

# Data modeling: CSCI E-106

Applied Linear Statistical Models

Chapter 6 – Multiple Regression I

# Multiple Regression

- Multiple regression analysis is one of the most widely used of all statistical methods.
- a variety of multiple regression models
- basic statistical results in matrix form

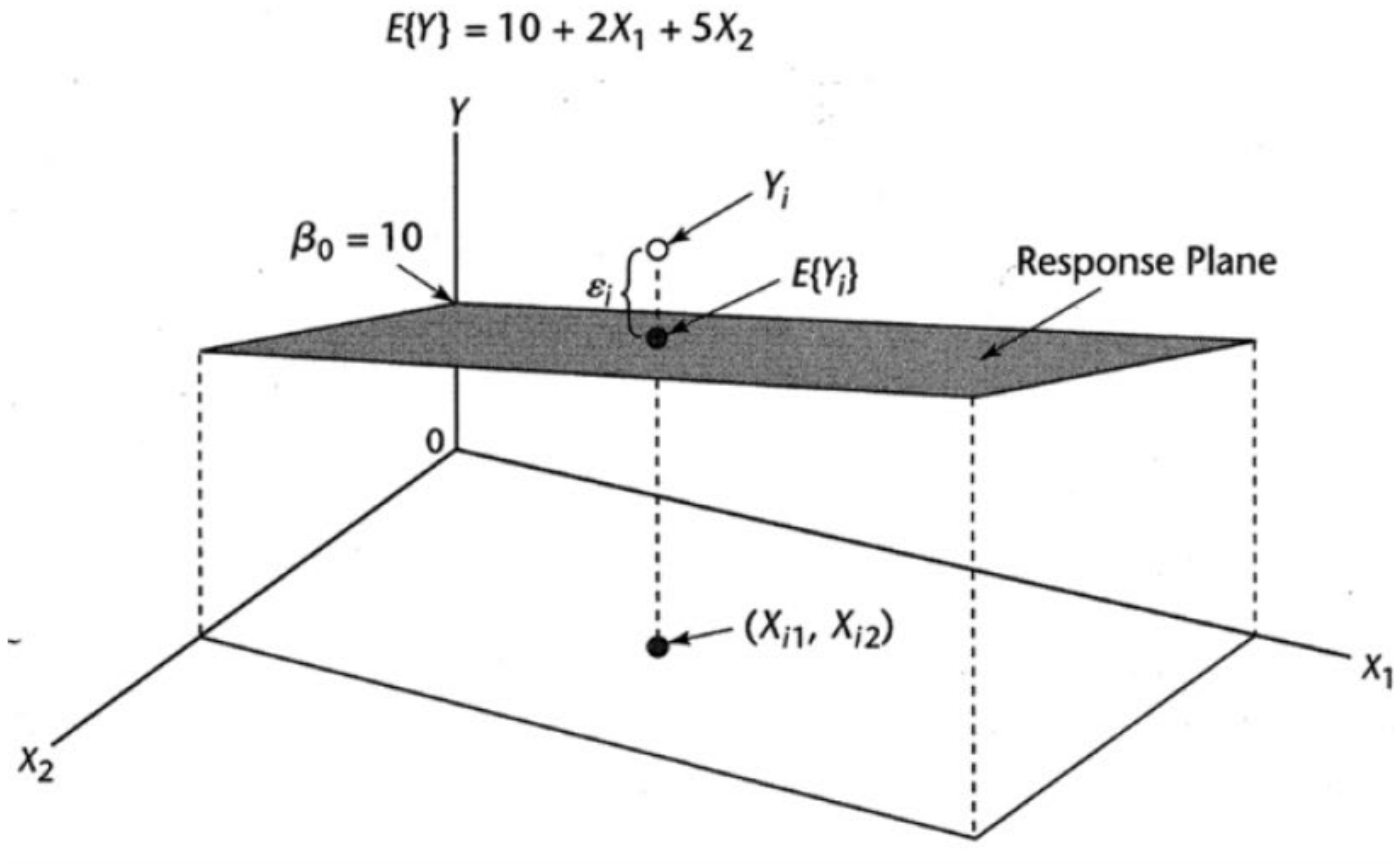
# First-Order Model with Two Predictor Variables

- Two predictor variables:  $X_1$ ;  $X_2$

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

- first-order model with two predictor variables: linear in the predictor variables.
  - $Y_i$  denotes as usual the response in the  $i$ th trial,
  - $X_{i1}$  and  $X_{i2}$  are the values of the two predictor variables in the  $i$ th trial.
  - Parameters of the model are  $\beta_0$ ,  $\beta_1$  and  $\beta_2$ , and the error term is  $\varepsilon_i$ .
- Assume  $E\{\varepsilon_i\} = 0 \Rightarrow E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2$
- *called a regression surface or a response surface*

# First-Order Model with Two Predictor Variables, cont'd



**Figure :** Response Function is a plane-Sales Promotion Example.

# Meaning of Regression Coefficients

- The parameter  $\beta_1$  indicates the change in the mean response  $E\{Y\}$  per unit increase in  $X_1$  when  $X_2$  is held constant.
- Likewise,  $\beta_2$  indicates the change in the mean response per unit increase in  $X_2$  when  $X_1$  is held constant
- When the effect of  $X_1$  on the mean response does not depend on the level of  $X_2$ , and correspondingly the effect of  $X_2$  does not depend on the level of  $X_1$ , the two predictor variables are said to have additive effects or not to interact.
- The parameters  $\beta_1$  and  $\beta_2$  are sometimes called partial regression coefficients because they reflect the partial effect of one predictor variable when the other predictor variable is included in the model and is held constant.

# Meaning of Regression Coefficients, cont'd

- $\beta_0$ : intercept in the regression plane;  $X_1 = 0, X_2 = 0$
- $\beta_1$ : the change in the mean response with  $\Delta X_1 = 1$  and  $X_2 = \text{constant}$ ;  $\frac{\partial E\{Y\}}{\partial X_1} = \beta_1$
- $\beta_2$ : the change in the mean response with  $X_1 = \text{constant}$  and  $\Delta X_2 = 1$ ;  $\frac{\partial E\{Y\}}{\partial X_2} = \beta_2$
- $\beta_1, \beta_2$ : **partial regression coefficients**  $\therefore$  they reflect the partial effect
- $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$ : additive or do not interact

# First-Order Model with More than Two Predictor Variables

- The first-order regression model with  $p - 1$  predictor variables:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i \\ &= \beta_0 + \sum_{k=1}^{p-1} \beta_k X_{ik} + \varepsilon_i \\ &= \sum_{k=0}^{p-1} \beta_k X_{ik} + \varepsilon_i, \quad \text{where } X_{i0} \equiv 1 \end{aligned}$$

- Assuming that  $E\{\varepsilon_i\} = 0$ , the response function (hyperplane) :

$$\Rightarrow E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1}$$

# First-Order Model with More than Two Predictor Variables, cont'd

- This response function is a hyperplane, which is a plane in more than two dimensions. It is no longer possible to picture this response surface
- $\beta_k$ : the change in the mean response  $E\{Y\}$  with  $\Delta X_k = 1$  and all other predictor variables are held constant
- additive and do not interact



# General linear Regression Model

- The general linear regression model with **normal error terms**:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i, \quad i = 1, \dots, n \\ &= \beta_0 X_{i0} + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i \quad (X_{i0} \equiv 1) \\ &= \sum_{k=0}^{p-1} \beta_k X_{ik} + \varepsilon_i, \quad \text{where } X_{i0} \equiv 1 \end{aligned}$$

- Parameters:  $\beta_0, \beta_1, \dots, \beta_{p-1}$
- known constants:  $X_{i1}, X_{i2}, \dots, X_{ip-1}$
- $\varepsilon_i$ : independent  $N(0, \sigma^2)$

# General linear Regression Model, cont'd

- **p - 1 Predictor Variables:** When  $X_1, \dots, X_{p-1}$  represent p - 1 different predictor variables, there are no interaction effects between the predictor variables.
- **Qualitative Predictor Variables:** such as gender (male, female) or disability status(not disabled, partially disabled, fully disabled).
  - Indicator (dummy) variables are used to identify classes of a qualitative variable.
  - Example: Y is the length of hospital stay;  $X_1$  is age, and  $X_2$  is gender

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$$

$X_{i1}$ : patient's age

$$X_{i2}: \begin{cases} 1, & \text{where patient female} \\ 0, & \text{where patient male} \end{cases}$$

# Qualitative Predictor Variables

- The response function:  $E\{Y\} = \beta_0 + \beta_1 X_1 + \beta_2 X_2$
- The response function for male patients:  $X_2 = 0$   
 $E\{Y\} = \beta_0 + \beta_1 X_1$
- The response function for female patients:  $X_2 = 1$

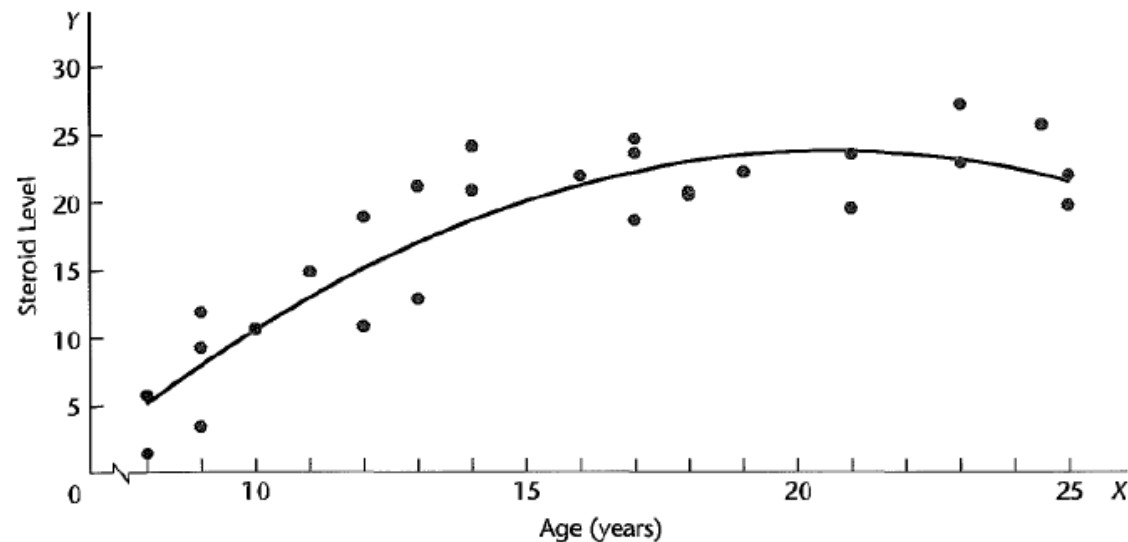
$$E\{Y\} = (\beta_0 + \beta_2) + \beta_1 X_1$$

# Polynomial Regression

- Special cases of the general regression model
- Contain squared and higher order terms of the predicted variables makes the response function curvilinear.

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \varepsilon_i$$

let  $X_i = X_{i1}$  and  $X_i^2 = X_{i2} \Rightarrow Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i$



# Transformed Variables

- complex, curvilinear response functions, yet still are special cases of the general linear regression model.
- Examples:

$$\log Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \varepsilon_i \quad (Y'_i = \log Y_i)$$

$$Y_i = \frac{1}{\beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \varepsilon_i} \quad (Y'_i = \frac{1}{Y_i})$$

# Interaction Effects and Combination of Cases

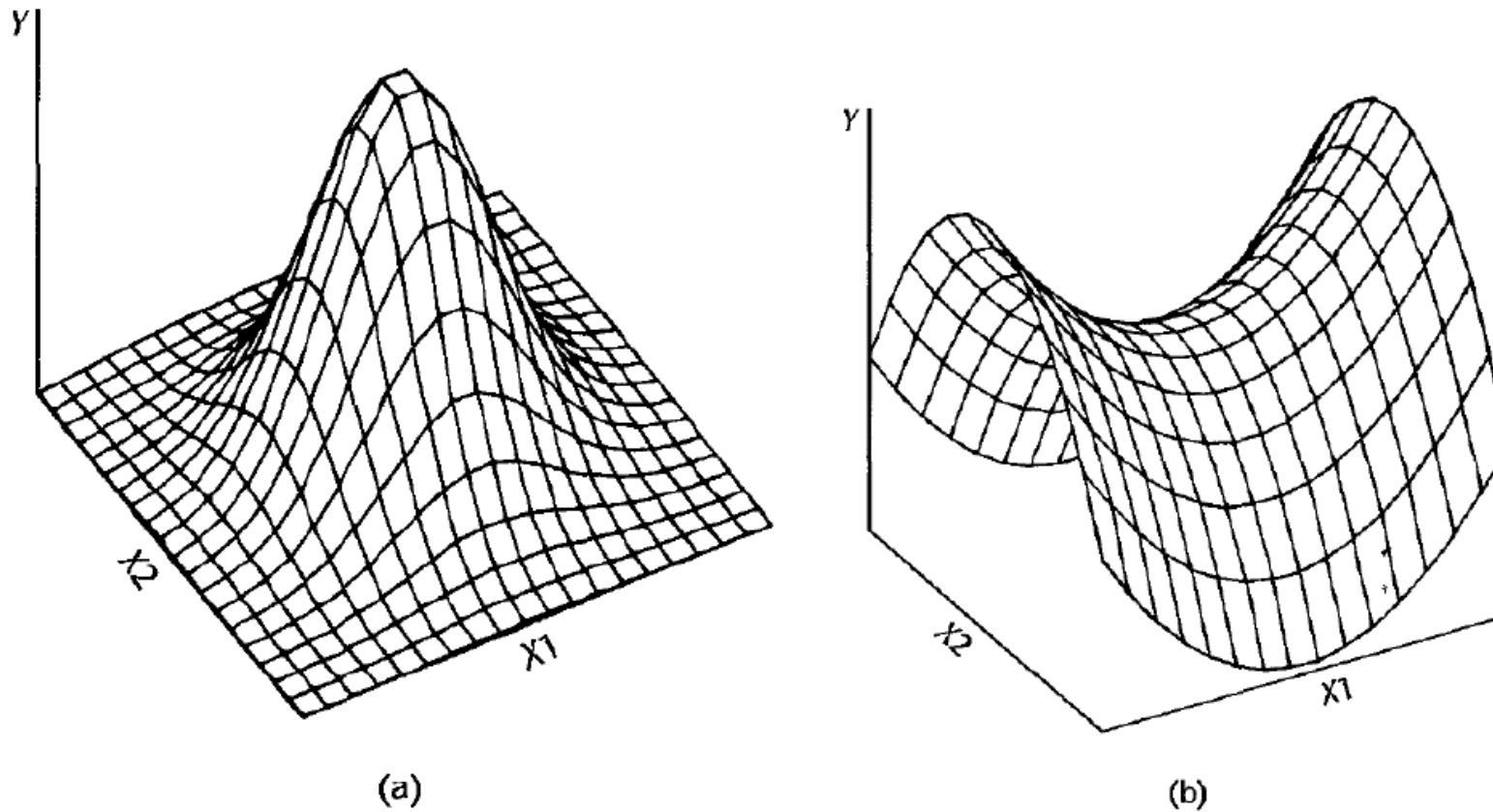
An example of a nonadditive regression model with  $X_1, X_2$ : (complex)

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i1} X_{i2} + \varepsilon_i \\ &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \varepsilon_i, \quad (X_{i3} = X_{i1} X_{i2}) \end{aligned}$$

By cross-product term:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}^2 + \beta_3 X_{i2} + \beta_4 X_{i2}^2 + \beta_5 X_{i1} X_{i2} + \varepsilon_i \\ &= \beta_0 + \beta_1 Z_{i1} + \beta_2 Z_{i2} + \beta_3 Z_{i3} + \beta_4 Z_{i4} + \beta_5 Z_{i5} + \varepsilon_i \end{aligned}$$

# Interaction Effects and Combination of Cases, cont'd



**Figure :** Additional Examples of Response Functions.

# Meaning of Linear in General Linear Regression Model

- A regression model is **linear in the parameters**:

$$Y_i = c_{i0}\beta_0 + c_{i1}\beta_1 + c_{i2}\beta_2 + \cdots + c_{i,p-1}\beta_{p-1} + \varepsilon_i$$

where  $c_{ik}$ ,  $k = 0, \dots, p - 1$  are coefficients involving the predictor variables

- Illustration: **nonlinear**

$$Y_i = \beta_0 \exp(\beta_1 X_i) + \varepsilon_i$$



# General Linear Regression Model in Matrix Terms

The general linear regression model:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i, \quad i = 1, \dots, n$$

$$\begin{aligned} \underset{n \times 1}{\mathbf{Y}} &= \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} & \underset{n \times p}{\mathbf{X}} &= \begin{bmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1,p-1} \\ 1 & X_{21} & X_{22} & \cdots & X_{2,p-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{n,p-1} \end{bmatrix} \\ \underset{p \times 1}{\boldsymbol{\beta}} &= \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{p-1} \end{bmatrix} & \underset{n \times 1}{\boldsymbol{\varepsilon}} &= \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} \end{aligned}$$

# General Linear Regression Model in Matrix Terms, cont'd

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$$\Rightarrow \underset{n \times 1}{Y} = \underset{n \times p}{X} \underset{p \times 1}{\beta} + \underset{n \times 1}{\varepsilon}$$

- $Y$ : vector of responses;
- $\beta$ : vector of parameters
- $X$ : matrix of constants
- $\varepsilon$ : vector of independent normal random variables;  
 $E\{\varepsilon\} = \mathbf{0}$ ;  $\underset{n \times n}{\sigma^2\{\varepsilon\}} = \sigma^2 I$
- Expectation and variance-covariance matrix of  $Y$ :

$$\underset{n \times 1}{E\{Y\}} = X\beta; \quad \underset{n \times 1}{\sigma^2\{Y\}} = \sigma^2 I$$

# Estimation of Regression Coefficients

- The general linear regression model:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \varepsilon_i, \quad i = 1, \dots, n$$

- The **least squares criterion**: the values  $\beta_0, \dots, \beta_{p-1}$  minimize  $Q$

$$Q = \sum_{i=1}^n (Y_i - \beta_0 - \beta_1 X_{i1} - \cdots - \beta_{p-1} X_{i,p-1})^2$$

# Estimation of Regression Coefficients, cont'd

- the vector of the least squares estimated regression coefficients:
- The normal equations:

$$\underset{p \times 1}{\mathbf{b}} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix}$$
$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$$

- LSE:

$$\underset{p \times 1}{\mathbf{b}} = \underset{p \times p}{(\mathbf{X}'\mathbf{X})^{-1}} \underset{p \times 1}{\mathbf{X}'\mathbf{Y}}$$

# Estimation of Regression Coefficients, cont'd

- The method of MLE leads to the same estimators of normal error regression model
- The likelihood function:

$$L(\boldsymbol{\beta}, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}}} \exp \left[ -\frac{1}{2\sigma^2} \sum_{i=1}^n (Y_i - \beta_0 - \beta_1 X_{i1} - \cdots - \beta_{p-1} X_{i,p-1})^2 \right]$$

Maximizing the likelihood function with respect to  $\beta_0, \beta_1, \dots, \beta_{p-1}$  leads to the estimators  $\mathbf{b}$

# Fitted Values and Residuals

- The vector of  $\hat{Y}_i$  and the vector of  $e_i = Y_i - \hat{Y}_i$ :

$$\begin{aligned}\hat{\mathbf{Y}}_{n \times 1} &= \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix} = \mathbf{X}\mathbf{b} = \mathbf{H}\mathbf{Y} \quad (\mathbf{H}_{n \times n} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}') \\ \mathbf{e}_{n \times 1} &= \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \mathbf{Y} - \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{X}\mathbf{b} = (\mathbf{I} - \mathbf{H})\mathbf{Y} \quad (= (\mathbf{I} - \mathbf{H})\boldsymbol{\varepsilon})\end{aligned}$$

# Fitted Values and Residuals, cont'd

the variance-covariance matrix of the residuals:

$$\sigma^2_{n \times n}\{\mathbf{e}\} = \sigma^2(\mathbf{I} - \mathbf{H})$$

$$\Rightarrow \text{(estimated by)} \quad s^2_{n \times n}\{\mathbf{e}\} = MSE(\mathbf{I} - \mathbf{H})$$

# Analysis of Variance Results

- The sums of squares for ANOVA in matrix terms:

$$SSTO = Y'Y - \left(\frac{1}{n}\right) Y'JY = Y' \left[ I - \left(\frac{1}{n}\right)J \right] Y$$

$$SSE = e'e = (Y - Xb)'(Y - Xb) = Y'Y - b'X'Y = Y'(I - H)Y$$

$$SSR = b'X'Y - \left(\frac{1}{n}\right) Y'JY = Y' \left[ H - \left(\frac{1}{n}\right)J \right] Y$$

$$MSR = \frac{SSR}{p - 1}$$

$$MSE = \frac{SSE}{n - p}$$



# Analysis of Variance Results, cont'd

**Table :** ANOVA Table for General Linear Regression Model Model(6.19).

Source of Variation	SS	df	MS
Regression	$SSR = \mathbf{b}'\mathbf{X}'\mathbf{Y} - (\frac{1}{n})\mathbf{Y}'\mathbf{J}\mathbf{Y}$	$p - 1$	$MSR = \frac{SSR}{p-1}$
Error	$SSE = \mathbf{Y}'\mathbf{Y} - \mathbf{b}'\mathbf{X}'\mathbf{Y}$	$n - p$	$MSE = \frac{SSE}{n-p}$
Total	$SSTO = \mathbf{Y}'\mathbf{Y} - (\frac{1}{n})\mathbf{Y}'\mathbf{J}\mathbf{Y}$	$n - 1$	

- $E\{MSE\} = \sigma^2$

- $p - 1 = 2$ :

$$E\{MSR\} = \sigma^2 + \frac{1}{2} \left[ \beta_1^2 \sum (X_{i1} - \bar{X}_1)^2 + \beta_2^2 \sum (X_{i2} - \bar{X}_2)^2 + 2\beta_1\beta_2 \sum (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2) \right]$$

if  $\beta_1 = 0 = \beta_2 \Rightarrow E\{MSR\} = \sigma^2$ , otherwise  $E\{MSR\} > \sigma^2$

# F Test for Regression Relation

- Test whether there is a regression relation between  $Y$  and  $X$ :

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$$

$$H_a : \text{not all } \beta_k \text{ } (k = 1, \dots, p - 1) \text{ equal zero}$$

$$\Rightarrow \text{test statistic: } F^* = \frac{MSR}{MSE}$$

- The **decision rule** to control the Type I error at  $\alpha$ :

If  $F^* \leq F(1 - \alpha; p - 1, n - p)$ , conclude  $H_0$

If  $F^* > F(1 - \alpha; p - 1, n - p)$ , conclude  $H_a$

# Coefficient of Multiple Determination

- The coefficient of multiple determination:  $R^2$

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO}$$

- Measures the proportionate reduction of total variation in  $Y$  associated with  $X_1, \dots, X_{p-1}$
- $0 \leq R^2 \leq 1$
- Adding more  $X$  variable  $\Rightarrow R^2 \uparrow$ 
  - $SSE$  can never become larger with more  $X$  variables
  - $SSTO$  is always the same of a given set of responses

# Coefficient of Multiple Determination, cont'd

- The adjusted coefficient of multiple determination:  $R_a^2$

$$R_a^2 = 1 - \frac{\frac{SSE}{n-p}}{\frac{SSTO}{n-1}} = 1 - \left( \frac{n-1}{n-p} \right) \frac{SSE}{SSTO}$$

- $R_a^2$  becomes smaller when another  $X$  is introduced into the model  
( $\because SSE \downarrow$ )
- Coefficient of Multiple Correlation:  $R$

$$R = \sqrt{R^2}$$

# Inferences about Regression Parameters

Unbiased:  $E\{\mathbf{b}\} = \boldsymbol{\beta}$

The variance-covariance matrix  $\sigma^2\{\mathbf{b}\}$ :

$$\sigma^2\{\mathbf{b}\}_{p \times p} = \begin{bmatrix} \sigma^2\{b_0\} & \sigma\{b_0, b_1\} & \cdots & \sigma\{b_0, b_{p-1}\} \\ \sigma\{b_1, b_0\} & \sigma^2\{b_1\} & \cdots & \sigma\{b_1, b_{p-1}\} \\ \vdots & \vdots & & \vdots \\ \sigma\{b_{p-1}, b_0\} & \sigma\{b_{p-1}, b_1\} & \cdots & \sigma^2\{b_{p-1}\} \end{bmatrix}$$
$$= \sigma^2\{\mathbf{b}\}_{p \times p} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

# Inferences about Regression Parameters, cont'd

The estimated variance-covariance matrix  $s^2\{\mathbf{b}\}$ :

$$s^2_{p \times p}\{\mathbf{b}\} = \begin{bmatrix} s^2\{b_0\} & s\{b_0, b_1\} & \cdots & s\{b_0, b_{p-1}\} \\ s\{b_1, b_0\} & s^2\{b_1\} & \cdots & s\{b_1, b_{p-1}\} \\ \vdots & \vdots & & \vdots \\ s\{b_{p-1}, b_0\} & s\{b_{p-1}, b_1\} & \cdots & s^2\{b_{p-1}\} \end{bmatrix}$$
$$= MSE(\mathbf{X}'\mathbf{X})^{-1}$$

# Interval Estimation of $\beta_k$

- For the normal error regression model:

$$\frac{b_k - \beta_k}{s\{b_k\}} \sim t(n - p) \quad k = 0, 1, \dots, p - 1$$

- The confidence limits for  $\beta_k$  with  $1 - \alpha$  confidence coefficient:

$$b_k \pm t(1 - \alpha/2; n - p)s\{b_K\}$$

# Interval Estimation of $\beta_k$ , cont'd

- Tests for  $\beta_k$ :

$$H_0 : \beta_k = 0 \quad H_a : \beta_k \neq 0$$

$$\Rightarrow t^* = \frac{b_k}{s\{b_k\}}$$

$\Rightarrow$  The decision rule:

If  $|t^*| \leq t(1 - \alpha/2; n - p)$ , conclude  $H_0$

Otherwise conclude  $H_a$



# Joint Inferences

- The Bonferroni joint confidence intervals for  $g$  parameters with  $1 - \alpha$ : ( $g \leq p$ )

$$b_k \pm Bs\{b_k\}$$

$$B = t(1 - \alpha/2g; n - p)$$

(Chap. 7: tests concerning subsets of the regression parameters)

# Interval Estimation of $E\{Y_h\}$

- Given values of  $X_1, \dots, X_{p-1}$ :  $X_{h,1}, \dots, X_{h,p-1}$

$$\underset{p \times 1}{\mathbf{X}_h} = \begin{bmatrix} 1 \\ X_{h1} \\ \vdots \\ X_{h,p-1} \end{bmatrix}$$

- The mean response  $E\{Y_h\}$ :

$$E\{Y_h\} = \mathbf{X}_h' \boldsymbol{\beta}$$

# Interval Estimation of $E\{Y_h\}$ , cont'd

- The estimated mean response  $\hat{Y}_h$ :

$$\begin{aligned}\hat{Y}_h &= \mathbf{X}_h' \mathbf{b} \\ \Rightarrow E\{\hat{Y}_h\} &= \mathbf{X}_h' \boldsymbol{\beta} = E\{Y_h\} \quad (\textit{Unbiased}) \\ \sigma^2\{\hat{Y}_h\} &= \sigma^2 \mathbf{X}_h' (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}_h = \sigma^2\{\hat{Y}_h\} = \mathbf{X}_h' \boldsymbol{\sigma}^2 \{\mathbf{b}\} \mathbf{X}_h\end{aligned}$$

- The estimated variance  $s^2\{\hat{Y}_h\}$ :

$$s^2\{\hat{Y}_h\} = \text{MSE}(\mathbf{X}_h' (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}_h) = \mathbf{X}_h' \mathbf{s}^2 \{\mathbf{b}\} \mathbf{X}_h$$

- The  $1 - \alpha$  confidence limits for  $E\{Y_h\}$ :

$$\hat{Y}_h \pm t(1 - \alpha/2; n - p) s\{\hat{Y}_h\}$$

# Confidence region for regression surface

- The Working-Hotelling confidence band for the regression line
- Boundary points of the confidence region at  $X_h$ :

$$\hat{Y}_h \pm Ws\{\hat{Y}_h\}$$

$$W^2 = pF(1 - \alpha; p, n - p)$$

# Simultaneous Confidence Intervals for Several Mean Responses

- Estimate of  $E\{Y_h\}$  corresponding to different  $X_h$  vectors with  $1 - \alpha$ :

- Working-Hotelling confidence region bounds:

$$\hat{Y}_h \pm Ws\{\hat{Y}_h\}$$

- Bonferroni simultaneous confidence intervals: (g interval estimates)

$$\hat{Y}_h \pm Bs\{\hat{Y}_h\}$$
$$B = t\left(1 - \frac{\alpha}{2g}; n - p\right)$$

# Prediction of New Observation $Y_{h(\text{new})}$

- The  $1 - \alpha$  prediction limits for a new observation  $Y_{h(\text{new})}$  at  $X_h$ :
  - $\hat{Y}_h \pm t(1 - \frac{\alpha}{2}; n - p) s\{pred\}$
  - where  $s^2\{pred\} = \text{MSE} + s^2\{\hat{Y}_h\} = \text{MSE}(1 + X_h'(X'X)^{-1}X_h)$
- Prediction of mean of m new observations at  $X_h$ :
  - $\hat{Y}_h \pm t(1 - \frac{\alpha}{2}; n - p) s\{predmean\}$
  - Where  $s^2\{predmean\} = \frac{\text{MSE}}{m} + s^2\{\hat{Y}_h\} = \text{MSE}(\frac{1}{m} + X_h'(X'X)^{-1}X_h)$

# Prediction of g New Observation

- g new observations at g different levels  $X_h$  with family confidence coefficient  $1 - \alpha$  :

$$\hat{Y}_h \pm Ss\{pred\}$$

$$\text{where } S^2 = g F(1 - \alpha ; g, n - p)$$

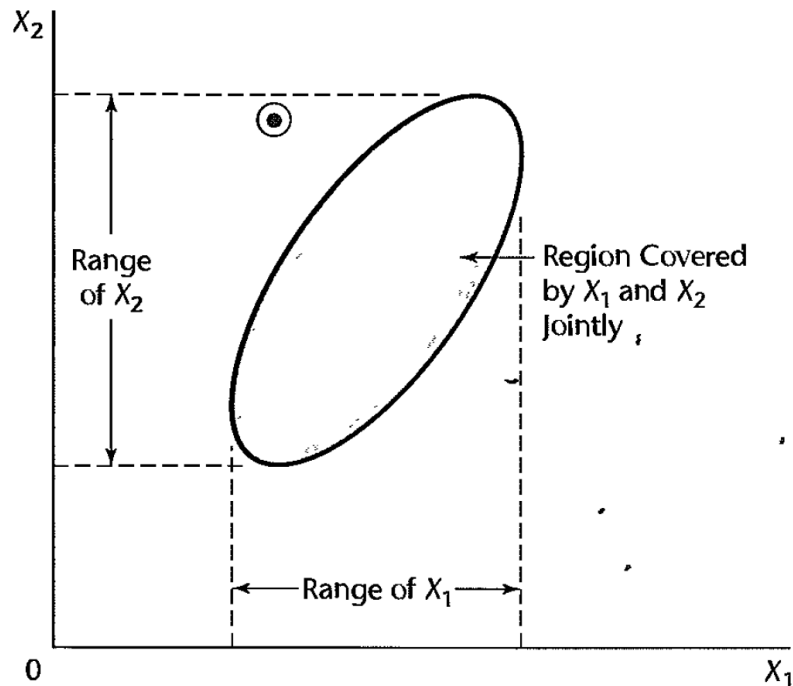
- Bonferroni simultaneous prediction limits:

$$\hat{Y}_h \pm Bs\{pred\}$$

$$\text{where } B = t\left(1 - \frac{\alpha}{2g}; n - p\right)$$

# Caution about Hidden Extrapolations

- Danger: the model may not be appropriate when it is **extended outside the region of the observations**.
- In multiple regression, it is particularly easy to lose track of this region since the levels of  $X_1, \dots, X_{p-1}$  jointly define the region. Thus, one cannot merely look at the ranges of each predictor variable.

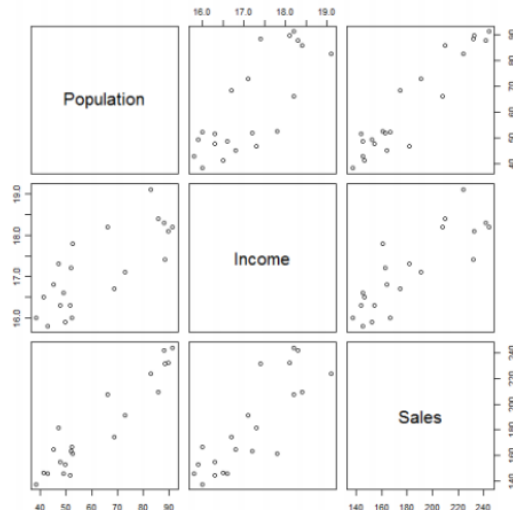


- The circled dot is within the ranges of the predictor variables  $X_1$  and  $X_2$  individually, yet is well outside the joint region of observations.
- It is easy to spot this extrapolation when there are only two predictor variables, but it becomes much more difficult when the number of predictor variables is large.
- We discuss in Chapter 10 a procedure for identifying hidden extrapolations when there are more than two predictor variables.



# Diagnostics and Remedial Measures

- Diagnostics play an important role in the development and evaluation of multiple regression models.
- Most of the diagnostic procedures for simple linear regression that we described in Chapter 3 carry over directly to multiple regression.
- Some important ones will be discussed in Chapters 10 and 11.



(b) Correlation Matrix

	SALES	TARGETPOP	DISPOINC
SALES	1.000	.945	.836
TARGETPOP		1.000	.781
DISPOINC			1.000

# Diagnostics and Remedial Measures, cont'd

- A complement to the scatter plot matrix that may be useful at times is the correlation matrix.
- This matrix contains the coefficients of simple correlation  $r_{Y,X1}$ ,  $r_{Y,X2}$ ,  $\dots$ ,  $r_{Y,Xp-1}$  between  $Y$  and each of the predictor variables.
- As well as all of the coefficients of simple correlation among the predictor variables  $r_{X1,X2}$ ,  $r_{X1,X3}$ , and etc.
- The format of the correlation matrix follows that of the scatter plot matrix:

$$\begin{bmatrix} 1 & r_{Y1} & r_{Y2} & \cdots & r_{Y,p-1} \\ r_{Y1} & 1 & r_{12} & \cdots & r_{1,p-1} \\ \vdots & \vdots & \vdots & & \vdots \\ r_{Y,p-1} & r_{1,p-1} & r_{2,p-1} & \cdots & 1 \end{bmatrix}$$

# Diagnostics and Remedial Measures, cont'd

- Scatter Plots
- Residual Plots
- Correlation Test for Normality
- Test for Constancy of Error Variance
- F Test for Lack of Fit
- Box-Cox transformations

# Diagnostics and Remedial Measures, cont'd

All measures below discussed in Chapter 3 for simple linear regression can be carried over:

- Scatter Plots
- Residual Plots
- Correlation Test for Normality
- Test for Constancy of Error Variance
  - Brown-Forsythe Test
  - Breusch-Pagan Test
- F Test for Lack of Fit
- Box-Cox transformations

# F test of lack of fit

As discussed Chapter 3, to test whether the multiple regression response function

$$E\{Y\} = \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1}$$

is an appropriate response surface.

- Repeat observations
- SSE is decomposed into Pure Error (PE) and Lack of Fit (LOF) components

# F test of lack of fit, cont'd

Testing:

$$H_0 : E\{Y\} = \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1}$$

$$H_a : E\{Y\} \neq \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1}$$

The test statistic:

$$F^* = \frac{SSLE}{c - p} \div \frac{SSPE}{n - c} = \frac{MSLF}{MSPE}$$

$\Rightarrow$  If  $F^* \leq F(1 - \alpha; c - p; n - c)$ , conclude  $H_0$

If  $F^* > F(1 - \alpha; c - p; n - c)$ , conclude  $H_a$

# Example: Dwaine Studio

```
> cor(DwaineStudio)
```

```
      X1      X2      Y
X1 1.0000000 0.7812993 0.9445543
X2 0.7812993 1.0000000 0.8358025
Y  0.9445543 0.8358025 1.0000000
```

```
> anova(f)
```

Analysis of Variance Table

Response: Y

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
X1	1	23371.8	23371.8	192.8962	4.64e-11 ***
X2	1	643.5	643.5	5.3108	0.03332 *
Residuals	18	2180.9	121.2		

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

```
>
```

```
> f<-lm(Y~X1+X2,data=DwaineStudio)
```

```
> summary(f)
```

Call:

lm(formula = Y ~ X1 + X2, data = DwaineStudio)

Residuals:

Min	1Q	Median	3Q	Max
-18.4239	-6.2161	0.7449	9.4356	20.2151

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	-68.8571	60.0170	-1.147	0.2663
X1	1.4546	0.2118	6.868	2e-06 ***
X2	9.3655	4.0640	2.305	0.0333 *

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 11.01 on 18 degrees of freedom  
Multiple R-squared: 0.9167, Adjusted R-squared: 0.9075  
F-statistic: 99.1 on 2 and 18 DF, p-value: 1.921e-10

## Example: Dwaine Studio, cont'd

- `f1<-lm(Y~.,data=DwaineStudio)` , will give you the previous slide model
- `f1<-lm(Y~.^2,data=DwaineStudio)`, will give you the model with interaction term
- `f1<-lm(Y~X1+X2+X1:X2,data=DwaineStudio)`, different way of fitting model with the interaction term