Module 10: Linear Regression, the g-prior, and model selection

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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

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

Multivariate Setup

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

- $\boldsymbol{y}$ is the response variable

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

- $\mathbf{x}_i$ is the ith row of the design matrix $X_{n \times p}$.

Consider the regression coefficients

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

Multivariate Setup

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

$$\boldsymbol{\beta} \sim MVN(\beta_0, \Sigma_o)$$

Recall the posterior can be shown to be

$$\boldsymbol{\beta} \mid \boldsymbol{y}, X, \sigma^2 \sim MVN(\boldsymbol{\beta}_n, \Sigma_n)$$

where

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

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

How do we specify a prior on β_0 and Σ_o?

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:

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

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

1. 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

$$\beta_n = E[\beta \mid \boldsymbol{y}, \boldsymbol{X}, \sigma^2] \tag{1}$$

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

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

$$\Sigma_n = \mathrm{Var}[\beta \mid \boldsymbol{y}, \boldsymbol{X}, \sigma^2] \tag{4}$$

$$= \left(\frac{X^T X}{g\sigma^2} + \frac{X^T X}{\sigma^2} \right)^{-1} = \frac{g}{g+1}\sigma^2 (X^T X)^{-1} \tag{5}$$

$$= \frac{g}{g+1}\mathrm{Var}[\hat{\beta}_{ols}] \tag{6}$$

Variance component σ^2

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

$$y \mid X, \beta, \sigma^2 \sim MVN(X\beta, \sigma^2 I) \tag{7}$$
$$1/\sigma^2 = \lambda \sim \text{Gamma}(\nu_0/2, \nu_0\sigma_0^2/2) \tag{8}$$

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).

[1] This 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)[2]

Run the sampler for S iterations.

[2]Here, β_1 should not be confused as the first component of the vector of β as here we are taking a draw from the Gibbs sampler.

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.[3]

[3] See Exercise 7.6 for the data description.

Model specification

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

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

$$\lambda \sim \text{Gamma}(\nu_0/2, \nu_0 \sigma_o^2/2) \tag{11}$$

Regression model on the g-prior

Fit a regression model using the g-prior with g = n, $\nu_0 = 2$ and $\sigma_0^2 = 1$. Obtain posterior confidence intervals for all of the parameters.

Regression model on the g-prior

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

Regression model on the g-prior

Therefore samples from the joint posterior $p(\sigma^2, \beta \mid \boldsymbol{y}, \boldsymbol{X}, \sigma^2)$ 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.

Regression model on the g-prior

```
#library(knitr)
#rm(list=ls())
azd_data = read.table("data/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       No
## 2     7 195 70   33 25.1 0.163  55      Yes
## 3     5  77 82   41 35.8 0.156  35       No
## 4     0 165 76   43 47.9 0.259  26       No
## 5     0 107 60   25 26.4 0.133  23       No
## 6     5  97 76   27 35.6 0.378  52      Yes
```

Regression model on the g-prior

```
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

```r
# 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] 0.8784369 0.8223900 0.7946847 0.7525878 0.8365229 0.
```

Monte carlo

```
# updated posterior mean and variance
# from using the g-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)))
```

```
##                 npreg            bp          skin           bmi       ped
## 2.5%  -0.051440018 -0.000798163 -0.003680508 0.005785437 0.1080511 0
## 97.5%  0.009515118  0.014099574  0.016031888 0.035282060 0.5689523 0
```

```
#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

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

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 $\boldsymbol{z}$.

Assume a prior $p(\boldsymbol{z})$.

Then

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

Bayesian model selection

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

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

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 $p(\boldsymbol{Y} \mid \boldsymbol{X}, \boldsymbol{z})$ for *each* model under consideration.

Bayesian model selection

We must compute

$$p(y \mid X, \boldsymbol{z}) = \int \int p(y, \beta, \sigma^2, \mid X, \boldsymbol{z}) \; d\beta \; d\sigma^2 \tag{12}$$

$$\propto \int \int p(y \mid X, \boldsymbol{z}) p(\beta \mid X, \boldsymbol{z}) p(\sigma^2) \; d\beta \; d\sigma^2. \tag{13}$$

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

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

Back to the g-prior

Given the g-prior

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

$p(y \mid X, \boldsymbol{z})$ 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

$$\frac{p(y \mid X, \boldsymbol{z}_a)}{p(y \mid X, \boldsymbol{z}_b)} = (1+n)^{(p_{z_b} - p_{z_a})/2} \times \left(\frac{s^2_{z_a}}{s^2_{z_b}} \right)^{1/2} \tag{14}$$

$$\times \left(\frac{s^2_{z_b} + SSR_g^{z_b}}{s^2_{z_a} + SSR_g^{z_a}} \right)^{(n+1)/2} \tag{15}$$

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.

Bayesian Model Averaging

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

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

Bayesian model averaging

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 $\boldsymbol{z}$ has a high posterior probability.

Generate a new value of $\boldsymbol{z}$ via

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

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

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

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

Bayesian model averaging

Note: we may also want to obtain posterior samples of $\boldsymbol{\beta}$ 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).

Bayesian model averaging

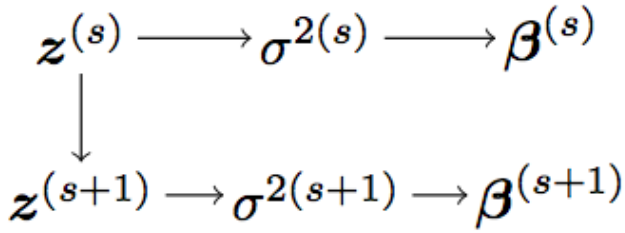

Figure 1: Start with $\boldsymbol{z}^{(s)}$. Then in random order update z_j from its full conditional.

Bayesian model averaging

Generate

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

1. Set $\boldsymbol{z} = \boldsymbol{z}^{(s)}$
2. For $j \in \{1, \ldots, p\}$ in random order, replace z_j with a sample from
$$p(z_j \mid \boldsymbol{z}_{-j}, \boldsymbol{Y}, \boldsymbol{X})$$
3. Set $\boldsymbol{z}^{(s+1)} = \boldsymbol{z}^{(s)}$
4. Sample $\sigma^{2(s)} \sim p(\sigma^2 \mid \boldsymbol{z}^{(s+1)}, \boldsymbol{Y}, \boldsymbol{X})$
5. Sample $\boldsymbol{\beta}^{(s+1)} \sim p(\boldsymbol{\beta} \mid \boldsymbol{z}^{(s+1)}, \sigma^{2(s+1)}, \boldsymbol{Y}, \boldsymbol{X})$

Back to diabetes data (Exercise 9.2, b)

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.)

Back to diabetes data (Exercise 9.2, b)

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

```
## a function to compute the marginal probability
lpy.X <- function(y, X, g=length(y), nu0=1,
                  s20=try(summary(lm(y~ -1+X))$sigma^2, silent=TRUE)){
  n = dim(X)[1]
  p = dim(X)[2]
  if (p==0) { Hg = 0; s20 = mean(y^2)}
  if (p>0){ Hg = (g/(g+1)) * X %*% solve(t(X) %*% X) %*% t(X) }
  SSRg = t(y) %*% ( diag(1, nrow=n) - Hg ) %*% y -
    .5*( n*log(pi) + p*log(1+g) + (nu0+n)*log(nu0*s20 + SSRg) -
           nu0*log(nu0*s20)) +
    lgamma( (nu0+n)/2 ) - lgamma(nu0/2)
}
```

Back to diabetes data (Exercise 9.2, b)

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

1. For $j \in \{1, \ldots, p\}$ in random order, draw z_j from $p(z_j \mid \boldsymbol{z}_{-j}, \boldsymbol{y}, \boldsymbol{X})$.
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

```
## 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 = (lpy.p - lpy.c) * (-1)^(zp[j]==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(y^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 ~ -1+Xs[,z==1,drop=F]))$sigma^2                    }

  SSRg = t(ys) %*% ( diag(1,nrow=n) - Hg ) %*% ys
  s2 = 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]) %*% ys

  E = rnorm(p, 0, sqrt(s2))
  beta.z = E %*% chol(Vb) + c(Eb)
```

Results

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

```
pprob_Z = apply(Z,2,mean)
pprob_Z = data.frame(matrix(pprob_Z,nr=1,nc=p))
names(pprob_Z) = names(azd_data[c(-2,-8)])
row.names(pprob_Z) = 'posterior including probability'

pprob_Z
```

```
##                                 npreg bp skin bmi ped age
## posterior including probability     1  1    1   1   1   1
```

```
#kable(pprob_Z)
```

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)))
```

```
##                [,1]          [,2]         [,3]        [,4]      [,5]
## 2.5%  -0.038197705 -0.0006085138 -0.002280803 0.003181347 0.3057129
## 97.5%  0.001302531  0.0138583425  0.013989194 0.030664721 0.4677377
```