Module 11: Linear Regression, the g-prior, and model selection

Rebecca C. Steorts

Hoff, Chapter 9

Agenda

- Review of the Multivariate setup
- The g-prior
- ▶ Application to diabetes (Hoff, 9.2)
- ► Bayesian model selection (g-prior)
- ► Bayesian model averaging

Notation

- $ightharpoonup X_{n \times p}$: regression features or covariates (design matrix)
- $\mathbf{x}_{p\times 1}$: ith row vector of the regression covariates
- $\mathbf{y}_{n\times 1}$: response variable (vector)
- \triangleright $\beta_{p\times 1}$: vector of regression coefficients

Multivariate Setup

Let's assume that we have data points (x_i, y_i) available for all i = 1, ..., n.

 \triangleright y is the response variable

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}_{n \times 1}$$

x_i is the *i*th row of the design matrix $X_{n \times p}$.

Consider the regression coefficients

$$\beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}_{p \times 1}$$

Multivariate Setup

$$y \mid X, \beta, \sigma^2 \sim MVN(X\beta, \sigma^2 I)$$

 $\beta \sim MVN(\beta_0, \Sigma_0)$

Recall the posterior can be shown to be

$$\beta \mid \mathbf{y}, \mathbf{X} \sim MVN(\beta_n, \Sigma_n)$$

where

$$\beta_n = E[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\Sigma_o^{-1} + (X^T X)^{-1} / \sigma^2)^{-1} (\Sigma_o^{-1} \beta_0 + \mathbf{X}^T \mathbf{y} / \sigma^2)$$

$$\Sigma_n = \text{Var}[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\Sigma_n^{-1} + (X^T X)^{-1}/\sigma^2)^{-1}$$

How do we specify β_0 and Σ_0 ?

The g-prior

To do the *least amount of calculus*, we can put a *g-prior* on β .

The g-prior on β has the following form:

$$\beta \mid \mathbf{X} \sim MVN(0, g \ \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}),$$

where g is a constant, such as g = n.

The prior also happens to be invariant and is widely studied for regression problems (Zellner, 1986).

We will find that

- g shrinks the coefficients and can prevent overfitting to the data
- 2. if g=n, then as n increases, inference approximates that using $\hat{\beta}_{ols}$

The g-prior

Under the g-prior, it follows that

$$\beta_n = E[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2]$$

$$= \left(\frac{X^T X}{g \sigma^2} + \frac{X^T X}{\sigma^2}\right)^{-1} \frac{X^T y}{\sigma^2}$$
(2)

$$= \frac{g}{g+1} (X^T X)^{-1} X^T y = \frac{g}{g+1} \hat{\beta}_{ols}$$
 (3)

$$\Sigma_{n} = \operatorname{Var}[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^{2}]$$

$$= \left(\frac{X^{T}X}{g\sigma^{2}} + \frac{X^{T}X}{\sigma^{2}}\right)^{-1} = \frac{g}{g+1}\sigma^{2}(X^{T}X)^{-1}$$

$$= \frac{g}{g+1}\operatorname{Var}[\hat{\beta}_{ols}]$$
(6)

Variance component σ^2

What about a prior on $1/\sigma^2 = \lambda$

$$y \mid X, \beta, \sigma^2 \sim MVN(X\beta, \sigma^2 I)$$
 (7)

$$1/\sigma^2 = \lambda \sim \text{Gamma}(\nu_0/2, \nu_0 \sigma_0^2/2)$$
 (8)

Then the posterior can be shown to be

$$p(\sigma^2 \mid y, X) \sim \text{InverseGamma}([\nu_0 + n]/2, [\nu_0 \sigma_0^2 + SSR_g]/2).$$

1

where SSR_g is somewhat complicated (see Hoff for details, p. 158).

¹This is left as an exercise to be done on your own.

Variance component σ^2

The joint distribution can be written as

$$p(\sigma^2, \beta \mid y, X) = p(\sigma^2 \mid y, X) \times p(\beta \mid y, X, \sigma^2)$$

Goal: simulate $(\sigma^2, \beta) \sim p(\sigma^2, \beta \mid y, X)$

Starting value (β_0, σ_0^2)

1. Simulate

$$\sigma^2 \sim p(\sigma^2 \mid y, X)$$

Give us (σ_1^2, β_0)

2. Use this updated value of σ_1^2 to simulate

$$\beta \sim p(\beta \mid y, X, \sigma_1^2)$$

Gives us (σ_1^2, β_1)

Run the sampler for S iterations.

Application to diabetes (Exercise 9.2, part a)

Suppose we have data on health-related variables of a population of 532 women.

Our goal is to model the conditional distribution of glucose level (glu) as a linear combination of the other variables, excluding the variable diabetes.²

²See Exercise 7.6 for the data description.

Model specification

$$y \mid X, \beta, \sigma^2 \sim MVN(X\beta, \lambda^{-1}I)$$
 (9)

$$\beta \mid \lambda \sim MVN(0, g(X^TX)^{-1}) \tag{10}$$

$$\lambda \sim \mathsf{Gamma}(\nu_0/2, \nu_0 \lambda^{-1}/2) \tag{11}$$

We will use the g-prior, where

- 1. g = n
- 2. $\nu_0 = 1$
- 3. $\sigma_0^2 = \lambda^{-1} = \hat{\sigma}_{ols} = 8.54$

Fit a regression model using the g-prior with g = n, ν_0 = 2 and σ_0^2 = 1. Obtain posterior confidence intervals for all of the parameters.

Section 9.2.2 (Hoff) shows that under the g prior, $p(\sigma^2 \mid \mathbf{y}, \mathbf{X})$ and $p(\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2)$ are inverse gamma and multivariate normal distributions respectively.

Therefore samples from the joint posterior $p(\sigma^2, \beta \mid \mathbf{y}, \mathbf{X}, \sigma^2)$ can be made with a Monte Carlo approximation.

We first center and scale all the variables so that there is no need to include an intercept in the model.

```
#library(knitr)
#rm(list=ls())
azd_data = read.table("azdiabetes.dat", header = TRUE)
head(azd_data)
```

```
npreg glu bp skin bmi ped age diabetes
##
## 1
        5
          86 68 28 30.2 0.364 24
                                        Nο
        7 195 70 33 25.1 0.163 55
                                       Yes
## 2
        5 77 82 41 35.8 0.156 35
                                        No
## 3
## 4
        0 165 76 43 47.9 0.259 26
                                        No
## 5
        0 107 60 25 26.4 0.133 23
                                        Nο
        5 97 76 27 35.6 0.378 52
                                       Yes
## 6
```

```
y = azd_data$glu
# remove glu and diabetes
X = as.matrix(azd_data[,c(-2,-8)])
head(X)
```

```
## npreg bp skin bmi ped age
## [1,] 5 68 28 30.2 0.364 24
## [2,] 7 70 33 25.1 0.163 55
## [3,] 5 82 41 35.8 0.156 35
## [4,] 0 76 43 47.9 0.259 26
## [5,] 0 60 25 26.4 0.133 23
## [6,] 5 76 27 35.6 0.378 52
```

Standardization

```
# standardize data to have mean 0 and variance 1
ys = scale(y)
Xs = scale(X)
n = dim(Xs)[1]
p = dim(Xs)[2]
```

Hyper-parameters

```
g = n
nu0 = 2
s20 = 1
```

Intermediate Matrices

```
# intermediate matrices
Hg = (g/(g+1)) * Xs %*% solve(t(Xs) %*% Xs) %*% t(Xs)
SSRg = t(ys) %*% ( diag(1,nrow=n) - Hg ) %*% ys
```

Monte carlo

```
# number of posterior samples
S = 1000

# generate posteriors
# we know that the sigma2 is
# an updated inverse gamma
s2 = 1/rgamma(S, (nu0+n)/2, (nu0*s20 + SSRg)/2)
head(s2)
```

[1] 0.8757964 0.8670699 0.8333923 0.8522915 0.8581030 0

Monte carlo

```
# updated posterior mean and variance
# from using the q-prior (see slide 7)
Vb = g*solve(t(Xs) %*% Xs)/(g+1)
Eb = Vb %*% t(Xs) %*% ys
E = matrix(rnorm(S*p, 0, sqrt(s2)), S, p)
# use cholesky factorization
beta s = t(t(E \% * \% chol(Vb)) + c(Eb))
# transform coefficients to the original scale
sd X = apply(X,2,sd)
Beta a = sweep(beta s,2,sd X,FUN = "/")
```

The 95% posterior confidence intervals

```
# 95% credible interval

(Beta_CIa = apply(Beta_a, 2, quantile, c(0.025, 0.975)))
```

```
#kable(data.frame(Beta_CIa))
```

Model selection

- Often we have a large number of covariates.
- Using all of them induces poor statistical performance.
- How can we reduce the covariates and have good inference and prediction?
- ▶ Common method: Backwards and stepwise regression (slow).

Model selection

Suppose that we believe some of the regression coefficients are 0.

Come up with a prior distribution that reflects the probability of this occuring.

Consider

$$y_i = z_1 b_1 x_{i,1} + \dots z_p b_p x_{i,p},$$

where b_p is a real number and z_j indicate which regression coefficients are nonzero.

Note: $\beta_j = b_j \times z_j$.

Bayesian model selection

Bayesian model selection works by obtaining a posterior distribution for z.

Assume a prior p(z).

Then

$$p(z \mid Y, X) = \frac{p(z)p(Y \mid X, z)}{\sum_{z} p(z)p(Y \mid X, z)}$$

Bayesian model selection

Suppose we want to compare two models z_a and z_b . Consider

$$odds(z_a, z_b \mid \mathbf{Y}, \mathbf{X}) = \frac{p(z_a \mid \mathbf{Y}, \mathbf{X})}{p(z_b \mid \mathbf{Y}, \mathbf{X})} = \frac{p(z_a)}{p(z_b)} \times \frac{p(\mathbf{Y} \mid \mathbf{X}, z_a)}{p(\mathbf{Y} \mid \mathbf{X}, z_b)}$$

This is posterior odds = prior odds \times "Bayes factor"

"Bayes factor": how much do the data favor model z_a over model z_b

To obtain a posterior distribution over models, we must compute $p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z})$ for each model under consideration.

Bayesian model selection

We must compute

$$p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}) = \int \int p(\mathbf{Y}, \beta, \sigma^2, | \mathbf{X}, \mathbf{z})$$

$$\int \int p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}) p(\beta \mid \mathbf{X}, \mathbf{z}) p(\sigma^2).$$
(12)

To do the least amount of calculus, we can put a g-prior on eta

$$\boldsymbol{\beta} \mid \boldsymbol{X}, \boldsymbol{z} \sim MVN(0, g \ \sigma^2(\boldsymbol{X}^T \boldsymbol{X})^{-1}).$$

Back to the g-prior

Given the g-prior

$$\beta \mid \mathbf{X}, \mathbf{z} \sim MVN(0, g \ \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}),$$

 $p(Y \mid X, z)$ can be worked out in closed form (details p. 165).

Go through the details on your own.

Back to the g-prior

This results in being able to compute

$$\frac{p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}_a)}{p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}_b)} = (1+n)^{(p_{z_b} - p_{z_a})/2} \times \left(\frac{s_{z_a}^2}{s_{z_b}^2}\right)^{1/2} \times \left(\frac{s_{z_b}^2 + SSR_g^{z_b}}{s_{z_a}^2 + SSR_g^{z_a}}\right)^{(n+1)/2} \tag{14}$$

We have a ratio of the marginal probabilities, giving us a balance between model complexity and model fit.

Suppose p_{z_b} is large compared to p_{z_a} .

This causes a penalization of model z_b

Note that a large value of $SSR_g^{z_a}$ compared with $SSR_g^{z_b}$ will penalize model z_a .

29 / 47

Suppose that we have an estimate of β from which we can make predictions.

We may also want a list of relatively high probablity models. We can use a Markov chain to search through the space of models for values of z with high posterior probability.

Suppose p is large. Then 2^p models to consider.

Instead let's use a Gibbs sampler to search through the space of models for values where z has a high posterior probability.

Generate a new value of z via

$$p(z_j \mid \boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{z}_{-j}).$$

The full conditional that $z_j = 1$ can be written as $o_j/(o_j + 1)$.

$$o_j = \frac{p(z_j = 1 \mid \boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{z}_{-j})}{p(z_j = 0 \mid \boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{z}_{-j})}$$
(16)

$$= \frac{p(z_j = 1)p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}_{-j}, z_j = 1)}{p(z_j = 0)p(\mathbf{Y} \mid \mathbf{X}, \mathbf{z}_{-j}, z_j = 0)}$$
(17)

Note: we may also want to obtain posterior samples of β and σ^2 .

Using the conditional distributions from Section 9.2, we can sample from these directly.

The Gibbs sampling scheme requires using Section 9.2 and 9.3 (covered in lab).

$$egin{aligned} oldsymbol{z}^{(s)} & \longrightarrow \sigma^{2(s)} & \longrightarrow oldsymbol{eta}^{(s)} \ & \downarrow & & \\ oldsymbol{z}^{(s+1)} & \longrightarrow \sigma^{2(s+1)} & \longrightarrow oldsymbol{eta}^{(s+1)} \end{aligned}$$

Figure 1: Start with $\mathbf{z}^{(s)}$. Then in random order update z_j from its full conditional.

Generate

$$\{\mathbf{z}^{(s+1)}, \sigma^{2(s+1)}, \boldsymbol{\beta}^{(s+1)}\}$$
:

- 1. Set $z = z^{(s)}$
- 2. For $j \in \{1, \dots, p\}$ in random order, replace z_j with a sample from

$$p(z_j \mid \boldsymbol{z}_{-j}, \boldsymbol{Y}, \boldsymbol{X})$$

- 3. Set $z^{(s+1)} = z^{(s)}$
- 4. Sample $\sigma^{2(s)} \sim p(\sigma^2 \mid \boldsymbol{z}^{(s+1)}, \boldsymbol{Y}, \boldsymbol{X})$
- 5. Sample $\boldsymbol{\beta}^{(s+1)} \sim p(\boldsymbol{\beta} \mid \boldsymbol{z}^{(s+1)}, \sigma^{2(s+1)}, \boldsymbol{Y}, \boldsymbol{X})$

Let's perform Bayesian model averaging (as described in Section 9.3)

Obtain $P(\beta_j \neq 0 \mid y)$ as well as posterior confidence intervals for all of the parameters. Compare our results to that in part (a.)

The following function 1py.X calculates the log of $p(y \mid X)$, which we will use in implementing the Gibbs sampler for Bayesian model averaging.

Let z be the random binary vector of variable indicators. Generating samples of $p(z, \sigma^2, \beta)$ from the joint posterior distribution is achieved with the following steps:

- 1. For $j \in \{1, ..., p\}$ in random order, draw z_j from $p(z_j \mid \mathbf{z}_{-j}, \mathbf{y}, \mathbf{X})$.
- 2. Sample $\sigma^2 \sim p(\sigma^2 \mid \boldsymbol{z}, \boldsymbol{y}, \boldsymbol{X})$.
- 3. Sample $\beta \sim p(\beta \mid \boldsymbol{z}, \sigma^2, \boldsymbol{y}, \boldsymbol{X})$.

MCMC setup

```
g = n
nu0 = 1 # unit information prior
z = rep(1, p)
# picking a starting value for the marginal probability
lpy.c = lpy.X(ys, Xs[,z==1,drop=FALSE])
S = 10
Z = matrix(NA, S, p)
B = matrix(0, S, p)
```

Gibbs sampler

L-+- - - P %-0/ -L-1 (IIL) + - (PL)

```
## Gibbs sampler
for(s in 1:S){
  # if(s %% 100 ==0) {print(s)}
  \# sample z
 for (j in sample(1:p)){
    zp = z
    zp[j] = 1 - zp[j]
   lpy.p = lpy.X(ys,Xs[, zp==1, drop=FALSE])
   r = (lpv.p - lpv.c) * (-1)^(zp[i]==0)
    zp[j] = rbinom(1, 1, 1/(1+exp(-r)))
   if(z[j] == zp[j]) \{lpy.c = lpy.p\}
 }
 Z[s.] = z
  # sample s2
 pm = sum(z==1) # number of nonzero variables in the model
 if (pm==0){
   Hg = 0
    s20 = mean(v^2)
 if (pm>0){
    Hg = (g/(g+1)) * Xs[,z=1,drop=F] %% solve(t(Xs[,z=1,drop=F]) %%
      Xs[,z=1,drop=F]) %*% t(Xs[,z=1,drop=F])
    # estimated residual variance from OLS
    s20=summary(lm(ys \sim -1+Xs[,z==1,drop=F]))sigma^2
                                                                                            }
 SSRg = t(ys) %*% ( diag(1,nrow=n) - Hg ) %*% ys
 s2 = \frac{1}{rgamma}(1, (nu0+n)/2, (nu0*s20 + SSRg)/2)
  \# Sigma2[s] = s2
  # sample beta
 Vb = g * solve(t(Xs[,z=1,drop=F]) %*% Xs[,z=1,drop=F])/(g+1)
 Eb = Vb \% t(Xs[z=1.drop=F]) \% vs
 E = rnorm(p, 0, sqrt(s2))
```

Let z be the random binary vector of variable indicators. Generating samples of $p(z, \sigma^2, \beta)$ from the joint posterior distribution is achieved with the following steps:

- 1. For $j \in \{1, ..., p\}$ in random order, draw z_j from $p(z_j \mid \mathbf{z}_{-j}, \mathbf{y}, \mathbf{X})$.
- 2. Sample $\sigma^2 \sim p(\sigma^2 \mid \boldsymbol{z}, \boldsymbol{y}, \boldsymbol{X})$.
- 3. Sample $\beta \sim p(\beta \mid \boldsymbol{z}, \sigma^2, \boldsymbol{y}, \boldsymbol{X})$.

MCMC setup

```
g = n
nu0 = 1 # unit information prior
z = rep(1, p)
# picking a starting value for the marginal probability
lpy.c = lpy.X(ys, Xs[,z==1,drop=FALSE])
S = 10
Z = matrix(NA, S, p)
B = matrix(0, S, p)
```

Gibbs sampler

L-+- - - P %-0/ -L-1 (IIL) + - (PL)

```
## Gibbs sampler
for(s in 1:S){
  # if(s %% 100 ==0) {print(s)}
  \# sample z
 for (j in sample(1:p)){
    zp = z
    zp[j] = 1 - zp[j]
   lpy.p = lpy.X(ys,Xs[, zp==1, drop=FALSE])
   r = (lpv.p - lpv.c) * (-1)^(zp[i]==0)
    zp[j] = rbinom(1, 1, 1/(1+exp(-r)))
   if(z[j] == zp[j]) \{lpy.c = lpy.p\}
 }
 Z[s.] = z
  # sample s2
 pm = sum(z==1) # number of nonzero variables in the model
 if (pm==0){
   Hg = 0
    s20 = mean(v^2)
 if (pm>0){
    Hg = (g/(g+1)) * Xs[,z=1,drop=F] %% solve(t(Xs[,z=1,drop=F]) %%
      Xs[,z=1,drop=F]) %*% t(Xs[,z=1,drop=F])
    # estimated residual variance from OLS
    s20=summary(lm(ys \sim -1+Xs[,z==1,drop=F]))sigma^2
                                                                                            }
 SSRg = t(ys) %*% ( diag(1,nrow=n) - Hg ) %*% ys
 s2 = \frac{1}{rgamma}(1, (nu0+n)/2, (nu0*s20 + SSRg)/2)
  \# Sigma2[s] = s2
  # sample beta
 Vb = g * solve(t(Xs[,z=1,drop=F]) %*% Xs[,z=1,drop=F])/(g+1)
 Eb = Vb \% t(Xs[z=1.drop=F]) \% vs
 E = rnorm(p, 0, sqrt(s2))
```

Results

The posterior probability $\Pr(\beta_j \neq 0 \mid \mathbf{y})$ is listed below for each predictor. Clearly all predictors are highly relevant to the response.

Results

The 95% posterior confidence intervals for all the parameters from Bayesian model averaging are listed below. The results are similar to those in part (a) because all the predictors are included in each iteration of Gibbs sampler all the time.

```
# transform coefficients to the original scale
#sd_X = apply(X,2,sd)
Beta_b = sweep(B,2,sd_X,FUN = "/")
# 95% credible interval
(Beta_CIb = apply(Beta_b, 2, quantile, c(0.025, 0.975)))
```

```
## 2.5% -0.042519364 0.001655628 0.000852291 0.008325769 0.1528408
## 97.5% -0.005436068 0.011930977 0.012194821 0.032696996 0.5228464
## [,6]
## 2.5% 0.01926098
## 97.5% 0.02791644
```

Preparation for Final Exam

- ► May 1, 7 10 PM, Old Chem 116 PM
- Similar format to other exams
- Closed note, closed book
- No calculators
- ► No pseudo-code

Material

- The exam will be cumulative
- ► There will be an emphasis on what we covered after Exam II
- You must take the final exam to pass the course
- No make up exams will be given

Material after Exam II

(Modules 8 - 11)

- Gibbs sampling
- Data augmentation (latent variable models)
- Gaussian mixture models (with latent variables)
- Entity resolution lecture
- Multivariate distributions and multivariate modeling
- Missing data
- Linear regression
- ► The g-prior
- Model selection

You have many practice exercises posted on this material and the cumulative material with solutions.