Linear Regression (part 2)

Predictive Modeling & Statistical Learning

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Multiple Linear Regression by Ordinary Least Squares

Regression with various predictors

- ► Multiple Linear Regression
- ightharpoonup p predictors x_1, x_2, \ldots, x_p
- one response variable y
- ▶ Do not confuse Multiple with Multivariate
- Multivariate Regression implies several responses (i.e. y₁, ..., y_q)

Introduction

Suppose we observe a quantitative response Y and p different predictors, X_1, X_2, \ldots, X_p .

We assume a linear relationship of the form:

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + \varepsilon$$

Advertising Data

```
# file in folder data/ of github repo
Advertising <- read.csv("data/Advertising.csv", row.names = 1)</pre>
```

```
Warning in file(file, "rt"): cannot open file
'../../data/Advertising.csv': No such file or directory
Error in file(file, "rt"): cannot open the connection
Error in head(Advertising, n = 8): object 'Advertising'
not found
```

(first 8 rows)

Data set Advertising

Response:

► Y: Sales

Predictors:

► X₁: TV

 $ightharpoonup X_2$: Radio

 $ightharpoonup X_3$: Newspaper

Linear model:

Sales =
$$\beta_0 + \beta_1 \text{ TV} + \beta_2 \text{ Radio} + \beta_3 \text{ Newspaper} + \epsilon$$

Given the actual data values, we may write the model as:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + \varepsilon_i$$

for
$$i = 1, \ldots, n$$

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$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + \varepsilon_i$$

for $i = 1, \ldots, n$

It will be more convenient to use vector-matrix notation:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

If we consider an intercept term β_0 , then we have:

$$\mathbf{y}_{n\times 1} = \mathbf{X}_{n\times (p+1)} \times \mathbf{\beta}_{(p+1)\times 1} + \mathbf{\varepsilon}_{n\times 1}$$

which can also be represented by:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ 1 & x_{31} & \cdots & x_{3p} \\ \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

If the data is **mean-centered** (i.e. $\bar{X}_1 = \cdots = \bar{X}_p = 0$)

$$\mathbf{y}_{n \times 1} = \mathbf{X}_{n \times p} \times \boldsymbol{\beta}_{p \times 1} + \boldsymbol{\varepsilon}_{n \times 1}$$

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$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ x_{21} & \cdots & x_{2p} \\ x_{31} & \cdots & x_{3p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

OLS Estimation

OLS Estimation

Assuming a linear model

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + \varepsilon$$

the challenge involves finding parameter estimates denoted by $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$ that provide the "best" approximation for Y:

$$Y \approx \hat{\beta_0} + \hat{\beta_1} X_1 + \dots + \hat{\beta_p} X_p$$

or more commonly

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \dots + \hat{\beta}_p X_p$$

Matrix Notation

Model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Estimation: fitted (or predicted) values

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}\mathbf{b}$$

Residuals: observed - predicted

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$$

Matrix Notation

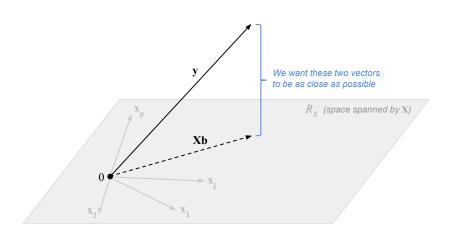
We want to calculate $b=\hat{\beta}$ such that \hat{y} is a good approximation of y.

The idea is to choose $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$ that minimize the *size* of the residuals:

$$e = y - \hat{y} = y - Xb$$

What criteria should be used to minimize the *size* of the residuals?

Geometric illustration



Matrix Notation

Our wish is to minimize the residuals for all i = 1, 2, ..., n:

$$e_i = y_i - \hat{y}_i$$

Among the the possible criteria to minimize we have:

- $ightharpoonup min \left\{ \sum_{i=1}^n e_i^2 \right\} \quad L_2$ -norm
- $ightharpoonup min \left\{ \sum_{i=1}^{n} |e_i| \right\} \quad L_1$ -norm
- $ightharpoonup min \{max(e_i)\}$ L_{∞} -norm
- ► etc

Matrix Notation

Least Squares involves minimizing the sum of squares $(L_2$ -norm):

$$\min\left\{\sum_{i=1}^n e_i^2\right\}$$

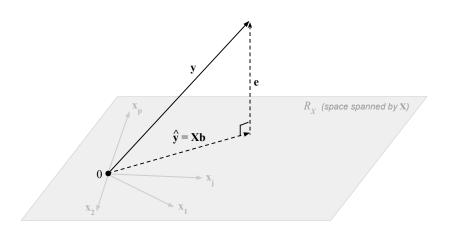
This sum is better known as the Residual Sum of Squares (RSS)

$$RSS = \sum_{i=1}^{n} e_i^2$$

In vector-matrix notation:

$$RSS = \mathbf{e}^\mathsf{T}\mathbf{e} = \|\mathbf{e}\|^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2$$

Least Squares Geometry



OLS Geometric Idea

Geometrically speaking

- lacktriangle the response lies in an n-dimensional space: $\mathbf{y} \in \mathbb{R}^n$
- \blacktriangleright the vector of parameters lies in a p-dimesional space: $\pmb{\beta} \in \mathbb{R}^p$
- ▶ in OLS, the response is projected orthogonally onto the model space spanned by X
- ightharpoonup the fit is represented by projection $\hat{y} = Xb$
- ▶ the difference between the fit and the data is the residual vector e
- ▶ the residual vector lies in an (n-p)-dimensional space: $\mathbf{b} \in \mathbb{R}^{(n-p)}$

Least Squares Minimization

OLS Criterion:

$$\min\left\{\sum_{i=1}^{n} e_i^2\right\} = \min\left\{\|\mathbf{e}\|^2\right\}$$

This means that the "best" b is the one which minimizes the RSS:

$$RSS(\mathbf{b}) = \sum_{i=1}^{n} e_i^2 = \mathbf{e}^\mathsf{T} \mathbf{e} = (\mathbf{y} - \mathbf{X}\mathbf{b})^\mathsf{T} (\mathbf{y} - \mathbf{X}\mathbf{b})$$

Differentiating $RSS(\mathbf{b})$ with respect to \mathbf{b} yields:

$$\frac{RSS(\mathbf{b})}{\partial \mathbf{b}} = -2\mathbf{X}^\mathsf{T} \mathbf{y} + 2\mathbf{X}^\mathsf{T} \mathbf{X} \mathbf{b}$$

Differentiating $RSS(\mathbf{b})$ with respect to \mathbf{b} yields:

$$\frac{RSS(\mathbf{b})}{\partial \mathbf{b}} = -2\mathbf{X}^\mathsf{T}\mathbf{y} + 2\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{b}$$

Equating to zero we have the so-called *normal equations*:

$$\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{b} = \mathbf{X}^\mathsf{T}\mathbf{y}$$

Assuming that the matrix X^TX is nonsingular (invertible), the unique ordinary least squares (OLS) estimator of β is given by:

$$\mathbf{b} = (\mathbf{X}^\mathsf{T} \mathbf{X})^{-1} \mathbf{X}^\mathsf{T} \mathbf{y}$$

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The fitted values are

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

What conditions are needed for X^TX to be invertible?

```
# number of observations
n <- nrow(Advertising)</pre>
## Error in nrow(Advertising): object 'Advertising' not
found
# model matrix
X <- as.matrix(Advertising[ ,c('TV', 'Radio', 'Newspaper')])</pre>
## Error in as.matrix(Advertising[, c("TV", "Radio",
"Newspaper")]): object 'Advertising' not found
X <- cbind(Intercept = rep(1, n), X)</pre>
## Error in cbind(Intercept = rep(1, n), X): object 'n'
not found
# response variable
y <- Advertising$Sales
## Error in eval(expr, envir, enclos): object
```

$$\mathbf{b} = (\mathbf{X}^\mathsf{T} \mathbf{X})^{-1} \mathbf{X}^\mathsf{T} \mathbf{y}$$

```
# coefficients
b <- solve(t(X) %*% X) %*% t(X) %*% y
## Error in t(X): object 'X' not found
b
## Error in eval(expr, envir, enclos): object 'b' not found</pre>
```

Predicted (fitted) values:

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

```
# fitted
fitted <- X %*% b
## Error in eval(expr, envir, enclos): object 'X' not
found</pre>
```

Observed -vs- Predicted (fitted) values

```
## Error in plot(y, fitted, las = 1, type = "n", xlab = "y
observed", ylab = "y fitted"): object 'y' not found
## Error in int_abline(a = a, b = b, h = h, v = v, untf =
untf, ...): plot.new has not been called yet
## Error in points(y, fitted, pch = 19, col = "#55555555",
cex = 1.5): object 'y' not found
## Error in text.default(20, 24, label = "identity line",
col = "#88888855"): plot.new has not been called yet
```

The fitted values are

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

Let $\mathbf{H} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}$, then:

$$\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$$

where H is commonly known as the **hat matrix**.

What's so special about H?

$$\hat{y} = Hy$$

```
# equivalent with the Hat matrix
H <- X %*% solve(t(X) %*% X) %*% t(X)

## Error in eval(expr, envir, enclos): object 'X' not found

y_hat <- H %*% y

## Error in eval(expr, envir, enclos): object 'H' not found</pre>
```

Review: projection Matrices

Let $L \subseteq \mathbb{R}^n$ be a linear subspace, i.e. $L = span\{\mathbf{v_1}, \dots, \mathbf{v_k}\}$ for some $\mathbf{v_1}, \dots, \mathbf{v_k} \in \mathbb{R}^n$.

If $V \in \mathbb{R}^{n imes k}$ contains $\mathbf{v_1}, \dots, \mathbf{v_k}$ on its columns, then

$$span\{\mathbf{v_1},\ldots,\mathbf{v_k}\}=\{a_1\mathbf{v_1}+\cdots+a_k\mathbf{v_k}:a_1,\ldots,a_k\in\mathbb{R}\}=\operatorname{col}(V)$$

The function $F: \mathbb{R}^n \to \mathbb{R}^n$ that projects points onto L is called the projection map onto L. This is actually a linear function, $F(\mathbf{x}) = P_L \mathbf{x}$, where $P_L \in \mathbb{R}^{n \times n}$ is the projection matrix onto L.

Review: projection Matrices

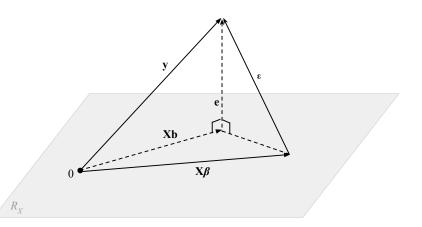
A projection matrix $P_L \in \mathbb{R}^{n \times n}$

- ▶ is a linear transformation
- ightharpoonup is symmetric: $P_L = P_L^{\mathsf{T}}$
- ightharpoonup is idempotent: $P_L^2 = P_L$
- ► Furthermore:
 - $P_L \mathbf{x} = \mathbf{x}$ for all $\mathbf{x} \in L$
 - $P_L \mathbf{x} = \mathbf{0}$ for all $\mathbf{x} \perp L$

The Hat matrix

- ► H is a linear transformation
- ightharpoonup H is symmetric: $H = H^T$
- ightharpoonup H is idempotent: $H=H^2$
- The hat matrix is an orthogonal projector or projection matrix
- $lackbox{ } \mathbf{Q} = \mathbf{I} \mathbf{H}$ is the orthogonal complement or "counterpart" of \mathbf{H}

Least Squares Geometry

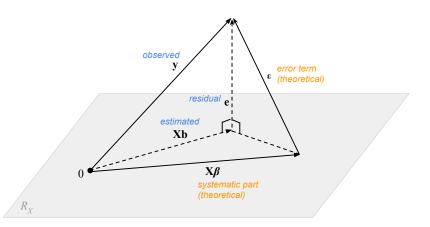


About the Hat matrix H

The theoretical model $y=X\beta+\varepsilon$ defines a decomposition of y in two unknown terms:

- $X\beta \in \mathbb{R}_X$
- $m{arepsilon} \in \mathbb{R}^n$

Least Squares Geometry



About the Hat matrix H

The theoretical model $y = X\beta + \varepsilon$ defines a decomposition of y in two unknown terms:

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About the Hat matrix H

The theoretical model $y = X\beta + \varepsilon$ defines a decomposition of y in two unknown terms:

- $X\beta \in \mathbb{R}_X$
- $m{\epsilon} \in \mathbb{R}^n$

The OLS method proposes a solution y = Xb + e that minimizes the "length" of the residual vector e by orthogonally projecting y as Xb in the spanned space of X, and by projecting ε as e in the subspace to \mathbb{R}_X .

Residuals and Theoretical Errors

The *residuals* $e = y - \hat{y}$ are the OLS estimates of the unobservable erros ε .

The residual vector can also be written as:

$$e = y - Xb = (I - H)\varepsilon = Q\varepsilon$$

Example: Advertising Data

$$e = y - Xb = (I - H)\varepsilon = Q\varepsilon$$

```
# residuals
residuals <- y - y_hat
## Error in eval(expr, envir, enclos): object 'y' not
found</pre>
```

Computation

OLS Solution

The vector of OLS estimates b is given by $(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$

In R, you may calculate b with something like this:

```
# beta coefficients
XtXi <- solve(t(X) %*% X)
b <- XtXi %*% t(X) %*% y</pre>
```

OLS Solution

Although this works, computationally it is not the best way to compute b.

Most computer programs don't compute $(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}$ directly. Instead, they typically use the QR decomposition.

QR Decomposition

Any matrix X can be written as:

$$X = QR$$

where:

- ▶ Q is an $n \times p$ orthogonal matrix: $Q^TQ = QQ^T = I$
- $ightharpoonup \mathbf{R}$ is a $p \times p$ upper triangular matrix

OLS solution via QR Decomposition

$$\begin{split} \mathbf{b} &= (\mathbf{X}^\mathsf{T} \mathbf{X})^{-1} \mathbf{X}^\mathsf{T} \mathbf{y} \\ &= \left((\mathbf{Q} \mathbf{R})^\mathsf{T} \mathbf{Q} \mathbf{R} \right)^{-1} (\mathbf{Q} \mathbf{R})^\mathsf{T} \mathbf{y} \\ &= (\mathbf{R}^\mathsf{T} \mathbf{Q}^\mathsf{T} \mathbf{Q} \mathbf{R})^{-1} \mathbf{R}^\mathsf{T} \mathbf{Q}^\mathsf{T} \mathbf{y} \\ &= (\mathbf{R}^\mathsf{T} \mathbf{R})^{-1} \mathbf{R}^\mathsf{T} \mathbf{Q}^\mathsf{T} \mathbf{y} \\ &= \mathbf{R}^{-1} (\mathbf{R}^{-\mathsf{T}} \mathbf{R}^\mathsf{T}) \mathbf{Q}^\mathsf{T} \mathbf{y} \\ &= \mathbf{R}^{-1} \mathbf{Q}^\mathsf{T} \mathbf{y} \end{split}$$

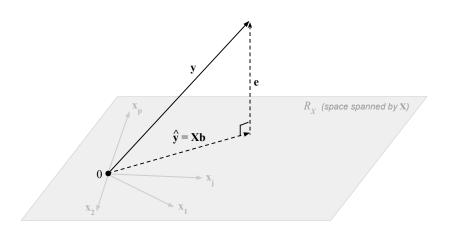
OLS solution via QR Decomposition

$$b = (\mathbf{X}^\mathsf{T} \mathbf{X})^{-1} \mathbf{X}^\mathsf{T} \mathbf{y}$$
$$= \mathbf{R}^{-1} \mathbf{Q}^\mathsf{T} \mathbf{y}$$

- ightharpoonup we don't really want to invert R
- we just want to recognize that we have a new system:

$$Rb = Q^Ty$$

In practice you apply some backsubstitution routine to solve such system (you'll do that in the lab)



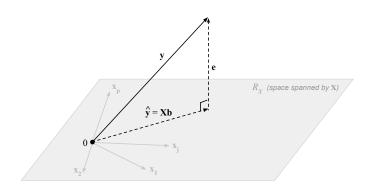
Assuming that the data is mean-centered, then the lengths of the vectors in \mathbb{R}^n can be interpreted in term of variances.

The Pythagoras theorem applied to the square triangle can be written as:

$$\mathbf{y}^\mathsf{T}\mathbf{y} = \mathbf{e}^\mathsf{T}\mathbf{e} + \mathbf{b}^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{b}$$

equivalently:

$$\|\mathbf{y}\|^2 = \|\mathbf{X}\mathbf{b}\|^2 + \|\mathbf{e}\|^2$$



$$\|\mathbf{y}\|^2 = \|\mathbf{X}\mathbf{b}\|^2 + \|\mathbf{e}\|^2$$

The Pythagoras theorem:

$$\mathbf{y}^\mathsf{T}\mathbf{y} = \mathbf{e}^\mathsf{T}\mathbf{e} + \mathbf{b}^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{X}\mathbf{b}$$

can be reexpressed as:

$$\sum (y_i)^2 = \sum (y_i - \hat{y}_i)^2 + \sum (\hat{y}_i)^2$$

Dividing by n, we put things in terms of variances:

$$\frac{1}{n}\sum_{i}(y_i)^2 = \frac{1}{n}\sum_{i}(y_i - \hat{y}_i)^2 + \frac{1}{n}\sum_{i}(\hat{y}_i)^2$$

Variance Decomposition

$$\underbrace{\frac{1}{n}\sum(y_i)^2}_{\text{total variance}} = \underbrace{\frac{1}{n}\sum(y_i - \hat{y}_i)^2}_{\text{residual variance}} + \underbrace{\frac{1}{n}\sum(\hat{y}_i)^2}_{\text{explained variance}}$$

Multiple Correlation Coefficient

We define the coefficient of multiple correlation as

$$R^2 = cor^2(\mathbf{y}, \hat{\mathbf{y}}) = cor^2(\mathbf{y}, \mathbf{Xb})$$

 \mathbb{R}^2 can be expressed in various forms:

$$R^2 = \frac{cov^2(\mathbf{y}, \hat{\mathbf{y}})}{var(\mathbf{y})var(\hat{\mathbf{y}})} = \frac{var(\hat{\mathbf{y}})}{var(\mathbf{y})} = \frac{\text{explained variance}}{\text{total variance}}$$

Multiple Correlation

$$R^2 = cor^2(\mathbf{y}, \hat{\mathbf{y}}) = cor^2(\mathbf{y}, \mathbf{Xb})$$

```
# coefficient of mulitple correlation
R2 <- cor(y, y_hat)
## Error in is.data.frame(y): object 'y_hat' not found
R2
## Error in eval(expr, envir, enclos): object 'R2' not found</pre>
```

 \mathbb{R}^2 is the proportion of the variability in \mathbf{y} explained by the model

Multiple Correlation Coefficient

 R^2 describes the fraction of the total variance of ${\bf y}$ that is explained by $\hat{{\bf y}}$

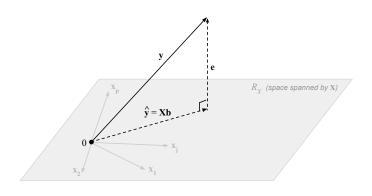
By minimzing $\sum_{i=1}^{n} e_i^2$, we actually maximize R^2 . What does this mean?

Multiple Correlation Coefficient

 R^2 describes the fraction of the total variance of ${\bf y}$ that is explained by $\hat{{\bf y}}$

By minimzing $\sum_{i=1}^{n} e_i^2$, we actually maximize R^2 . What does this mean?

In other words, the OLS fit provides a linear combination of the predictors that has maximum correlation with the response variable \mathbf{y} .

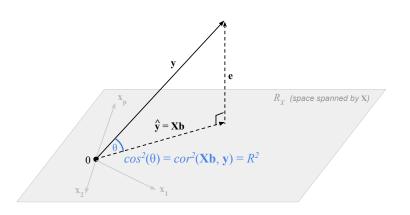


$$\|\mathbf{y}\|^2 = \|\mathbf{X}\mathbf{b}\|^2 + \|\mathbf{e}\|^2$$

$$\|\mathbf{y}\|^{2} = \|\hat{\mathbf{y}}\|^{2} + \|\mathbf{e}\|^{2}$$

$$\sum_{i=1}^{n} (y_{i} - \bar{y})^{2} = \sum_{i=1}^{n} (\hat{y}_{i} - \bar{y})^{2} + \sum_{i=1}^{n} e_{i}^{2}$$

$$R^{2} = \frac{\|\hat{\mathbf{y}}\|^{2}}{\|\mathbf{y}\|^{2}} = \cos^{2}(\mathbf{y}, \hat{\mathbf{y}})$$



About R^2

- $ightharpoonup R^2$ is one way to measure the quality of the fit.
- ▶ It doesn't tell you how accurate the coefficients are.
- ▶ It is a measure of resubstitution error. (not of generalization error)
- ▶ It depends on the number of predictors *p*.
- It is interesting from the theoretical-geometric point of view.
- ▶ But in practice it does not say much about the predictive performance of a model.

Some Comments

- ► There is nothing in the Least Squares method that requires statistical inference: formal tests of null hypotheses or confidence intervals.
- ► In its simplest for, regression analysis can be performed without statistical inference.
- ▶ We will study the inferential framework in the next slides.

References

- ► An Introduction to Statistical Learning by James et al (2013). Springer.
- Statistical Regression and Classification by Norman Matloff (2017). CRC Press.
- ▶ Linear Models with R by Julian Faraway (2015). CRC Press.
- ▶ Modern Regression Methods by Thomas Ryan (2009). Wiley.
- ▶ A Modern Approach to Regression with R by Simon Sheather (2009). Springer.
- ► Modern Multivariate Statistical Techniques by Julian Izenman (2008). Springer.
- ▶ Data Mining and Statistics for Decision Making by Stephane Tuffery (2011). Chapter 11: Classification and prediction methods. Wiley.

References (French Literature)

- Probabilites, analyse des donnees et statistique by Gilbert Saporta (2011). Chapter 17: La regression multiple et le modele lineaire general. Editions Technip, Paris.
- ➤ Statistique: Methodes pour decrire, expliquer et prevoir by Michel Tenenhaus (2008). Chapter 5: La Regression Multiple. Dunod, Paris.
- ▶ Regression avec R by Cornillon and Matzner-Lober (2011). Springer.
- ➤ Statistique Exploratoire Multidimensionnelle by Lebart et al (2004). Chapter 3, section 3.2: Regression multiple, modele lineaire. Dunod, Paris.
- ► Traitement des donnees statistiques by Lebart et al. (1982). Unit 3: Modele Lineaire. Dunod, Paris.