# Linear Regression (part 2)

Intro 2 Statistical Learning

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# Multiple Linear Regression by Ordinary Least Squares

# Regression with various predictors

- Multiple Linear Regression
- ightharpoonup p predictors  $x_1$ ,  $x_2$ , ...,  $x_p$
- one response variable y
- ▶ Do not confuse *Multiple* with *Multivariate*
- Multivariate Regression implies several responses (i.e. y<sub>1</sub>, ..., y<sub>q</sub>)

## 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("Advertising.csv", row.names = 1)</pre>
```

```
TV
          Radio
                 Newspaper
                           Sales
   230.1
           37.8
                     69.2
                           22.1
    44.5 39.3
                     45.1 10.4
   17.2
           45.9
                    69.3
                           9.3
4
   151.5 41.3
                     58.5
                           18.5
5
   180.8
        10.8
                     58.4 12.9
6
                           7.2
   8.7
           48.9
                     75.0
    57.5
           32.8
                     23.5
                            11.8
   120.2
           19.6
                     11.6
                            13.2
```

(first 8 rows)

# Data set Advertising

#### Response:

▶ Y: Sales

#### Predictors:

► X<sub>1</sub>: 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 
$$i = 1, \dots, n$$

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  $i = 1, \ldots, n$ 

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

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

If we consider an intercept term  $\beta_0$ , 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.  $\bar{X}_1 = \cdots = \bar{X}_p = 0$ )

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

which can also be represented by:

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

# **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

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

## Matrix Notation

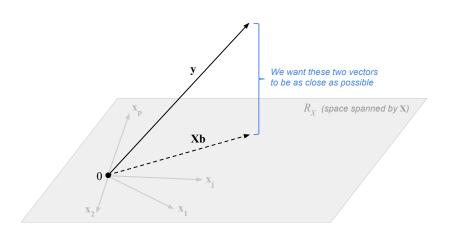
We want to calculate  $b=\hat{\beta}$  such that  $\hat{y}$  is a good approximation of y.

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
- $ightharpoonup min \{max(e_i)\}$   $L_{\infty}$ -norm
- etc

## Matrix Notation

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

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

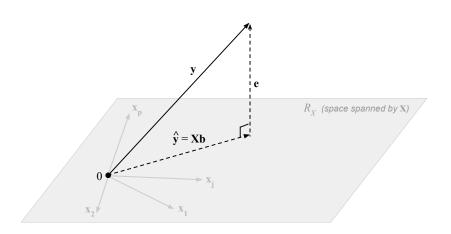
This sum is better known as the Residual Sum of Squares (RSS)

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

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

- ▶ the response lies in an n-dimensional space:  $\mathbf{y} \in \mathbb{R}^n$
- ▶ the vector of parameters lies in a p-dimesional space:  $\beta \in \mathbb{R}^p$
- ▶ in OLS, the response is projected orthogonally onto the model space spanned by X
- lacktriangle the fit is represented by projection  $\hat{\mathbf{y}} = \mathbf{X}\mathbf{b}$
- 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  $\beta$  is given by:

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

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

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

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)

# model matrix
X <- as.matrix(Advertising[ ,c('TV', 'Radio', 'Newspaper')])
X <- cbind(Intercept = rep(1, n), X)

# response variable
y <- Advertising$Sales</pre>
```

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

```
# coefficients
b <- solve(t(X) %*% X) %*% t(X) %*% y
b

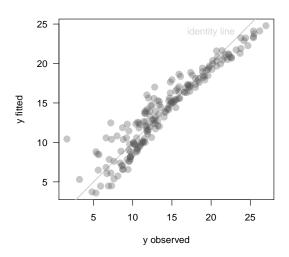
## [,1]
## Intercept 2.938889369
## TV 0.045764645
## Radio 0.188530017
## Newspaper -0.001037493
```

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 <- X %*% b
```

# Observed -vs- Predicted (fitted) values



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)
y_hat <- H %*% y
```

# 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

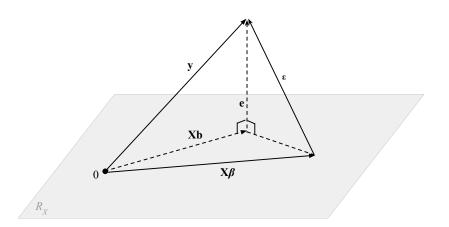
### A projection matrix $P_L \in \mathbb{R}^{n \times n}$

- ▶ is a linear transformation
- is symmetric:  $P_L = P_L^{\mathsf{T}}$
- 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
- ${f Q} = {f I} {f H}$  is the orthogonal complement or "counterpart" of  ${f H}$

# Least Squares Geometry

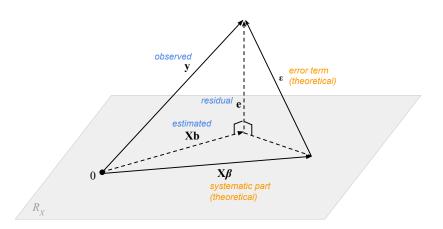


## About the Hat matrix H

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

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

#### 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:

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

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  $\varepsilon$  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  $\varepsilon$ .

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</pre>

## Computation

#### **OLS Solution**

The vector of OLS estimates b is given by  $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ In R, you may calculate b with something like this:

```
# beta coefficients

XtXi <- solve(t(X) %*% X)

b <- XtXi %*% t(X) %*% y
```

#### **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:

$$\mathbf{X} = \mathbf{Q}\mathbf{R}$$

#### where:

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

#### OLS solution via QR Decomposition

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

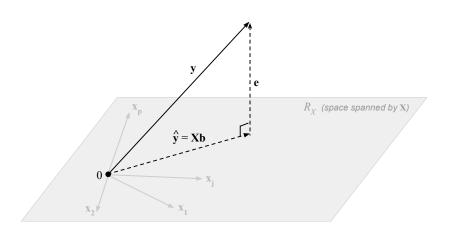
#### OLS solution via QR Decomposition

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

- 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)



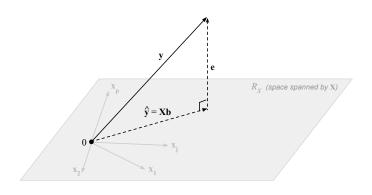
Assuming that the data is mean-centered, then the lengths of the vectors in  $\mathbb{R}^n$  can be interpreted in term of variances.

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)
R2
## [,1]
## [1,] 0.947212</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  $\hat{{\bf y}}$ 

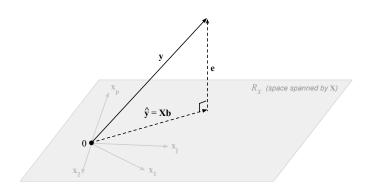
By minimzing  $\sum_{i=1}^{n} e_i^2$ , we actually maximize  $R^2$ . What does this mean?

## 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  $\mathbf{y}$ .

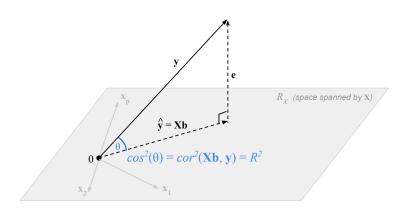


$$\|\mathbf{y}\|^2 = \|\mathbf{X}\mathbf{b}\|^2 + \|\mathbf{e}\|^2$$

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

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

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



#### 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 form, regression analysis can be performed without statistical inference.
- ▶ We will study the inferential framework in the next slides.

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