Tutorial Notes 9 of MATH3424

1 Summary of course material

1. Collinearity: the existence of strong linear relationships among the predictor variables

   Typical indications of collinearity

   (a) High R^2, but low p-value for the coefficient estimates.

   (b) Significant estimates F statistic, but low p-value for the coefficient estimates.

   (c) If the estimated coefficient is contrary to prior expectation (which people are confident to be correct).

2. Detection of Collinearity:

   Variance Inflation Factor (VIF): Let R_j^2 be the square of the multiple correlation coefficient that results when the predictor variable X_j is regressed against all the other predictor variables. The variance inflation for X_j is

   only valid in standard linear

   $$\mathrm{VIF}_j = \frac{1}{1-R_j^2}, \quad j = 1, \cdots, p$$

   $$\mathrm{VIF}_j = \left[\left(\frac{\tilde{X}'\tilde{X}}{n-1}\right)^{-1}\right]_{jj}$$

   (a) $\mathrm{VIF}_j \to 1$, X_j is linearly independent of other predictor variables.

   (b) VIF_j large, X_j has a strong linear relationship with the other predictor variables

   (c) VIF exceeding 10 would imply that collinearity may be causing problems.

   (d) $\overline{\mathrm{VIF}} = \frac{1}{p}\sum_{j=1}^{p}\mathrm{VIF}_j$: another index of collinearity

   $$\tilde{Y} = \begin{bmatrix} \tilde{y}_1 \\ \vdots \\ \tilde{y}_n \end{bmatrix} \quad \tilde{X}_j = \begin{bmatrix} \tilde{x}_{j1} \\ \vdots \\ \tilde{x}_{jn} \end{bmatrix}$$

3. Ridge Regression:

   (a) Assume the standardized form of the regression model is given by

   $\tilde{X}_j$, $j=1,\cdots,p$
   $\tilde{Y}$ has sample mean 0 and sample variance 1.

   $$\tilde{Y} = \theta_1\tilde{X}_1 + \theta_2\tilde{X}_2 + \cdots + \theta_p\tilde{X}_p + \varepsilon'$$

   $$\mathbb{E}\tilde{Y} = \tilde{X}\theta$$

   The estimating equations for ridge regression coefficients are

   $$\begin{cases} (1+k)\theta_1 + r_{12}\theta_2 + \cdots + r_{1p}\theta_p = r_{1y}, \\ r_{21}\theta_1 + (1+k)\theta_2 + \cdots + r_{2p}\theta_p = r_{2y}, \\ \quad\vdots \\ r_{p1}\theta_1 + r_{p2}\theta_2 + \cdots + (1+k)\theta_p = r_{py}, \end{cases}$$

   $$s_x = \sqrt{\frac{1}{n-1}\sum(x_i-\bar{x})^2}$$

   where k is the bias parameter, r_{ij} is the correlation between ith and jth predictor variables and $\cancel{r_{ij}}$ r_{iy} is the correlation between ith predictor variable and response variable.

   $$(\underbrace{r_x}_{p\times p} + kI_p)\theta = \underbrace{r_{xY}}_{p\times 1}$$

For x, y

$$r_{xy} \stackrel{\text{def}}{=} \frac{\sum(x_i-\bar{x})(y_i-\bar{y})}{(n-1)s_x s_y} = \frac{1}{n-1}\sum\frac{(x_i-\bar{x})}{s_x}\frac{(y_i-\bar{y})}{s_y}$$

$$\mathbb{E}(\hat\theta) = \mathbb{E}\left[\left(\frac{\tilde X'\tilde X}{n-1}+kI_p\right)^{-1}\frac{\tilde X'\tilde Y}{n-1}\right] = \left(\frac{\tilde X'\tilde X}{n-1}+kI_p\right)^{-1}\frac{\tilde X'}{n-1}\mathbb{E}(\tilde Y)$$

$$= \left(\frac{\tilde X'\tilde X}{n-1}+kI_p\right)^{-1}\frac{\tilde X'\tilde X}{n-1}\theta$$

$$\mathbb{E}(\hat\theta-\theta) = \left(\frac{\tilde X'\tilde X}{n-1}+kI\right)^{-1}\left(\frac{\tilde X'\tilde X}{n-1}-\frac{\tilde X'\tilde X}{n-1}-kI\right)\theta = -k\underline{\left(\frac{\tilde X'\tilde X}{n-1}+kI\right)^{-1}}\theta$$

The solution is given by

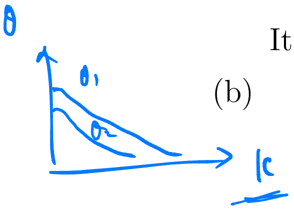
$$\hat\theta = \left(\frac{\tilde X'\tilde X}{n-1}+kI_p\right)^{-1}\frac{\tilde X'\tilde Y}{n-1}$$

when k is large.

$$\mathbb{E}(\hat\theta-\theta) \approx -k\cdot(kI)^{-1}\theta = -\theta$$

$$\mathbb{E}(\hat\theta) \approx 0.$$

It is a biased estimator of θ. (Why?)



(b)

$$\text{Total Variance}(k) = \sum_{j=1}^{p}\text{Var}(\hat\theta_j(k)) = \sigma^2\sum_{j=1}^{p}\frac{\lambda_j}{(\lambda_j+k)^2}$$

(c) Ridge trace to detect collinearity

(d) Selection of bias parameter k: Fixed Point/Iterative Method/Ridge Trace

Remarks on Ridge Regression:

Ridge regression estimates can be obtained by the method of penalized least squares (Why?). The penalized least squares criterion combines the usual sum of squared errors with a pentlty for large regression coefficients:

penalty

$$S(\theta_1,\cdots,\theta_p) = \sum_{i=1}^{n}\left(\tilde y_i - \sum_{j=1}^{p}\theta_j\tilde x_{ij}\right)^2 + (n-1)k\sum_{j=1}^{p}\theta_j^2$$

$$S(\theta_1,\cdots,\theta_p) = \|\tilde Y-\tilde X\theta\|_2^2 + (n-1)k\|\theta\|_2^2$$

$$= (\tilde Y-\tilde X\theta)'(\tilde Y-\tilde X\theta) + (n-1)k\,\theta'\theta$$

$$\frac{\partial S(\theta)}{\partial\theta} = -2\tilde X'(\tilde Y-\tilde X\theta) + 2(n-1)k\theta = 0$$

$$\tilde X'\tilde Y = (n-1)k\theta + \tilde X'\tilde X\theta = (\tilde X'\tilde X + (n-1)kI)\theta$$

$$\hat\theta = (\tilde X'\tilde X + (n-1)kI)^{-1}\tilde X'\tilde Y$$

$$= \left(\frac{\tilde X'\tilde X}{n-1}+kI\right)^{-1}\frac{\tilde X'\tilde Y}{n-1}$$

2 Questions

2.1

Chemical shipment. The data to follow, taken on 20 incoming shipments of chemicals in drums arriving at a warehouse, show number of drums in shipment (X_1), total weight of shipment (X_2, in hundred pounds), and number of minutes required to handle shipment (Y).

i:	1	2	3	...	18	19	20
X_{i1}:	7	18	5	...	21	6	11
X_{i2}:	5.11	16.72	3.20	...	15.21	3.64	9.57
Y_i:	58	152	41	...	155	39	90

(a) Fit the original data by OLS and find the fitted values.

```
Call:
lm(formula = Y ~ ., data = df)

Residuals:
    Min      1Q  Median      3Q     Max 
-8.8353 -3.5591 -0.0533  2.4018 15.1515 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   3.3243     3.1108   1.069      0.3    
X1            3.7681     0.6142   6.135 1.10e-05 ***
X2            5.0796     0.6655   7.632 6.89e-07 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 5.618 on 17 degrees of freedom
Multiple R-squared:  0.9869,	Adjusted R-squared:  0.9854 
F-statistic: 641.6 on 2 and 17 DF,  p-value: < 2.2e-16
```

Figure 1: summary of linear regression by OLS

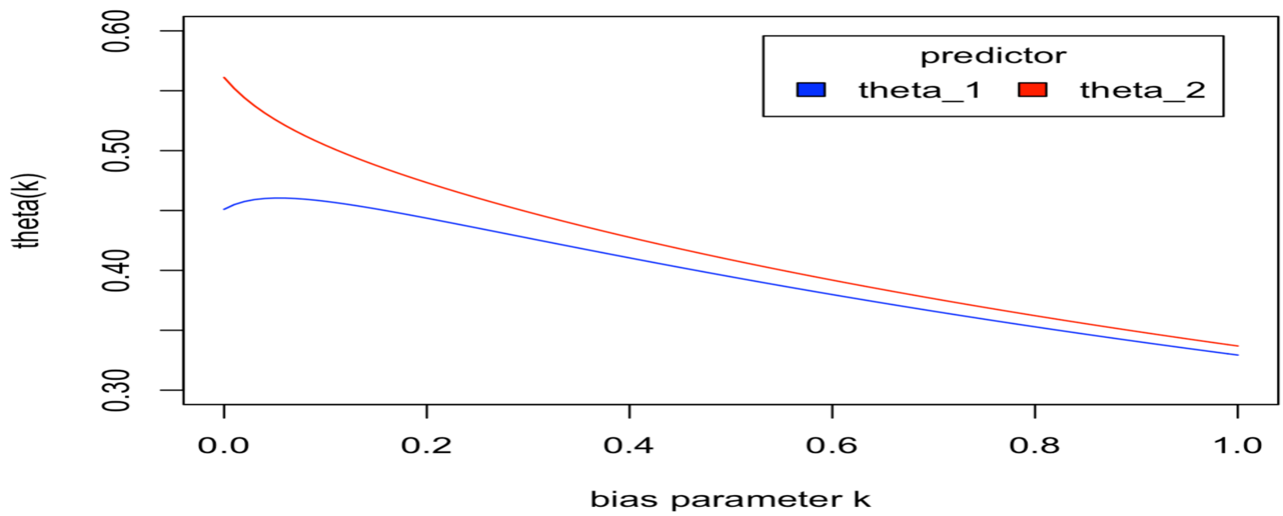
```
        1         2         3         4         5         6         7         8         9        10        11        12        13 
 55.65775 156.08097  38.41952  91.78733 100.54737  42.68637 202.09731  72.94678 117.55927  46.34368 123.35921  96.84849  45.18459 
       14        15        16        17        18        19        20 
 81.30495  56.83527 130.24902 133.56918 159.71512  44.42265  93.38515 
```

Figure 2: fitted value by OLS

(b) Make a ridge trace plot for k values ranging from 0 to 1 with standardized data.

```r
df <- read.table("T9.txt", header = FALSE)
colnames(df) <- c("Y","X1","X2")
df_scale <- as.data.frame(scale(df))
X <- as.matrix(df_scale[,-1])
Y <- as.matrix(df_scale[,1])
n <- length(Y);p <- 2
k_seq <- seq(0,1,length.out = 101)
theta_res <- matrix(0, length(k_seq), p)
for (i in 1:101){
  theta_res[i,c(1,2)]<-solve(t(X)%*%X/(n-1)+k_seq[i]*diag(p))%*%(t(X)%*%Y/(n-1))
  }
theta_res <- cbind(k_seq,theta_res)
plot(theta_res[,1],theta_res[,2], type = "l", col="blue",
     ylim = c(0.3,0.6),xlab = "bias parameter k", ylab = "theta(k)")
lines(theta_res[,1],theta_res[,3], type = "l", col="red")
legend("topright", inset=.05, title="predictor",
       c("theta_1","theta_2"), fill=c("blue","red"), horiz=TRUE)
```

$$\left(\frac{\tilde{X}'\tilde{X}}{n-1} + kI\right)^{-1} \frac{\tilde{X}'\tilde{Y}}{n-1}$$



Now given below are the estimated ridge standardized regression coefficients, the variance inflation factors, ~~and R^2~~ for selected bias parameters k.

k	.000	.005	.01	.05	.07	.09	.10	.20
$\hat{\theta}_1$	.451	.453	.455	.460	.460	.459	.458	.444
$\hat{\theta}_2$	.561	.556	.552	.526	.517	.508	.504	.473
$\mathrm{VIF}_1 = \mathrm{VIF}_2$	7.03	6.20	5.51	2.65	2.03	1.61	1.46	.71

(c) Why are the VIF_1 values the same as the VIF_2 values here?

$$\tilde{Y} \sim \tilde{X}_1 + \tilde{X}_2 \qquad \mathrm{VIF}_1 = \frac{1}{1-\underline{R_1^2}}$$

$$\boxed{R^2 = |\mathrm{Cor}(X, Y)|^2.} \qquad \mathrm{VIF}_2 = \frac{1}{1-\underline{R_2^2}}$$

$$\mathrm{VIF}_j = \left(\frac{\tilde{X}'\tilde{X}}{n-1} + kI\right)^{-1} \frac{\tilde{X}'\tilde{X}}{n-1} \left(\frac{\tilde{X}'\tilde{X}}{n-1} + kI\right)^{-1}$$

$$\mathrm{VIF}_j = \left(\frac{\tilde{X}'\tilde{X}}{n-1}\right)^{-1}, \quad k=0$$

(d) Suggest a reasonable value for the bias parameter k based on the information provided above. What is the estimation of k given by fixed point method?

$$k = \frac{p\,\underline{\hat{\sigma}^2(0)}}{\sum_{j=1}^{p}[\hat{\theta}_j(0)]^2} = 0.05326$$

(e) Transform the estimated standardized regression coefficients using the bias parameter you suggest in part (d) back to the original variables and obtain the fitted values for the 20 cases. How similar are these fitted values to those obtained with the ordinary least squares fit in part (a)?

$$\hat{\beta}_j = \frac{s_y}{s_{x_j}} \cdot \hat{\theta}_j$$

```
m_simple <- lm(Y~.,df)
summary(m_simple)
std <- diag(sqrt(var(df)))
mean_XY <- colMeans(df)
ratio <- std[1]/std[-1]
theta_est <- theta_res[theta_res[,1]==0.05,-1]
beta_est <- ratio*theta_est
beta_0_est <- mean_XY[1]-sum(beta_est*mean_XY[-1])
X_o <- as.matrix(df[,-1])
Y_o <- as.matrix(df[,1])
fitted_ridge <- as.numeric(X_o%*%beta_est+beta_0_est)
names(fitted_ridge) <- c(1:length(fitted_ridge))
fitted_ridge
```

Figure 3: fitted value by ridge

```
        1         2         3         4         5         6         7         8         9        10        11        12        13
 55.65775 156.08097  38.41952  91.78733 100.54737  42.68637 202.09731  72.94678 117.55927  46.34368 123.35921  96.84849  45.18459
       14        15        16        17        18        19        20
 81.30495  56.83527 130.24902 133.56918 159.71512  44.42265  93.38515
```

Figure 4: fitted value by OLS

```
        1         2         3         4         5         6         7         8         9        10        11        12        13
 56.54120 154.14860  39.75123  92.61263  99.88431  43.75176 198.86197  73.37879 117.40364  47.18078 123.15542  96.73016  46.40789
       14        15        16        17        18        19        20
 82.15683  57.95908 128.98746 132.72810 158.49749  45.69351  93.16915
```

Figure 5: fitted value by ridge

2.2

We know from Chapter 3 that in standard multiple linear regression $\mathrm{Cov}(\hat{\beta}) = \sigma^2(X'X)^{-1}$. Show that $\mathrm{Var}(\hat{\beta}_j) \propto \sigma^2 \cdot \mathrm{VIF}_j$ for $j = 1, \cdots, p$.

Hint: You might need to use the following matrix inverse formula for block matrix:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}$$

$$\mathrm{Var}(\hat{\beta}_j) \propto \sigma^2 \cdot \frac{1}{1-R_j^2}$$

$$\mathrm{Var}(\hat{\beta}_j) = \sigma^2 \cdot \frac{1}{(n-1)s_j^2} \cdot \frac{1}{1-R_j^2}$$

$$s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_j - \bar{x})^2$$