# Data modeling: CSCI E-106

**Applied Linear Statistical Models** 

Chapter 10 – Building the Regression Model II: Diagnostic

## Overview

- a number of refined diagnostics for checking the adequacy of a regression model
  - detecting improper functional form for a predictor variable
  - outliers
  - influential observations
  - multicollinearity

## Added Variable Plots

#### **Previous**

- Chap. 3,6: check whether a curvature effect for that variable is required in the model
- the residual plots vs. the predictor variables: determine whether it would be helpful to add one or more of these variables to the model

#### Limitation:

 not properly show the nature of the marginal effect of a predictor variable, given the other predictor variables in the model

- partial regression plots or adjusted variable plots; provide graphic information about the marginal importance of a predictor variable  $X_k$ , given the other predictor variables already in the model
- In an added-variable plot, both Y and  $X_k$  under consideration are regressed against the other predictor variables and residuals are obtained for each.
- the plot of these residuals:
  - the marginal importance of this variable in reducing the residual variability
  - provide information about the nature of the marginal regression relation for  $X_k$  under consideration for possible inclusion in the regression model

• Illustration: the regression effect for  $X_1$ , given that  $X_2$  is already in the model

regress Y on X<sub>2</sub>

$$\hat{Y}_{i}(X_{2}) = b_{0} + b_{2}X_{i2} 
e_{i}(Y|X_{2}) = Y_{i} - \hat{Y}_{i}(X_{2})$$

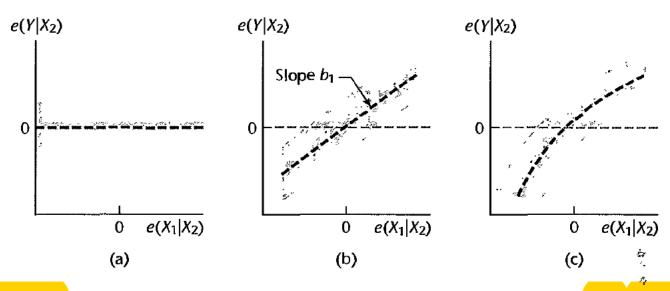
regress X<sub>1</sub> on X<sub>2</sub>

$$\hat{X}_{i1}(X_2) = b_0^* + b_2^* X_{i2}$$

$$e_i(X_1|X_2) = X_{i1} - \hat{X}_{i1}(X_2) \bigcirc$$

 $\Rightarrow$ added variable for predictor variable  $X_1$ :

Plot 
$$e(Y|X_2)$$
 vs  $e(X_1|X_2)$ 

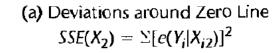


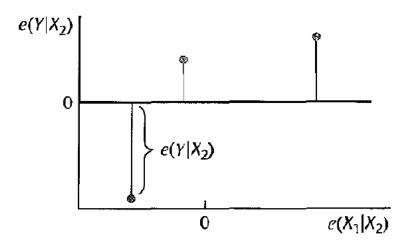
- Figure (a) shows a horizontal band, indicating that  $X_1$  contains no additional information useful for predicting Y beyond that contained in  $X_2$ , so that it is not helpful to add  $X_1$  to the regression model.
- Figure (b) shows a linear band with a nonzero slope. This plot indicates that a linear term in  $X_1$  may be a helpful addition to the regression model already containing  $X_2$ .
- Figure (c) shows a curvilinear band, indicating that the addition of  $X_1$  to the regression model may be helpful and suggesting the possible nature of the curvature effect by the pattern shown.

### Added-variable plots:

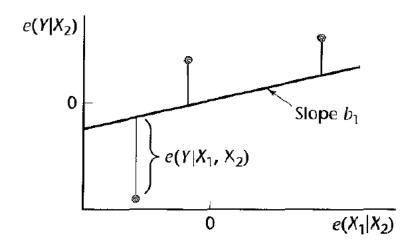
- providing information about the possible nature of the marginal relationship for a predictor variable, given the other variables already in the regression model
- the strength of the relationship
- useful for uncovering outlying data points that may have a strong influence in estimating the relationship of the predictor variable  $X_k$  to the response variable

FIGURE 10.2 Illustration of Deviations in an Added-Variable Plot.





(b) Deviations around Line with Slope  $b_1$  $SSE(X_1, X_2) = \sum [e(Y_i|X_{i1}, X_{i2})]^2$ 



- $SSE(X_2)$
- $SSE(X_1, X_2)$
- Difference  $(SSE(X_2) SSE(X_1, X_2))$ :  $SSR(X_1|X_2)$ ; provides information about the marginal strength of the linear relation of  $X_1$  to the response variable, given that  $X_2$  is in the model

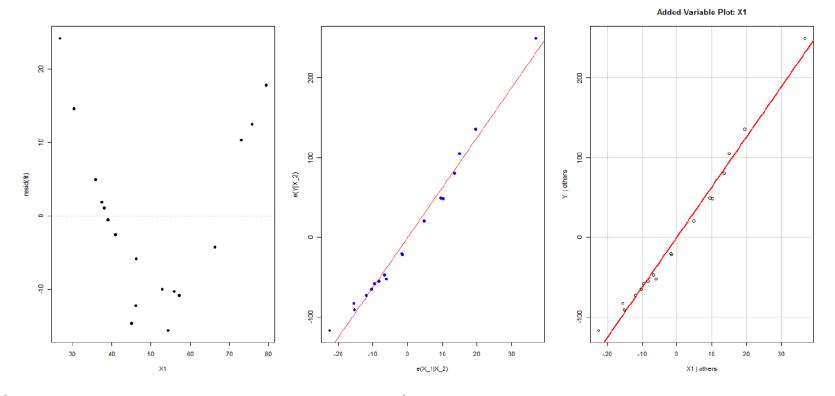
#### Example:

	Average Annual Income	Risk Aversion	Amount of Life Insurance Carried
Manager	(thousand dollars)	Score	(thousand dollars)
i	$X_{i1}$	$X_{i2}$	$Y_i$
1	45.01	6	91
2	57.20	4	162
3	26.85	5	11
	• • •		• • •
16	46.13	4	91
17	30.37	3	14
18	39.06	5	63

- $r_{12} = 0.254$
- $\hat{Y} = -205.72 + 6.288X_1 + 4.738X_2$
- Residual plot: a linear relation for  $X_1$  is not appropriate in the model already containing  $X_2$

## R Code

```
attach(Dataset_10TA01)
fit < -lm(Y^X1+X2)
par(mfrow=c(1,3))
plot(X1,resid(fit),pch=16)
abline(0,0,lty=2,col="gray")
## Method 1:
plot(resid(Im(Y^X2)) \sim resid(Im(X1^X2)), col="blue", pch=16, xlab="e(X_1|X_2)", ylab="e(Y|X_2)")
abline(lm(resid(lm(Y~X2))~resid(lm(X1~X2))),col="red")
## Method 2: using avPlot()
library(car)
avPlot( model=lm( Y~X1+X2 ), variable=X1 )
```



- $\hat{Y}(X_2) = 50.70 + 15.54X_2$ ;  $\hat{X}_1(X_2) = 40.779 + 1.718X_2$
- Plots: through (0,0);  $b_1 = 6.2880$ ;
- suggest the curvilinear relation between Y and  $X_1|X_2$  is strongly positive; a slight concave upward shape
- $R_{Y1|2}^2 = 0.984$

#### **Comments:**

- An added-variable plot only suggests the nature of the functional relation in which a predictor variable should be added to the regression model but does not provide an analytic expression of the relation.
- Added-variable plots need to be used with caution for identifying the nature of the marginal effect of a predictor variable.
  - may not show the proper form of the marginal effect of a predictor variable if the functional relations for some or all of the predictor variables already in the regression model are misspecified
  - the relations of the predictor variable to the response variable are complex
  - high multicollinearity among the predictor variables

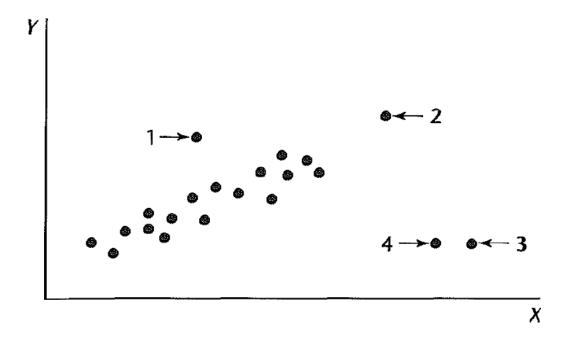
• Any fitted multiple regression function can be obtained from a sequence of fitted partial regressions. Ex: having  $e(Y|X_2)$ ,  $e(X_1|X_2)$ 

```
\Rightarrow e(Y|X_2) = 6.2880[e(X_1|X_2)]
\Rightarrow [\hat{Y} - \hat{Y}(X_2)] = 6.2880[X_1 - \hat{X}_1(X_2)]
\Rightarrow \hat{Y} = -205.72 + 6.2880X_1 + 4.737X_2
```

## Identifying Outlying Y Observations

#### Outlying or Extreme:

- the observations for these cases are well separated from the remainder of the data
- large residuals; have dramatic effects



- Outlying: Y value, X values or both
- Not all outlying cases have a strong influence on the fitted regression function.
- A basic step: determine if the regression model under consideration is heavily influenced by one or a few cases in the data set

Two refined measures for identifying cases with outlying *Y* observations:

Residuals, Semistudentized Residuals:

$$e_i = Y_i - \hat{Y}_i; \quad e_i^* = \frac{e_i}{\sqrt{MSE}}$$

• Hat matrix:  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \Rightarrow \hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$ 

$$m{e} = (m{I} - m{H}) m{Y}$$
  
 $\Rightarrow \sigma^2 \{ m{e} \} = \sigma^2 (m{I} - m{H})$   
 $\sigma^2 \{ e_i \} = \sigma^2 (1 - h_{ii}), \quad h_{ii}$ : the *i*th elements on the diagonal of  $m{H}$   
 $\sigma \{ e_i, e_j \} = -h_{ij} \sigma^2, \quad i \neq j$   
 $\Rightarrow s^2 \{ e_i \} = MSE(1 - h_{ii}), \quad s\{ e_i, e_j \} = -h_{ij} MSE$ 

• 
$$h_{ii} = X_i'(X'X)^{-1}X_i$$
,  $X_i = [1X_{i,1} \cdots X_{i,p-1}]'$ 

#### Small data set: n = 4

	(a) Data and Basic Results							
i,	(1) X <sub>11</sub>	(2) X <sub>12</sub>	(3) •Y <sub>i</sub>	(4) Ŷ,	(5) e <sub>i</sub>		5) )::	(7) s <sup>2</sup> {e <sub>i</sub> }
1 2 3 4	14 19 12 11	25 32 22 15	301 327 246 187	282.2 332.3 260.0 186.5	18.8 <b>5</b> .3 14.0 . <b>5</b>	.95 .66	377 513 514 996	3 <b>52.</b> 0 28.0 194.6 .2
	(E	) H				(c) s <sup>2</sup>	{e}	
.1	877 .1727 727 .9513 553 —.1284 157 .0044	1284 .6614	0157 .0044 .0117 .9996		352.0 99.3 261.8 9.0	-99.3 28.0 73.8 -2.5	<b>2</b> 61.8 	9.0 -2.5 -6.7 .2

- $\hat{Y} = 80.93 5.84X_1 + 11.32X_2$
- MSE = 574.9
- $s^2\{e_1\} = 574.9(1 0.3877) = 352.0$

• Deleted Residuals: The difference between  $Y_i$  and  $\hat{Y}_{i(i)}$ : (PRESS prediction error)

delted residual: 
$$d_i = Y_i - \hat{Y}_{i(i)} = \frac{e_i}{1 - h_{ii}}$$

- h<sub>ii</sub>: the larger will be the deleted residuals as compared to the ordinary residual
- the estimated variance of  $d_i$ :

$$s^{2}\{d_{i}\} = MSE_{(i)}(1 + \mathbf{X}'_{i}(\mathbf{X}'_{(i)}\mathbf{X}_{(i)})^{-1}\mathbf{X}_{i}) = \frac{MSE_{(i)}}{1 - h_{ii}}$$

$$\Rightarrow \frac{d_{i}}{s\{d_{i}\}} \sim t((n-1) - p)$$

Studentized Deleted Residuals:

$$t_{i} = \frac{d_{i}}{s\{d_{i}\}} = \frac{e_{i}}{\sqrt{MSE_{(i)}(1 - h_{ii})}}$$

$$\left((n - p)MSE = (n - p - 1)MSE_{(i)} + \frac{e_{i}^{2}}{1 - h_{ii}}\right)$$

$$\Rightarrow t_{i} = e_{i} \left[\frac{n - p - 1}{SSE(1 - h_{ii}) - e_{i}^{2}}\right]^{1/2}$$

 h<sub>ii</sub>: the larger will be the deleted residuals as compared to the ordinary residual

• the estimated variance of  $d_i$ :

$$s^{2}\{d_{i}\} = MSE_{(i)}(1 + \mathbf{X}'_{i}(\mathbf{X}'_{(i)}\mathbf{X}_{(i)})^{-1}\mathbf{X}_{i}) = \frac{MSE_{(i)}}{1 - h_{ii}}$$

$$\Rightarrow \frac{d_{i}}{s\{d_{i}\}} \sim t((n-1) - p)$$

- Test for Outliers: whose studentized deleted residuals are large in absolute value
  - If the regression model is appropriate, so that no case is outlying. Each  $t_i \sim t(n-p-1)$ .
  - $|t_i|$ : the appropriate Bonferroni critical value:  $t(1 \alpha/2n; n p 1)$

### Body fat example

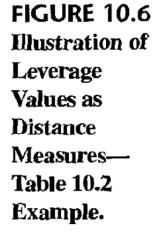
	(1)	(2)	(3)
· <b>I</b> :	$e_l$	$h_{il}$	$t_l$
			,
1	-1.683	.201	<b>730</b>
2	3.643	.059	1.534
3	-3.176	.372	<u>-1.656</u>
4	-3.158	111،	-1.348
5	.000	.248	.000
6	361	.129	148
7	.716	.156	.298
5 6 7 8 9	4:01:5	.096	1.760
9	2.655	.115	1.117
10	-2.475	.110	-1.034
11 12 13	.336	.120	.137
12	2.226	.109	.923
13	-3.947	.1 <b>78</b>	-1.825
14	3.447	.148	1.524
15	.571	.333	.267
16	.642	.095	.25.8
1.7	851	.106	.344
18	<b>783</b>	.197	.335
19	-2.857	.067	-1.176
18 19 20	1.040	.050	.409

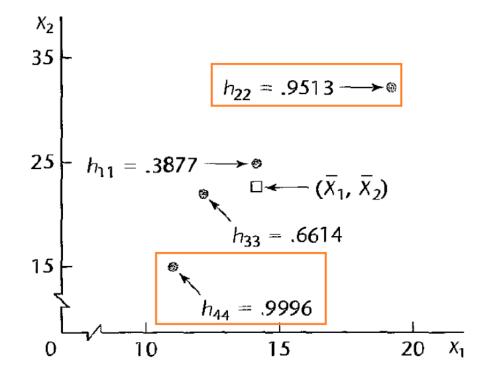
• 
$$|t| < 3.252 = t(1 - \alpha/2n; n - p - 1)$$

 The Bonferroni procedure provides a Conservative test for the presence of an outlier.

## Identifying Outlying X Observations

- Using **H** for identifying outlying X
- $0 \le h_{ii} \le 1$   $\sum_{i=1}^{n} h_{ii} = p$
- $h_{ii}$ : called *leverage*; measure the distance between  $X_i$  and  $\bar{X}$ 
  - large  $h_{ii} \Rightarrow X_i$  distant from the center of all  $X_s$

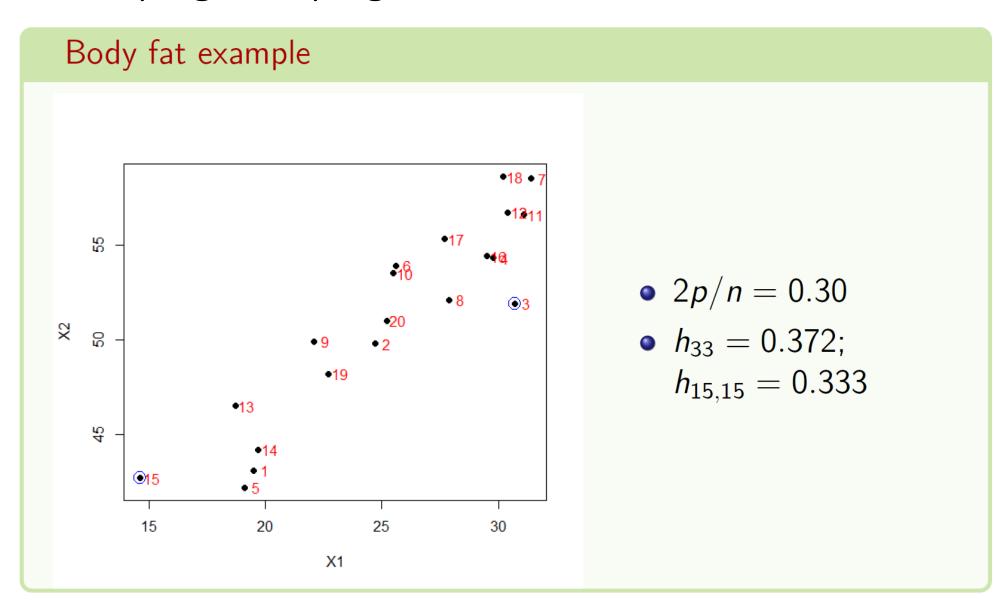




- If  $X_i$  is outlying $\Rightarrow$  has a large leverage  $h_{ii}$
- $\hat{Y}_i$ : a linear combination of Y ( $\hat{Y} = HY$ )
- $h_{ii}$ : the weight of  $Y_i \Rightarrow$  the larger is  $h_{ii}$ , the more important is  $Y_i$  in determining  $\hat{Y}_i$
- The larger is  $h_{ii}$ , the smaller is  $\sigma^2\{e_i\}$ .
- $h_{ii}=1\Rightarrow \sigma^2\{e_i\}=0$
- Rule:

$$h_{ii} > 2\bar{h} = 2\frac{\sum h_{ii}}{n} = 2\frac{p}{n} \quad (\frac{2p}{n} \le 1)$$

very high leverage:  $h_{ii} > 0.5$ moderate leverage:  $h_{ii} : 0.2 \sim 0.5$ 



```
attach(Dataset 07TA01)
fit < -Im(Y^X1+X2+X3)
n < -length(Y); p = 3
plot(X2^X1, pch=16)
text(X1+0.5, X2,
labels=as.character(1:length(X1)),col="red")
hii<-hatvalues(fit)
index<-hii>2*p/n
points(X1[index], X2[index], cex=2.0, col="blue")
```

### **DFFITS** measure

• Influence on single fitted value: DFFITS-measure the influence that case i has on  $\hat{Y}_i$ 

$$(DFFITS)_i = rac{\hat{Y}_i - \hat{Y}_{i(i)}}{\sqrt{MSE_{(i)}h_{ii}}} = t_i \left(rac{h_{ii}}{1 - h_{ii}}
ight)^{1/2}$$

• Rule:

 $\left\{ \begin{array}{l} |DFFITS| > 1 \quad \text{for small to medium data sets} \\ |DFFITS| > 2\sqrt{p/n} \quad \text{for large data sets} \end{array} \right.$ 

• If  $X_i$  is an outlier and has a high  $h_{ii}$ ,  $(DFFITS)_i$  will tend to be large absolutely.

### Cook's Distance

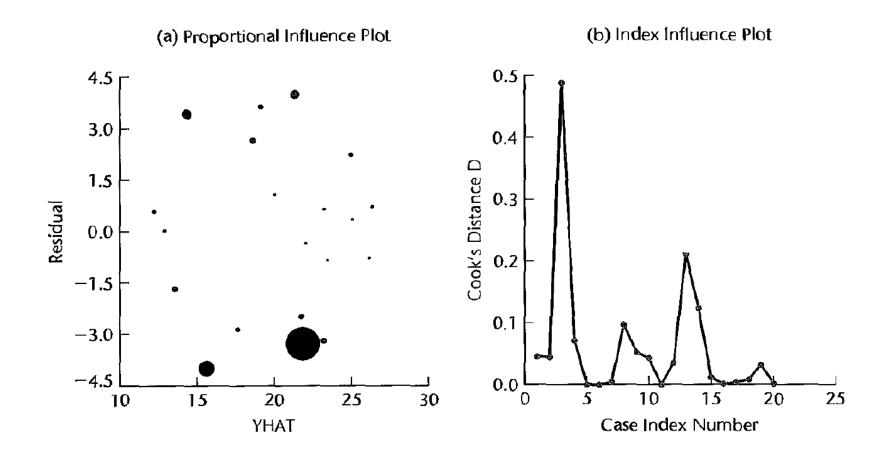
 Influence on all fitted value: Cook's distance-consider the influence of the ith case on all n fitted values

$$D_{i} = \frac{\sum_{j=1}^{n} (\hat{Y}_{i} - \hat{Y}_{j(i)})^{2}}{\rho MSE} = \frac{(\hat{\boldsymbol{Y}} - \hat{\boldsymbol{Y}}_{(i)})'(\hat{\boldsymbol{Y}} - \hat{\boldsymbol{Y}}_{(i)})}{\rho MSE}$$
$$= \frac{e_{i}^{2}}{\rho MSE} \left[ \frac{h_{ii}}{(1 - h_{ii})^{2}} \right]$$

- the size of  $e_i$
- $\bullet$   $e_i \uparrow \text{ or } h_{ii} \uparrow \Rightarrow D_i \uparrow$
- Rule:  $D_i \sim F(p, n-p)$

little influence :  $P(F(p, n-p) \le D_i) > 0.1$  or 0.2 major influence :  $P(F(p, n-p) \le D_i) > 0.5$ 

## Cook's Distance, cont'd



## **DFBETAS**

• Influence on regression coefficients: DFBETAS-the difference between  $b_k$  and  $b_{k(i)}$ 

$$(DFBETAS)_{k(i)} = rac{b_k - b_{k(i)}}{\sqrt{MSE_{(i)}c_{kk}}}, \quad k = 0, 1, \dots, p-1$$

where  $c_{kk}$ : the kth diagonal element of  $(\mathbf{X}'\mathbf{X})^{-1}$ 

• Rule:

 $\begin{cases} |\mathit{DFBETAS}| > 1 & \text{for small to medium data sets} \\ |\mathit{DFBETAS}| > 2\sqrt{n} & \text{for large data sets} \end{cases}$ 

## DFBETAS, cont'd

```
# Body fat example (Table 10.4)
> influence.measures(fit)
Influence measures of
         lm(formula = Y \sim X1 + X2):
      dfb.1
               dfb.X1
                         dfb.X2
                                    dffit cov.r
                                                  cook.d
                                                           hat inf
  -3.05e-01 -1.31e-01 2.32e-01 -3.66e-01 1.361 4.60e-02 0.2010
   1.73e-01 1.15e-01 -1.43e-01 3.84e-01 0.844 4.55e-02 0.0589
  -8.47e-01 -1.18e+00 1.07e+00 -1.27e+00 1.189 4.90e-01 0.3719
  -1.02e-01 -2.94e-01 1.96e-01 -4.76e-01 0.977 7.22e-02 0.1109
  -6.37e-05 -3.05e-05 5.02e-05 -7.29e-05 1.595 1.88e-09 0.2480
   3.97e-02 4.01e-02 -4.43e-02 -5.67e-02 1.371 1.14e-03 0.1286
7 -7.75e-02 -1.56e-02 5.43e-02 1.28e-01 1.397 5.76e-03 0.1555
   2.61e-01 3.91e-01 -3.32e-01 5.75e-01 0.780 9.79e-02 0.0963
9 -1.51e-01 -2.95e-01 2.47e-01 4.02e-01 1.081 5.31e-02 0.1146
10 2.38e-01 2.45e-01 -2.69e-01 -3.64e-01 1.110 4.40e-02 0.1102
11 -9.02e-03 1.71e-02 -2.48e-03 5.05e-02 1.359 9.04e-04 0.1203
12 -1.30e-01 2.25e-02 7.00e-02 3.23e-01 1.152 3.52e-02 0.1093
13 1.19e-01 5.92e-01 -3.89e-01 -8.51e-01 0.827 2.12e-01 0.1784
14 4.52e-01 1.13e-01 -2.98e-01 6.36e-01 0.937 1.25e-01 0.1480
15 -3.00e-03 -1.25e-01 6.88e-02 1.89e-01 1.775 1.26e-02 0.3332
16 9.31e-03 4.31e-02 -2.51e-02 8.38e-02 1.309 2.47e-03 0.0953
17 7.95e-02 5.50e-02 -7.61e-02 -1.18e-01 1.312 4.93e-03 0.1056
18 1.32e-01 7.53e-02 -1.16e-01 -1.66e-01 1.462 9.64e-03 0.1968
19 -1.30e-01 -4.07e-03 6.44e-02 -3.15e-01 1.002 3.24e-02 0.0670
20 1.02e-02 2.29e-03 -3.31e-03 9.40e-02 1.224 3.10e-03 0.0501
```

## DFBETAS, cont'd

#### Some final comments:

- Analysis of outlying and influential cases: a necessary component of good regression analysis
  - neither automatic nor foolproof
  - require good judgment by the analyst
- Methods described: ineffective
- Extensions of the single-case diagnostic procedures: computational requirements

## Variance Inflation Factor-VIF

#### Some problems: multicollinearity

- Adding or deleting X: change the regression coefficients
- Extra sum of squares: depending upon which other  $X_k$  variables are already included in the model
- $X_k$  highly correlated with each other  $\Rightarrow s\{b_k\} \uparrow$
- the estimated regression coefficients individually may not be statistically significant

#### informal diagnostics for multicollinearity:

- 1. Large changes in  $b_k$  when  $X_k$  is added or deleted, or when an observation is altered or deleted
- 2. Nonsignificant results in individual tests on the regression coefficients for important predictor variables.
- 3. Estimated regression coefficients with an algebraic sign that is the opposite of that expected from theoretical consideration or prior experience.
- 4. Large  $r_{xx}$
- 5. Wide confidence interval for  $\beta_k$

#### Important limitations:

- do not provide quantitative measurements
- may not identify the nature of the multicollinearity
- sometimes the observed behavior may occur without multicollinearity being present

### Variance Inflation Factor (VIF)

- a formal method: detecting multicollinearity; widely accepted
- measure how much the variances of b<sub>k</sub>s are inflated as compared to when the predictor variables are not linearly related.
- Illustration:
- Variance-covariance matrix of **b**:  $\sigma^2\{b\} = \sigma^2(X'X)^{-1}$

Using the standardized regression model:

Variance-covariance matrix of  $b^*$ :  $\sigma^2\{b^*\} = (\sigma^*)^2 r_{xx}^{-1}$ 

 $(\sigma^*)^2$  = the error term variance for the transformed model  $(VIF)_k$  = the kth diagonal element of  $r_{\chi\chi}^{-1}$ 

$$\Rightarrow \sigma^{2}\{b_{k}^{*}\} = (\sigma^{*})^{2}(VIF)_{k} = \frac{(\sigma^{*})^{2}}{1 - R_{k}^{2}}$$

$$VIF \text{ for } b_{k}^{*}: (VIF)_{k} = (1 - R_{k}^{2})^{-1}, \quad k = 1, 2, \dots, p - 1$$

$$R_{k}^{2}: X_{k} \text{ is regressed on the } p - 2 \text{ other } X_{k'} \text{s}$$

- $R_k^2 = 0 \Rightarrow (VIF)_k = 1$ :  $X_k$  is not linearly related to  $X_{k'}$ s
- $R_k^2 \neq 0 \Rightarrow (VIF)_k > 1$ : indicate inflated variance for  $b_k^*$  as a result of the intercorrelations among the X variables

Perfect linear association with  $X_k s \Rightarrow R_k^2 = 1 \Rightarrow VIF_k$  and  $\sigma^2\{b_k^*\}$  are unbounded

Rule: largest VIF value among all  $Xs \Rightarrow$  as an indicator of the severity of multicollinearity

$$\max\{VIF_1, ..., VIF_{p-1}\} > 10$$

• If  $\overline{\it VIF} > 1 \Rightarrow$  serious multicollinearity problems

$$: E\left\{\sum_{k=1}^{p-1} (b_k^* - \beta_k^*)^2\right\} = (\sigma^*)^2 \sum_{k=1}^{p} (VIF)_k$$

 $\Rightarrow$ large  $\overline{VIF} \Rightarrow$  larger differences between  $b_k^*$  and  $\beta_k^*$ 

• If no linearly  $R_k^2 \equiv 0 \Rightarrow (VIF)_k = 1$ 

$$\Rightarrow E\left\{\sum_{k=1}^{p-1} (b_k^* - \beta_k^*)^2\right\} = (\sigma^*)^2 (p-1)$$

$$\Rightarrow \overline{VIF} = \frac{(\sigma^*)^2 \sum_{k=1}^{p} (VIF)_k}{(\sigma^*)(p-1)} = \frac{\sum_{k=1}^{p} (VIF)_k}{(p-1)}$$

Variable	<b>b</b> **	(VIF) <sub>k</sub>
$X_1$	4.2637	708.84
$X_2$	<b>-2.9287</b>	564.34
<i>X</i> <sub>3</sub>	-1.5614	104.61

Maximum  $(VIF)_k = 708.84$   $(\overline{VIF}) = 459.26$ 

Figure : VIF-Body Fat Example with three Xs

- $VIF_3 = 105$
- $r_{13}^2 = 0.458^2 = 0.209764$ ,  $r_{23}^2 = 0.085^2$ : not large
- $X_3$ :  $R_3^2 = 0.990$ ; strong related to  $X_1, X_2$

### Body Fat Example:

```
> summary(fit)
Call:
Im(formula = Y \sim X1 + X2 + X3)
Residuals:
        1Q Median
                      30 Max
-3.7263 -1.6111 0.3923 1.4656 4.1277
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 117.085 99.782 1.173 0.258
X1
            4.334
                     3.016 1.437 0.170
X2
            -2.857
                     2.582 -1.106
                                  0.285
            -2.186
                     1.595 -1.370 0.190
X3
Residual standard error: 2.48 on 16 degrees of freedom
Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641
```

F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

```
Analysis of Variance Table
Response: Y
     Df Sum Sq Mean Sq F value Pr(>F)
       1 352.27 352.27 57.2768 1.131e-06 ***
       1 33.17 33.17 5.3931 0.03373 *
       1 11.55 11.55 1.8773 0.18956
Residuals 16 98.40 6.15
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> vif(fit)
  X1
           X2
                     X3
708.8429 564.3434 104.6060
```

15-Jul-19 40

> anova(fit)

#### Comments

- Some program: using  $1/VIF_k = 1 R_k^2 < 0.01$  (0.001, 0.001)
- Limitation: cannot distinguish between several simultaneous multicollinearities
- Other methods: more complex than VIF