Linear Regression

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Multiple Regression:

General Linear Tests

General Linear Tests

$\mathcal{I}$ and $\mathcal{J}$ are two non-overlapping index sets:

- **Full model**: with both $X_{\mathcal{I}}$ and $X_{\mathcal{J}}$
- **Reduced model**: with only $X_{\mathcal{I}}$
- Test whether $X_{\mathcal{J}}$ may be dropped out of the full model:

$$H_0 : \beta_j = 0, \text{ for } \textbf{all } j \in \mathcal{J} \quad vs. \quad H_a : \text{not all } \beta_j : j \in \mathcal{J} \text{ is zero}$$

- H_0 corresponds to the reduced model with only $X_{\mathcal{I}}$.

F Test

Compare SSE under the full model with SSE under the reduced model by an F ratio:

$$F^* = \frac{\frac{SSE(R)-SSE(F)}{df_R - df_F}}{\frac{SSE(F)}{df_F}} = \frac{MSR(X_{\mathcal{J}}|X_{\mathcal{I}})}{MSE(F)}$$

- Under H_0 (i.e., the reduced model):

$$F^* \sim_{H_0} F_{df_R - df_F, df_F}$$

- Reject H_0 at level α iff the observed $F^* > F(1-\alpha; df_R - df_F, df_F)$.

Multiple Regression:

General Linear Tests

Examples

F-test for Regression Relation

- Full model with $X_1, \cdots, X_{p-1}$:

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

- Reduced model with no X variable:

$$Y_i = \beta_0 + \epsilon_i, \;\; i = 1, \cdots, n, \quad SSE(R) = SSTO, \; df_R = n - 1$$

- $SSE(R) - SSE(F) = SSTO - SSE(F) = SSR(F)$, and

  $df_R - df_F = (n-1) - (n-p) = p - 1 = d.f.(SSR(F))$

- $F^* = \frac{SSR(F)/(p-1)}{SSE(F)/(n-p)} = \frac{MSR(F)}{MSE(F)}$

Test whether a Single $\beta_k = 0$

Body Fat: for the model with all three predictors, test whether the midarm circumference (X_3) can be dropped.

- Full model: $SSE(F) = 98.40$ with d.f. 16:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i, \quad i = 1, \cdots, 20.$$

- Reduced model: $SSE(R) = 109.95$ with d.f. 17:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i, \quad i = 1, \cdots, 20.$$

- $F^* = \frac{11.55/1}{98.40/16} = 1.88$; Pvalue=$P(F_{1,16} > 1.88) = 0.189$, so X_3 can be dropped.

Equivalence between F-test and T-test

- $H_0 : \beta_k = 0 \;\; vs. \;\; H_a : \beta_k \neq 0$
- T-test:
$$T^* = \frac{\hat{\beta}_k}{s\{\hat{\beta}_k\}} \underset{H_0}{\sim} t_{(n-p)},$$
where $\hat{\beta}_k$ is the LS estimator of β_k and $s\{\hat{\beta}_k\}$ is its standard error. At level α, reject H_0 when $|T^*| > t(1-\alpha/2; n-p)$.
- $F^* = (T^*)^2$ and $F(1-\alpha; 1, n-p) = (t(1-\alpha/2; n-p))^2 \rightarrow$ F-test and two-sided T-test are equivalent.

For one-sided alternatives, we still need the T-tests.

Test whether Several $\beta_k = 0$

Body Fat: Test whether both X_2 and X_3 can be dropped from the model with all three predictors:

- Full model: $SSE(F) = 98.40$ with d.f. 16:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \epsilon_i, \quad i = 1, \cdots, 20.$$

- Reduced model: $SSE(R) = 143.12$ with d.f. 18:

$$Y_i = \beta_0 + \beta_1 X_{i1} + \epsilon_i, \quad i = 1, \cdots, 20.$$

- $F^* = \frac{44.72/2}{98.40/16} = 3.635$; Pvalue$= P(F_{2,16} > 3.635) = 0.0499$

Test Equality of Several β_ks

- Full model: $Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i$
- For $q \leq p-1$: $H_0 : \beta_1 = \cdots = \beta_q$ *vs.* $H_a : \beta_1, \cdots, \beta_q$ are not all equal
- Reduced model: $Y_i = \beta_0 + \beta_c (X_{i1} + \cdots + X_{iq}) + \cdots + \beta_{p-1} X_{i,p-1} + \epsilon_i$
- β_c denotes the common value of $\beta_1, \cdots, \beta_q$ under H_0, and $X_1 + \cdots + X_q$ is the corresponding (new) X variable. $SSE(R)$ has d.f. $n-(p-q+1)$.
- $F^* = \frac{(SSE(R)-SSE(F))/(q-1)}{SSE(F)/(n-p)} \underset{H_0}{\sim} F_{q-1,n-p}$

Multiple Regression: Regression Coefficients as Partial Coefficients

Coefficient of Partial Determination

Proportional reduction in SSE by adding one X variable into a model: ($j \notin \mathcal{I}$)

$$R^2_{Y,j|\mathcal{I}} := \frac{SSE(X_{j\cup\mathcal{I}}) - SSE(X_{\mathcal{I}})}{SSE(X_{\mathcal{I}})} = \frac{SSR(X_j|X_{\mathcal{I}})}{SSE(X_{\mathcal{I}})}$$

- Between 0 and 1
- Example: $R^2_{Y,1|2} = \frac{SSR(X_1|X_2)}{SSE(X_2)}$ is the proportional reduction in SSE by including X_1 into the model with X_2.

Body Fat

A researcher measured the amount of body fat (Y) of 20 healthy females 25 to 34 years old, together with three (potential) predictor variables, triceps skinfolds thickness (X_1), thigh circumference (X_2), and midarm circumference (X_3). The amount of body fat was obtained by a cumbersome and expensive procedure requiring immersion of the person in water. Thus it would be helpful if a regression model with some or all of these predictors could provide reliable estimates of body fat as these predictors are easy to measure.

Boy Fat: Model 3

```
Call:
lm(formula = Y ~ X1 + X2, data = fat)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) -19.1742     8.3606  -2.293   0.0348 *
X1            0.2224     0.3034   0.733   0.4737
X2            0.6594     0.2912   2.265   0.0369 *
---
Residual standard error: 2.543 on 17 degrees of freedom
Multiple R-squared: 0.7781,     Adjusted R-squared: 0.7519
F-statistic:  29.8 on 2 and 17 DF,  p-value: 2.774e-06

Analysis of Variance Table
Response: Y
Df Sum Sq Mean Sq F value    Pr(>F)
X1         1 352.27  352.27 54.4661 1.075e-06 ***
X2         1  33.17   33.17  5.1284    0.0369 *
Residuals 17 109.95    6.47
```

Boy Fat: Model 4

```
lm(formula = Y ~ X1 + X2 + X3, data = fat)

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
X3            -2.186      1.595  -1.370    0.190
---
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)
X1         1 352.27  352.27 57.2768 1.131e-06 ***
X2         1  33.17   33.17  5.3931   0.03373 *
X3         1  11.55   11.55  1.8773   0.18956
Residuals 16  98.40    6.15
```

Body Fat

$$R^2_{Y,2|1} = \frac{SSR(X_2|X_1)}{SSE(X_1)} = \frac{33.17}{33.17 + 11.55 + 98.40} = 23.2\%.$$

$$R^2_{Y,3|12} = \frac{SSR(X_3|X_1, X_2)}{SSE(X_1, X_2)} = \frac{11.55}{11.55 + 98.40} = 10.5\%.$$

When X_2 is added to the model containing X_1, SSE is reduced by 23.2%; When X_3 is added to the model containing X_1, X_2, SSE is reduced by 10.5%.

Extra Sum of Squares as SSR and Interpretation of Coefficient of Partial Determination

It can be shown that:

- $SSR(X_j|X_{\mathcal{I}})$ is the SSR when regressing the residuals $e(Y|X_{\mathcal{I}}) = Y - \hat{Y}(X_{\mathcal{I}})$ to the residuals $e(X_j|X_{\mathcal{I}}) = X_j - \hat{X}_j(X_{\mathcal{I}})$.
- $R^2_{Y,j|\mathcal{I}}$ is the coefficient of simple determination between the two sets of residuals.
- $R^2_{Y,j|\mathcal{I}}$ thus measures linear association between Y and X_j after the linear effects of $X_{\mathcal{I}}$ have been adjusted for.

Example: $R^2_{Y,1|2}$

- Regress Y on X_2: $e_i(Y|X_2) = Y_i - \widehat{Y}_i(X_2), \;\; i = 1, \cdots n.$
- Regress X_1 on X_2: $e_i(X_1|X_2) = X_{i1} - \widehat{X}_{i1}(X_2), \;\; i = 1, \cdots n.$
- $R^2_{Y1|2}$ equals to the coefficient of simple determination between $e_i(Y|X_2)$ and $e_i(X_1|X_2)$.
- It measures the linear association between Y and X_1 after the linear effects of X_2 have been adjusted for.

Partial Correlations

The **signed** square-root of a coefficient of partial determination is called a partial correlation.

- The sign is the same as the sign of the corresponding fitted regression coefficient (in the larger model).
- Partial correlation is the correlation coefficient between the two respective sets of residuals.

Body Fat

- $r_{Y2|1} = \sqrt{0.232} = 0.482$, since in Model 3, $\hat{\beta}_2 > 0$.
- $r_{Y3|12} = -\sqrt{0.105} = -0.324$, since in Model 4, $\hat{\beta}_3 < 0$.

LS Fitted Regression Coefficients as Partial Coefficients

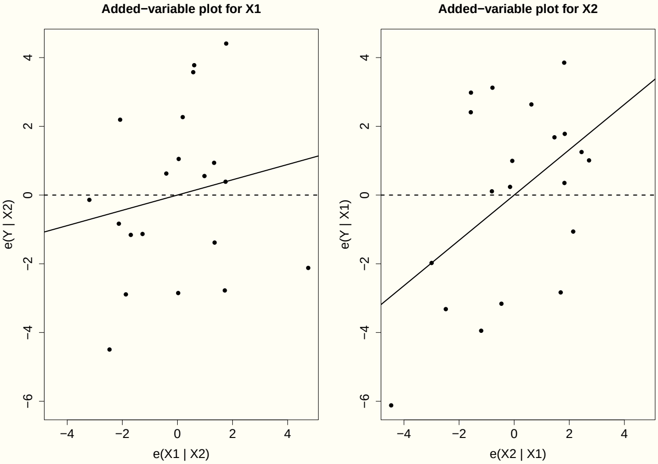
The LS fitted regression coefficients $\hat{\beta}$ are indeed partial coefficients.

- Consider $p-1$ X variables in the model. Let $\hat{\beta}_j$ be the LS fitted regression coefficient for X_j.
- Then $\hat{\beta}_j$ equals to the LS fitted regression coefficient when regressing the residuals $e(Y|X_{-(j)}) = Y - \hat{Y}(X_{-(j)})$ to the residuals $e(X_j|X_{-(j)}) = X_j - \hat{X}_j(X_{-(j)})$, where $X_{-(j)} = \{X_l : 1 \leq l \neq j \leq p\}$.

Added-Variable Plots

- Both the response variable Y and X_j are regressed onto the rest of the X variables, denoted by $X_{-(j)}$, in the model.
- The residuals reflect the part of Y (X_j) that is not linearly associated with the rest of the X variables.
- The plot of these two sets of residuals against each other:
    - shows the marginal importance of X_j in reducing the residual variability in Y after accounting for the linear effects in the rest of the X variables.
    - provides information about the nature of the marginal effect of X_j on Y, e.g., linear or curvilinear.

Figure: Body Fat $Y \sim X_1, X_2$: Added-variable plots



- Added-variable plot for X_1 (given X_2) implies that X_1 is of not much additional help in explaining Y when X_2 is already in the model. This is consistent with $R^2_{Y1|2} = 3.1\%$.
- Added-variable plot for X_2 (given X_1) shows that X_2 is of some help in explaining Y when X_1 is already in the model. From previous slides, $R^2_{Y2|1} = 23.2\%$. It also shows that a linear term of X_2 in the model is adequate.

Standardization

Standardization

X values could differ substantially in order of magnitude. This could lead to:

- Regression coefficients not comparable
- Numerical instability in inverting $\mathbf{X}'\mathbf{X}$

A regression model can be *reparametrized* into a *standardized regression model* through centering and rescaling.

Transformed X Variables

$$X_{ik}^* = \frac{1}{\sqrt{n-1}}\left(\frac{X_{ik} - \overline{X}_k}{s_k}\right), \quad i = 1, \cdots, n, \; k = 1, \cdots, p-1,$$

where

$$\overline{X}_k = \frac{1}{n}\sum_{i=1}^{n} X_{ik}, \quad s_k = \sqrt{\frac{\sum_{i=1}^{n}(X_{ik} - \overline{X}_k)^2}{n-1}}$$

are sample mean and sample standard deviation of X_k, respectively.

The transformed X variables are centered and are on the same scale:

- Their sample means equal zero.
- Their sample standard deviations equal $\frac{1}{\sqrt{n-1}}$.

Moreover, standardization does not change pairwise sample correlations.

Standardized Regression Model

Standardized Regression Model

Rewrite the regression model in terms of standardized variables:

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

where

$$\beta_k^* = \sqrt{n-1} s_k \beta_k \quad , k = 1, \cdots, p-1,$$

$$\beta_0^* = \beta_0 + \sum_{k=1}^{p-1} \beta_k \bar{X}_k$$

is a *reparametrization* of the original model.

Standardized Model: Design Matrix

$$\underset{n\times p}{\mathbf{X}^*} = \begin{bmatrix} 1 & X^*_{11} & \cdots & X^*_{1,p-1} \\ 1 & X^*_{21} & \cdots & X^*_{2,p-1} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & X^*_{n1} & \cdots & X^*_{n,p-1} \end{bmatrix}$$

Standardized Model: $\mathbf{X}'\mathbf{X}$

$$\underset{p\times p}{\mathbf{X}^{*\prime}\mathbf{X}^{*}} = \begin{bmatrix} n & 0 & 0 & \cdots & 0 \\ 0 & 1 & r_{12} & \cdots & r_{1,p-1} \\ 0 & r_{21} & 1 & \cdots & r_{2,p-1} \\ 0 & \vdots & \cdots & \vdots & \\ 0 & r_{p-1,1} & r_{p-1,2} & \cdots & 1 \end{bmatrix} = \begin{bmatrix} n & \mathbf{0}^T \\ \mathbf{0} & \underset{(p-1)\times(p-1)}{\mathbf{r}_{XX}} \end{bmatrix},$$

where $\mathbf{r}_{XX}$ is the sample correlation matrix of the X variables.

$$(\mathbf{X}^{*\prime}\mathbf{X}^{*})^{-1} = \begin{bmatrix} \frac{1}{n} & \mathbf{0}^T \\ \mathbf{0} & \mathbf{r}_{XX}^{-1} \end{bmatrix}$$

Sample Correlation Matrix $\mathbf{r}_{XX}$

Its (k, l)-element r_{kl} is the sample correlation coefficient between X_k and X_l:

$$r_{kl} = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(X_{ik} - \overline{X}_k)(X_{il} - \overline{X}_l)}{s_k s_l}, \quad 1 \leq k, l \leq p - 1.$$

- All elements are unit-less numbers between -1 and 1.
- All diagonal elements are one.
- Symmetric: $r_{kl} = r_{lk}$

Standardized Model: $\mathbf{X}'\mathbf{Y}$

$$\underset{p\times 1}{\mathbf{X}^{*\prime}\mathbf{Y}} = \begin{bmatrix} n\bar{Y} \\ \sqrt{n-1}s_Y r_1 \\ \sqrt{n-1}s_Y r_2 \\ \vdots \\ \sqrt{n-1}s_Y r_{p-1} \end{bmatrix} = \sqrt{n-1}s_Y \begin{bmatrix} \frac{n}{\sqrt{n-1}s_Y}\bar{Y} \\ \underset{(p-1)\times 1}{\mathbf{r}_{XY}} \end{bmatrix},$$

where r_k is the sample correlation coefficient between Y and X_k:

$$r_k = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(X_{ik} - \overline{X}_k)(Y_i - \overline{Y})}{s_k s_Y}, \quad k = 1, \cdots p-1$$

Standardized Model: Least Squares Estimator

$$\underset{p\times 1}{\hat{\boldsymbol{\beta}}^{*}} = \begin{bmatrix} \hat{\beta}_0^* \\ \hat{\beta}_1^* \\ \hat{\beta}_2^* \\ \vdots \\ \hat{\beta}_{p-1}^* \end{bmatrix} = \begin{bmatrix} \bar{Y} \\ \sqrt{n-1}\, s_Y \mathbf{r}_{XX}^{-1} \mathbf{r}_{XY} \end{bmatrix}$$

These are called the *fitted standardized regression coefficients*.

$$E(\hat{\boldsymbol{\beta}}^{*}) = \boldsymbol{\beta}^{*}, \quad \boldsymbol{\sigma}^{\mathbf{2}}\{\hat{\boldsymbol{\beta}}^{*}\} = \sigma^2(\mathbf{X}^{*\prime}\mathbf{X}^{*})^{-1} = \sigma^2 \begin{bmatrix} \frac{1}{n} & \mathbf{0}^T \\ \mathbf{0} & \mathbf{r}_{XX}^{-1} \end{bmatrix}$$

Relationships with the Original Model

- Fitted regression coefficients:

$$
\begin{aligned}
\hat{\beta}_k^* &= \sqrt{n-1}\, s_k \hat{\beta}_k, \quad k = 1, \cdots, p-1 \\
\hat{\beta}_0^* &= \hat{\beta}_0 + \sum_{k=1}^{p-1} \hat{\beta}_k \bar{X}_k (= \bar{Y})
\end{aligned}
$$

- Fitted values, residuals, and sums of squares are the same as the original model.

Uncorrelated X Variables

Uncorrelated X Variables

- $\mathbf{r}_{XX} = \mathbf{I}_{p-1}$
- Fitted standardized regression coefficients:

$$\hat{\beta}_k^* = \sqrt{n-1} s_Y \times r_k, \quad k = 1, \cdots, p-1$$

- Variance-covariance matrix:

$$\boldsymbol{\sigma}^2\{\hat{\boldsymbol{\beta}}^*\} = \sigma^2 \begin{bmatrix} \frac{1}{n} & \mathbf{0}^T \\ \mathbf{0} & \mathbf{I}_{p-1} \end{bmatrix}$$

If the X variables in the model are uncorrelated with each other, then the effect of one X variable does not depend on other X variables:

- The fitted regression coefficient of an X variable is not affected by other X variables.
- The fitted regression coefficients are uncorrelated with each other.
- The contribution of an X variable in reducing the error sum of squares equals its marginal effect:

$$SSR(X_j|X_{-(j)}) = SSR(X_j).$$

Example: Crew Productivity

A study on the effect of work crew size (X_1) and level of bonus pay (X_2) on productivity (Y). The levels of X_1 and X_2 are chosen such that they are uncorrelated (this is called an *orthogonal design*).

case	X1	X2	Y
	crew-size	bonus-pay	productivity
1	4	2	42
2	4	2	39
3	4	3	48
4	4	3	51
5	6	2	49
6	6	2	53
7	6	3	61
8	6	3	60

Crew Productivity: Model 1

```
Call:
lm(formula = Y ~ X1, data = data)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)   23.500     10.111   2.324   0.0591 .
X1             5.375      1.983   2.711   0.0351 *
---
Residual standard error: 5.609 on 6 degrees of freedom
Multiple R-squared: 0.5505,     Adjusted R-squared: 0.4755
F-statistic: 7.347 on 1 and 6 DF,  p-value: 0.03508

> anova(fit1)
Analysis of Variance Table
Response: Y
Df Sum Sq Mean Sq F value  Pr(>F)
X1         1 231.12 231.125   7.347 0.03508 *
Residuals  6 188.75  31.458
```

Crew Productivity: Model 2

```
Call:
lm(formula = Y ~ X2, data = data)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)   27.250     11.608   2.348   0.0572 .
X2             9.250      4.553   2.032   0.0885 .
---
Residual standard error: 6.439 on 6 degrees of freedom
Multiple R-squared: 0.4076,     Adjusted R-squared: 0.3088
F-statistic: 4.128 on 1 and 6 DF,  p-value: 0.08846

> anova(fit2)
Analysis of Variance Table
Response: Y
Df Sum Sq Mean Sq F value  Pr(>F)
X2         1 171.12 171.125  4.1276 0.08846 .
Residuals  6 248.75  41.458
```

Crew Productivity: Model 3

```
Call:
lm(formula = Y ~ X1 + X2, data = data)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)   0.3750     4.7405   0.079 0.940016
X1            5.3750     0.6638   8.097 0.000466 ***
X2            9.2500     1.3276   6.968 0.000937 ***
---
Residual standard error: 1.877 on 5 degrees of freedom
Multiple R-squared: 0.958,      Adjusted R-squared: 0.9412
F-statistic: 57.06 on 2 and 5 DF,  p-value: 0.000361

> anova(fit3)
Analysis of Variance Table
Response: Y
Df  Sum Sq Mean Sq F value    Pr(>F)
X1         1 231.125 231.125  65.567 0.0004657 ***
X2         1 171.125 171.125  48.546 0.0009366 ***
Residuals  5  17.625   3.525
```

Multicollinearity

Multicollinearity

Multicollinearity refers to the situation when the X variables are *intercorrelated* among themselves.

- This term is often reserved for the situation when the inter-correlation/collinearity among the X variables is high.
- This means there exists a nonzero vector $\mathbf{c}$ such that
  $\underset{n\times p}{\mathbf{X}}\underset{p\times 1}{\mathbf{c}} \approx \mathbf{0}_n$.
- Consequently, the matrix $\underset{p\times p}{\mathbf{X}'\mathbf{X}}$ would be nearly singular.

Body Fat

Variables: Y : body fat, X_1: triceps skinfolds thickness, X_2: thigh circumference, X_3: midarm circumference

Sample correlation matrix:

	X1	X2	X3	Y
X1	1.0000000	0.9238425	0.4577772	0.8432654
X2	0.9238425	1.0000000	0.0846675	0.8780896
X3	0.4577772	0.0846675	1.0000000	0.1424440
Y	0.8432654	0.8780896	0.1424440	1.0000000

Compare Models

Variables in Model	$\hat{\beta}_1$	$\hat{\beta}_2$	$s\{\hat{\beta}_1\}$	$s\{\hat{\beta}_2\}$	MSE
Model 1: X_1	0.8572	-	0.1288	-	7.95
Model 2: X_2	-	0.8565	-	0.1100	6.3
Model 3: X_1, X_2	0.2224	0.6594	0.3034	0.2912	6.47
Model 4: X_1, X_2, X_3	4.334	-2.857	3.016	2.582	6.15

- The fitted regression coefficient for X_1 (X_2) varies drastically depending on which other X variables are in the model.
- The standard errors of the fitted regression coefficients are inflated when more X variables are added to the model.

- X_1 and X_2 are highly correlated with each other **and** with the response variable Y.
- When X_2 is already in the model, the additional contribution from X_1 in explaining Y is small since X_2 contains much of the same information in terms of explaining Y:

$$SSR(X_1) = 352.27, \quad SSR(X_1|X_2) = 3.47$$

Boy Fat: Model 4

```
lm(formula = Y ~ X1 + X2 + X3, data = fat)

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
X3            -2.186      1.595  -1.370    0.190
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Response: Y
Df Sum Sq Mean Sq F value    Pr(>F)
X1         1 352.27  352.27 57.2768 1.131e-06 ***
X2         1  33.17   33.17  5.3931   0.03373 *
X3         1  11.55   11.55  1.8773   0.18956
Residuals 16  98.40    6.15
```

None of the X variables is statistically significant by the T test.

However, the F-test of regression relation is highly significant.

- The reduced model for each individual T test contains all other X variables and thus may be non-significant due to multicollinearity.
- The reduced model for the F test contains no X variable.
- The three T tests together are not equivalent to testing whether there is a regression relation between Y and the set of X variables (i.e., F test).

Effects of Multicollinearity

With multicollinearity, the estimated regression coefficients tend to have large sampling variability (i.e., large standard errors) $\Longrightarrow$

- Wide confidence intervals
- It's possible that none of the regression coefficients is statistically significant, but there is a significant regression relation between the response variable and the entire set of X variables.

However, multicollinearity does not prevent us from getting a good fit of the data.

With multicollinearity:

- The regression coefficient of an X variable depends on which other X variables also in the model.
- So regression coefficient does not reflect any inherent effect of the corresponding X variable, but reflects only a marginal effect given whatever other X variables also in the model.
- Similarly, the reduction in the total variation in Y ascribed to an X variable must be interpreted as a margin reduction given other X variables also in the model.

Variance Inflation Factor

Quantify Multicollinearity

$$\boldsymbol{\sigma}^{\mathbf{2}}\{\hat{\boldsymbol{\beta}}^*\} = \sigma^2 \begin{bmatrix} \frac{1}{n} & \mathbf{0}^T \\ \mathbf{0} & \mathbf{r}_{XX}^{-1} \end{bmatrix}$$

- The kth diagonal element of the inverse correlation matrix $\mathbf{r}_{XX}^{-1}$ is called the **variance inflation factor (VIF)** for $\hat{\beta}_k^*$, denoted by VIF_k:

$$\boldsymbol{\sigma}^2\{\hat{\beta}_k^*\} = VIF_k \sigma^2, \quad k = 1, \cdots, p-1$$

It can be shown that $VIF_k = \frac{1}{1-R_k^2}$, where R_k^2 is the coefficient of multiple determination when X_k is regressed onto the rest X variables:

- $VIF_k \geq 1$
- If X_k is uncorrelated with the rest X variables, then $R_k^2 = 0$ and $VIF_k = 1 \Longrightarrow$ no variance inflation
- If $R_k^2 > 0$, then $VIF_k > 1 \Longrightarrow$ an inflated variance of $\hat{\beta}_k^*$ due to intercorrelation between X_k and the rest X variables
- If X_k has a perfect linear association with the rest X variables, then $R_k^2 = 1$ and $VIF_k = \infty \Longrightarrow$ LS estimator not well defined

Diagnostic of Multicollinearity by VIF

In practice, the largest VIF, $\max_k VIF_k$, greater than 10 is often taken as an indication of high multicollinearity.

Body Fat

$$\mathbf{r}_{XX} = \begin{bmatrix} 1.00 & 0.92 & 0.46 \\ 0.92 & 1.00 & 0.08 \\ 0.46 & 0.08 & 1.00 \end{bmatrix}, \quad \mathbf{r}_{XX}^{-1} = \begin{bmatrix} 708.84 & -631.92 & -270.99 \\ -631.92 & 564.34 & 241.49 \\ -270.99 & 241.49 & 104.61 \end{bmatrix}$$

X_1 and X_2 are highly correlated, X_1 and X_3 are moderately correlated, and X_2 and X_3 are not much correlated.

$$R_1^2 = 0.9986, \quad R_2^2 = 0.9982, \quad R_3^2 = 0.9904$$

Each X variable is highly intercorrelated with the rest X variables.

Identifiability

Unidentifiability

A model is *unidentifiable* if its parameters can not be uniquely estimated. For regression models, unidentifiability occurs when

- columns of the design matrix $\underset{n \times p}{\mathbf{X}}$ are linearly dependent (i.e., perfect collinearity) $\Longrightarrow$ $rank(\mathbf{X}) < p$
- $\Longrightarrow$ $\underset{p \times p}{\mathbf{X}'\mathbf{X}}$ is not invertible
- $\Longrightarrow$ LS estimator is not well defined because the normal equation $\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$ has many solutions
- $\Longrightarrow$ there exist many vectors that minimize the least squares criterion.

What Causes Unidentifiability?

Possible causes include:

- More variables than cases, i.e., $p > n \Longrightarrow$ select a smaller subset of variables
- A feature is recorded by two different units and both are included in the model $\Longrightarrow$ remove redundancy
- Some linear combinations of variables are included in the model $\Longrightarrow$ eliminate them

By default, R will fit the largest identifiable model by removing variables in the reverse order of appearance in the model formula.

Example

case	X1	X2	Y
1	2	6	24
2	8	9	82
3	6	8	66
4	10	10	98

- X variables (including the column of 1) are perfectly correlated since $X_2 = 5 + 0.5X_1$.
- There are infinitely many response functions that fit this data equally "best".

```
Call:
lm(formula = Y ~ X1, data = data)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)   7.1429     3.5341   2.021  0.18066
X1            9.2857     0.4949  18.764  0.00283 **
---
Residual standard error: 2.928 on 2 degrees of freedom
Multiple R-squared: 0.9944,     Adjusted R-squared: 0.9915
F-statistic: 352.1 on 1 and 2 DF,  p-value: 0.002828

Call:
lm(formula = Y ~ X2, data = data)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) -85.7143     8.2956  -10.33  0.00924 **
X2           18.5714     0.9897   18.76  0.00283 **
---
Residual standard error: 2.928 on 2 degrees of freedom
Multiple R-squared: 0.9944,     Adjusted R-squared: 0.9915
F-statistic: 352.1 on 1 and 2 DF,  p-value: 0.002828
```

```
Call:
lm(formula = Y ~ X1 + X2, data = data)

Coefficients: (1 not defined because of singularities)
Estimate Std. Error t value Pr(>|t|)
(Intercept)   7.1429     3.5341   2.021  0.18066
X1            9.2857     0.4949  18.764  0.00283 **
X2                NA         NA      NA       NA
---
Residual standard error: 2.928 on 2 degrees of freedom
Multiple R-squared: 0.9944,     Adjusted R-squared: 0.9915
F-statistic: 352.1 on 1 and 2 DF,  p-value: 0.002828
```

R discards X_2 and fits a model only using X_1.

Polynomial Regression

Polynomial Regression

One of the most commonly used models to describe a curvilinear regression relation:

- very flexible and easy to fit
- higher than third-order terms are rarely employed in practice because of
  - high sampling variability
  - *overfitting*: fit the observed data well, but do not generalize well to new observations

Centering

In practice, centered X variables $\tilde{X}_k = X_k - \bar{X}_k$ are often used in polynomial regression models:

- Centering reduces the correlation between the linear term and the quadratic term substantially and thus improves numerical accuracy.
- Centering does not change the fitted regression function.

Second-Order Model with One Predictor

$$
\begin{aligned}
Y_i &= \beta_0 + \beta_1(X_i - \overline{X}) + \beta_2(X_i - \overline{X})^2 + \epsilon_i, \qquad i = 1, \cdots, n \\
&= \beta_0 + \beta_1 \tilde{X}_i + \beta_2 \tilde{X}_i^2 + \epsilon_i, \qquad \tilde{X}_i = X_i - \overline{X}
\end{aligned}
$$

The response function is a *parabola*:

$$
y = \beta_0 + \beta_1 \tilde{x} + \beta_2 \tilde{x}^2
$$

- β_0 is the mean response when $\tilde{x} = 0$ (i.e. $x = \overline{X}$).
- β_1 is called the *linear effect coefficient* and β_2 is called the *quadratic effect coefficient*.

Second-Order Model with Two Predictors

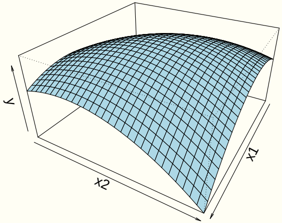
$$Y_i = \beta_0 + \beta_1 \tilde{X}_{i1} + \beta_2 \tilde{X}_{i2} + \beta_{11} \tilde{X}_{i1}^2 + \beta_{22} \tilde{X}_{i2}^2 + \beta_{12} \tilde{X}_{i1} \tilde{X}_{i2} + \epsilon_i, i = 1, \cdots, n$$

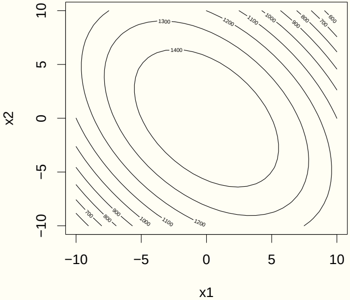
- response surface is a *conic section*:

$$y = \beta_0 + \beta_1 \tilde{x}_1 + \beta_2 \tilde{x}_2 + \beta_{11} \tilde{x}_1^2 + \beta_{22} \tilde{x}_2^2 + \beta_{12} \tilde{x}_1 \tilde{X}_2$$

- separate *linear and quadratic terms* for each predictor
- a cross-product term representing the interaction between the two predictors
- β_{12} is called the *interaction effect coefficient*

A quadratic response surface: $y = 1500 - 4x_1^2 - 3x_2^2 - 3x_1 x_2$





The contour plot shows combinations of (x_1, x_2) that yield the same value of y.

Extension: Second-Order Model with K Predictors

$$Y_i = \beta_0 + \sum_{k=1}^{K} \beta_k \tilde{X}_{ik} + \sum_{k=1}^{K} \beta_{kk} \tilde{X}_{ik}^2 + \sum_{1 \le k < k' \le K} \beta_{kk'} \tilde{X}_{ik} \tilde{X}_{ik'} + \epsilon_i, i = 1, \cdots, n$$

- response function:

$$y = \beta_0 + \sum_{k=1}^{K} \beta_k \tilde{x}_k + \sum_{k=1}^{K} \beta_{kk} \tilde{x}_k^2 + \sum_{1 \le k < k' \le K} \beta_{kk'} \tilde{x}_k \tilde{x}_{k'}$$

- β_ks are *linear effect coefficients*; β_{kk}s are *quadratic effect coefficients*.
- $\{\beta_{kk'} : 1 \le k < k' \le K\}$ are *interaction effect coefficients* between the respective pairs of predictors.

Third-Order Model with One Predictor

$$\begin{aligned} Y_i &= \beta_0 + \beta_1(X_i - \overline{X}) + \beta_2(X_i - \overline{X})^2 + \beta_3(X_i - \overline{X})^3 + \epsilon_i, \quad i = 1, \cdots, n \\ &= \beta_0 + \beta_1 \tilde{X}_i + \beta_2 \tilde{X}_i^2 + \beta_3 \tilde{X}^3 + \epsilon_i, \qquad \tilde{X}_i = X_i - \overline{X} \end{aligned}$$

The response function is a cubic polynomial:

$$y = \beta_0 + \beta_1 \tilde{x} + \beta_2 \tilde{x}^2 + \beta_3 \tilde{x}^3$$

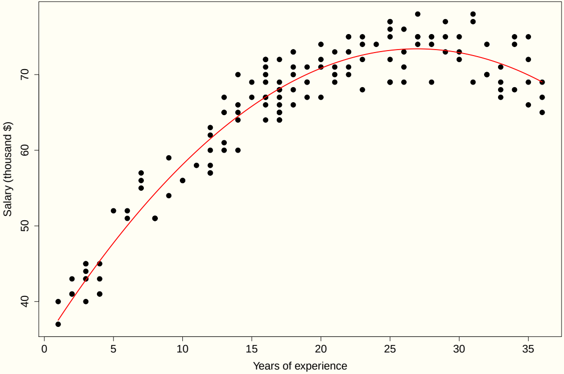
Polynomial Regression:

Example

Salary

Professional organizations regularly survey their members for information concerning salaries, pensions, and conditions of employment. One goal is to relate salary to years of experience. This data has years of experience (X) and salary (Y) on 143 cases.

Salary: Scatter Plot



Salary: Second-Order Model

```
> salary.c=salary
# Correlation coefficient between X and X^2 is 0.965 for the original variable "year of experience",
# and is -0.0414 for the centered variable
> salary.c[,"Experience"]=salary[,"Experience"]-mean(salary[,"Experience"]) ## center the X variable
> fitc=lm(Salary~ Experience+I(Experience^2), data=salary.c) ## fit a second-order model
> summary(fitc)

Call:
lm(formula = Salary ~ Experience + I(Experience^2), data = salary.c)
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)     69.927208   0.323090  216.43   <2e-16 ***
Experience       0.861177   0.024957   34.51   <2e-16 ***
I(Experience^2) -0.053316   0.002477  -21.53   <2e-16 ***
---
Residual standard error: 2.817 on 140 degrees of freedom
Multiple R-squared: 0.9247,     Adjusted R-squared: 0.9236
F-statistic: 859.3 on 2 and 140 DF,  p-value: < 2.2e-16
```

Salary: Third-Order Model

```
Call:
lm(formula = Salary ˜ Experience + I(Experienceˆ2) + I(Experienceˆ3),
data = salary.c)

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)     69.9484745  0.3224575  216.92   <2e-16 ***
Experience       0.9364986  0.0603531   15.52   <2e-16 ***
I(Experienceˆ2) -0.0537196  0.0024866  -21.60   <2e-16 ***
I(Experienceˆ3) -0.0003957  0.0002888   -1.37    0.173
---
> anova(fit3)
Analysis of Variance Table
Response: Salary
Df Sum Sq Mean Sq   F value Pr(>F)
Experience        1 9962.9  9962.9 1263.1043 <2e-16 ***
I(Experienceˆ2)   1 3677.9  3677.9  466.2810 <2e-16 ***
I(Experienceˆ3)   1   14.8    14.8    1.8764  0.173
Residuals       139 1096.4     7.9
```

First test whether the third-order term may be dropped.

- full model: third-order model vs. reduced model: second-order model
- $SSR(X^3|X, X^2) = 14.8$ with d.f. 1
- $SSE(X, X^2, X^3) = 1096.4$ with d.f. 139
- F-statistic $= 1.876$
- pvalue $= 0.173$
- Therefore, the third-order term is not significant and may be dropped

Then test whether the second-order term may be dropped.

- full model: second-order model vs. reduced model: first-order model
- $SSR(X^2|X) = 3677.9$ with d.f. 1
- $SSE(X, X^2) = SSE(X, X^2, X^3) + SSR(X^3|X, X^2) = 1111.2$ with d.f. 140
- F-statistic $= 466.28$
- pvalue $< 2e-16$
- Therefore, the second-order term is very significant and should be retained.