Chapter 2: Estimation

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Regression Analysis

- y: **response** , output
- $x = (x_1, x_2, \ldots, x_p)$: **predictors** , input
- Goal: model the relationship between y and $x_1, \ldots, x_p$

Example.

- General form: $y = f(x) + \epsilon$
- $f(\cdot)$: underlying truth. **Unknown**
- y: **continuous**
- $x_1, \ldots, x_p$: continuous, discrete, categorical
- Usually we are given a set of data

$$(x_{11}, \ldots, x_{1p}, y_1), \cdots, (x_{n1}, \ldots, x_{np}, y_n)$$

Galapagos Example

- Interested in how the number of species of tortoise on a Galapagos Island depends on other features of the island
- y: number of species of tortoise
- $x_1, \ldots, x_5$: area of the island, highest elevation of the island, distance from the nearest island, distance from Santa Cruz Island, area of the adjacent island

Galapagos Example

```
## Load the data
> library(faraway)
> data(gala)
## Check out the data
> gala
          Species Endemics  Area Elevation Nearest ...
Baltra         58       23 25.09       346     0.6 ...
Bartolome      31       21  1.24       109     0.6 ...
Caldwell        3        3  0.21       114     2.8 ...
Champion       25        9  0.10        46     1.9 ...
Coamano         2        1  0.05        77     1.9 ...
...
```

Other Analyses

Linear Regression Analysis

- There is no way to estimate $f(\cdot)$ directly given a finite number of samples.

- We have to put some **restrictions/structure** on $f(\cdot)$.

- **Assume**

$$f(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

  where β_j's are **unknown parameters** and β_0 is the intercept.

- Estimation of $f(\cdot) \overset{\textbf{reduced}}{\Longrightarrow}$ Estimation of β_j's

What Does "Linear" Mean?

A linear model is **linear in parameters** , not linear in predictors. Formally, a function g is linear in β if

$$g(a \cdot \beta + a^* \cdot \beta^*) = a \cdot g(\beta) + a^* \cdot g(\beta^*)$$

where $a, a^* \in \mathbb{R}$ and $\beta, \beta^* \in \mathbb{R}^p$.

Examples:

With $x = (x_1, x_2, x_3)$,

$$f(x) \quad = \quad \beta_0 + \beta_1 e^{x_1} + \beta_2 \ln(x_2) + \beta_3 x_1 x_3 \quad \text{is a linear model}$$

With $x = (x_1)$,

$$f(x) \quad = \quad \beta_0 + \beta_1 x_1^{\beta_2} \quad \text{is not a linear model}$$

Transformation

$f(x) = \beta_0 x_1^{\beta_1}$ is not a linear model. However, notice that

$$\ln f(x) = \ln \beta_0 + \beta_1 \ln x_1$$

Hence if we let $f^*(x) = \ln f(x), \beta_0^* = \ln \beta_0, \beta_1^* = \beta_1$, we have

$$f^*(x) = \beta_0^* + \beta_1^* \ln x_1$$

which is a linear model.

Implications

- Linear models are less restrictive than you might think
- They can be made **very flexible** by transformation of the response and the predictors.
- Linear models are not just straight lines, they can be curved (e.g., $y = ax^2 + bx + c$).

Simple Linear Regression

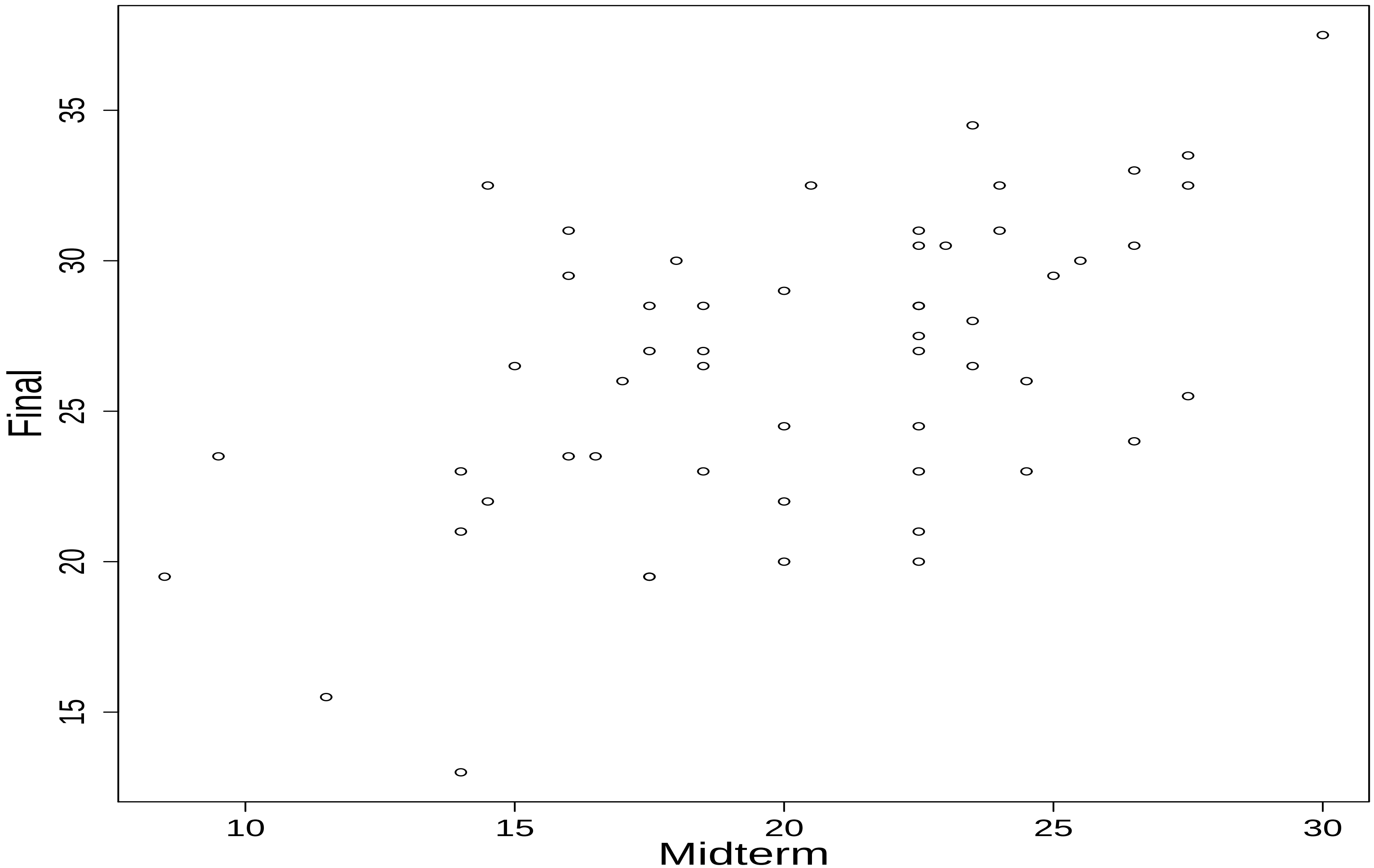
- $p = 1$, only one predictor variable
- The model is:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad i = 1, \ldots, n$$

Example

- Scores from previous Stats 500
- y: final score
- x: midterm score
- $y = \beta_0 + \beta_1 x + \epsilon$

Stats 500 Data

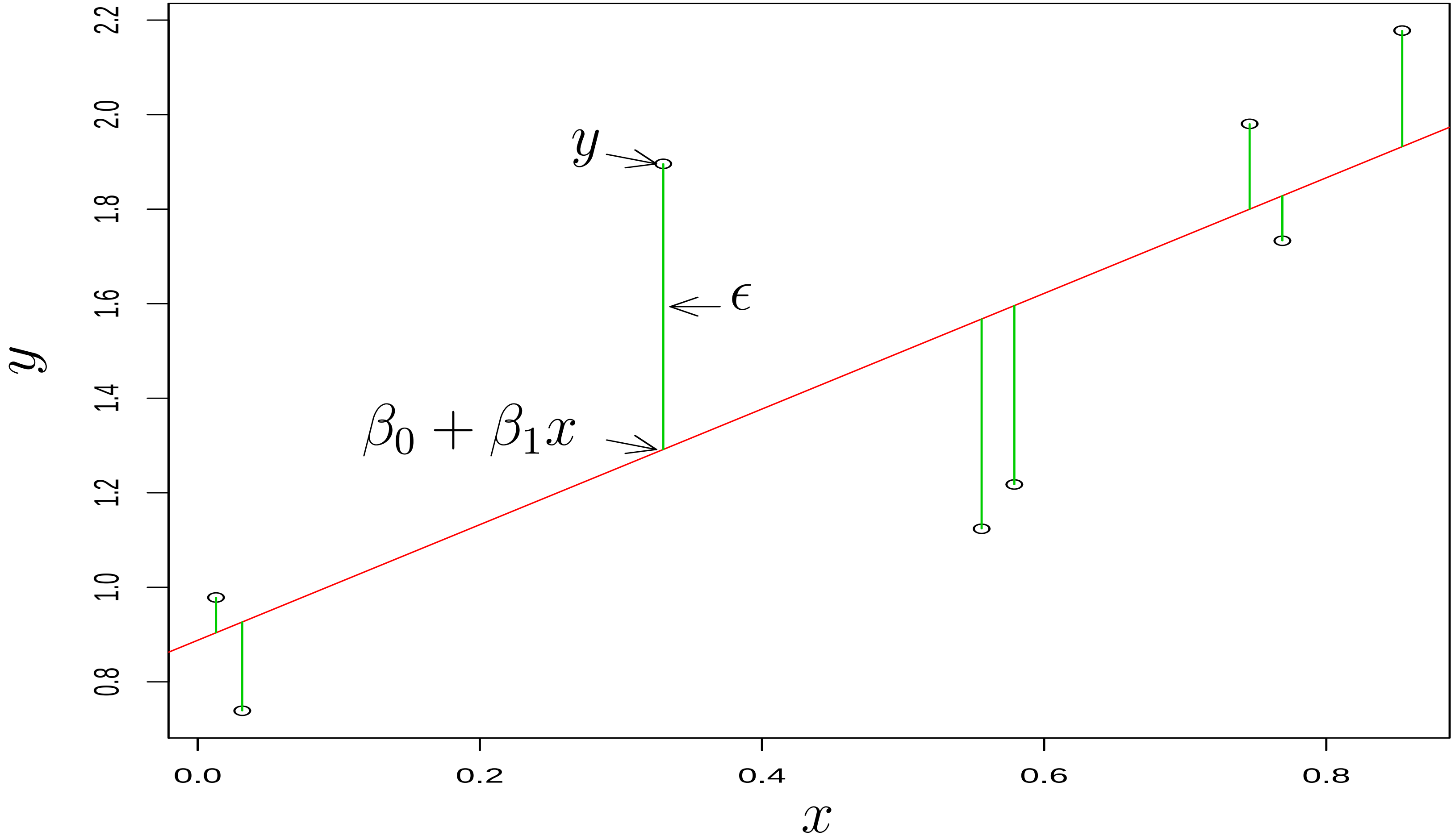


Simple Linear Regression Ctd

- Goal: given $(y_i, x_i),\ i = 1, \ldots, n$, estimate β_0, β_1
- ϵ_i is the error term; can always assume $E\epsilon = 0$.
- Minimize errors - how do we define that?
- One criterion is **least squares** :

$$\min_{\beta_0,\beta_1} \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Least Squares Estimate



Estimating β_0, β_1

Differentiate the criterion with respect to β_0, β_1 and set the derivatives equal to 0, we get:

$$\begin{aligned} \frac{\partial}{\partial \beta_0} &= (-2)\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) = 0 \\ \frac{\partial}{\partial \beta_1} &= (-2)\sum_{i=1}^{n} x_i(y_i - \beta_0 - \beta_1 x_i) = 0 \end{aligned}$$

Estimating β_0, β_1 Ctd

Solving for β_0 and β_1, we have:

$$\begin{aligned} \hat{\beta}_{\mathbf{1}} &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ \hat{\beta}_{\mathbf{0}} &= \bar{y} - \hat{\beta}_1 \bar{x} \end{aligned}$$

where

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i, \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i.$$

"**Hat** " notation is used for estimates.

Yet another interpretation

Letting

$$s_y = SD(y) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2}, \; s_x = SD(x) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$r = Cor(x, y) = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{s_x \cdot s_y}$$

we can rewrite the line equation (simple algebra) as

$$\frac{y - \bar{y}}{s_y} = r\frac{x - \bar{x}}{s_x},$$

or, if x and y are standardized first (mean 0, sd 1), simply

$$y = rx.$$

Two regression lines

- Suppose x and y have both been standardized.
- Regress y on x: $y = rx$
- Regress x on y: $x = ry$

Regression effect : predictions always “regress” towards the mean

- Regression effect is usually uninteresting
- Example: husband’s and wife’s education

Multiple Linear Regression

Model: $y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$

predictors = `p`

parameters = `p+1`

Assume $E(\epsilon_i) = 0, \quad i = 1, \ldots, n$

Matrix Notation

Let

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & x_{ij} & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{pmatrix}$$

$$\beta = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}, \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

Then we can write the model for the data as:

$$y_{n\times 1} = X_{n\times(p+1)}\beta_{(p+1)\times 1} + \epsilon_{n\times 1}$$

This is the same model in more compact notation.

Estimating β

- Observe y and X. How do we estimate β?
- Minimize the errors (ϵ)
- Least squares criterion:

$$
\begin{aligned}
\min_{\beta} \sum_{i=1}^{n} \epsilon_i^2 &= \epsilon^T \epsilon \\
&= (y - X\beta)^T (y - X\beta) \\
&= y^T y - 2y^T X\beta + \beta^T X^T X\beta
\end{aligned}
$$

Estimating β Ctd

Differentiating the criterion with respect to β and setting the derivative equal to 0, we get the **normal equation** :

$$X^T X\hat{\beta} = X^T y \Rightarrow \hat{\beta} = \left(X^T X\right)^{-1} X^T y$$

- X full rank $\Leftrightarrow$ $X^T X$ invertible

Fitted Model

- Fitted values: $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \cdots + \hat{\beta}_p x_{ip}$
- Fitted model: $\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p$
- **Residuals** : $\hat{\epsilon}_i = y_i - \hat{y}_i$
- Residual sum of squares (**RSS**): $\sum_{i=1}^n \hat{\epsilon}_i^2$

Hat Matrix

- $X\hat{\beta} = X\left(X^T X\right)^{-1} X^T y = Hy$, where

$$H = X\left(X^T X\right)^{-1} X^T$$

  is called the **"Hat"** matrix.

- Fitted values: $\hat{y} = Hy$
- Residuals: $\hat{\epsilon} = y - \hat{y} = (I - H)y$
- H is a **projection matrix** .

Projection Matrix

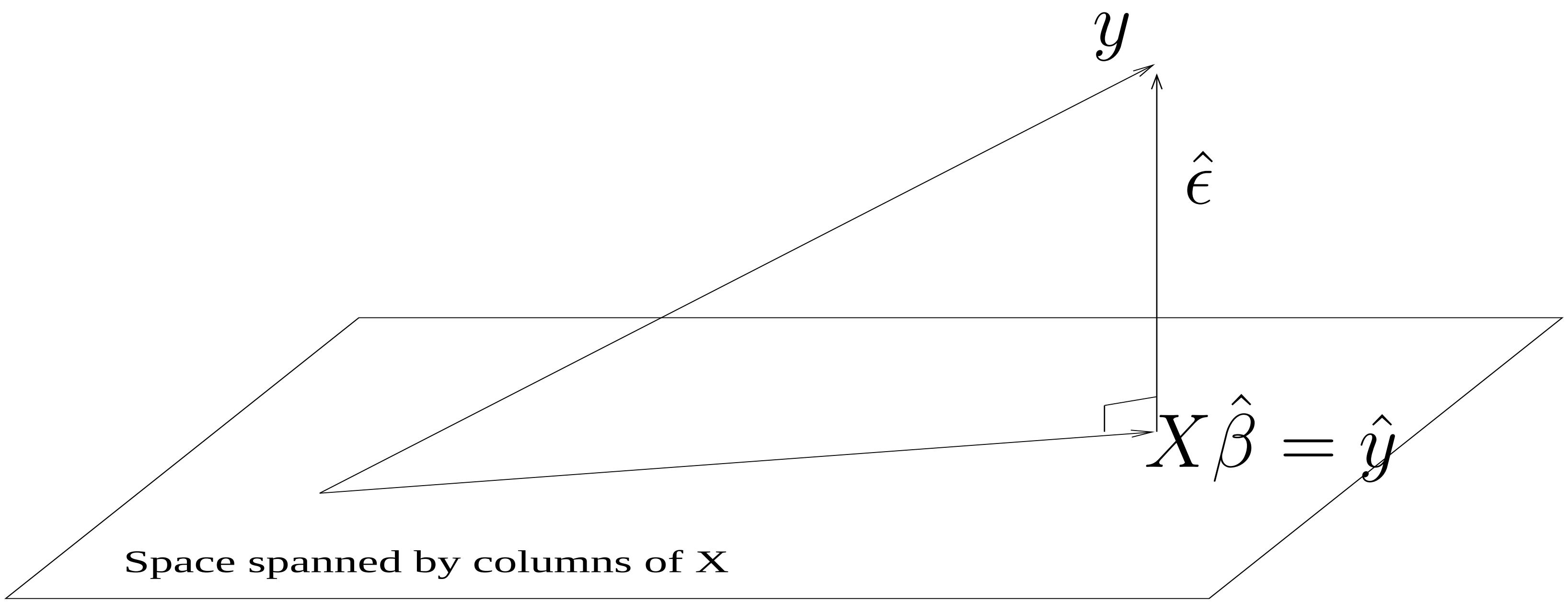
Definition: H is a projection matrix if

- $H^T = H$ (H is **symmetric**).
- $HH = H$ (H is **idempotent**).

Does $X\left(X^TX\right)^{-1}X^T$ satisfy these two conditions?

The projection matrix H projects $y_{n\times 1}$ onto the column space of $X_{n\times(p+1)}$, which leads to the **vector space interpretation** of least squares estimate.

Vector Space Interpretation



$\min_\beta (y - X\beta)^T (y - X\beta)$ can be interpreted as minimizing the Euclidean distance between y and the linear space spanned by the columns of X.

Properties of $\hat{\beta}$

- **Unbiased** : $E(\hat{\beta}) = \beta$. Check:

- $\mathrm{Var}(\hat{\beta}) =?$ **Assume** $\mathrm{Var}(\epsilon) = \sigma^2 I$, then

$$\begin{aligned} \mathrm{Var}(\hat{\beta}) &= (X^T X)^{-1}\sigma^2 \\ \mathrm{Var}(\hat{\beta}_j) &= (X^T X)^{-1}_{jj}\sigma^2 \end{aligned}$$

Properties of $\hat{\beta}$ Ctd

- σ^2 can also be estimated:

$$\hat{\sigma}^2 = \frac{\sum_i (y_i - \hat{y}_i)^2}{n - (p+1)},$$

  where $n - (p+1)$ is the **degrees of freedom** .

- **Unbiased** : $E(\hat{\sigma}^2) = \sigma^2$

Galapagos Example

```
## Get the X matrix
> dim(gala)
[1] 30  7
> n = dim(gala)[1]
> p = dim(gala)[2] - 2
> x = cbind(1, as.matrix(gala[, 3:7]))
> ## Compute the inverse of (X^T X)
> xtx = t(x) %*% x
> xtxi = solve(xtx)
> beta = xtxi %*% t(x) %*% gala[,1]
```

```
> beta
                  [,1]
           7.068220709
Area      -0.023938338
Elevation  0.319464761
Nearest    0.009143961
Scruz     -0.240524230
Adjacent  -0.074804832
> ## Residual sum of squares
> rss = sum((gala[,1] - x %*% beta)^2)
> sigma2 = rss / (n - (p+1))
> sigma = sqrt(sigma2)
> sigma
[1] 60.97519
```

COV

```
> ## Use the lm() function
> temp = lm(Species ~ Area + Elevation + Nearest
             + Scruz + Adjacent, data=gala)
> summary(temp)
Call:
lm(formula = Species ~ Area + Elevation + Nearest +
Scruz +  Adjacent,  data = gala)
Residuals:
     Min        1Q   Median       3Q      Max
-111.679  -34.898   -7.862   33.460  182.584
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  7.068221  19.154198   0.369 0.715351
Area        -0.023938   0.022422  -1.068 0.296318
```

```
Elevation     0.319465   0.053663   5.953 3.82e-06 ***
Nearest       0.009144   1.054136   0.009 0.993151
Scruz        -0.240524   0.215402  -1.117 0.275208
Adjacent     -0.074805   0.017700  -4.226 0.000297 ***
---
Signif. codes:   0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 60.98 on 24 degrees of freedom
Multiple R-Squared: 0.7658,     Adjusted R-squared: 0.7171
F-statistic:  15.7 on 5 and 24 DF,  p-value: 6.838e-07
```

Goodness of Fit

- Measure how well the model fits with the data
- Residual sum of squares (**RSS**): $\sum_i (y_i - \hat{y}_i)^2$
  Seems reasonable, but what about units?

Goodness of Fit Ctd

- **Coefficient of determination** :

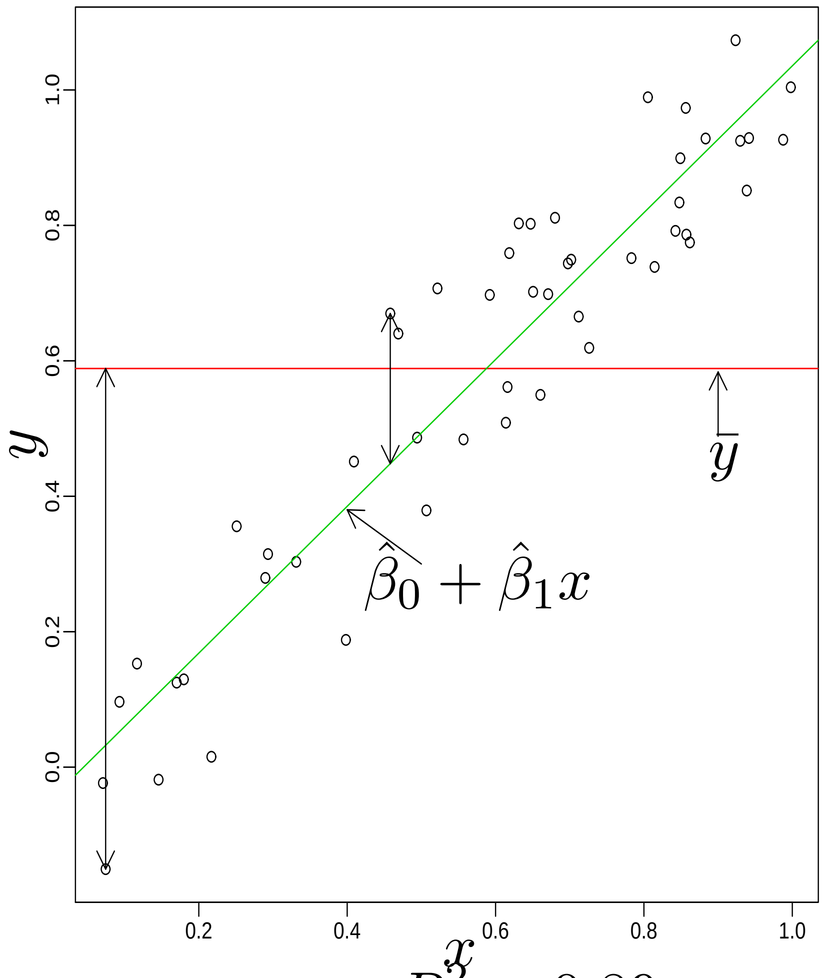
$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

Alternative expression:

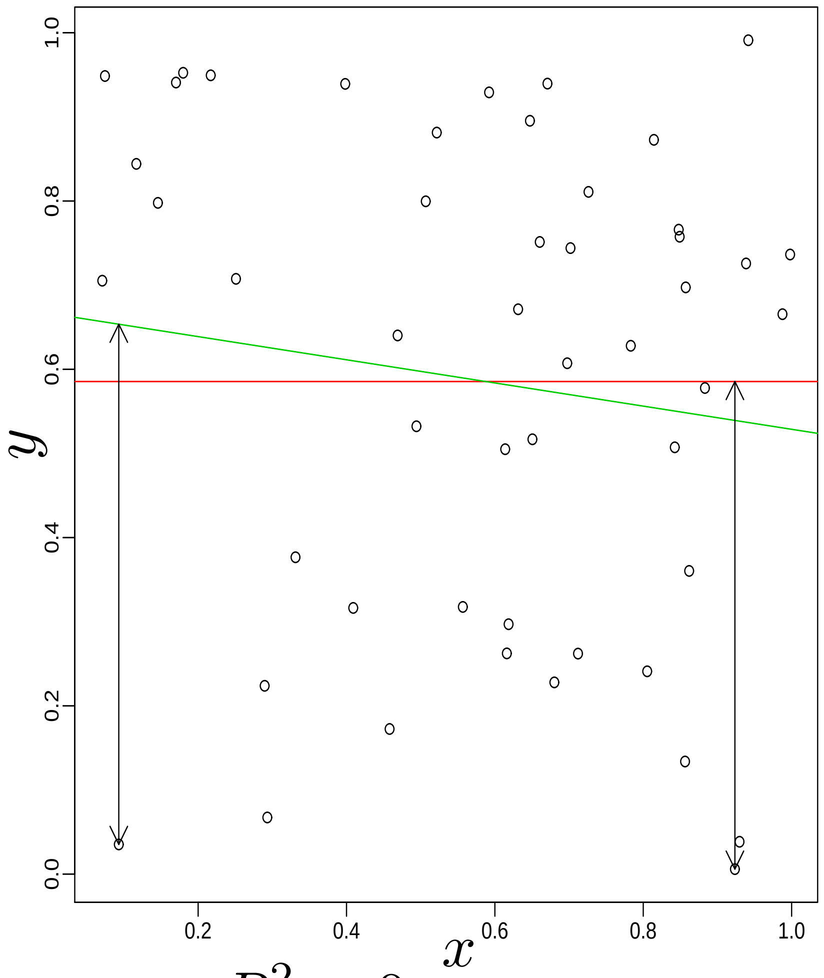
$$R^2 = \frac{\sum_i (\hat{y}_i - \bar{y})^2}{\sum_i (y_i - \bar{y})^2}$$

- $0 \leq R^2 \leq 1$. Why?
- R^2 "close" to 1 indicates good fit.

Intuition



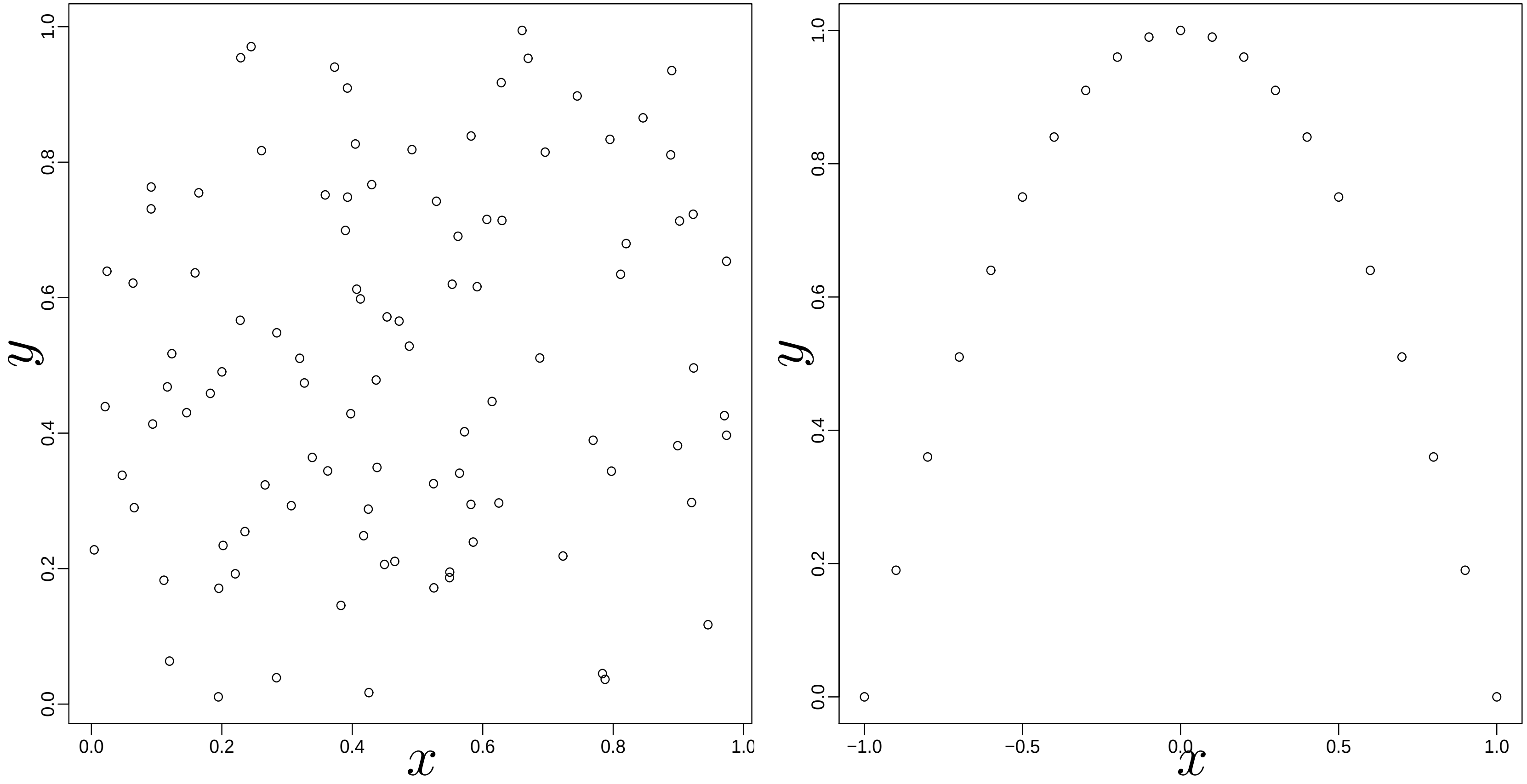
$R^2 = 0.89$



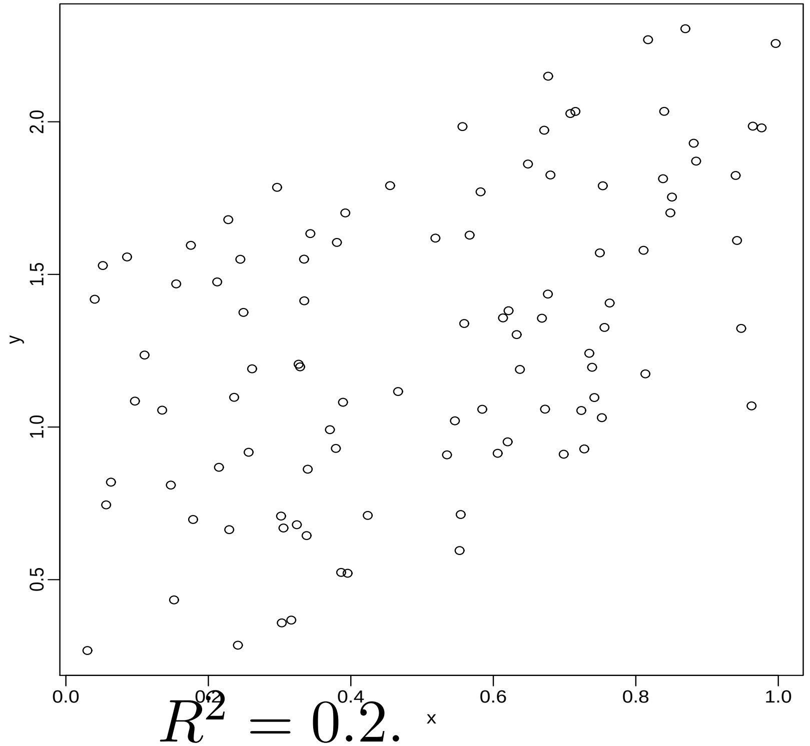
$R^2 = 0$

Remarks on R^2

- R^2 near 0 could be



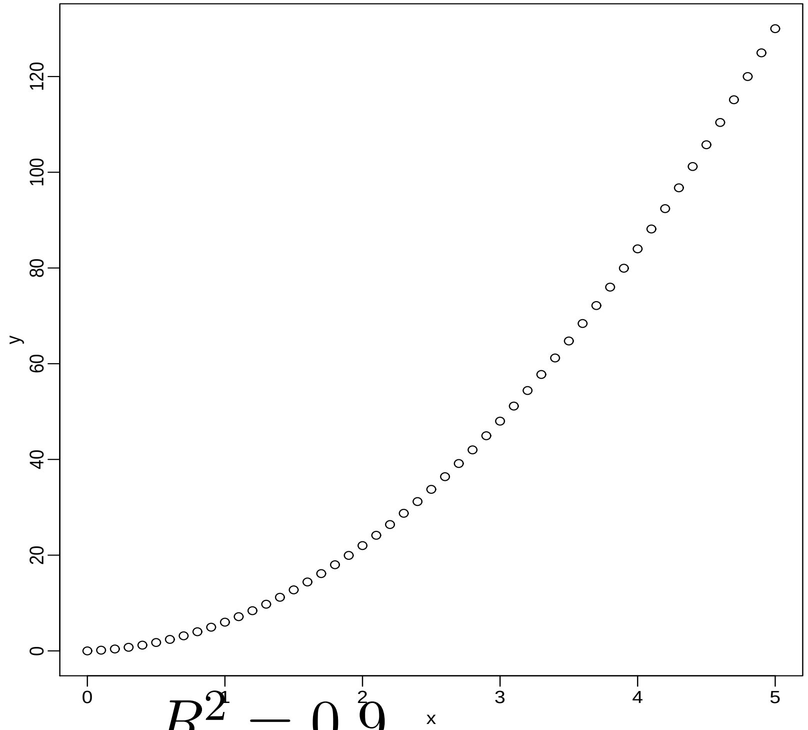
- Small R^2 does not mean that y and X are not linearly related (can have slight trend with high variance).



$R^2 = 0.2.$

- Likewise,

  R^2 close to 1 does not mean the linear model is correct.



$R^2 = 0.9.$

The Gauss-Markov Theorem

- Why use the least squares estimate $\hat{\beta}$?
- Theorem: Suppose $y = X\beta + \epsilon$, X is of full-rank, $E(\epsilon) = 0$ and $\text{Var}(\epsilon) = \sigma^2 I$. Consider $\psi = c^T\beta$. Then among all **unbiased linear** estimates of ψ, $\hat{\psi} = c^T\hat{\beta}$ has the **minimum variance** and is unique.
- Example: Let $c^T = (1, x_1, \ldots, x_p)$, then $\psi = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$.
- Best Linear Unbiased Estimate (**BLUE**)

What Can Go Wrong?

- $X^T X$ could be singular (happens if predictors are linearly dependent or if $p > n$)
- Assumed $\mathrm{Var}(\epsilon) = \sigma^2 I$
- Best only among linear, unbiased estimates

Ch 6 & 9