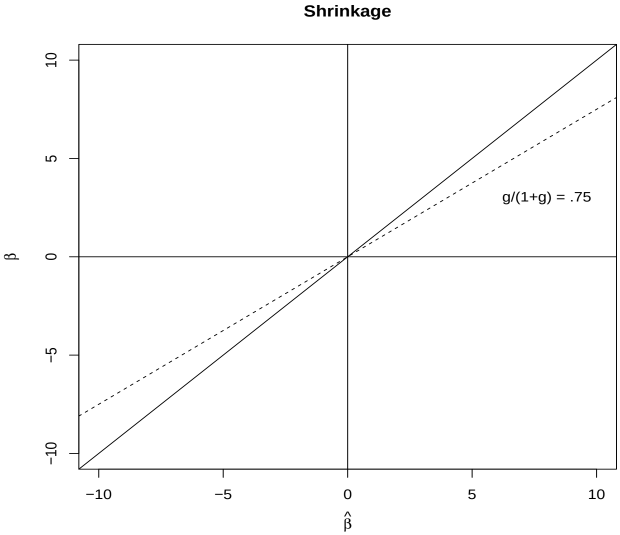
- Choice of g?
- $\frac{g}{1+g}$ weight given to the data
- Fixed g effect does not vanish as $n \to \infty$
- Use $g = n$ or place a prior diistribution on g

Shrinkage

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



Ridge Regression

- If X^TX 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:

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

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

$$\boldsymbol{\beta} \mid \phi, \lambda, Y \sim N\left((\lambda I_p + X^TX)^{-1}X^TY, \frac{1}{\phi}(\lambda I_p + X^TX)^{-1}\right)$$

- induces shrinkage as well!

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- 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

$$\gamma_j = 0 \Leftrightarrow \beta_j = 0$$
$$\gamma_j = 1 \Leftrightarrow \beta_j \neq 0$$

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

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Centered model:

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

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which leads to marginal likelihood of γ that is proportional to

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

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

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

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 $\mathcal{M}_\gamma$. 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 ϕ (gamma)

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- Find determinant of $\phi(\mathbf{I}_n + g\mathbf{P}_{\mathbf{X}_\gamma})$
- 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!)

Posteriors

$$\alpha \mid \phi, y \sim \mathrm{N}\left(\bar{y}, \frac{1}{n\phi}\right)$$

$$\boldsymbol{\beta}_\gamma \mid \gamma, \phi, g, y \sim \mathrm{N}\left(\frac{g}{1+g}\hat{\boldsymbol{\beta}}_\gamma, \frac{g}{1+g}\frac{1}{\phi}\left[\mathrm{X}_\gamma{}^T\mathrm{X}_\gamma\right]^{-1}\right)$$

$$\phi \mid \gamma, y \sim \mathrm{Gamma}\left(\frac{n-1}{2}, \frac{\mathrm{TotalSS} - \frac{g}{1+g}\mathrm{RegSS}}{2}\right)$$

$$p(\gamma \mid y) \propto p(y \mid \gamma)p(\gamma)$$

$$\mathrm{TotalSS} \equiv \sum_i (y_i - \bar{y})^2 \qquad \mathrm{RegSS} \equiv \hat{\boldsymbol{\beta}}_\gamma^T \mathrm{X}_\gamma^T \mathrm{X}_\gamma \hat{\beta}\gamma$$

$$R^2_\gamma = \frac{\mathrm{RegSS}}{\mathrm{TotalSS}} = 1 - \frac{\mathrm{ErrorSS}}{\mathrm{TotalSS}}$$

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

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

  Express as a function of Bayes factors and prior odds!
- Use MCMC over Γ - Gibbs, Metropolis Hastings if p is large
- slow convergence/poor mixing with high correlations

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  Express as a function of Bayes factors and prior odds!
- Use MCMC over Γ - Gibbs, Metropolis Hastings if p is large
- slow convergence/poor mixing with high correlations
- Metropolis Hastings algorithms more flexibility (swap pairs of variables)
- Do we need to run MCMC over γ, $\boldsymbol{\beta}_\gamma$, α, and ϕ?

Choice of g: Bartlett's Paradox

The Bayes factor for comparing γ to the null model:

$$BF(\gamma : \gamma 0) = (1 + g)^{(n-1-p_\gamma)/2}(1 + g(1 - R_\gamma^2))^{-(n-1)/2}$$

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- What happens to BF as $g \to \infty$?

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- why is this a paradox?

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- Let $F = \frac{R^2_\gamma/p_\gamma}{(1-R^2_\gamma)/(n-1-p_\gamma)}$

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- BF converges to a fixed constant $(1+g)^{n-1-p_\gamma/2}$ (does not go to infinity

"Information Inconsistency" see Liang et al JASA 2008

Mixtures of g priors & Information consistency

- Need $BF \to \infty$ if $\mathrm{R}^2_\gamma \to 1$
- Put a prior on g

$$BF(\gamma : \gamma_0) = \frac{C \int (1+g)^{(n-1-p_\gamma)/2}(1+g(1-R^2_\gamma))^{-(n-1)/2}\pi(g)dg}{C}$$

- interchange limit and integration as $R^2 \to 1$ want

$$\mathrm{E}_g[(1+g)^{(n-1-p_\gamma)/2}]$$

  to diverge
- hyper-g prior (Liang et al JASA 2008)

$$p(g) = \frac{a-2}{2}(1+g)^{-a/2}$$

  or $g/(1+g) \sim Beta(1,(a-2)/2)$
- prior expectation converges if $a > n + 1 - p_\gamma$
- Consider minimal model $p_\gamma = 1$ and $n = 3$ (can estimate intercept, one coefficient, and σ^2, then $a > 3$ integral exists
- For $2 < a \leq 3$ integral diverges and resolves the information paradox!

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- robust prior (Bayarri et al Annals of Statistics 2012

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- Zellner-Siow Cauchy prior $1/g \sim G(1/2, n/2)$
- robust prior (Bayarri et al Annals of Statistics 2012
- Intrinsic prior (Womack et al JASA 2015)

All have prior tails for β that behave like a Cauchy distribution and (the latter 4) marginal likelihoods that can be computed using special hypergeometric functions (${}_2F_1$, Appell F_1)

USair Data

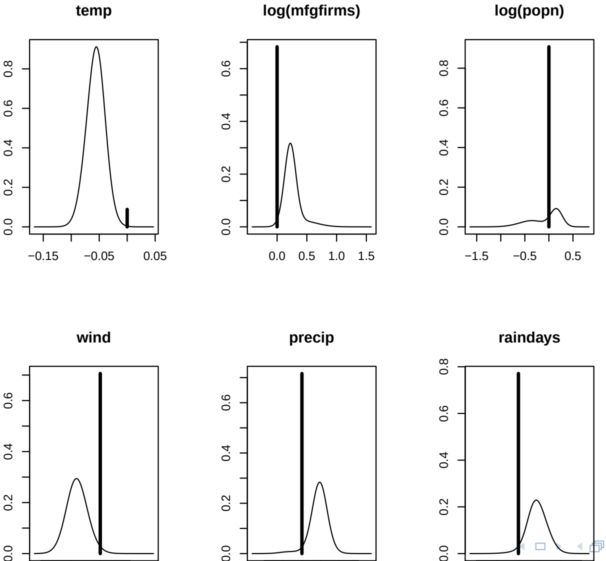
```
> library(BAS)
> data(usair, package="HH")
> poll.bma = bas.lm(log(SO2) ~ temp + log(mfgfirms) +
+                                 log(popn) + wind +
+                                 precip + raindays,
+                     data=usair,
+                     prior="JZS",  #Jeffrey-Zellner-Siow
+                     alpha=nrow(usair), # n
+                     n.models=2^6,
+                     modelprior = uniform(),
+                     method="deterministic")
```

Summary

```
> summary(poll.bma)
                 P(B != 0 | Y) model 1   model 2   model 3   model
Intercept           1.00000000 1.00000 1.0000000 1.0000000 1.000000
temp                0.91158530 1.00000 1.0000000 1.0000000 1.000000
log(mfgfirms)       0.31718916 0.00000 0.0000000 0.0000000 1.000000
log(popn)           0.09223957 0.00000 0.0000000 0.0000000 0.000000
wind                0.29394451 0.00000 0.0000000 0.0000000 1.000000
precip              0.28384942 0.00000 1.0000000 0.0000000 1.000000
raindays            0.22903262 0.00000 0.0000000 1.0000000 0.000000
BF                          NA 1.00000 0.3286643 0.2697945 0.265587
PostProbs                   NA 0.29410 0.0967000 0.0794000 0.078100
R2                          NA 0.29860 0.3775000 0.3714000 0.542700
dim                         NA 2.00000 3.0000000 3.0000000 5.000000
logmarg                     NA 3.14406 2.0313422 1.8339656 1.818248
```

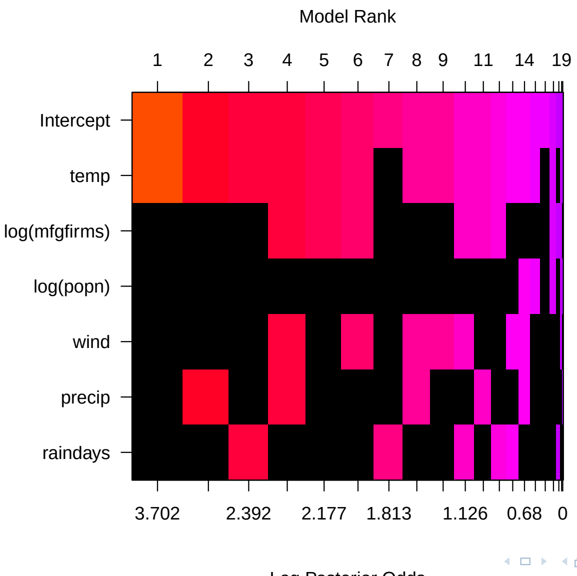
Plots

```
> beta = coef(poll.bma)
> par(mfrow=c(2,3));  plot(beta, subset=2:7,ask=F)
```



Posterior Distribution with Uniform Prior on Model Space

```
> image(poll.bma, rotate=FALSE)
```

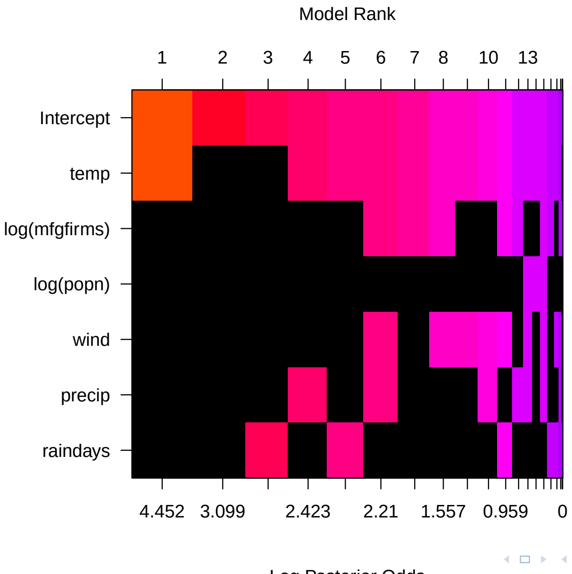


Posterior Distribution with BB(1,1) Prior on Model Space

```
> poll.bb.bma = bas.lm(log(SO2) ~ temp + log(mfgfirms) +
+                               log(popn) + wind +
+                               precip + raindays,
+                    data=usair,
+                    prior="JZS",
+                    alpha=nrow(usair),
+                    n.models=2^6,  #enumerate
+                    modelprior=beta.binomial(1,1))
```

BB(1,1) Prior on Model Space

```
> image(poll.bb.bma, rotate=FALSE)
```



Summary

- Choice of prior on β_γ
- g-priors or mixtures of g (sensitivity)
- priors on the models (sensitivity)
- posterior summaries - select a model or "average" over all models

Diabetes Example from Hoff $p = 64$

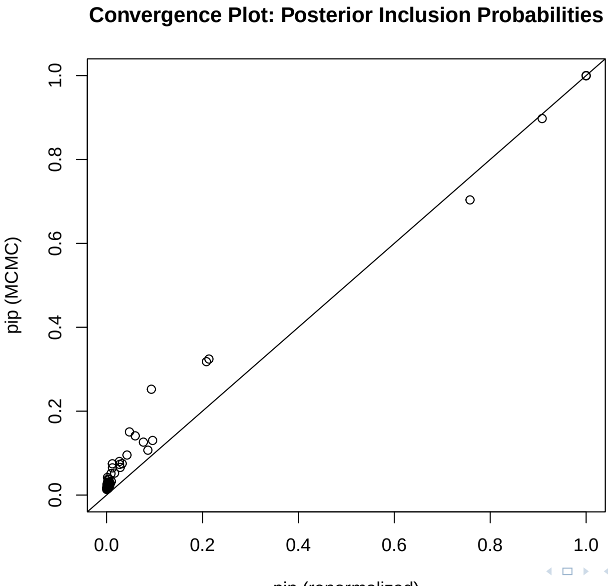
```
> set.seed(8675309)
> source("yX.diabetes.train.txt")
> diabetes.train = as.data.frame(diabetes.train)
> source("yX.diabetes.test.txt")
> diabetes.test = as.data.frame(diabetes.test)
> colnames(diabetes.test)[1] = "y"
> str(diabetes.train)
'data.frame':        342 obs. of  65 variables:
 $ y       : num  -0.0147 -1.0005 -0.1444 0.6987 -0.2222 ...
 $ age     : num  0.7996 -0.0395 1.7913 -1.8703 0.113 ...
 $ sex     : num  1.064 -0.937 1.064 -0.937 -0.937 ...
 $ bmi     : num  1.296 -1.081 0.933 -0.243 -0.764 ...
 $ map     : num  0.459 -0.553 -0.119 -0.77 0.459 ...
 $ tc      : num  -0.9287 -0.1774 -0.9576 0.256 0.0826 ...
 $ ldl     : num  -0.731 -0.402 -0.718 0.525 0.328 ...
 $ hdl     : num  -0.911 1.563 -0.679 -0.757 0.171 ...
 $ tch     : num  -0.0544 -0.8294 -0.0544 0.7205 -0.0544 ...
 $ ltg     : num  0.4181 -1.4349 0.0601 0.4765 -0.6718 ...
```

MCMC with BAS

```
> library(BAS)
> diabetes.bas = bas.lm(y ~ ., data=diabetes.train,
+                              prior = "JZS",
+                              method="MCMC",
+                              n.models = 10000,
+                              MCMC.iterations=150000,
+                              thin = 10,
+                              initprobs="eplogp",
+                              force.heredity=FALSE)
> system.time(bas.lm(y ~ ., data=diabetes.train,
+                        prior = "JZS",
+                        method="MCMC", n.models = 10000,
+                        MCMC.iterations=150000,
+                        thin = 10,  initprobs="eplogp",
+                        force.heredity=FALSE))
   user  system elapsed
  6.464   0.261   6.729
>
```

Diagnostics

```
> diagnostics(diabetes.bas, type="pip")
```

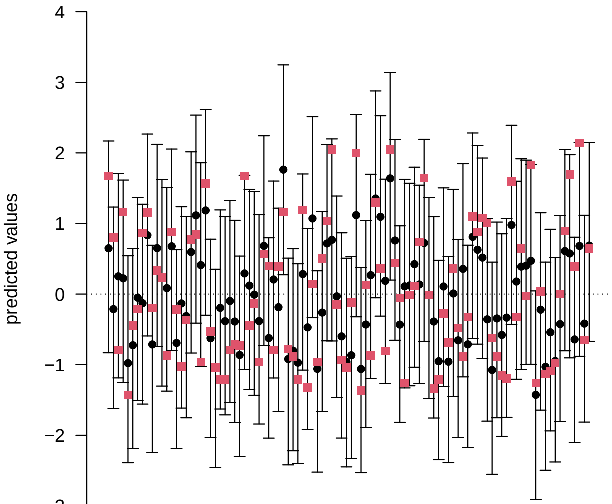


Prediction

```
> pred.bas = predict(diabetes.bas,
+                    newdata=diabetes.test,
+                    estimator="BMA",
+                    se=TRUE)
> mean((pred.bas$fit- diabetes.test$y)^2)
[1] 0.4552798
> ci.bas = confint(pred.bas);
> coverage = mean(diabetes.test$y > ci.bas[,1] & diabetes.te
> coverage
[1] 1
```

95% prediction intervals

```
> plot(ci.bas); points(diabetes.test$y, col=2, pch=15)
NULL
```



Selection and Prediction

- BMA - optimal for squared error loss Bayes
- HPM: Highest Posterior Probability model (not optimal for prediction) but for selection
- MPM: Median Probabilty model (select model where PIP $>$ 0.5) (optimal under certain conditions; nested models)
- BPM: Best Probability Model - Model closest to BMA under loss (usually includes more predictors than HPM or MPM)

Selection

```
> pred.bas = predict(diabetes.bas,
+                    newdata=diabetes.test,
+                    estimator="BPM",
+                    se=TRUE)
> #MSE
> mean((pred.bas$fit- diabetes.test$y)^2)
[1] 0.4740667
> #Coverage
> ci.bas = confint(pred.bas)
> mean(diabetes.test$y > ci.bas[,1] &
+      diabetes.test$y < ci.bas[,2])
[1] 0.98
```

Alternatives to MCMC

- "Stochastic Search" (no guarantee samples represent posterior)

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-
- If $p > n$, can use a generalized inverse, but requires care for prior on γ!

Model averaging versus Model Selection – what are objectives?

Effect Estimation

- Coefficients in each model are adjusted for other variables in the model
- OLS: leave out a predictor with a non-zero coefficient then estimates are biased!
- Model Selection in the presence of high correlation, may leave out "redundant" variables;
- improved MSE for prediction (Bias-variance tradeoff)
- in BMA all variables are included, but coefficients are shrunk to 0
- Care needed for "causal" questions and confounder adjustment! With confounding, should not use plain BMA. Need to change prior to include potential confounders (advanced topic)