# Stat 206: Linear Models

## Lecture 9

October 26, 2015

# Standardization

Different $X$ variables often have different units which could make their values vastly different.

- Regression coefficients are not in the same scale and thus are hard to interpret.
- Elements of $\mathbf{X}'\mathbf{X}$ differ substantially in order of magnitude, causing numerical instability when finding its inversion.
- A regression model can be reparametrized into a standardized regression model through centering and rescaling.
- This process is called standardization, a.k.a. correlation transformation.

# Example

A data set with a response variable $Y$ in dollars, two predictor variables $X_1$ in thousand dollars and $X_2$ in cents. The fitted regression function:

$$\hat{Y} = 200 + 20,000X_1 + 0.2X_2.$$

- $X_1$ has a much larger fitted regression coefficient than $X_2$. However, this is caused by using different currency units.
- The effect of a \$1,000 increase in $X_1$ (corresponding to 1-unit increase) when $X_2$ is kept fixed would be an increase of \$20,000 in the mean response, while the effect of a \$1,000 increase in $X_2$ (corresponding to 100,000-unit increase) when $X_1$ is kept fixed is also a \$20,000 increase in the mean response.

# Correlation Transformation

Define transformed variables:

$$
\begin{aligned}
Y_i^* &= \frac{1}{\sqrt{n-1}}\left(\frac{Y_i - \overline{Y}}{s_Y}\right), \quad i = 1, \cdots, n, \\
X_{ik}^* &= \frac{1}{\sqrt{n-1}}\left(\frac{X_{ik} - \overline{X}_k}{s_{X_k}}\right), \quad k = 1, \cdots, p-1,
\end{aligned}
$$

where

$$
\begin{aligned}
\overline{Y} &= \frac{1}{n}\sum_{i=1}^{n} Y_i, \quad \overline{X}_k = \frac{1}{n}\sum_{i=1}^{n} X_{ik} \quad (k = 1, \cdots, p-1), \\
s_Y &= \sqrt{\frac{\sum_{i=1}^{n}(Y_i - \overline{Y})^2}{n-1}}, \quad s_{X_k} = \sqrt{\frac{\sum_{i=1}^{n}(X_{ik} - \overline{X}_k)^2}{n-1}},
\end{aligned}
$$

are sample means and sample standard deviations, respectively.

- The sample means of the transformed variables are
  .
- The sample standard deviations of the transformed variables are .
- So all variables are and are
  .
- Correlation transformation the pairwise (sample) correlations among the $X$ variables, the (sample) correlations between the $X$ variables and the response variable.

- The sample means of the transformed variables are all zero.
- The sample standard deviations of the transformed variables are all $\frac{1}{\sqrt{n-1}}$.
- So all variables are centered and are on the same scale.
- Correlation transformation does not change the pairwise (sample) correlations among the $X$ variables, nor does it change the (sample) correlations between the $X$ variables and the response variable.

# Standardized Regression Model

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

where

$\beta_k^* =$ $(k = 1, \cdots, p-1)$, $\boldsymbol{\epsilon}_i^* =$ , $i = 1, \cdots, n$

and

$\mathbf{E}\{\boldsymbol{\epsilon}^*\} = \mathbf{0}_n, \quad \boldsymbol{\sigma^2}\{\boldsymbol{\epsilon}^*\} = \sigma^{*2}\mathbf{I}_n, \quad$ *with* $\quad \sigma^* =$ .

- The intercept parameter is omitted, as its LS estimator will always be . *Why?*

# Standardized Regression Model

$$Y_i^* = \beta_1^* X_{i1}^* + \beta_2^* X_{i2}^* + \cdots + \beta_{p-1}^* X_{i,p-1}^* + \epsilon_i^*, \quad i = 1, \cdots n, \qquad (2)$$

where

$$\beta_k^* = \frac{s_{X_k}}{s_Y}\beta_k \ \ (k = 1, \cdots, p-1), \quad \boldsymbol{\epsilon}_i^* = \frac{\boldsymbol{\epsilon}_i}{\sqrt{n-1}s_Y}, \ \ i = 1, \cdots, n$$

and

$$\mathbf{E}\{\boldsymbol{\epsilon}^*\} = \mathbf{0}_n, \quad \boldsymbol{\sigma}^{\mathbf{2}}\{\boldsymbol{\epsilon}^*\} = \sigma^{*2}\mathbf{I}_n, \quad \textit{with} \quad \sigma^* = \frac{1}{\sqrt{n-1}s_Y}\sigma.$$

- The intercept parameter $\beta_0^*$ is omitted, as its LS estimator will always be zero. *Why?*

# Design Matrix of Standardized Model

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

This matrix only has $p-1$ columns, since the regression intercept is omitted in the standardized model.

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

is the sample correlation matrix of the $X$ variables.

# Correlation Matrix

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

- All its elements are numbers
  .
- Its diagonal elements are , since the correlation of a variable with itself is .
- Correlation matrix is a matrix:

# Correlation Matrix

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

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

- All its elements are unit-less numbers in between $-1$ and 1.
- Its diagonal elements are all one, since the correlation of a variable with itself is one, i.e., $r_{kk} \equiv 1$ for $k = 1, \cdots, p-1$.
- Correlation matrix is a symmetric matrix: $r_{kl} = r_{lk}$.

# $\mathbf{X}'\mathbf{Y}$ Matrix of Standardized Model

Response vector of the standardized model:

$$\mathbf{Y}^* = \begin{bmatrix} Y_1^* \\ Y_2^* \\ \vdots \\ Y_n^* \end{bmatrix}.$$

$$\mathbf{X}^{*\prime}\mathbf{Y}^* = \underset{(p-1)\times 1}{\mathbf{r}_{XY}} = \begin{bmatrix} r_{Y1} \\ r_{Y2} \\ \vdots \\ r_{Y,p-1} \end{bmatrix},$$

where $r_{Yk}$ is the sample correlation coefficient between $Y$ and $X_k$:

$$r_{Yk} = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(X_{ik} - \overline{X}_k)(Y_i - \overline{Y})}{s_{X_k} s_Y}, \quad k = 1, \cdots p-1.$$

# LS Estimators of Standardized Model

$$\underset{(p-1)\times 1}{\hat{\boldsymbol{\beta}}^*} = \begin{bmatrix} \hat{\beta}_1^* \\ \hat{\beta}_2^* \\ \vdots \\ \hat{\beta}_{p-1}^* \end{bmatrix} = \mathbf{r}_{XX}^{-1}\mathbf{r}_{XY}.$$

- These are called *fitted standardized regression coefficients*.
- Relationships with the LS estimators of the original model:

$$\begin{aligned} \hat{\beta}_k &= \frac{s_Y}{s_{X_k}}\hat{\beta}_k^*, \quad k = 1, \cdots, p-1 \\ \hat{\beta}_0 &= \overline{Y} - \hat{\beta}_1\overline{X}_1 - \cdots - \hat{\beta}_{p-1}\overline{X}_{p-1}. \end{aligned}$$

  The relationships are the same as those between the true coefficients.

*What are the relationships between sums of squares in standardized model and those in the original model?*

# Body Fat

Sample means and sample standard deviations:

$$\overline{Y} = 20.20, \quad \overline{X}_1 = 25.30, \quad \overline{X}_2 = 51.17, \quad \overline{X}_3 = 27.62;$$

$$s_Y = 5.11. \quad s_{X_1} = 5.02, \quad s_{X_2} = 5.23, \quad s_{X_3} = 3.65.$$

Correlation matrices.

$$\mathbf{r}_{XX} = \begin{bmatrix} 1.00 & 0.92 & 0.46 \\ 0.92 & 1.00 & 0.08 \\ 0.46 & 0.08 & 1.00 \end{bmatrix}, \quad \mathbf{r}_{XY} = \begin{bmatrix} 0.84 \\ 0.88 \\ 0.14 \end{bmatrix}.$$

Least-squares estimators of the standardized model:

$$\hat{\boldsymbol{\beta}}^* = \begin{bmatrix} \hat{\beta}_1^* \\ \hat{\beta}_2^* \\ \hat{\beta}_3^* \end{bmatrix} = \mathbf{r}_{XX}^{-1}\mathbf{r}_{XY} = \begin{bmatrix} 4.26 \\ -2.93 \\ -1.56 \end{bmatrix}.$$

Least-squares estimators of the original model:

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Least-squares estimators of the original model:

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix} = \begin{bmatrix} 4.33 \\ -2.86 \\ -2.18 \end{bmatrix} = \begin{bmatrix} \frac{5.11}{5.02} \times 4.26 \\ \frac{5.11}{5.23} \times (-2.93) \\ \frac{5.11}{3.65} \times (-1.56) \end{bmatrix}.$$

# Multicollinearity

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

- This term is often reserved for the situation when the inter-correlation/collinearity among the $X$ variables is

  .

- $X$ variables being nearly collinear means that there exist constants $c_0, c_1, \cdots, c_{p-1}$ not all zero such that

$$c_0 + c_1 X_{i1} + \cdots + c_{p-1} X_{i,p-1} \approx 0, \quad i = 1, \cdots, n.$$

  i.e., there exists a nonzero vector $\mathbf{c}$ such that

  .

# 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 **very high**.
- $X$ variables being nearly collinear/highly intercorrelated means that there exist constants $c_0, c_1, \cdots, c_{p-1}$ not all zero such that

$$c_0 + c_1 X_{i1} + \cdots + c_{p-1} X_{i,p-1} \approx 0, \quad i = 1, \cdots, n.$$

i.e., there exists a nonzero vector $\mathbf{c}$ such that $\underset{n\times p}{\mathbf{X}}\ \underset{p\times 1}{\mathbf{c}} \approx \mathbf{0}_n$.

# Interpreting Regression Coefficients

- In presence of multicollinearity, the magnitude/sign of a coefficient

  interpreted as reflecting the comparative importance/direction-of-effect of the corresponding $X$ variable.

- **A regression coefficient should be interpreted as reflecting the**

  **of the corresponding $X$ variable, given whatever other $X$ variables also in the model.**

- To understand the effects of multicollinearity, we consider two extreme situations: (i) When the $X$ variables are not correlated with each other at all; (ii) When they are perfectly intercorrelated.

- In practice, it is usually somewhere in between (i) and (ii).

# Interpreting Regression Coefficients

- In presence of multi-collinearity, the magnitude/sign of a coefficient **can not be** interpreted as reflecting the comparative importance/direction-of-effect of the corresponding $X$ variable.
- **A regression coefficient should be interpreted as reflecting the marginal/partial effect of the corresponding $X$ variable, given whatever other $X$ variables also in the model.**
- To understand the effects of multicollinearity, we consider two extreme situations: (i) When the $X$ variables are not correlated with each other at all; (ii) When they are perfectly intercorrelated.
- In practice, it is usually somewhere in between (i) and (ii).

# Uncorrelated $X$ Variables

- Under standardized model:

$$\mathbf{X}^{*\prime}\mathbf{X}^{*} = \mathbf{r}_{XX} = \qquad , \quad \mathbf{X}^{*\prime}\mathbf{Y}^{*} = \qquad .$$

- LS estimators:

$$\hat{\beta}_j^{*} = \qquad , \quad j = 1, \cdots, p-1,$$

  are the between the response variable $Y$ and individual $X$ variables.

- Variance-covariance matrix:

$$\sigma^2\{\hat{\boldsymbol{\beta}}^{*}\} = \qquad .$$

- LS estimators under the original model:

# Uncorrelated $X$ Variables

- Under standardized model:

$$\mathbf{X}^{*\prime}\mathbf{X}^{*} = \mathbf{r}_{XX} = \mathbf{I}, \quad \mathbf{X}^{*\prime}\mathbf{Y}^{*} = \mathbf{r}_{YX}.$$

- LS estimators:

$$\hat{\beta}_j^{*} = r_{YX_j}, \quad j = 1, \cdots, p-1,$$

  are the ample correlation coefficients between the response variable $Y$ and individual $X$ variables.

- Variance-covariance matrix:

$$\boldsymbol{\sigma}^2\{\hat{\boldsymbol{\beta}}^{*}\} = \sigma^{*2}\mathbf{I}.$$

  So the LS estimators are uncorrelated.

- LS estimators under the original model:

$$\hat{\beta}_j = \frac{s_Y}{s_{X_j}}\hat{\beta}_j^{*} = \frac{s_Y}{s_{X_j}} r_{YX_j}, \quad \sigma^2\{\hat{\beta}_j\} = \frac{1}{(n-1)s_{X_j}^2}\sigma^2,$$

  and $\sigma^2\{\hat{\beta}_j, \hat{\beta}_k\} = 0$ if $j \neq k$.

When the $X$ variables are uncorrelated, the effect of an $X$ variable depend on other $X$ variables in the model.

- The LS fitted regression coefficient is
  by which other $X$ variables are in the model.
- The LS fitted regression coefficients are with each other.
- The marginal contribution of an $X$ variable in reducing the error sum of squares is the
  other $X$ variables in the model, i.e.

- This is a strong advocate for controlled experiments, since there it may be possible to use an *orthogonal design* where the levels of the $X$ variables are chosen such that their sample correlations are .

When the $X$ variables are uncorrelated, the effect of an $X$ variable does **not** depend on other $X$ variables in the model.

- The LS fitted regression coefficient is **not** affected by which other $X$ variables are in the model.
- The LS fitted regression coefficients are uncorrelated with each other.
- The marginal contribution of an $X$ variable in reducing the error sum of squares is the **same** with or without other $X$ variables in the model, i.e.

$$SSR(X_j|X_{\mathcal{I}}) = SSR(X_j).$$

- This is a strong advocate for controlled experiments, since there it may be possible to use an *orthogonal design* where the levels of the $X$ variables are chosen such that their sample correlations are (nearly) zero.

Consider the standardized models.

$$
\begin{aligned}
SSE(X_{\mathcal{I}}, X_j) &= \sum_{i=1}^{n}\left(Y_i^* - \sum_{k\in\mathcal{I}}\hat{\beta}_k^* X_{ik}^* - \hat{\beta}_j^* X_{ij}^*\right)^2 \\
&= \sum_{i=1}^{n}\left(Y_i^* - \sum_{k\in\mathcal{I}}\hat{\beta}_k^* X_{ik}^*\right)^2 - 2\sum_{i=1}^{n} Y_i^*\hat{\beta}_j^* X_{ij}^* \\
&+ \sum_{i=1}^{n}\left(\hat{\beta}_j^* X_{ij}^*\right)^2 \\
&= SSE(X_{\mathcal{I}}) + \sum_{i=1}^{n}\left(Y_i^* - \hat{\beta}_j^* X_{ij}^*\right)^2 - \sum_{i=1}^{n}(Y_i^*)^2 \\
&= SSE(X_{\mathcal{I}}) + SSE(X_j) - SSTO = SSE(X_{\mathcal{I}}) - SSR(X_j).
\end{aligned}
$$

*Use the facts that the X variables are uncorrelated and the LS estimators do not depend on the model being fitted. The SSE and SSR of the original model are those of the standardized models multiplied by* $(n-1)s_Y^2$*, so the above also holds for the original model.*

# Crew Productivity

A study on the effect of work crew size ($X_1$) and level of bonus pay ($X_2$) on productivity ($Y$).

| 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 |

Pairwise correlation matrix.

| | X1 | X2 | Y |
|---|---|---|---|
| X1 | 1.00 | 0.00 | 0.74 |
| X2 | 0.00 | 1.00 | 0.64 |
| Y | 0.74 | 0.64 | 1.00 |

$X_1$ and $X_2$ are uncorrelated.

# Crew Productivity: Model 1

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

Residuals:
   Min     1Q Median     3Q    Max
-6.750 -3.750  0.125  4.500  6.000

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 *
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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)

Residuals:
   Min     1Q Median     3Q    Max
-7.000 -4.688 -0.250  5.250  7.250

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 .
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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)

Residuals:
     1      2      3      4      5      6      7      8
 1.625 -1.375 -1.625  1.375 -2.125  1.875  0.625 -0.375

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 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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
```

# Perfectly Correlated $X$ variables

A set of $X$ variables is said to be *collinear* if one or several of them may be expressed as a linear combination of the other $X$ variables (including $\mathbf{1}_n$).

- The design matrix $\underset{n\times p}{\mathbf{X}}$ is . So the matrix $\underset{p\times p}{\mathbf{X}'\mathbf{X}}$ is .
- LS estimators are because the least-squares equation

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$$

  has solutions.
- This means that there exist vectors $\mathbf{b}$ that minimize the least squares criterion:

$$Q(\mathbf{b}) = \sum_{i=1}^{n} (Y_i - b_0 - b_1 X_{i1} - \cdots - b_{p-1} X_{i,p-1})^2 .$$

# Perfectly Correlated $X$ variables

A set of $X$ variables is said to be *collinear* if one or several of them may be expressed as a linear combination of the other $X$ variables (including $\mathbf{1}_n$).

- The design matrix $\underset{n\times p}{\mathbf{X}}$ is not of full column rank: $rank(\mathbf{X}) < p$. So the matrix $\underset{p\times p}{\mathbf{X}'\mathbf{X}}$ is not invertible.
- LS estimators are not well-defined because the least-squares equation

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$$

  has many solutions.
- This means that there exist many vectors $\mathbf{b}$ that minimize the least squares criterion:

$$Q(\mathbf{b}) = \sum_{i=1}^{n} (Y_i - b_0 - b_1 X_{i1} - \cdots - b_{p-1} X_{i,p-1})^2 .$$

- If $X$ variables are perfectly correlated, then there exists a nonzero vector $\underset{p\times 1}{\mathbf{c}}$ such that

$$\underset{n\times p}{\mathbf{X}}\ \underset{p\times 1}{\mathbf{c}} = \mathbf{0}_n.$$

- If $\mathbf{b}$ is a solution to the least-squares equation, i.e.,

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y},$$

then $\mathbf{b} + k\mathbf{c}$ is also a solution where $k \in \mathbb{R}$ is an arbitrary scalar since

$$\begin{aligned}\mathbf{X}'\mathbf{X}\left(\mathbf{b} + k\mathbf{c}\right) &= \mathbf{X}'\mathbf{X}\mathbf{b} + k\mathbf{X}'\mathbf{X}\mathbf{c} \\ &= \mathbf{X}'\mathbf{Y} + k\mathbf{X}'\mathbf{0}_n = \mathbf{X}'\mathbf{Y}.\end{aligned}$$

- Similarly, if $\mathbf{b}$ minimizes the least-squares criterion function $Q(\cdot)$, then $\mathbf{b} + k\mathbf{c}$ also minimizes $Q(\cdot)$ since

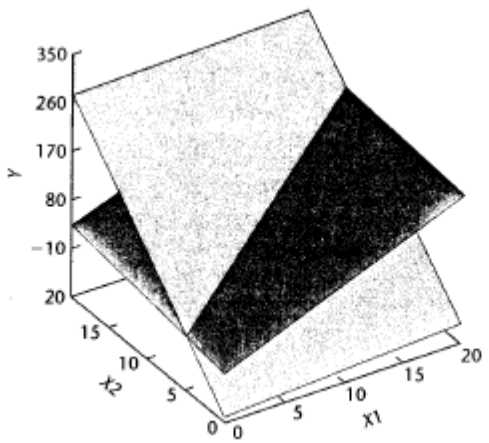
$$\begin{aligned}Q(\mathbf{b}) &= \left(\mathbf{Y} - \mathbf{X}\mathbf{b}\right)'\left(\mathbf{Y} - \mathbf{X}\mathbf{b}\right) \\ &= \left(\mathbf{Y} - \mathbf{X}(\mathbf{b} + k\mathbf{c})\right)'\left(\mathbf{Y} - \mathbf{X}(\mathbf{b} + k\mathbf{c})\right) = Q(\mathbf{b} + k\mathbf{c}).\end{aligned}$$

# Example

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

- $X$ variables are perfectly correlated since $X_2 = 5 + 0.5X_1$.
- There are infinitely many response functions that fit this data equally "best" (with $SSE = 17.14$).

**FIGURE 7.2**
**Two Response Planes That Intersect when $X_2 = 5 + .5X_1$.**



- The two response surfaces in the figure are completely different, but they have the same $y$ values on $X_2 = 5 + 0.5X_1$: $y = 7.14 + 9.29X_1$.
- Actually, any response surface that passes the intersecting line will fit the data equally well as these two, e.g.,

$$\widehat{Y} = 7.14 + 9.29X_1, \quad \widehat{Y} = -85.71 + 18.57X_2.$$

*Can you think about some others?*

```
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 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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)

Residuals:
      1       2       3       4
-1.7143  0.5714  3.1429 -2.0000

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
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

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
```

Here, R discards $X_2$ and fits a model only using $X_1$.

**When $X$ variables are perfectly correlated, we may still get a fit of the data.**

- The least-squares fitted values $\widehat{\mathbf{Y}}$ is and is the

  of the response vector $\mathbf{Y}$ to the linear subspace of $\mathbb{R}^n$ generated by the columns of the design matrix $\mathbf{X}$.
- Estimation of mean responses and predictions of new observations are still possible if they

  *What does this mean now?*
- However, the regression coefficients are

  .

**When $X$ variables are perfectly correlated, we may still get a good fit of the data**.

- The least-squares fitted values $\widehat{\mathbf{Y}}$ is uniquely defined and is the orthogonal projection of the response vector $\mathbf{Y}$ to the linear subspace of $\mathbb{R}^n$ generated by the columns of the design matrix $\mathbf{X}$.
- Estimation of mean responses and predictions of new observations are still possible if they are done within the region of the observations.
  *What does this mean now?* (See the next slides)
- However, the regression coefficients are not meaningful anymore without additional constraints.

# Estimation of Mean Response and Prediction

- Suppose $\mathbf{X}_h$ is a $p \times 1$ column vector satisfies:

$$\mathbf{X}_h' = \mathbf{c}'\mathbf{X} \quad (*)$$

  for some $n \times 1$ column vector $\mathbf{c}$, i.e., $\mathbf{X}_h^T$ is a linear combination of the rows of the design matrix $\mathbf{X}$, or equivalently, $\mathbf{X}_h$ is within the linear subspace of $\mathbb{R}^p$ generated by the rows of the design matrix $\mathbf{X}$ (the row space).

- The estimator of the mean response $E(Y_h)$ or the predicted value for $Y_h$ is:

$$\widehat{Y}_h = \mathbf{X}_h'\widehat{\boldsymbol{\beta}} = \mathbf{c}'\mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{c}'\widehat{\mathbf{Y}}, \quad \sigma^2\{\widehat{Y}_h\} = \mathbf{c}'\boldsymbol{\sigma}^2\{\widehat{\mathbf{Y}}\}\mathbf{c} = \sigma^2\mathbf{c}'\mathbf{H}\mathbf{c}.$$

- Although the LS estimators $\widehat{\boldsymbol{\beta}}$ is not uniquely defined, the fitted values vector $\widehat{\mathbf{Y}}$ is and so is $\widehat{Y}_h$ as long as $\mathbf{X}_h$ satisfies $(*)$.

# Example

```
> newX=data.frame(X1=3, X2=5+0.5*3)
> predict.lm(fit1, newX, interval="confidence",se.fit=TRUE)
$fit
  fit     lwr     upr
1  35 25.2425 44.7575

$se.fit
[1] 2.267787

$df
[1] 2

$residual.scale
[1] 2.9277

> predict.lm(fit2, newX,interval="confidence", se.fit=TRUE)
$fit
  fit     lwr     upr
1  35 25.2425 44.7575

$se.fit
[1] 2.267787

$df
[1] 2

$residual.scale
[1] 2.9277
```

```
> predict.lm(fit3, newX,interval="confidence",se.fit=TRUE)
$fit
  fit     lwr     upr
1  35 25.2425 44.7575

$se.fit
[1] 2.267787

$df
[1] 2

$residual.scale
[1] 2.9277

Warning message:
In predict.lm(fit3, newX, interval = "confidence", se.fit = TRUE) :
  prediction from a rank-deficient fit may be misleading
```

```
> newX=data.frame(X1=3, X2=5)
> predict.lm(fit1, newX, interval="confidence",se.fit=TRUE)
$fit
  fit     lwr     upr
1  35 25.2425 44.7575

$se.fit
[1] 2.267787

$df
[1] 2

$residual.scale
[1] 2.9277

> predict.lm(fit2, newX,interval="confidence", se.fit=TRUE)
$fit
       fit       lwr      upr
1 7.142857 -8.063107 22.34882

$se.fit
[1] 3.534091

$df
[1] 2

$residual.scale
[1] 2.9277
```

```
> predict.lm(fit3, newX,interval="confidence",se.fit=TRUE)
$fit
  fit     lwr     upr
1  35 25.2425 44.7575

$se.fit
[1] 2.267787

$df
[1] 2

$residual.scale
[1] 2.9277

Warning message:
In predict.lm(fit3, newX, interval = "confidence", se.fit = TRUE) :
  prediction from a rank-deficient fit may be misleading
```

# Effects of Multicollinearity

- With multicollinearity, the estimated regression coefficients tend to have sampling variability (i.e., standard errors). This leads to:
  - confidence intervals.
  - It's possible that of the regression coefficients is statistically significant, but at the same time there is a regression relation between the response variable and the entire set of $X$ variables.
- Multicollinearity does not prevent us from getting a of the data.
- Multicollinearity does not tend to affect inferences about mean response or prediction **if**

prediction

# Effects of Multicollinearity

- With multicollinearity, the estimated regression coefficients tend to have large sampling variability (i.e., large standard errors). This leads to:
  - Wide confidence intervals.
  - It's possible that none of the regression coefficients is statistically significant, but at the same time there is a significant regression relation between the response variable and the entire set of $X$ variables.
- Multicollinearity does not prevent us from getting a good fit of the data.
- Multicollinearity does not tend to affect inferences about mean response or prediction if these are done **within the region of the observations**, i.e., $\mathbf{X}_h' = \mathbf{c}'\mathbf{X}$ for some vector $\mathbf{c}$.

◂ prediction

# Interpretation of Regression Coefficients and ESS

In the presence of multicollinearity:

- The regression coefficient of an $X$ variable
  which other $X$ variables are also in the model.
- Therefore, a regression coefficient reflect any
  inherent effect of the corresponding $X$ variable on the
  response variable, but only a
  given whatever other $X$ variables are also in the model.
- Similarly, there is sum of squares that can be
  ascribed to any one $X$ variable.
- The reduction in the total variation in $Y$ ascribed to an $X$
  variable must be interpreted as a
  given other $X$ variables also included in the model.

# Interpretation of Regression Coefficients and ESS

In the presence of multicollinearity:

- The regression coefficient of an $X$ variable depends on which other $X$ variables are also in the model.
- Therefore, a regression coefficient does **not** reflect any inherent effect of the corresponding $X$ variable on the response variable, but only a marginal effect given whatever other $X$ variables are also in the model.
- Similarly, there is **no** unique sum of squares that can be ascribed to any one $X$ variable.
- 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 included in the model.

# Body Fat

Correlation matrices.

$$\mathbf{r}_{XX} = \begin{bmatrix} 1.00 & 0.92 & 0.46 \\ 0.92 & 1.00 & 0.08 \\ 0.46 & 0.08 & 1.00 \end{bmatrix}, \quad \mathbf{r}_{XY} = \begin{bmatrix} 0.84 \\ 0.88 \\ 0.14 \end{bmatrix}.$$

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

$$\mathbf{r}_{XX}^{-1} = \begin{bmatrix} 708.84 & -631.92 & -270.99 \\ -631.92 & 564.34 & 241.49 \\ -270.99 & 241.49 & 104.61 \end{bmatrix}$$

So,

Each predictor is with the rest of the predictors.

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$$\mathbf{r}_{XX}^{-1} = \begin{bmatrix} 708.84 & -631.92 & -270.99 \\ -631.92 & 564.34 & 241.49 \\ -270.99 & 241.49 & 104.61 \end{bmatrix}$$

So,

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

Each predictor is highly intercorrelated with the rest of the predictors.

| 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 regression coefficient for $X_1$ ($X_2$) depending on which other $X$ variables are included in the model.
- The standard errors of the fitted regression coefficients are becoming when more $X$ variables are included into the model.
- MSE tends to as additional $X$ variables are added into the model.

◂ R outputs

| 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 |
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| 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 regression coefficient for $X_1$ ($X_2$) varies drastically depending on which other $X$ variables are included in the model.
- The standard errors of the fitted regression coefficients are becoming inflated when more $X$ variables are included into the model.
- MSE tends to decrease as additional $X$ variables are added into the model.

◂ R outputs

- $SSR(X_1) = 352.27$, $SSR(X_1|X_2) = 3.47$.
- The reason why $SSR(X_1|X_2)$ is so small compared to $SSR(X_1)$ is that $X_1$ and $X_2$ are with each other and with the response variable $Y$.
    - When $X_2$ is already in the model, the marginal contribution from $X_1$ in explaining $Y$ is since $X_2$ contains much of the information as $X_1$ in terms of explaining $Y$.

- $SSR(X_1) = 352.27$, $SSR(X_1|X_2) = 3.47$.
- The reason why $SSR(X_1|X_2)$ is so small compared to $SSR(X_1)$ is that $X_1$ and $X_2$ are highly correlated with each other **and with the response variable** $Y$**.**
    - When $X_2$ is already in the model, the marginal contribution from $X_1$ in explaining $Y$ is small since $X_2$ contains much of the same information as $X_1$ in terms of explaining $Y$.

*What would happen if $X_1$ and $X_2$ were not correlated with $Y$, but were highly correlated among themselves?*

# Body Fat: Model 1

```
> summary(fit1)

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

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -1.4961     3.3192  -0.451    0.658
X1            0.8572     0.1288   6.656 3.02e-06 ***
---

Residual standard error: 2.82 on 18 degrees of freedom
Multiple R-squared: 0.7111,     Adjusted R-squared: 0.695
F-statistic:  44.3 on 1 and 18 DF,  p-value: 3.024e-06

> anova(fit1)
Analysis of Variance Table

Response: Y
          Df Sum Sq Mean Sq F value    Pr(>F)
X1         1 352.27  352.27  44.305 3.024e-06 ***
Residuals 18 143.12    7.95
```

back

# Body Fat: Model 2

```
> summary(fit2)

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

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -23.6345     5.6574  -4.178 0.000566 ***
X2            0.8565     0.1100   7.786  3.6e-07 ***

Residual standard error: 2.51 on 18 degrees of freedom
Multiple R-squared: 0.771,      Adjusted R-squared: 0.7583
F-statistic: 60.62 on 1 and 18 DF,  p-value: 3.6e-07

> anova(fit2)
Analysis of Variance Table

Response: Y
          Df Sum Sq Mean Sq F value  Pr(>F)
X2         1 381.97  381.97  60.617 3.6e-07 ***
Residuals 18 113.42    6.30
```

back

# Body Fat: Model 3

```
> summary(fit3)

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

> anova(fit3)
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
```

back

# Body Fat: Model 4

```
> summary(fit4)

Call:
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

> anova(fit4)
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
```

partial

multicollinearity

# Body Fat

The precision of predictions within the region of the observations does not tend to be worsened with additional correlated $X$ variables in the model.

```
> newX=data.frame(X1=25, X2=50, X3=29)
> predict.lm(fit1, newX, se.fit=TRUE)
$fit
       1
19.93356
$se.fit
[1] 0.6317416
...
> predict.lm(fit2, newX, se.fit=TRUE)
$fit
       1
19.19284
$se.fit
[1] 0.5758769
...
> predict.lm(fit3, newX, se.fit=TRUE)
$fit
       1
19.35566
$se.fit
[1] 0.6243083
...
> predict.lm(fit4, newX, se.fit=TRUE)
$fit
       1
19.19885
$se.fit
[1] 0.6194612
```