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
- p predictors $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_p}$
- one response variable $\mathbf{y}$
- Do not confuse *Multiple* with *Multivariate*
- Multivariate Regression implies several responses (i.e. $\mathbf{y_1}, \dots, \mathbf{y_q}$)

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:

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

Advertising Data

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

	TV	Radio	Newspaper	Sales
1	230.1	37.8	69.2	22.1
2	44.5	39.3	45.1	10.4
3	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	8.7	48.9	75.0	7.2
7	57.5	32.8	23.5	11.8
8	120.2	19.6	11.6	13.2

(first 8 rows)

Data set Advertising

Response:

- Y: Sales

Predictors:

- X_1: TV
- X_2: Radio
- X_3: Newspaper

Linear model:

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

Some vector-matrix notation

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

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

for $i = 1, \ldots, n$

Some vector-matrix notation

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

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

for $i = 1, \ldots, n$

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

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

Some vector-matrix notation

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

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

which can also be represented by:

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

Some vector-matrix notation

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

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

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

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

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

$$Y \approx \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_p X_p$$

or more commonly

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

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

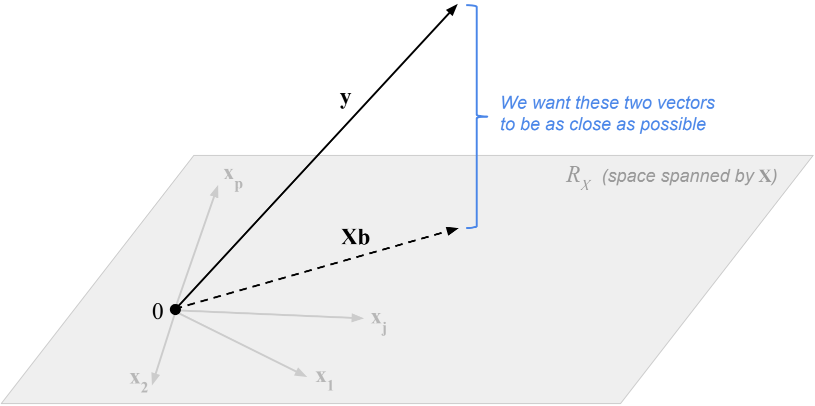
We want to calculate $\mathbf{b} = \hat{\boldsymbol{\beta}}$ such that $\hat{\mathbf{y}}$ is a good approximation of $\mathbf{y}$.

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

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

What criteria should be used to minimize the residuals?

Geometric illustration



Matrix Notation

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

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

Among the the possible criteria to minimize we have:

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

Matrix Notation

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

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

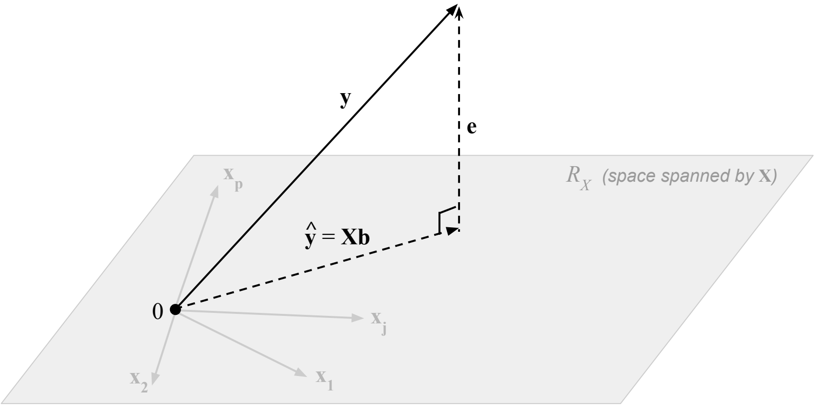
This sum is better known as the Residual Sum of Squares (RSS)

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

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

- the response lies in an n-dimensional space: $\mathbf{y} \in \mathbb{R}^n$
- the vector of parameters lies in a p-dimesional space: $\boldsymbol{\beta} \in \mathbb{R}^p$
- in OLS, the response is projected orthogonally onto the model space spanned by $\mathbf{X}$
- 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 $\mathbf{e}$
- the residual vector lies in an $(n-p)$-dimensional space: $\mathbf{b} \in \mathbb{R}^{(n-p)}$

Least Squares Minimization

OLS Minimization

OLS Criterion:

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

This means that the "best" $\mathbf{b}$ is the one which minimizes the RSS:

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

OLS Minimization

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

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

OLS Minimization

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*:

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

OLS Minimization

Assuming that the matrix $\mathbf{X}^\mathsf{T}\mathbf{X}$ is nonsingular (invertible), the unique ordinary least squares (OLS) estimator of $\boldsymbol{\beta}$ is given by:

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

OLS Minimization

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

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

The fitted values are

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

What conditions are needed for $\mathbf{X}^\top\mathbf{X}$ to be invertible?

Example: Advertising Data

```r
# 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
```

Example: Advertising Data

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

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

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

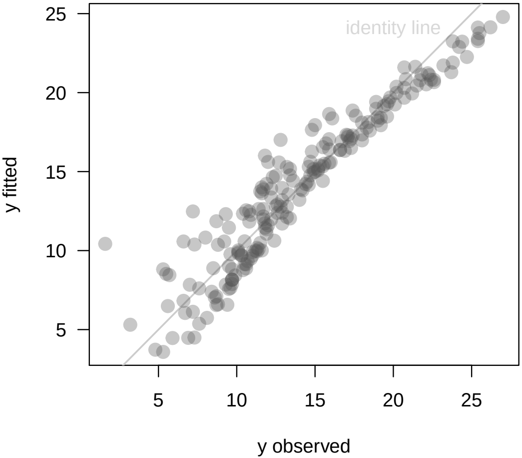
Example: Advertising Data

Predicted (fitted) values:

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

```
# fitted
fitted <- X %*% b
```

Observed -vs- Predicted (fitted) values



OLS Minimization

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 $\mathbf{H}$ is commonly known as the **hat matrix**.

What's so special about $\mathbf{H}$?

Example: Advertising Data

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

```
# 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. $L = span\{\mathbf{v_1}, \ldots, \mathbf{v_k}\}$ for some $\mathbf{v_1}, \ldots, \mathbf{v_k} \in \mathbb{R}^n$.

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

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

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

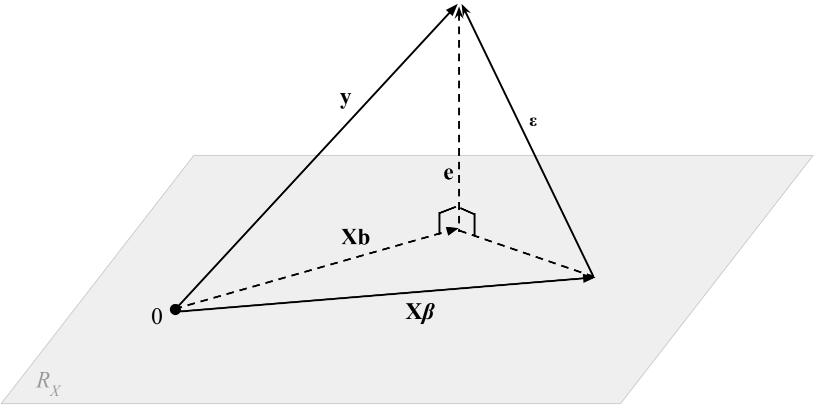
A projection matrix $P_L \in \mathbb{R}^{n\times n}$

- 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

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

Least Squares Geometry

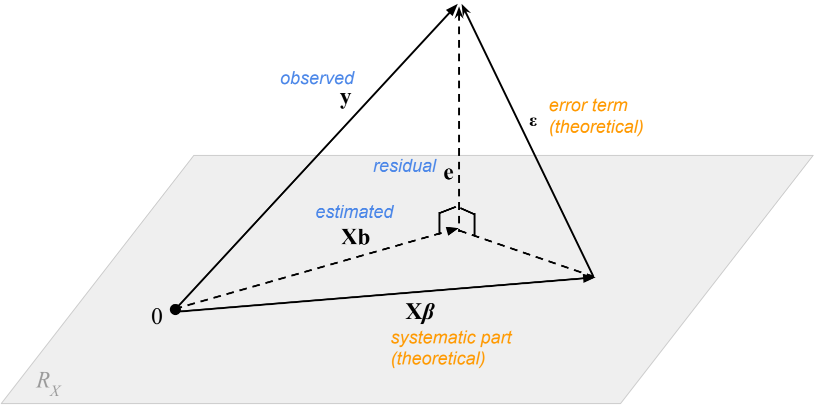


About the Hat matrix $\mathbf{H}$

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

- $X\boldsymbol{\beta} \in \mathbb{R}_X$
- $\boldsymbol{\varepsilon} \in \mathbb{R}^n$

Least Squares Geometry



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About the Hat matrix $\mathbf{H}$

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- $X\boldsymbol{\beta} \in \mathbb{R}_X$
- $\boldsymbol{\varepsilon} \in \mathbb{R}^n$

The OLS method proposes a solution $\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{e}$ that minimizes the “length” of the residual vector $\mathbf{e}$ by orthogonally projecting $\mathbf{y}$ as $\mathbf{X}\mathbf{b}$ in the spanned space of $\mathbf{X}$, and by projecting $\boldsymbol{\varepsilon}$ as $\mathbf{e}$ in the subspace to $\mathbb{R}_X$.

Residuals and Theoretical Errors

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

The residual vector can also be written as:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{b} = (\mathbf{I} - \mathbf{H})\boldsymbol{\varepsilon} = \mathbf{Q}\boldsymbol{\varepsilon}$$

Example: Advertising Data

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{b} = (\mathbf{I} - \mathbf{H})\boldsymbol{\varepsilon} = \mathbf{Q}\boldsymbol{\varepsilon}$$

```r
# residuals
residuals <- y - y_hat
```

Computation

OLS Solution

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

```r
# 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 $\mathbf{b}$.

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 $\mathbf{X}$ can be written as:

$$\mathbf{X} = \mathbf{QR}$$

where:

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

OLS solution via QR Decomposition

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

OLS solution via QR Decomposition

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

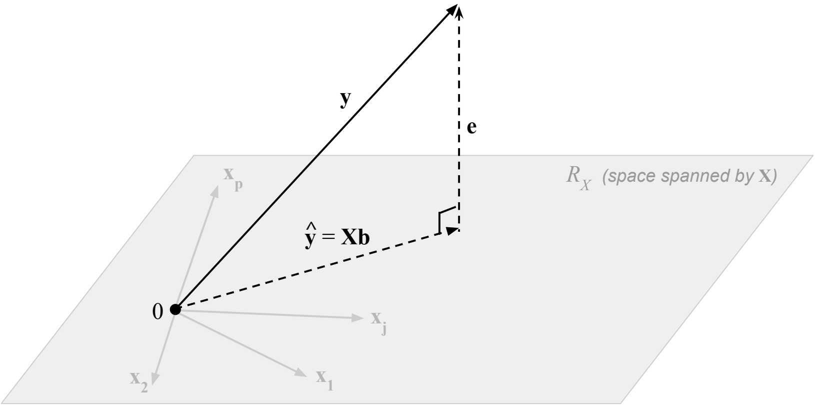
- we don't really want to invert $\mathbf{R}$
- we just want to recognize that we have a new system:

$$\mathbf{R}\mathbf{b} = \mathbf{Q}^\mathsf{T}\mathbf{y}$$

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

Assessing the Quality of the Fit

Assessing the quality of the fit



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

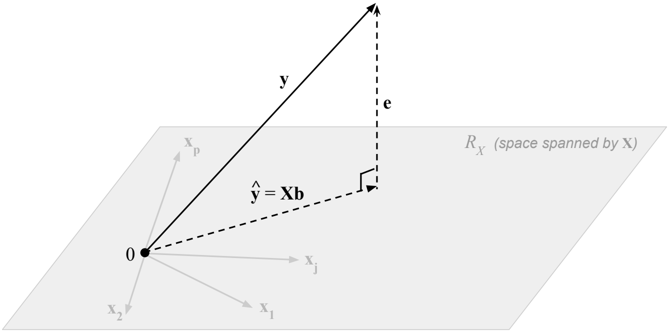
The Pythagoras theorem applied to the square triangle can be written as:

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

equivalently:

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

Assessing the quality of the fit



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

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:

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

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

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

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

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

```
# coefficient of mulitple correlation
R2 <- cor(y, y_hat)
R2

##           [,1]
## [1,] 0.947212
```

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 $\mathbf{y}$ that is explained by $\hat{\mathbf{y}}$

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

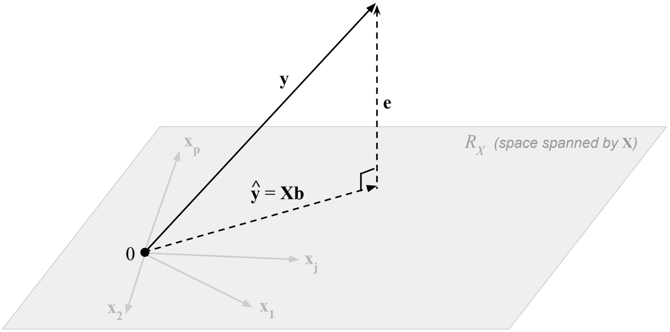
Multiple Correlation Coefficient

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

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 $\mathbf{y}$.

Assessing the quality of the fit



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

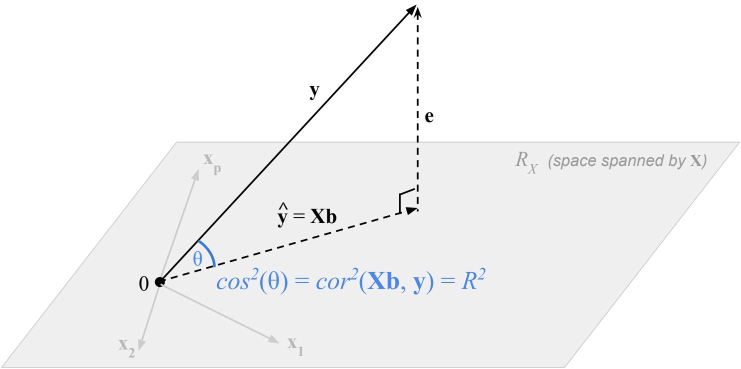
Assessing the quality of the fit

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

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

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

Assessing the quality of the fit



About R^2

- 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

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References (French Literature)

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- **Statistique: Methodes pour decrire, expliquer et prevoir** by Michel Tenenhaus (2008). *Chapter 5: La Regression Multiple*. Dunod, Paris.
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- **Traitement des donnees statistiques** by Lebart et al. (1982). *Unit 3: Modele Lineaire*. Dunod, Paris.