



STAT 571A — Advanced Statistical Regression Analysis

Chapter 6 NOTES Multiple Regression – I

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Multiple Linear Regression Model

- If $p-1 > 1$ predictor variables are under study, we expand the SLR model into a (“first-order”) **Multiple Linear Regression (MLR)** model:

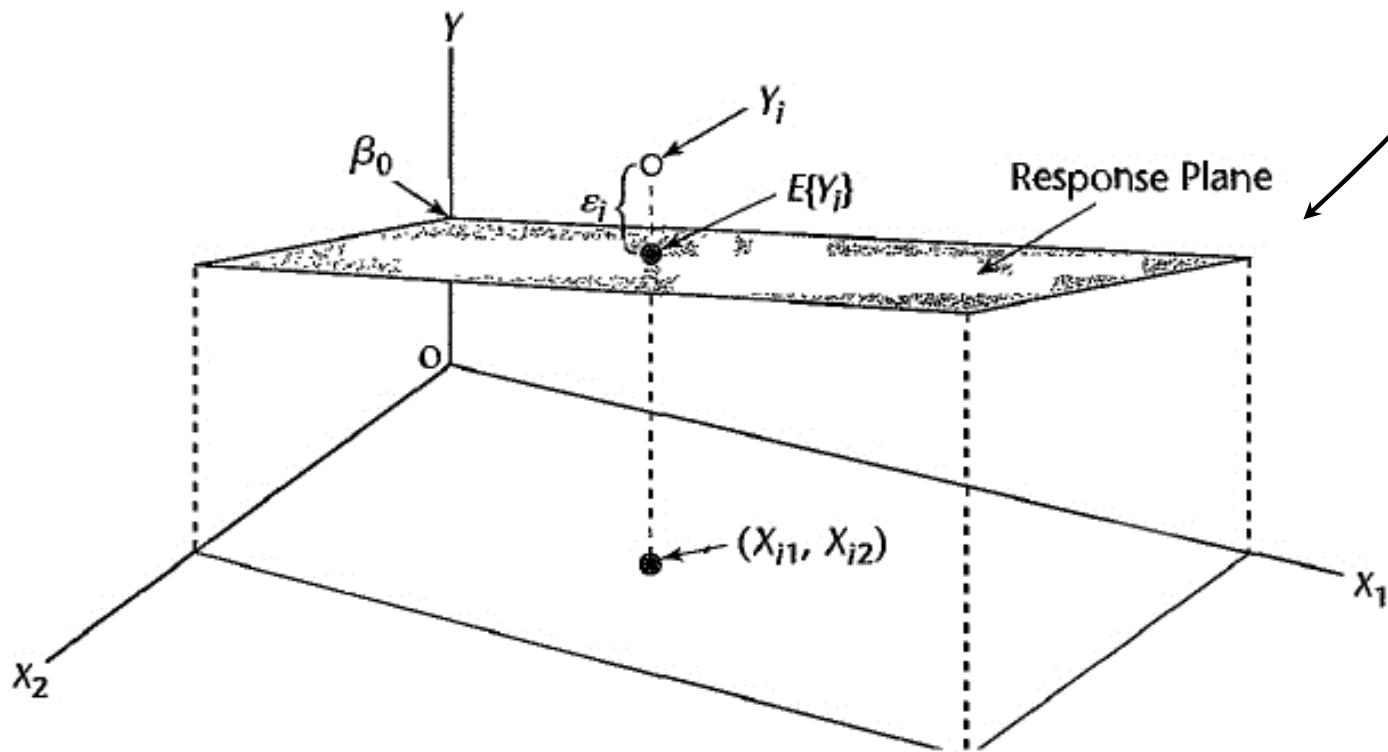
$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_{p-1} X_{i,p-1} + \varepsilon_i$$

where $\varepsilon_i \sim \text{i.i.d.} N(0, \sigma^2)$; $i = 1, \dots, n$.

- One can also write this as $Y_i = \beta_0 X_{i0} + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_{p-1} X_{i,p-1} + \varepsilon_i$, where $X_{i0} \equiv 1$.

MLR with $p=3$

- For instance take the case of $p = 3$ (two predictors): $E\{Y_i\} = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}$
- This is a plane in 3-D space (see Fig. 6.1).



MLR with $p=3$ (cont'd)

- Two predictors: $E\{Y_i\} = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2}$
- Interpret the β_k s as:
 - β_1 is change in $E\{Y\}$ for unit change in X_1 , when all other X_k 's (here, just X_2) are held fixed.
 - β_2 is change in $E\{Y\}$ for unit change in X_2 , when all other X_k 's (here, just X_1) are held fixed.
 - β_0 is the “Y-intercept,” as before.

Special MLR Models

- If one (or more) of the X_k 's is an indicator (=0 or =1), $E\{Y\}$ has a simplified interpretation. See equ. (6.10).
- If $X_k = X^k$, this is a **polynomial regression** (discussed in §8.1).
- Say X_1 and X_2 interact in how they affect $E\{Y\}$. Then we include a second-order **interaction** term:

$$E\{Y_i\} = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i1} X_{i2}$$

Response Surface Model

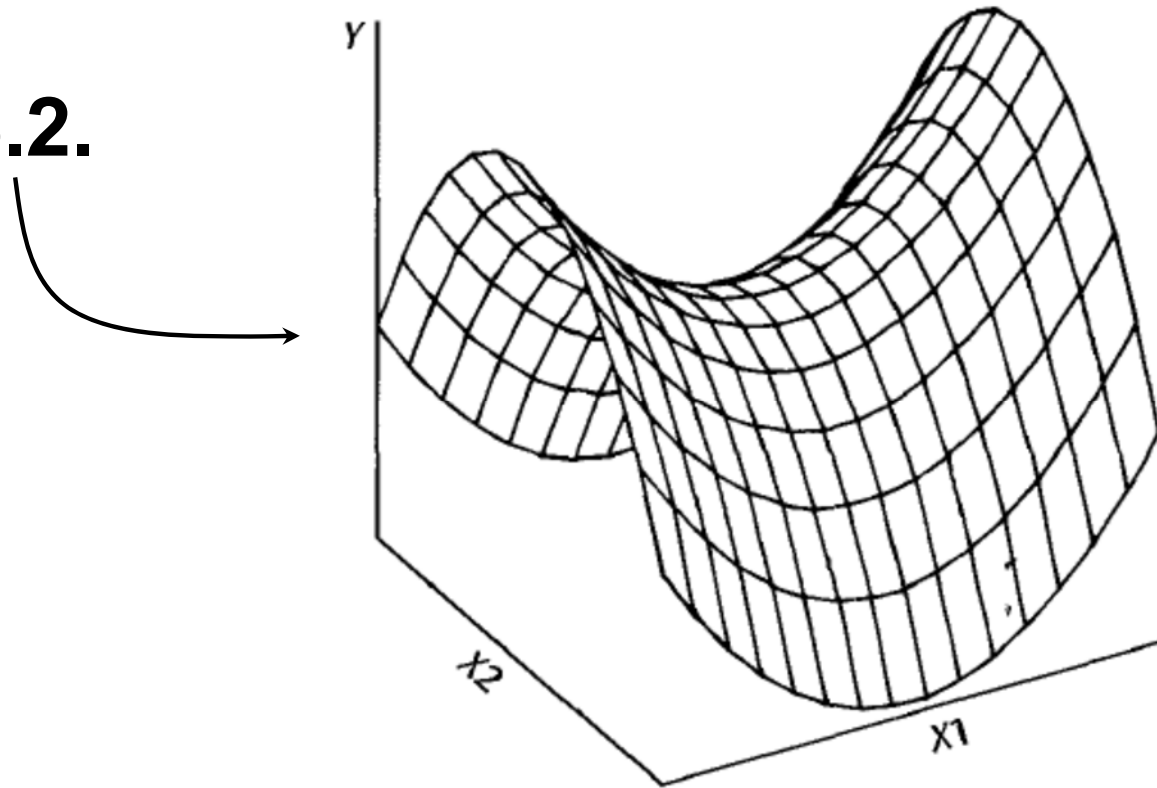
- We combine the second-order polynomial with second-order interactions to create a **response surface model**:

$$E\{Y_i\} = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i1}^2 + \beta_3 X_{i2} + \beta_4 X_{i2}^2 + \beta_5 X_{i1} X_{i2}$$

- (Why is this “linear”? Because all the β_k 's enter into $E\{Y\}$ at first-order!)

Response Surface (cont'd)

- The second-order response surface model produces a smoothly arcing surface in 3-D space.
- See Fig. 6.2.



§6.2: MLR Matrix Formulation

The MLR model (with any $p - 1 > 1$) is a straightforward extension of SLR, so the matrix equations are of essentially identical form.

$$\text{Recall } \mathbf{Y}_{n \times 1} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad \mathbf{E}\{\mathbf{Y}\} = \begin{bmatrix} E[Y_1] \\ E[Y_2] \\ \vdots \\ E[Y_n] \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\text{and now take } \mathbf{X}_{n \times p} = \begin{bmatrix} 1 & X_{11} & X_{12} & \dots & X_{1,p-1} \\ 1 & X_{21} & X_{22} & \dots & X_{2,p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{n,p-1} \end{bmatrix}$$

Matrix Formulation (cont'd)

If we let $\beta_{p \times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}$, we can write

the MLR model as a matrix expression:

$$Y_{n \times 1} = X_{n \times p} \beta_{p \times 1} + \epsilon_{n \times 1}$$

where $\epsilon \sim N_n(0, \sigma^2 I)$.

The mean response vector is $E\{Y\} = X\beta$
and the covariance matrix is $\sigma^2\{Y\} = \sigma^2 I$.

§6.3: LS Estimation

The LS normal equations can again be written simply as

$$(X'X)b = X'Y,$$

for $b = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{p-1} \end{bmatrix}$. The solution for b is clearly

$$b = (X'X)^{-1}X'Y$$

whenever $(X'X)^{-1}$ exists.

(Here again, these correspond to the MLE for β .)

§6.4: Fitted Values

The fitted values for the MLR are

$\hat{Y} = [\hat{Y}_1 \dots \hat{Y}_n]'$, which in matrix notation is again

$$\hat{Y} = Xb = HY.$$

The hat matrix remains $H = X(X'X)^{-1}X'$.

Also, the residual vector is still

$$e = Y - \hat{Y} = Y - HY = (I - H)Y,$$

with $\sigma^2\{e\} = (I - H)\sigma^2$ estimated via

$$s^2\{e\} = (I - H) \times \text{MSE}.$$

§6.5: MLR ANOVA

The MLR ANOVA table also looks similar to its SLR counterpart:

<u>Source</u>	<u>d.f.</u>	<u>SS</u>	<u>MS</u>
Regr.	$p-1$	$SSR=Y'(H - \frac{1}{n}J)Y$	$MSR=\frac{SSR}{p-1}$
<u>Error</u>	<u>$n-p$</u>	<u>$SSE=Y'(I - H)Y$</u>	<u>$MSE=\frac{SSE}{n-p}$</u>
Total	$n-1$	$SSTO=Y'(I - \frac{1}{n}J)Y$	

The expected means squares are $E\{MSE\} = \sigma^2$ and $E\{MSR\} = \sigma^2 + \theta^2(\beta)$ (see next slide).

E{MSR}

The expected mean square for MSR involves the expression $\theta^2(\beta)$, which is a complicated function of β such that $\theta^2(0) = 0$.

For instance, at $p=3$:

$$\theta^2(\beta) = \frac{1}{2} \left\{ \sum \sum \beta_k^2 (X_{ik} - \bar{X}_k)^2 + 2\beta_1\beta_2 \sum (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2) \right\}$$

This suggests that an F-test is available for testing $H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0 \rightarrow$

Full MLR F-Test

- To test $H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$ vs. H_a : any departure, construct the “full” F-statistic $F^* = MSR/MSE$ and reject H_0 when $F^* > F(1-\alpha; p-1, n-p)$.
- (At $p=2$ we clearly recover the SLR F-test of $H_0: \beta_1=0$.)
- The P-value is $P = P[F(p-1, n-p) > F^*]$.

Multiple R²

For the MLR model, the **Coefficient of Multiple Determination** mimics its SLR progenitor:

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

Again, $0 \leq R^2 \leq 1$.

Interpretation: R² is still the % of total variation in the Y_i's explained by the X_j's in the regression model.

Adjusted R^2

- With multiple X_k 's, however, R^2 exhibits irregularities.
- Notice that by adding a new X_k to the model, SSE cannot increase. Thus we can drive $R^2 \rightarrow 1$ simply by pushing $p \rightarrow n$.
- An **adjusted R^2** compensates by replacing the SS terms with MS terms:
$$R_a^2 = 1 - \{MSE/MSTO\}.$$
- Interpretation is essentially similar.

§6.6: MLR Inferences

The LS estimator \mathbf{b} is again unbiased:

$$E\{\mathbf{b}\} = \boldsymbol{\beta}.$$

Its sample covariance mtx. is again

$s^2\{\mathbf{b}\} = \text{MSE}(\mathbf{X}'\mathbf{X})^{-1}$. Take a closer look:

$$s^2\{\mathbf{b}\} = \begin{bmatrix} s^2\{b_0\} & s\{b_0, b_1\} & \dots & s\{b_0, b_{p-1}\} \\ s\{b_1, b_0\} & s^2\{b_1\} & \dots & s\{b_1, b_{p-1}\} \\ \vdots & \vdots & \vdots & \vdots \\ s\{b_{p-1}, b_0\} & s\{b_{p-1}, b_1\} & \dots & s^2\{b_{p-1}\} \end{bmatrix}$$

The covar. of b_0 and b_{p-1}

The var. of b_{p-1}

MLR inferences (cont'd)

So, each indiv. b_k has

$$T_k = \frac{b_k - \beta_k}{s\{b_k\}} \sim t(n-p)$$

($k = 0, \dots, p-1$). From this, a (pointwise) $1-\alpha$ conf. int. on β_k has the familiar form

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

Or, to test $H_0: \beta_k = 0$ vs. $H_a: \beta_k \neq 0$ find $t^* = b_k/s\{b_k\}$ & reject H_0 when $|t^*| > t(1 - \frac{\alpha}{2}; n-p)$.

(One-sided tests are similar.)

Bonferroni Adjustment

- But, **WATCH IT!** The t-based conf. int's and hypoth. tests are pointwise. If multiple b_k 's are assessed, need a multiplicity adjustment.
- For instance, **Bonferroni-adjusted simultaneous limits** on $g > 1$ different β_k 's are
$$b_k \pm B s\{b_k\}$$
for $B = t(1 - \frac{1}{2}\{\alpha/g\}; n-p)$ and $k = 1, \dots, g$.

§6.7: Inference on $E\{Y_h\}$

Given a future predictor vector $X_h = \begin{bmatrix} 1 \\ X_{h1} \\ \vdots \\ X_{h,p-1} \end{bmatrix}$,

an estimate of $E\{Y_h\}$ at this X_h is $\hat{Y}_h = X_h' b$.

We find $E\{\hat{Y}_h\} = X_h' \beta$ (unbiased!) with std. error $s\{\hat{Y}_h\} = \sqrt{\text{MSE}(X_h'(X'X)^{-1}X_h)}$.

A $1-\alpha$ conf. int. on $E\{Y_h\}$ then has the familiar form

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

Multiplicity Adjustment

Here again these are pointwise conf. int's.
If more than a single X_h is under study,
must apply a multiplicity adjustment.

Over a finite, pre-specified set of $g > 1$
 X_h 's, use the Bonferroni-adjusted intervals

$$\hat{Y}_h \pm B s\{\hat{Y}_h\}$$

where $B = t(1 - \frac{1}{2}\{\alpha/g\}; n-p)$ and $h = 1, \dots, g$.

Multiplicity Adjustment (cont'd)

Or, for an exact, simultaneous $1-\alpha$ **confidence (hyper-)band** on $E\{Y\}$ over all possible vectors X_h , use the WHS method:

$$\hat{Y}_h \pm W s\{\hat{Y}_h\}$$

for $W^2 = p F(1-\alpha; p, n-p)$.

WHS also applies (conservatively) for any $g > 1$ X_h 's, so always check: if $W \leq B$, use the WHS limits instead of Bonferroni.

(Can also use the WHS band, and only the WHS band, for *post hoc* intervals on $E\{Y_h\}$.)

MLR Prediction

For prediction of a future observation $Y_{h(\text{new})}$ at some $X_{h(\text{new})}$, use

$$\hat{Y}_{h(\text{new})} = X'_{h(\text{new})} \mathbf{b},$$

with

$$s\{\text{pred}\} = \sqrt{\text{MSE} \left(1 + X'_{h(\text{new})} (\mathbf{X}'\mathbf{X})^{-1} X_{h(\text{new})} \right)}.$$

The corresp. (pointwise) $1-\alpha$ **prediction interval** is then

$$\hat{Y}_{h(\text{new})} \pm t\left(1 - \frac{\alpha}{2}; n-p\right) s\{\text{pred}\}.$$

S-Method Prediction Intervals

As previously, the pointwise prediction interval is valid at only one $X_{h(\text{new})}$. For simultaneous prediction intervals at $g > 1$ future $X_{h(\text{new})}$'s, apply a modification of the WHS method due to Scheffé (called the “S-method”):

$$\hat{Y}_{h(\text{new})} \pm S s\{\text{pred}\}$$

where $S = \sqrt{g F(1-\alpha; g, n-p)}$,
for $h = 1, \dots, g$.

Bonferroni Prediction Intervals

Can also use Bonferroni intervals for multiplicity-adjusted predictions:

$$\hat{Y}_{h(\text{new})} \pm B s\{\text{pred}\}$$

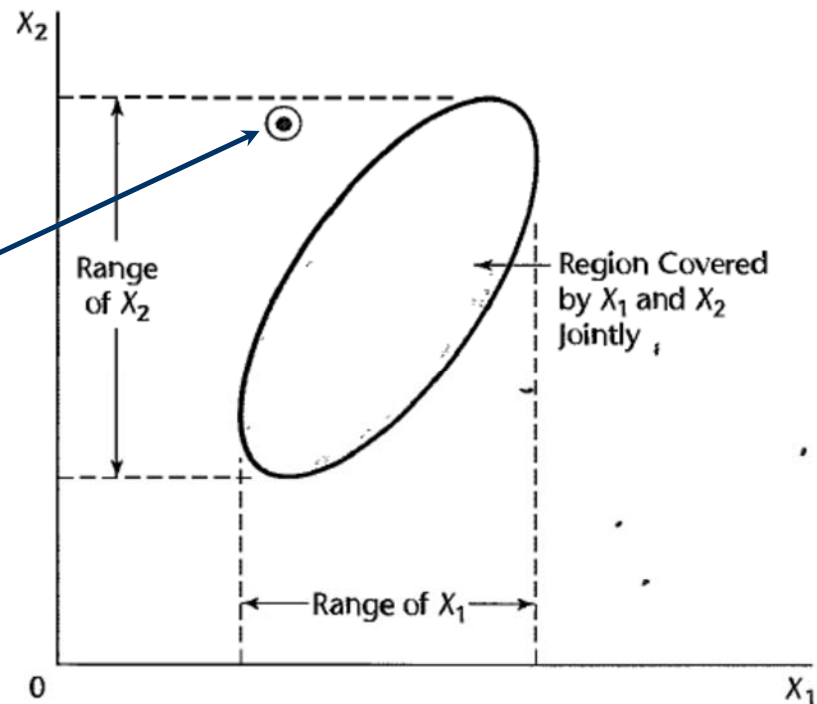
with $B = t(1 - 1/2\{\alpha/g\}; n-p)$ over $h = 1, \dots, g$.

Both the Scheffé and Bonferroni crit. points are conservative for any finite g , so check first: if $S \leq B$, use Scheffé's S -method, otherwise use Bonferroni.

Extrapolation

- As always, **be careful** with extrapolated X_h vectors.
- Ensure that the entire vector is within the range of the data.
- See Fig. 6.3 at p=3:

This point extrapolates, but that's not clear without a careful look at the data.



§6.8: Diagnostics

Preliminary diagnostics to assess an MLR fit include:

- Quick check of pairwise correlations among Y and each/all X_k 's: make sure no surprises are hiding (also see 'multicollinearity' discussion in §7.6).
- Should **always plot the data!** Try plotting Y vs. each X_k . Use a **scatterplot matrix** (see Fig. 6.4).
- Also try 3-D scatterplots of Y vs. pairs of X_k 's. If available, apply real-time rotation. (In R, use `plot3d()` function from external *rgl* package.)

MLR Residual Plots

Residual plots remain a mainstay:

- plot e_i vs. \hat{Y}_i (the usual resid. plot)
- plot $e_i = Y_i - \hat{Y}_i$ vs. X_{ik} at every $k = 1, \dots, p-1$
- graph histograms/boxplots of the e_i 's
- check NP plot of the e_i 's

(Same interpretations apply as in the SLR case.)

Brown-Forsythe Test

The Brown-Forsythe test for constant σ^2 remains valid with the MLR model:

- (a) Divide e_i 's into two groups: group 1 has e_i 's from small **fitted values, \hat{Y}_i ,**
- (b) and group 2 has e_i 's from large **fitted values, \hat{Y}_i .**
- (c) Then construct the t_{BF}^* -statistic as in §3.6. Conclude significant departure from homogeneous variance if
$$|t_{BF}^*| > t(1 - \frac{\alpha}{2}; n-2).$$
- (d) P-value is $2P[t(n-2) > |t_{BF}^*|]$.

Other Diagnostics/Remediation

- **To test for Lack of Fit (LOF), can apply F-tests similar to those seen in §3.7.**
 - **Need to have appropriate form(s) of replication among the X_k 's.**
 - **Can get tricky! See p. 235.**
- **If serious departures from normality or from variance homogeneity are observed, can apply Box-Cox power transformation to Y_i , as in §3.9.**

§6.9: MLR Example – Dwaine Studios (CH06FI05)

- Example: $p=3$ (two predictors) with
 - Y = portrait studio sales
 - X_1 = target popl'n below 16 yrs. old
 - X_2 = per cap. disposable income
- Data in Fig. 6.5.
- Start with: (a) scatterplot matrix, and (b) quick check of pairwise correlations.

Dwaine Studios (CH06FI05)

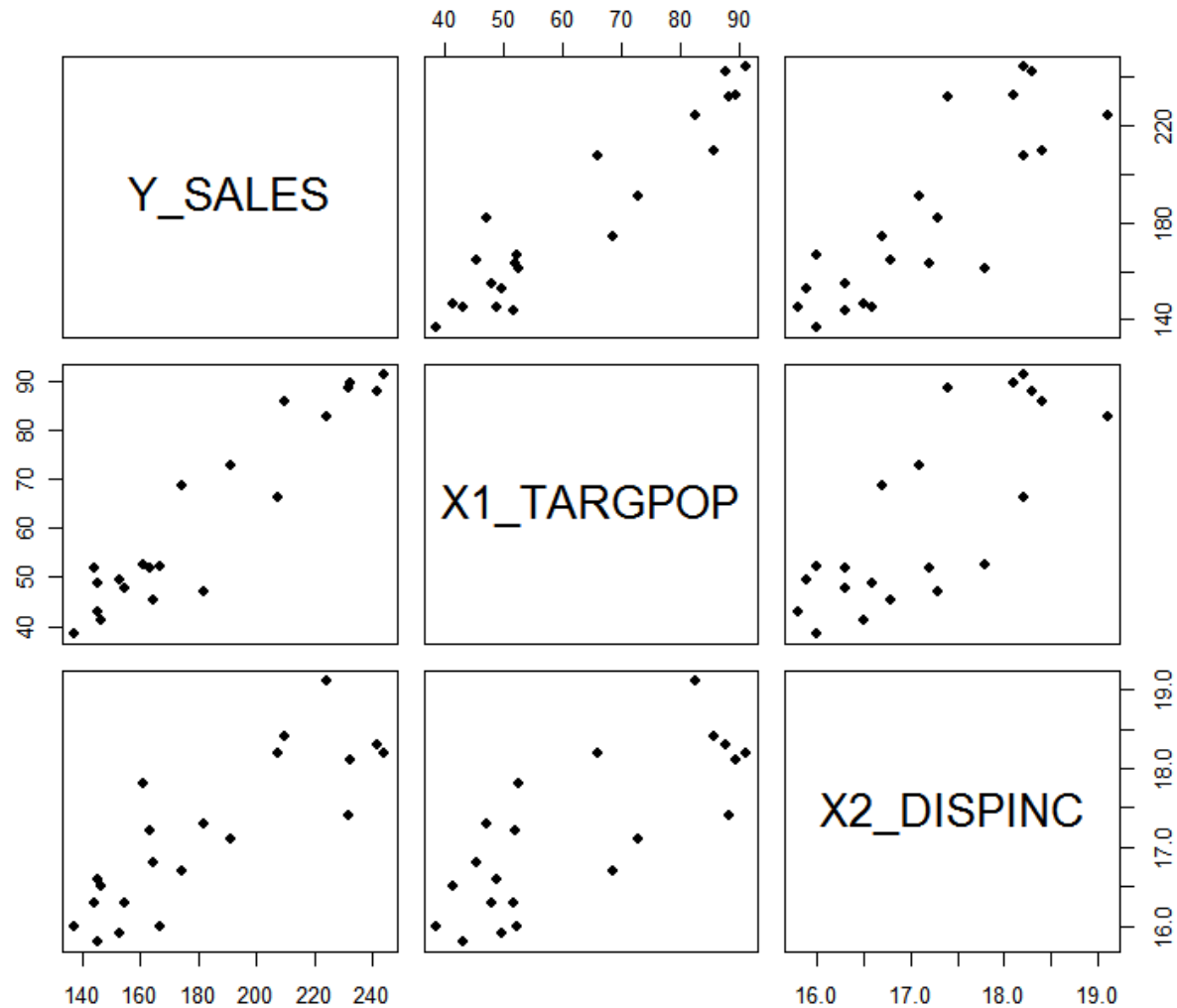
Scatterplot Matrix

For the **Scatterplot Matrix** in R, apply the **`pairs()`** command to a data frame containing the variables:

```
> CH06FI05.df = data.frame( Y_SALES,  
                             X1_TARGPOP, X2_DISPINC )  
  
> pairs( CH06FI05.df )
```


Dwaine Studios Data (CH06FI05)

Scatterplot Matrix



Dwaine Studios (CH06FI05)

Correlation Matrix

For the correlations between Y and the multiple X_k predictor variables, in R apply the `cor()` command to the data frame:

```
> cor( CH06FI05.df )
```

	Y_SALES	X1_TARGPOP	X2_DISPINC
Y_SALES	1.0000000	0.9445543	0.8358025
X1_TARGPOP	0.9445543	1.0000000	0.7812993
X2_DISPINC	0.8358025	0.7812993	1.0000000

Dwaine Studios (CH06FI05) (cont'd)

Fit MLR model with $p-1 = 2$ predictors:

```
> CH06FI05.lm = lm( Y_SALES ~  
                    X1_TARGPOP + X2_DISPINC )
```

```
> coef( CH06FI05.lm )  
      (Intercept)      X1_TARGPOP      X2_DISPINC  
      -68.85707           1.45456           9.36550
```

```
> summary( CH06FI05.lm )$r.squared  
$r.squared  
[1] 0.9167465
```

R^2 ←

```
> summary( CH06FI05.lm )$adj.r.squared  
$adj.r.squared  
[1] 0.9074961
```

R_a^2 ←

Dwaine Studios (CH06FI05) (cont'd)

Fit MLR model with $p-1 = 2$ predictors:

```
> CH06FI05.lm = lm( Y_SALES ~  
                    X1_TARGPOP + X2_DISPINC )  
> coef( CH06FI05.lm )
```

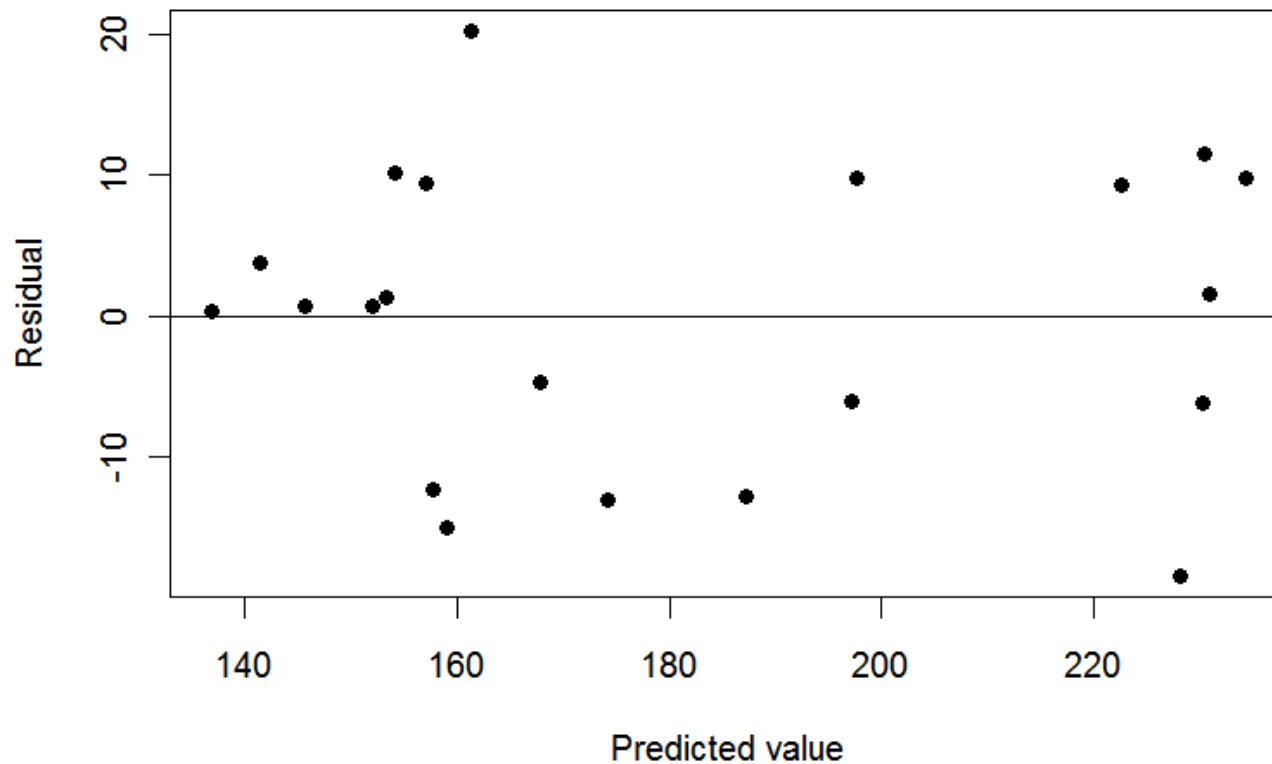
(Intercept)	X1_TARGPOP	X2_DISPINC
-68.85707	1.45456	9.36550

So, e.g., a unit (\$K) increase in $X_2 = \{\text{dispos. income}\}$ generates a \$9.3655K incr. in sales, **when $X_1 = \text{target popln. size}$ is held fixed.**

Dwaine Studios (CH06FI05) (cont'd)

Residual plot ($e_i = Y_i - \hat{Y}_i$ vs. \hat{Y}_i):

```
> plot( resid(CH06FI05.lm) ~ fitted(CH06FI05.lm) )  
> abline( h=0 )
```



Dwaine Studios (CH06FI05) (cont'd)

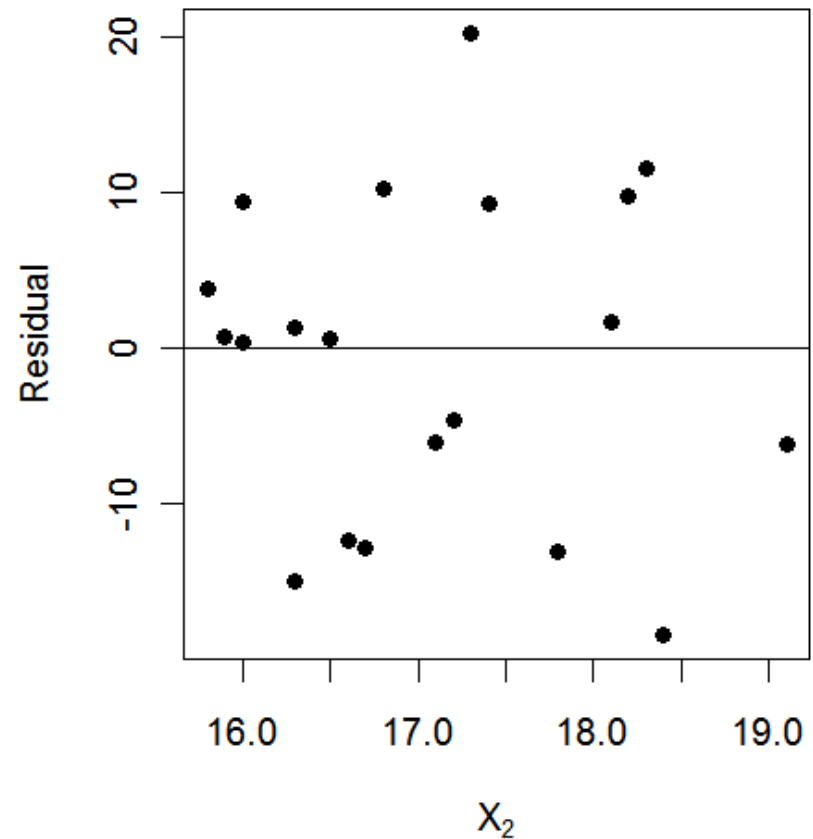
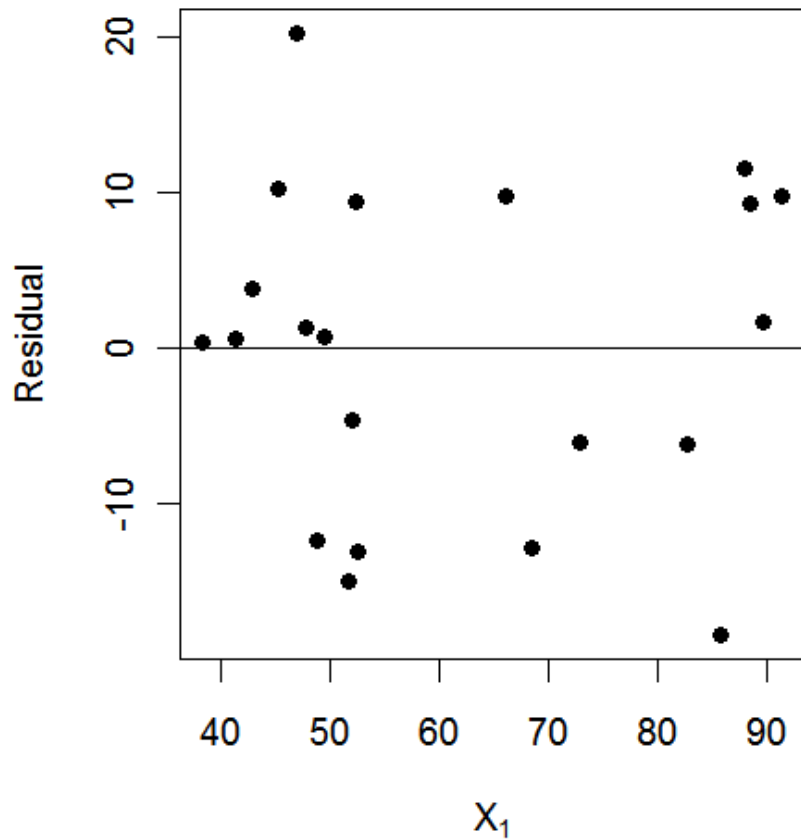
Per-predictor residual plots ($e_i = Y_i - \hat{Y}_i$ vs. each X_{ik}):

```
> par( mfrow=c(1,2) )
> plot( resid(CH06FI05.lm) ~ X1_TARGPOP,
        pch=19, xlab=expression(X[1]),
        ylab='Residual' )
> abline( h=0 )
> plot( resid(CH06FI05.lm) ~ X2_DISPINC,
        pch=19, xlab=expression(X[2]),
        ylab='Residual' )
> abline( h=0 )
```

Plots follow →

Dwaine Studios (CH06FI05) (cont'd)

Per-predictor residual plots (cf. Fig. 6.8):



Dwaine Studios (CH06FI05) (cont'd)

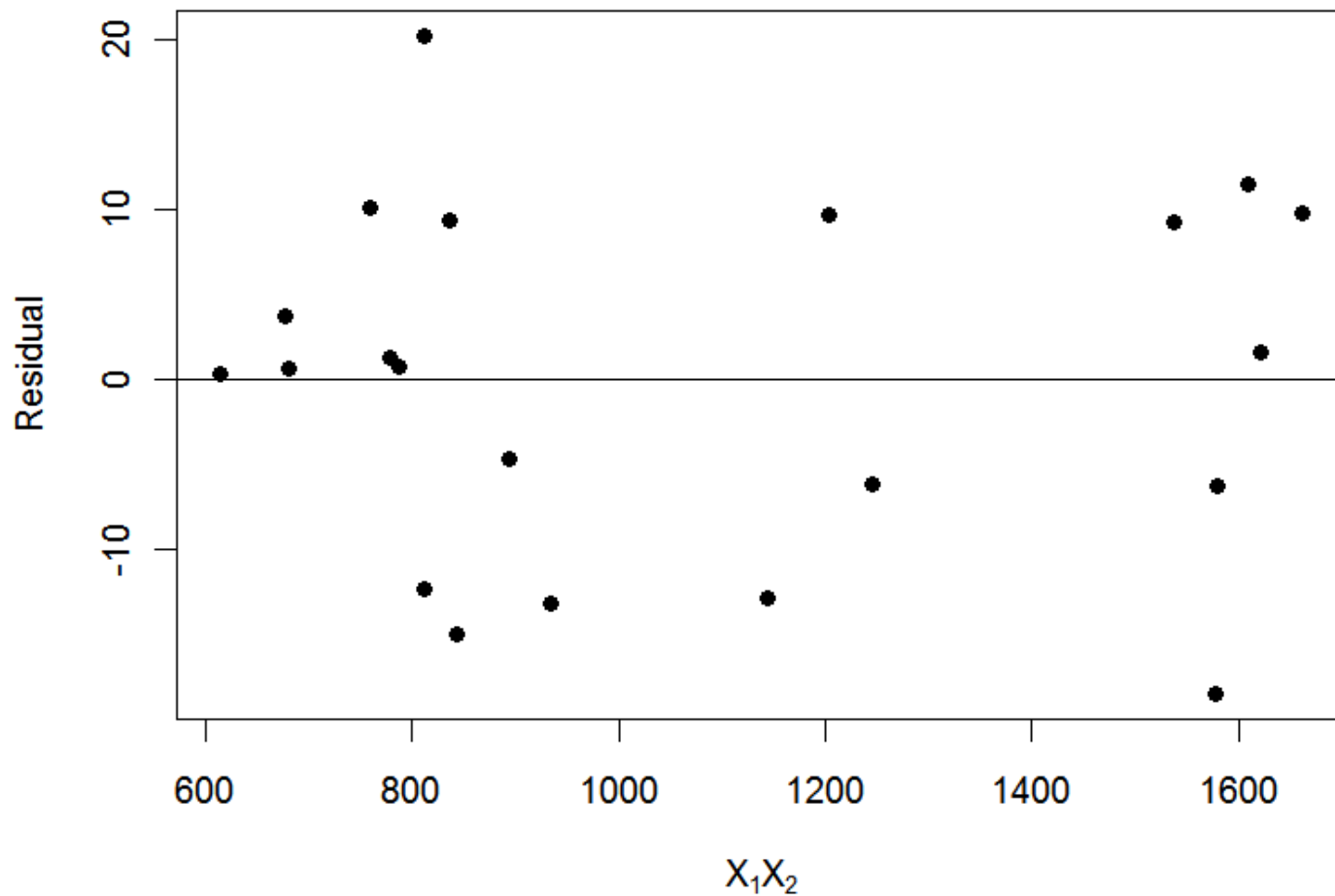
Can also plot residuals against functions of the X_{ik} s; e.g., plot e_i vs. potential interaction term $X_{i1}X_{i2}$:

```
> X3 = X1_TARGPOP * X2_DISPINC
> plot( resid(CH06FI05.lm) ~ X3,
        pch=19, ylab='Residual',
        xlab=expression(X[1]*X[2]) )
> abline( h=0 )
```

A systematic pattern in the plot suggests a need for the interaction term in the full MLR model →

Dwaine Studios (CH06FI05) (cont'd)

Interaction-predictor residual plot shows no systematic pattern (cf. Fig. 6.8d):



Dwaine Studios (CH06FI05) (cont'd)

ANOVA for testing full MLR model with $p-1 = 2$ predictors:

```
> anova( lm(Y_SALES ~ 1), CH06FI05.lm )
```

```
Model 1: Y_SALES ~ 1
```

```
Model 2: Y_SALES ~ X1_TARGPOP + X2_DISPINC
```

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	20	26196.2				
2	18	2180.9	2	24015	99.103	1.921e-10

$F^* = 99.1$ with highly signif. P-value = 1.9×10^{-10} .

Dwaine Studios (CH06FI05) (cont'd)

Pointwise conf. intervals on β_1 and β_2 are available via `confint(CH06FI05.lm)`. For Bonferroni-corrected **simultaneous conf. intervals**, adjust via the `level=` option:

```
> g = length( coef(CH06FI05.lm) ) - 1
> alpha = .10
> confint( CH06FI05.lm, level=1-(alpha/g) )[2:3,]
```

	[lower]	[upper]
X1_TARGPOP	1.0096226	1.899497
X2_DISPINC	0.8274411	17.903560

(cf. p. 245)

Dwaine Studios (CH06FI05) (cont'd)

- Pointwise **conf. intervals on $E\{Y_h\}$** at single future value of predictor vector

$$\mathbf{X}_h' = [\mathbf{X}_{h0} \ \mathbf{X}_{h1} \ \mathbf{X}_{h2}] = [1 \ 65.4 \ 17.6]:$$

- In R, need to define new data frame containing desired \mathbf{X}_h value(s):

```
> newdata.df = data.frame( X1_TARGPOP=65.4,  
                           X2_DISPINC=17.6 )
```

- Then, employ **predict.lm()** function:

```
> predict.lm( CH06FI05.lm, newdata=newdata.df,  
              se.fit=T, interval='confidence' )
```

Dwaine Studios (CH06FI05) (cont'd)

Output from `predict.lm()`:

```
> predict.lm( CH06FI05.lm, newdata=newdata.df,
              se.fit=T, interval='confidence' )
```

```
$fit
```

	fit	lwr	upr
1	191.1039	185.2911	196.9168

```
$se.fit
```

```
[1] 2.766798
```

```
$df
```

```
[1] 18
```

Lower and upper 95% limits

\hat{Y}_h

std. error, $s\{\hat{Y}_h\}$

Dwaine Studios (CH06FI05) (cont'd)

- Pointwise **prediction intervals on Y_h** at single future value of predictor vector $X_h' = [X_{0h} \ X_{1h} \ X_{2h}] = [1 \ 65.4 \ 17.6]$:
- In R, continue to employ **`predict.lm()`** function with **`newdata.df`** data frame, but change **`interval=`** option:

```
> predict.lm( CH06FI05.lm, newdata=newdata.df,
              se.fit=T, interval='prediction' )
```

Dwaine Studios (CH06FI05) (cont'd)

Prediction from `predict.lm()`:

```
> predict.lm( CH06FI05.lm, newdata=newdata.df,
              interval='prediction' )
```

	fit	lwr	upr
1	191.1039	167.2589	214.949

\hat{Y}_h

Lower and upper
95% prediction limits

This is a *pointwise* prediction interval. For *multiple* X_h 's, correction for simultaneity is required.

Dwaine Studios (CH06FI05) (cont'd)

Simultaneous **prediction intervals on Y_h** at $g = 2$ future values of predictor vector:

$$\mathbf{X}_h = \begin{bmatrix} 1 \\ 65.4 \\ 17.6 \end{bmatrix}, \begin{bmatrix} 1 \\ 53.1 \\ 17.7 \end{bmatrix}$$

```
> newdata.df = data.frame( X1_TARGPOP=c(65.4,53.1),  
                           X2_DISPINC=c(17.6,17.7) )  
  
> g = nrow( newdata.df )
```


Dwaine Studios (CH06FI05) (cont'd)

- Simultaneous **90% prediction intervals on Y_h**
- Begin with check of Scheffé vs. Bonferroni critical points:

```
> alpha = .10
> Spoint = sqrt( g*qf(1-alpha, g,
                    CH06FI05.lm$df.residual) )
[1] 2.290828
```

```
> Bpoint = qt( 1-(.5*(alpha/g)),
                CH06FI05.lm$df.residual )
[1] 2.100922
```

- $B = 2.10 \leq S = 2.29$, so apply Bonferroni adjustment

Dwaine Studios (CH06FI05) (cont'd)

Simultaneous **90% prediction intervals** on Y_h with Bonferroni critical point at $g=2$:

```
> newdata.df
```

	X1_TARGPOP	X2_DISPINC
1	65.4	17.6
2	53.1	17.7

```
> predict.lm( CH06FI05.lm, newdata=newdata.df,
               interval='prediction',
               level=1-(alpha/g)) )
```

	fit	lwr	upr
1	191.1039	167.2589	214.9490
2	174.1494	149.0867	199.2121