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Model Assumptions

Recall the major assumptions we have made in linear regression models

$$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik} + \epsilon_i, \quad i = 1, 2, \dots, n$$

are

- ▶ The relationship between the response and regressors is linear.
- ▶ The error terms ϵ_i have mean zero.
- ► The error terms ϵ_i have constant variance σ^2 (homoscedasticity)
- ▶ The error terms ϵ_i are normally distributed.
- ▶ The error terms ϵ_i and ϵ_j are uncorrelated for $i \neq j$.
- ▶ The regressors x_1, \dots, x_k are nonrandom.
- ▶ The regressors x_1, \dots, x_k are measured without error.
- The regressors are linearly independent.



Multiple linear regression model given a set of n-data is given by

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_k x_{ik} + \epsilon_i, \quad i = 1, \cdots, n$$

and the above equation can be written as

$$y = X\beta + \epsilon$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Using the least squares method, the estimator of $\beta = (\beta_0, \beta_1, \cdots, \beta_k)^T$ is given by

$$\boldsymbol{\hat{eta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

provided that $\mathbf{X}^T\mathbf{X}$ is invertiable.

This will requires that the columns of **X** be linearly independent.

When the predictor variables are dependent (correlated) with each other, then we will have the problem called multicollinearity.



Example

Suppose we have a regression model with the fitted value given by

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3$$

but $x_3 = 4x_1 + 3x_2$.

Then x_3 is redundant and carry no new information. Worst, it will make the estimated slopes in the regression model arbitrary as

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3$$

$$= \hat{\beta}_0 + (\hat{\beta}_1 + 4\hat{\beta}_3) x_1 + (\hat{\beta}_2 + 3\hat{\beta}_3) x_2$$

$$= \hat{\beta}_0 + (\hat{\beta}_2 - \frac{3}{4}\hat{\beta}_1) x_2 + (\hat{\beta}_3 + \frac{\hat{\beta}_1}{4}) x_3$$

$$= \dots$$

Examples of correlated predictor variables are:

- ► A person's height and weight in relation to the body mass index (BMI)
- Level of education and age of a person in relation to their annual salary
- Arm length, leg length, height, weight of a person in relation to their physical strength.



Suppose we have only two predictor variables x_1 and x_2 . Let us consider a regression model

$$y = \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

where x_1, x_2 and y are scaled to unit length, that is $\overline{x}_1 = \overline{x}_2 = 0$ with

$$x_{11}^2 + x_{21}^2 = 1 \ \ \text{and} \ \ x_{12}^2 + x_{22}^2 = 1.$$

Hence with

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}$$
 we see that $\mathbf{X}^T \mathbf{X} = \begin{bmatrix} 1 & r_{12} \\ r_{12} & 1 \end{bmatrix}$

where r_{12} is the correlation between x_1 and x_2

$$r_{12} = \frac{\sum (x_{i1} - \overline{x}_1)(x_{i2} - \overline{x}_2)}{\sqrt{\sum (x_{i1} - \overline{x}_1)^2 \sum (x_{i2} - \overline{x}_2)^2}}$$



From our previous discussion, we have

$$\operatorname{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1} = \frac{\sigma^2}{1 - r_{12}^2} \begin{bmatrix} 1 & -r_{12} \\ -r_{12} & 1 \end{bmatrix}$$

This gives

$$\operatorname{Var}(\hat{\beta}_1) = \frac{\sigma^2}{1 - r_{12}^2} = \operatorname{Var}(\hat{\beta}_2)$$

and

$$\operatorname{Cov}(\hat{\beta}_1, \hat{\beta}_2) = -\frac{r_{12}\sigma^2}{1 - r_{12}^2}.$$

From here we see that

$$\operatorname{Var}(\hat{\beta}_1) = \operatorname{Var}(\hat{\beta}_2) \to \infty$$

as $r_{12} \to 1$ (or -1).

The equation below

$$\operatorname{Var}(\hat{\beta}_1) = \operatorname{Var}(\hat{\beta}_2) \to \infty$$

as
$$r_{12}
ightarrow 1$$
 (or -1)

tell us that when there is a strong multicollinearity, i.e. when $|r_{12}| \approx 1$, we will have a large variances and covariances for the least squares estimators.

Hence a slightly different sample can lead to a vastly different estimates of the model parameters.

When there are more than two predictor variables, multicollinearity produces similar effect.



Another effect of having Multicollinearity in a model is that the parameters tend to be overestimates in magnitude.

For this, we look at $||\hat{\beta} - \beta||^2 = \sum_j (\hat{\beta}_j - \beta_j)^2$. Taking the expectation leads to

$$E\left(||\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}||^2\right) = \sum_{j} E\left[(\hat{\beta}_j - \beta_j)^2\right]$$

$$= \sum_{j} \operatorname{Var}(\hat{\beta}_j)$$

$$= \operatorname{Trace}\left(\operatorname{Var}(\hat{\boldsymbol{\beta}})\right)$$

$$= \sigma^2 \operatorname{Trace}\left((\mathbf{X}^T \mathbf{X})^{-1}\right)$$

$$= \frac{2\sigma^2}{1 - r_{12}^2}$$

The equation

$$E(||\hat{\beta} - \beta||^2) = \frac{2\sigma^2}{1 - r_{12}^2}$$

shows that when there is a strong multicollinearity, $\hat{\pmb{\beta}}$ is far from $\pmb{\beta}$ on average.

Also, we can show that

$$E\left(||\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}||^2\right) = E\left(||\hat{\boldsymbol{\beta}}||^2\right) - ||\boldsymbol{\beta}||^2$$

Therefore

$$E(||\hat{\beta}||^2) = ||\beta||^2 + \frac{2\sigma^2}{1 - r_{12}^2}$$

This implies that when there is a strong multicollinearity, the length of the vector $\hat{\beta}$ is on average, much larger than β .



Multicollinearity Diagnostics

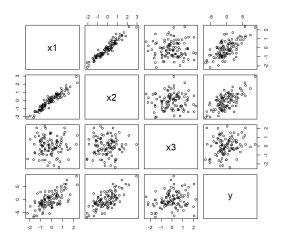
A very simple measure of multicollinearity is the inspection of the scatter plot and correlation matrix.

```
Multicol1<-read.csv("Multicol1.CSV", header=TRUE, sep=",")
x1<-Multicol1$x1
x2<-Multicol1$x2
x3<-Multicol1$x3
y<-Multicol1$y
plot(Multicol1)
#Calculate the correlation matrix
myCorr=cor(Multicol1)
myCorr
            x1
                         x2
                                      x3
x1 1.00000000 0.95257460 0.01582233 0.6732043
x2 0.95257460 1.00000000 0.02461845 0.6911211
x3 0.01582233 0.02461845 1.00000000 0.2165981
   0.67320428 0.69112108 0.21659812 1.0000000
```



Multicollinearity Diagnostics

Just like what we have seen in the covariance matrix, the scatter plot also indicates the collinearity of x_1 and x_2 .





The scatter plot and covariance matrix are bivariate method in the sense that they detect the relationship between two variables.

We now develop a method to detect whether there is a relationship between one predictor with a linear combination of the rest of the predictors.

For that, we regress each single predictor x_j , $j=1,\cdots,k$ on the remaining ones, i.e.

$$x_j \sim x_1 + \cdots + x_{j-1} + x_{j+1} + \cdots + x_k$$

and compute the corresponding coefficients of determination R_j^2 .



From

$$x_j \sim x_1 + \cdots + x_{j-1} + x_{j+1} + \cdots + x_k$$

the value of R_j^2 tells us how well is x_j describable by the other variables.

Hence a large value of R_j^2 indicates strong linear dependence of x_j on the other predictors.

This then implies that there is multicollinearity of the predictors in the model.



Instead of comparing each R_j^2 , we define the variance inflation factors (VIF) of the predictors as

$$VIF_j = \frac{1}{1 - R_j^2}$$

Notice that with VIF_i so defined,

 \blacktriangleright when x_i is nearly a combination of the other predictors:

$$R_j^2 \approx 1$$
 hence VIF_j is large

 \blacktriangleright when x_i is orthogonal to all the other predictors:

$$R_j^2 = 0$$
 hence $VIF_j = 1$



In general,

$$VIF_j = \frac{1}{1 - R_i^2}$$

the larger these factors are, the more worry you should be about having multicollinearity in the model. As a rule of thumb:

If $VIF_j > 4$ we should investigate, while

If $VIF_j > 10$ we should act and remediate.

Running the VIF on R

We see that x_1 and x_2 have a high VIF value, the result is in accordance to previous diagnostic analysis using scatter plot and the covariance matrix.



Dealing with Multicollinearity

When dealing with multicollinearity, these are the strategies that one can try:

- Collecting additional data to break up the multicollinearity in the existing data.
- Model respecification.
 - (i) If x_1, x_2 and x_3 are nearly linearly dependent, it may be possible to find some function such as $x = (x_1 + 2x_2)/x_3$ that preserves the original predictors but reduces the ill-conditioning.
 - (ii) Variable elimination: If x_1, x_2 and x_3 are nearly linearly dependent, eliminating one of the predictor (say x_1) may help in reducing the effect of multicollinearity.



As we have observed in the previous slide. When a data contains multicollinearity, the magnitude of β will be inflated (on average).

This implies that the confidence intervals for the slope parameters will tend to be wide and estimation of the slopes will be unstable.



The main idea behind ridge regression is to add a small bias to help shrinks the estimated coefficients towards zero to fix the magnitude inflation.

That is, we find the minimum of

$$S = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ji} \right)^2 + \lambda \sum_{j=1}^{k} (\beta_j)^2$$

The added term

$$\lambda \sum_{j=1}^{k} (\beta_j)^2$$

is the penalty that shrinks our coefficients.



In the minimization of S below

$$S = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ji} \right)^2 + \lambda \sum_{j=1}^{k} (\beta_j)^2$$

the parameter λ needs to fit the linear model and shrinking the coefficients.

The selection of λ will be done by using the smallest value of Generalized Cross Validation (GCV) value.



Remark:

We need to perform unit normal scaling on the columns of \boldsymbol{X} before performing ridge regression.

This is because the penalty term would be unfair to other predictors if they are not on the same scale.



Looking at the same data set Multicol1.csv, we create a unit normal scaling on the column of ${\bf X}$ as follows:

```
Multicol1<-read.csv("Multicol1.Csv", header=TRUE, sep=",")
x1<-Multicol1$x1
x2<-Multicol1$x2
x3<-Multicol1$x3
y<-Multicol1$y

#Standardize each variable(subtract mean, divided by sd)
Multicol1s=data.frame(scale(Multicol1))

xs1<-Multicol1s$x1
xs2<-Multicol1s$x2
xs3<-Multicol1s$x3
y<-Multicol1$$y
```

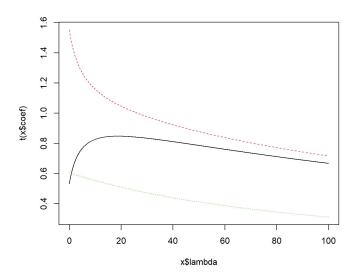


The ridge regression in R is performed as follows:

```
#Ridge Regression
install.packages('MASS')
library(MASS)

reg_seq=seq(0,100,0.001)
fit=lm.ridge(y~xs1+xs2+xs3, lambda = reg_seq)
plot(fit)
```

From the values we tried for various λ , we see how the coefficients shrink as λ grows larger:





Using select(fit) we obtain the following outputs:

```
> select(fit)
modified HKB estimator is 1.471051
modified L-W estimator is 0.9599733
smallest value of GCV at 9.806
```

We will use the smallest value of Generalized Cross Validation (GCV) to be the value of our λ . This gives $\lambda=9.806$ Running the ridge regression with this λ gives