# Machine Learning

# 1. Linear Regression

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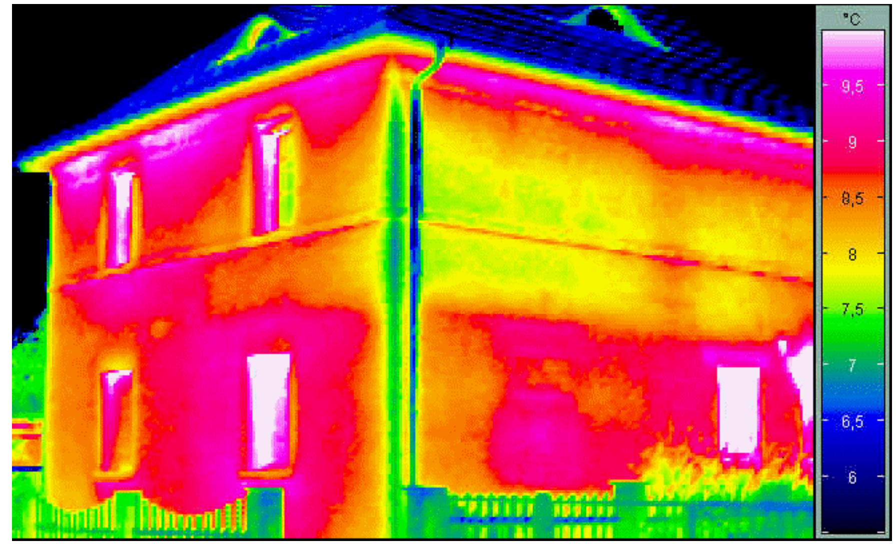
## Example

Example: how does gas consumption depend on external temperature? (Whiteside, 1960s).




weekly measurements of

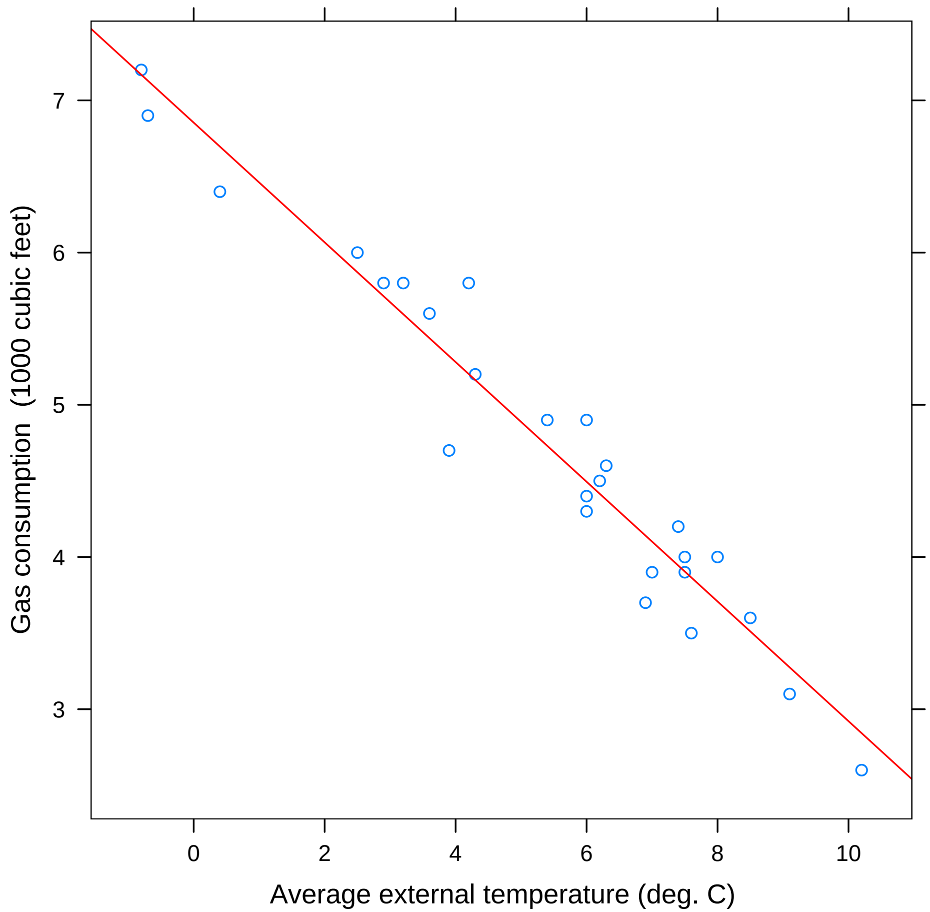
- average external temperature
- total gas consumption (in 1000 cubic feets)

A third variable encodes two heating seasons, before and after wall insulation.

How does gas consumption depend on external temperature?

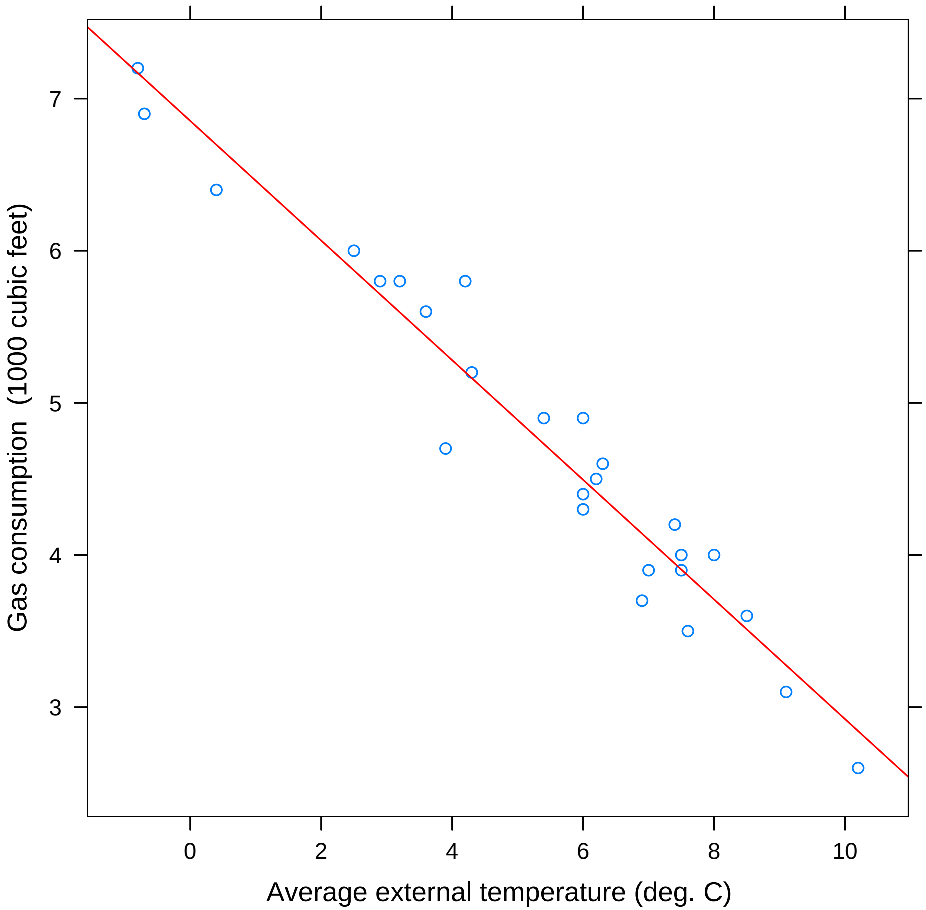
How much gas is needed for a given temperature ?

# Example

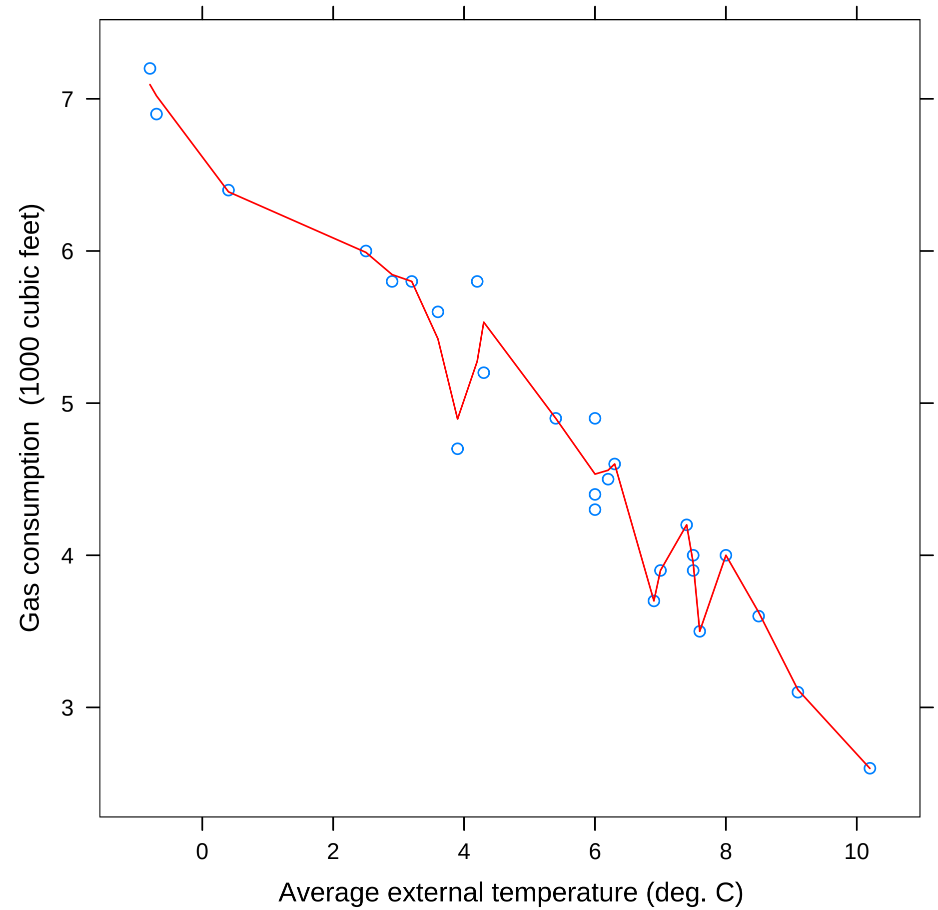



linear model

# Example




linear model




more flexible model

## Variable Types and Coding

The most common variable types:

**numerical / interval-scaled / quantitative**
where differences and quotients etc. are meaningful,
usually with domain $\mathcal{X} := \mathbb{R}$,
e.g., temperature, size, weight.

**nominal / discrete / categorical / qualitative / factor**
where differences and quotients are not defined,
usually with a finite, enumerated domain,
e.g., $\mathcal{X} := \{\text{red}, \text{green}, \text{blue}\}$
or $\mathcal{X} := \{\text{a}, \text{b}, \text{c}, \ldots, \text{y}, \text{z}\}$.

**ordinal / ordered categorical**
where levels are ordered, but differences and quotients are not defined,
usually with a finite, enumerated domain,
e.g., $\mathcal{X} := \{\text{small}, \text{medium}, \text{large}\}$

## Variable Types and Coding

Nominals are usually encoded as binary **dummy variables**:

$$\delta_{x_0}(X) := \begin{cases} 1, & \text{if } X = x_0, \\ 0, & \text{else} \end{cases}$$

one for each $x_0 \in \mathcal{X}$.

Example: $\mathcal{X} := \{\text{red}, \text{green}, \text{blue}\}$

Replace

one variable $X$ with 3 levels: $\text{red}, \text{green}, \text{blue}$

by

three variables $\delta_{\text{red}}(X)$, $\delta_{\text{green}}(X)$ and $\delta_{\text{blue}}(X)$ with 2 levels: 0, 1

| $X$ | $\delta_{\text{red}}(X)$ | $\delta_{\text{green}}(X)$ | $\delta_{\text{blue}}(X)$ |
|---|---|---|---|
| red | $1$ | $0$ | $0$ |
| green | $0$ | $1$ | $0$ |
| blue | $0$ | $0$ | $1$ |

## The Regression Problem Formally

Let

$X_1, X_2, \ldots, X_p$ be random variables called **predictors** (or **inputs**, **covariates**).
Let $\mathcal{X}_1, \mathcal{X}_2, \ldots, \mathcal{X}_p$ be their domains.
We write shortly

$$X := (X_1, X_2, \ldots, X_p)$$

for the vector of random predictor variables and

$$\mathcal{X} := \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_p$$

for its domain.

$Y$ be a random variable called **target** (or **output**, **response**).
Let $\mathcal{Y}$ be its domain.

$\mathcal{D} \subseteq \mathcal{X} \times \mathcal{Y}$ be a (multi)set of instances of the unknown joint distribution $p(X, Y)$ of predictors and target called **data**.
$\mathcal{D}$ is often written as enumeration

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

# The Regression Problem Formally

The task of regression and classification is
to predict $Y$ based on $X$,
i.e., to estimate

$$r(x) := E(Y \mid X = x) = \int y\, p(y|x) dy$$

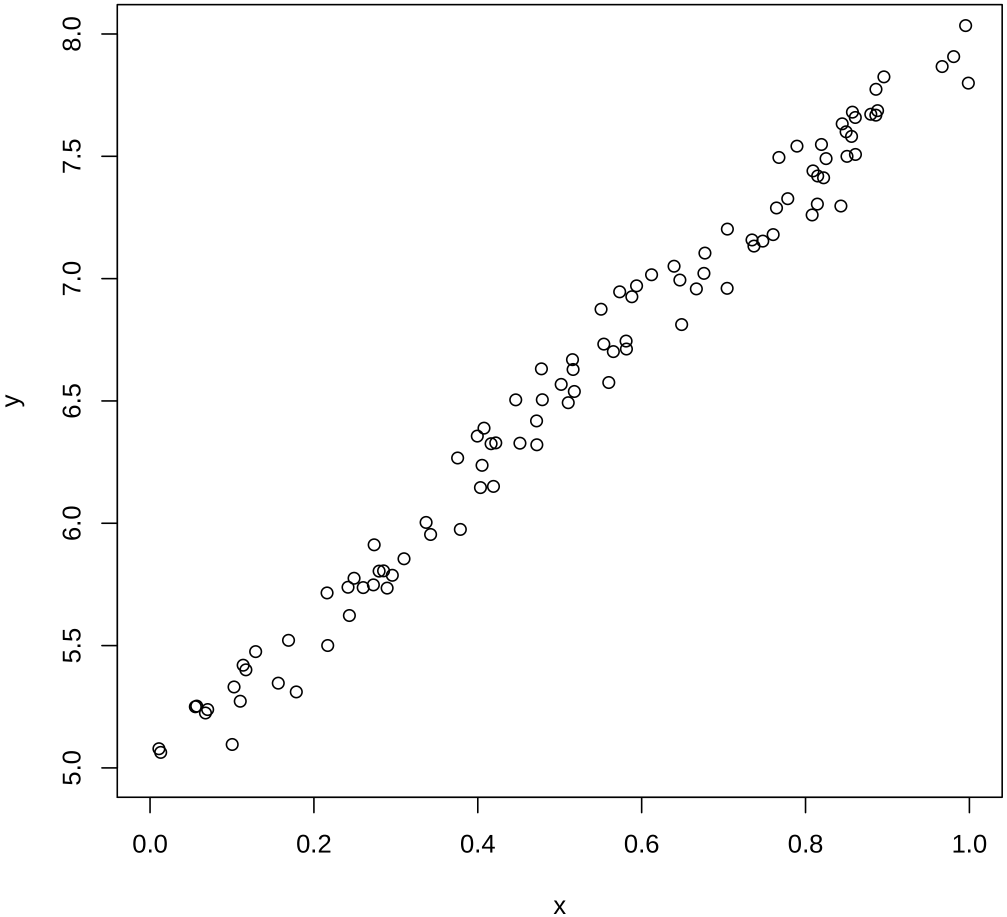
based on data (called **regression function**).

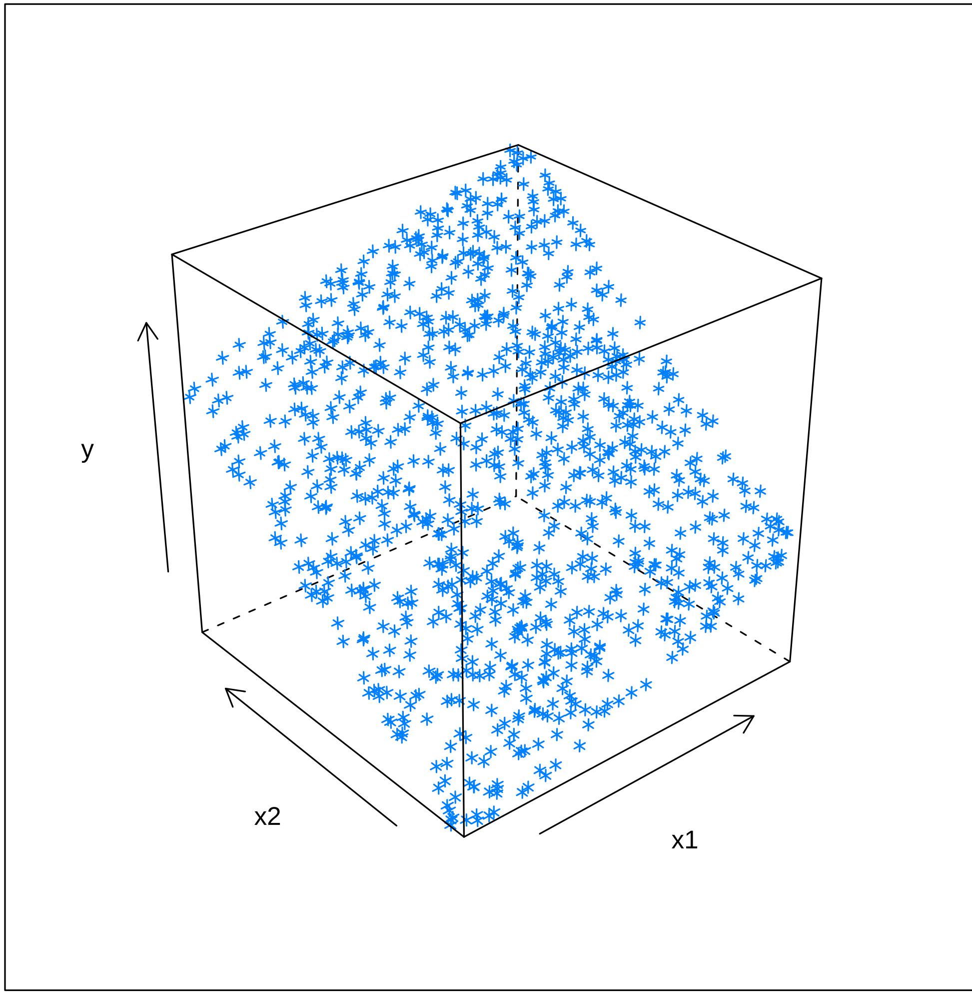
If $Y$ is numerical, the task is called **regression**.

If $Y$ is nominal, the task is called **classification**.

1. The Regression Problem
2. **Simple Linear Regression**
3. Multiple Regression
4. Variable Interactions
5. Model Selection
6. Case Weights

# Simple Examples: Single Predictor vs. Multiple Predictors



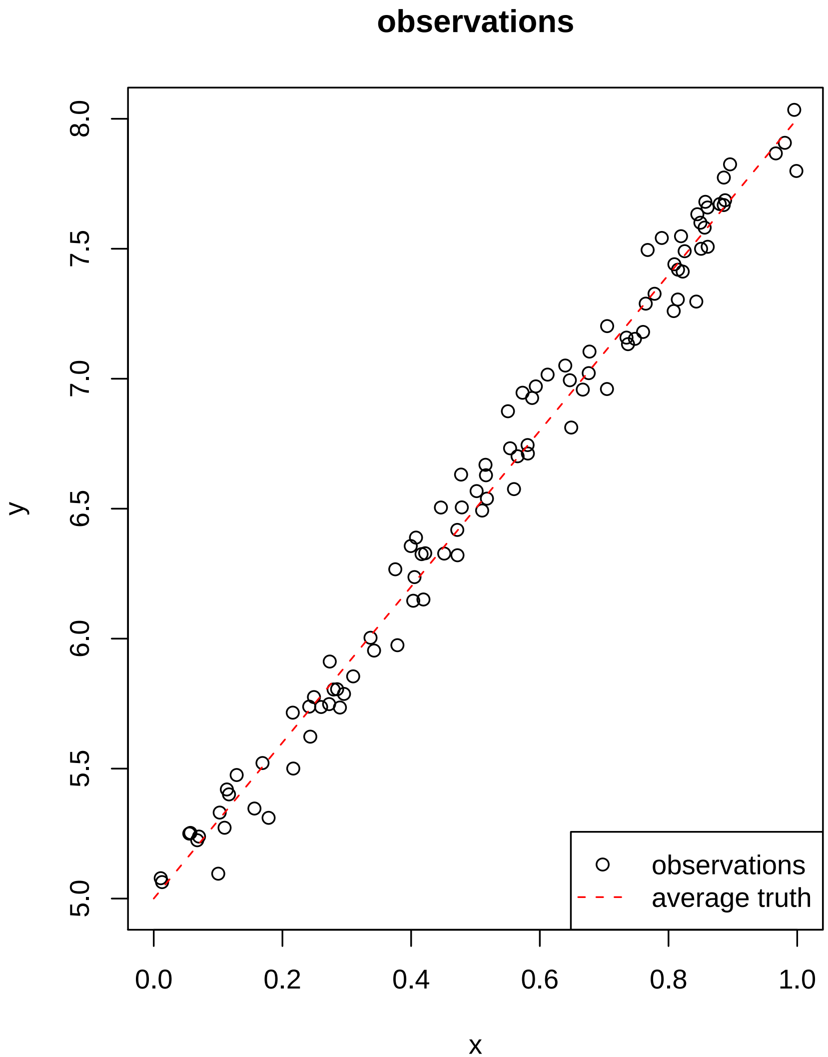

single predictor:

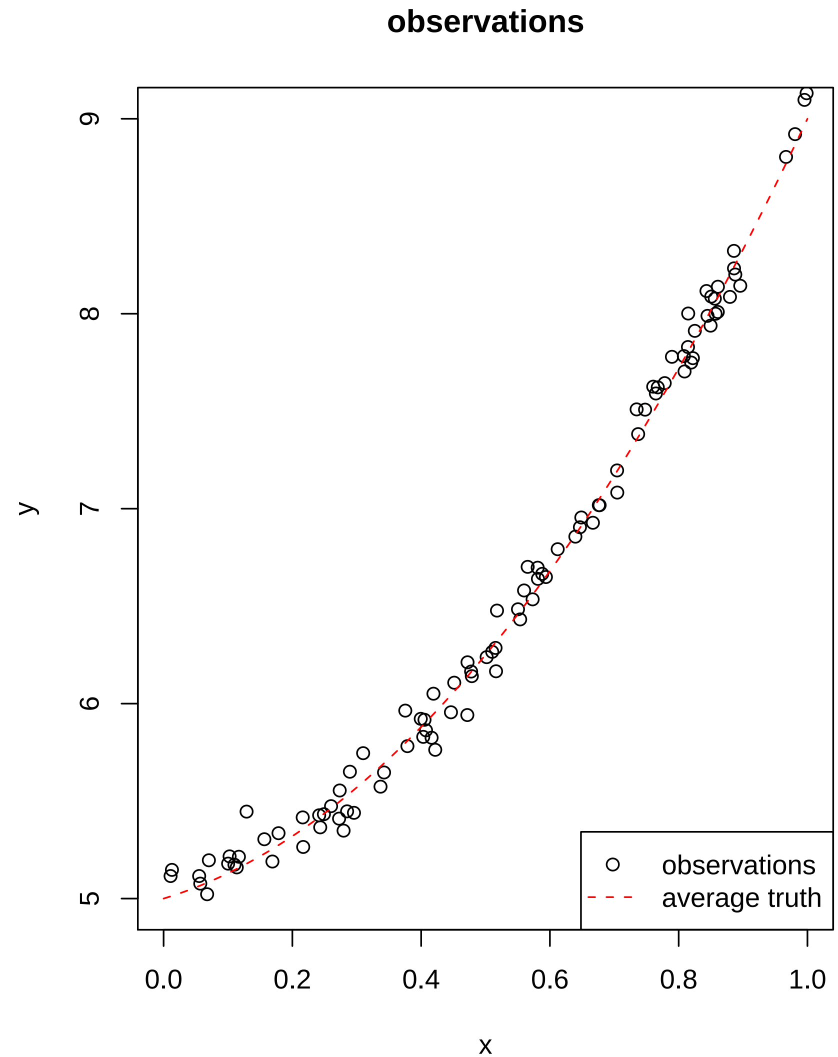
$$y = 3x + 5$$

multiple predictors:

$$y = x_1 + 2x_2 + 5$$

# Simple Examples: Regression Function



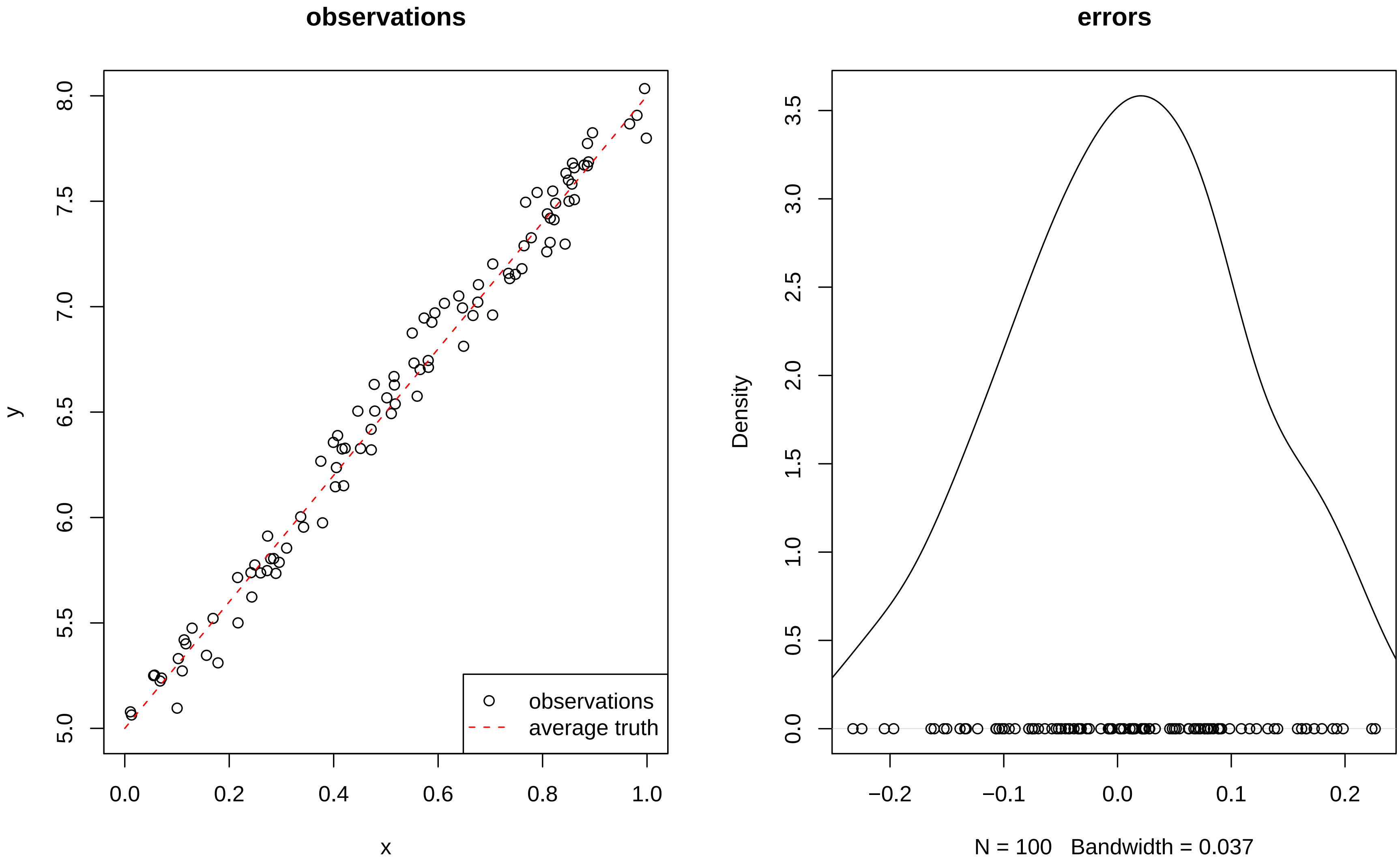

linear regression function:

$$y = 3x + 5$$

non-linear regression function:

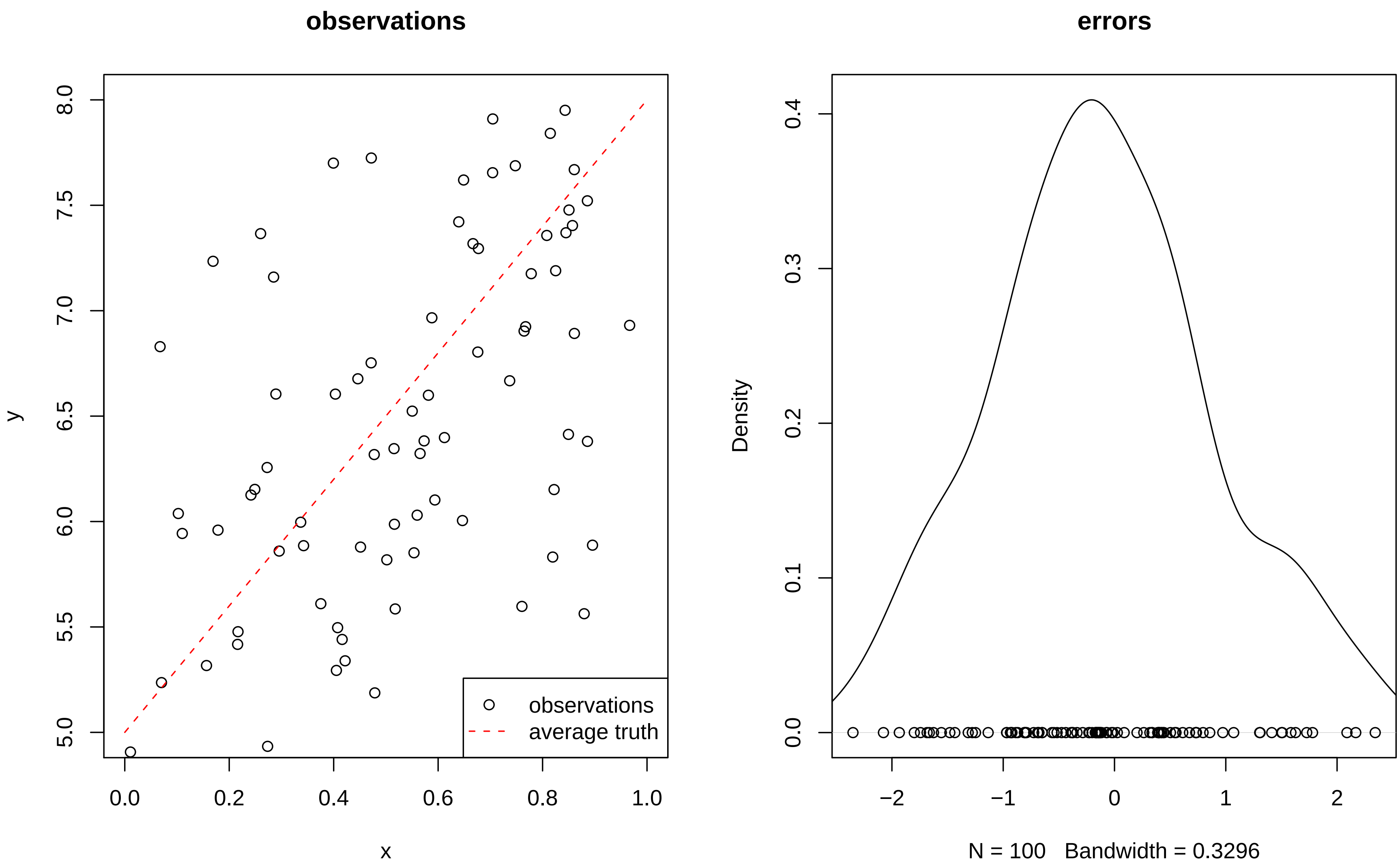
$$y = 3x^2 + x + 5$$

# Simple Examples: Size of Errors (1/2)



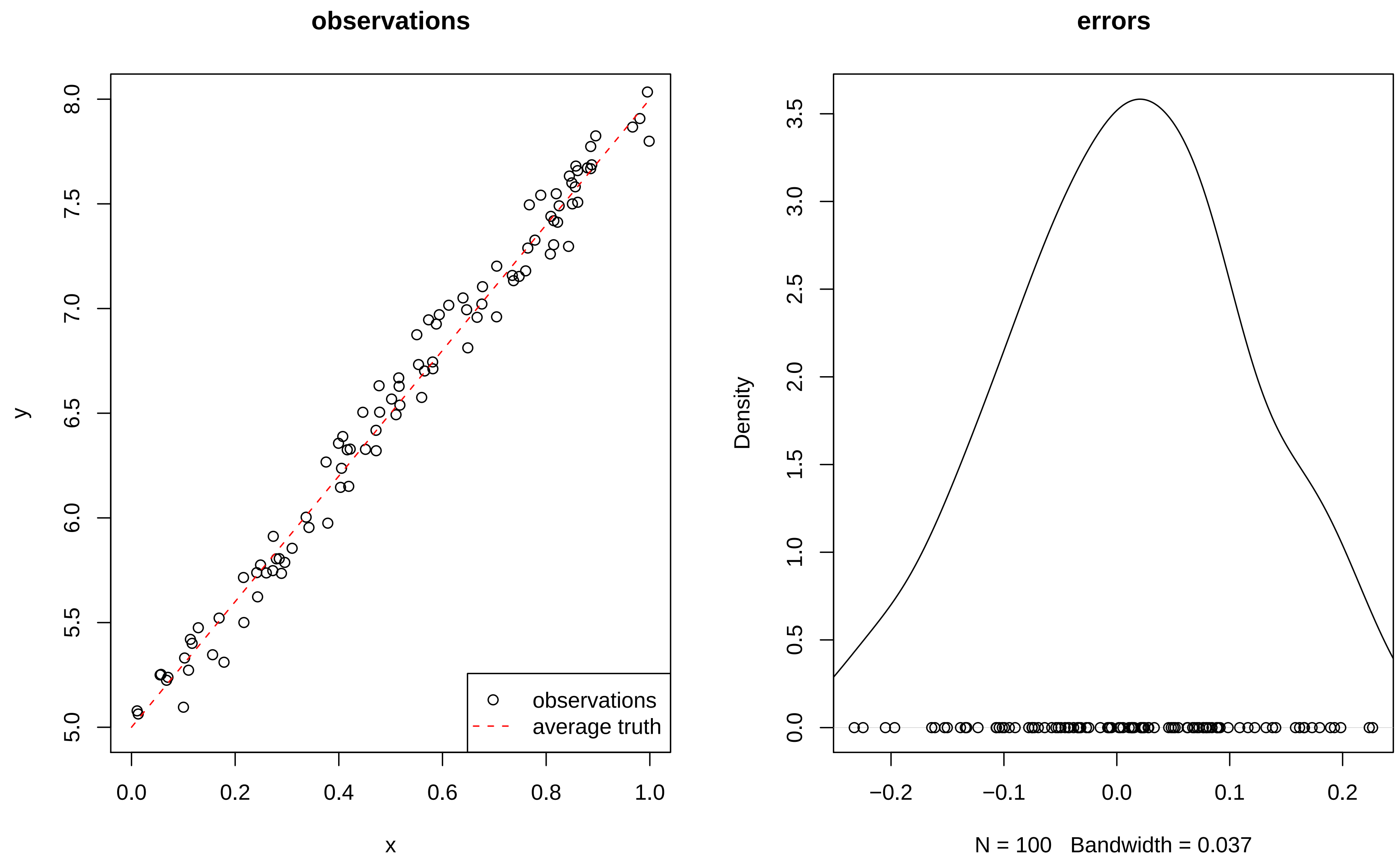

Small errors vs. . . .

# Simple Examples: Size of Errors (2/2)



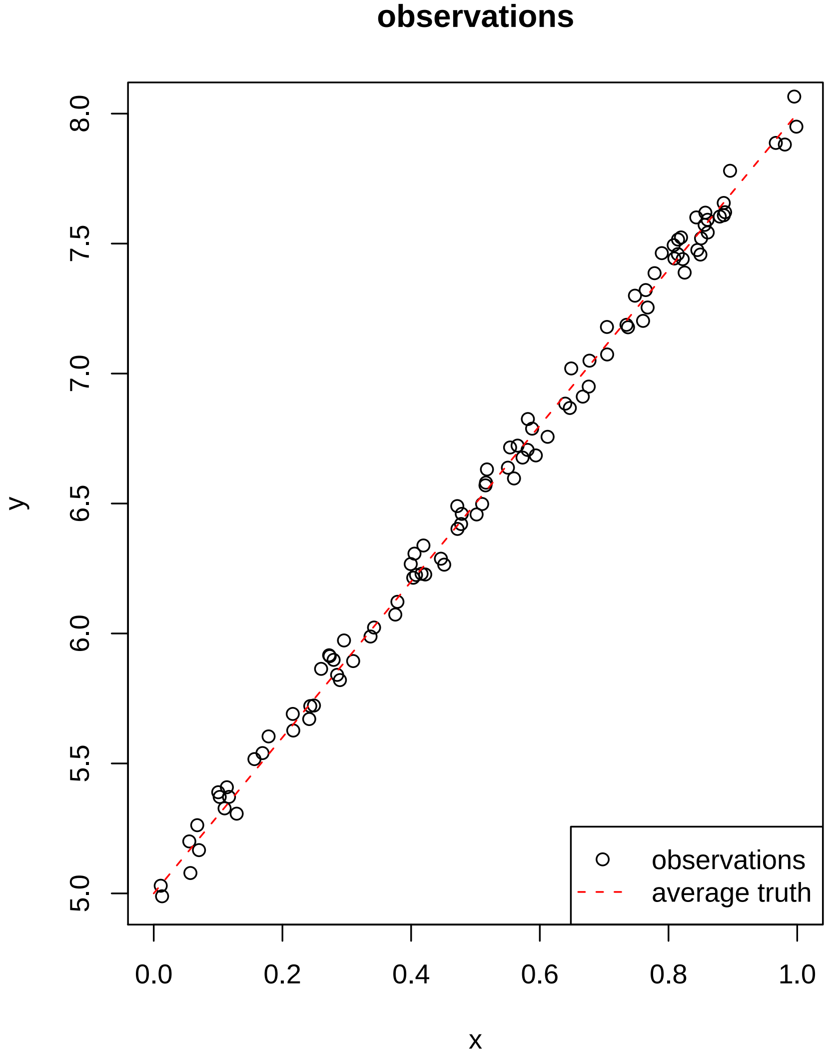

. . . large errors.

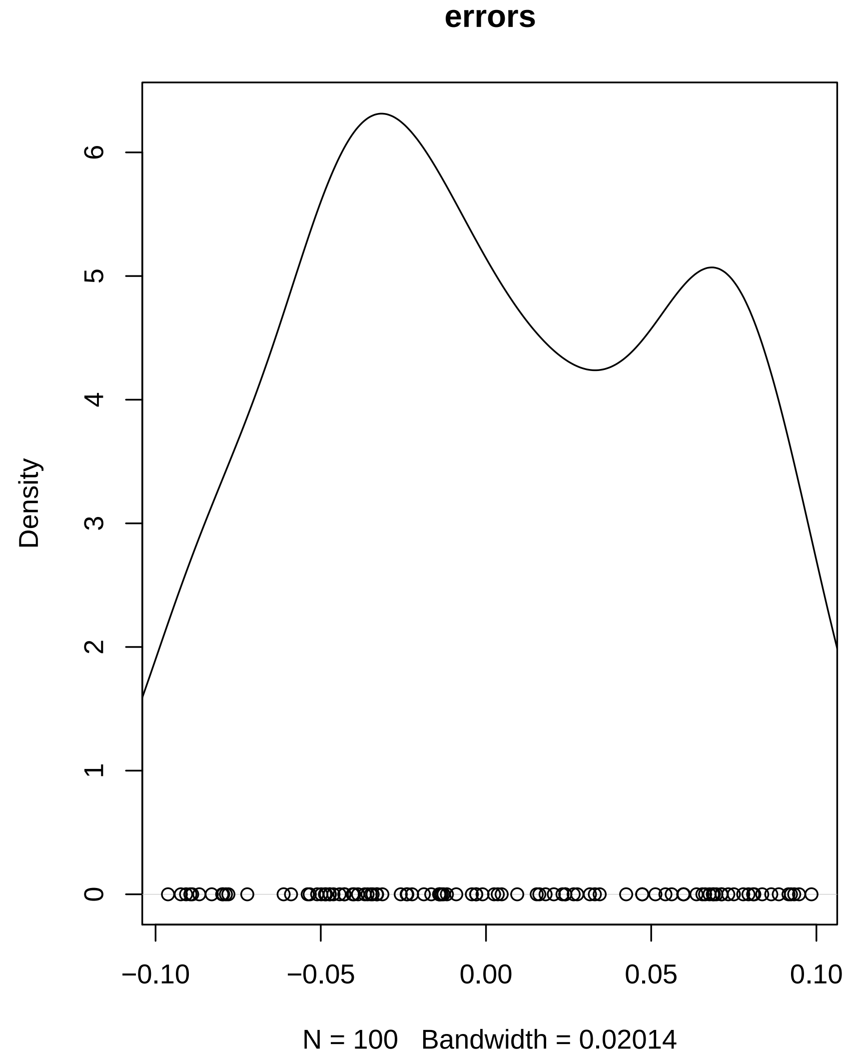
# Simple Examples: Distribution of Errors (1/2)




Normally distributed errors vs. . . .

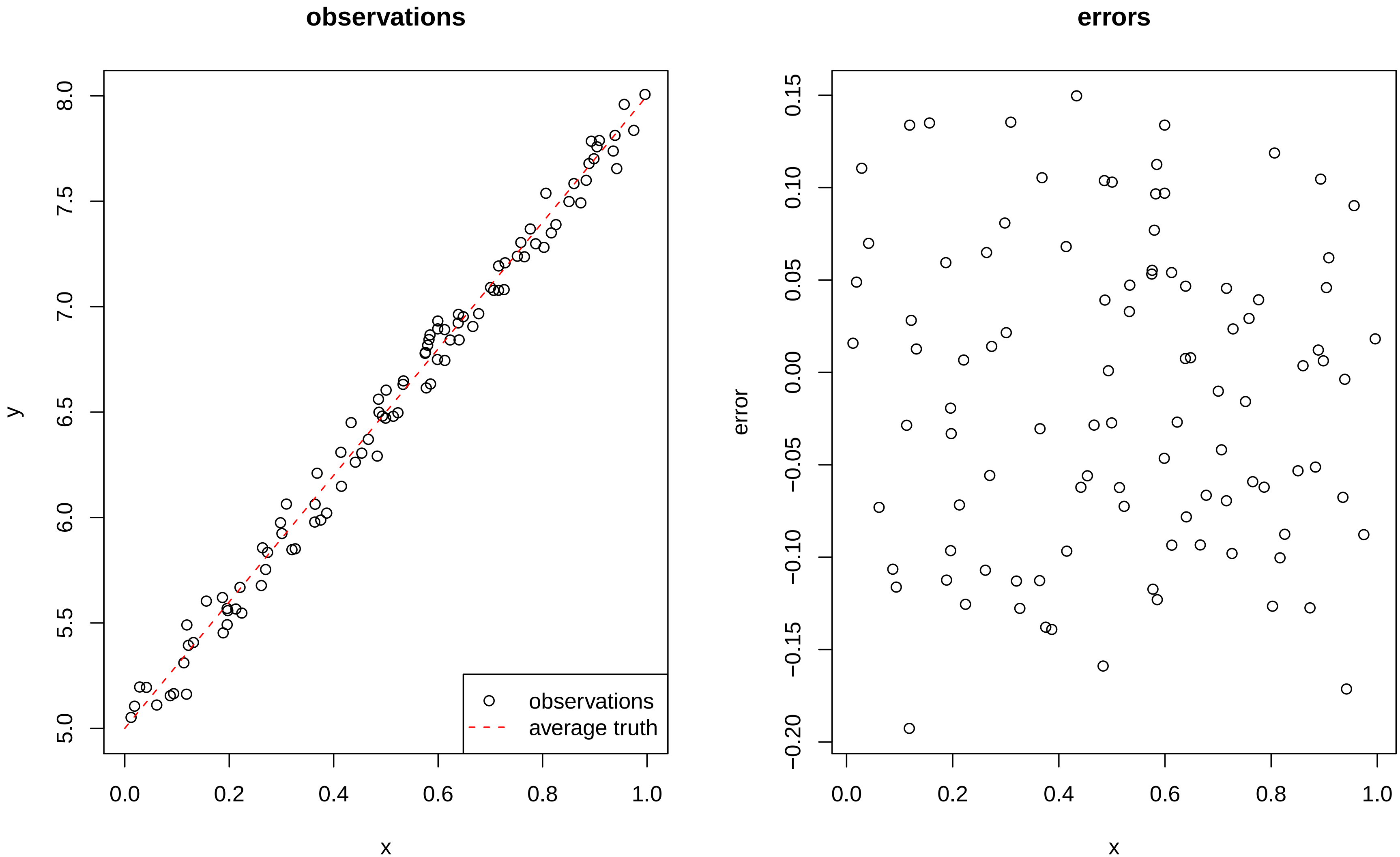
# Simple Examples: Distribution of Errors (2/2)



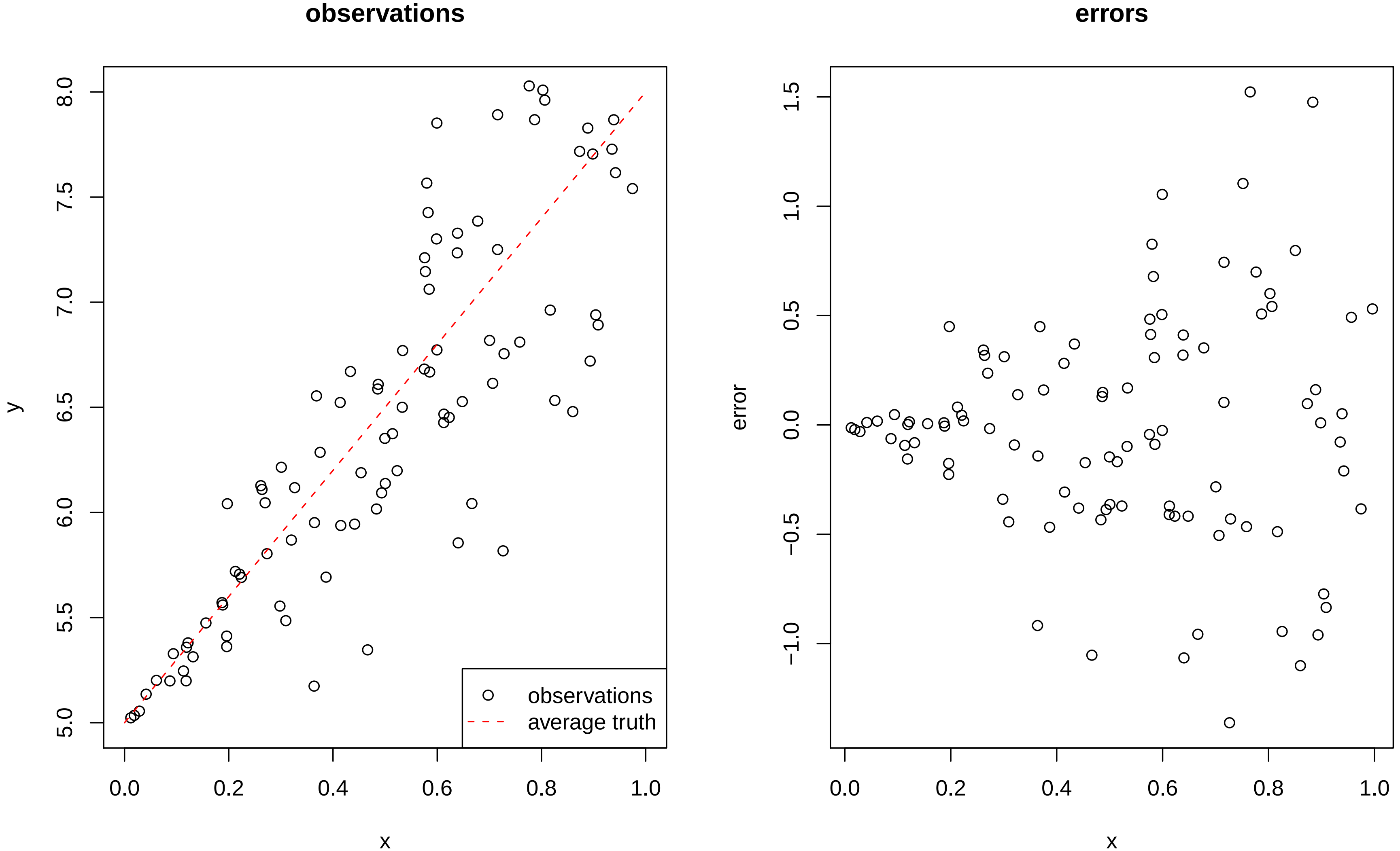

. . . uniformly distributed errors.

# Simple Examples: Homoscedastic vs. Heteroscedastic Errors (1/2)



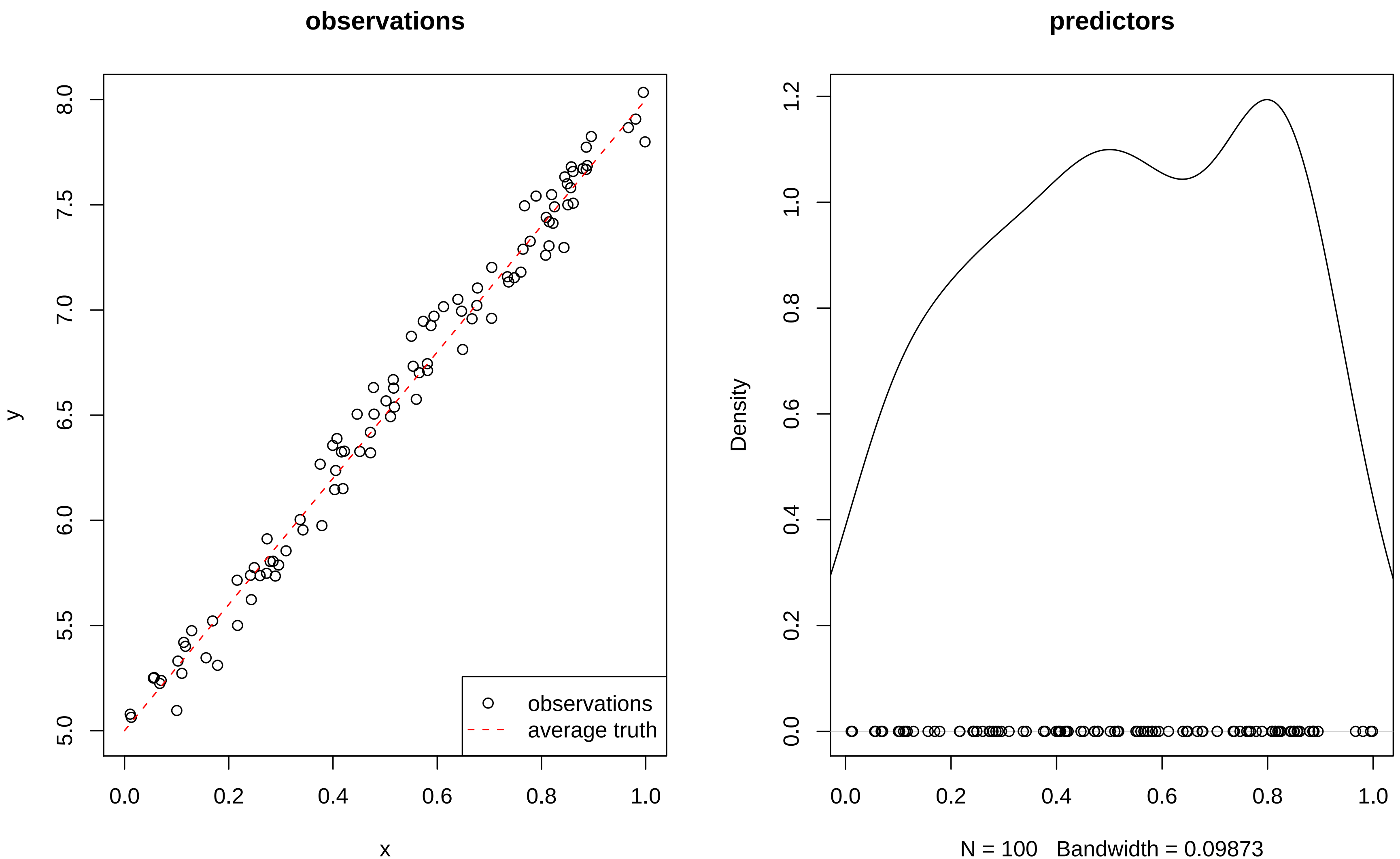

Errors do not depend on predictors (homoscedastic) vs. . . .

# Simple Examples: Homoscedastic vs. Heteroscedastic Errors (2/2)



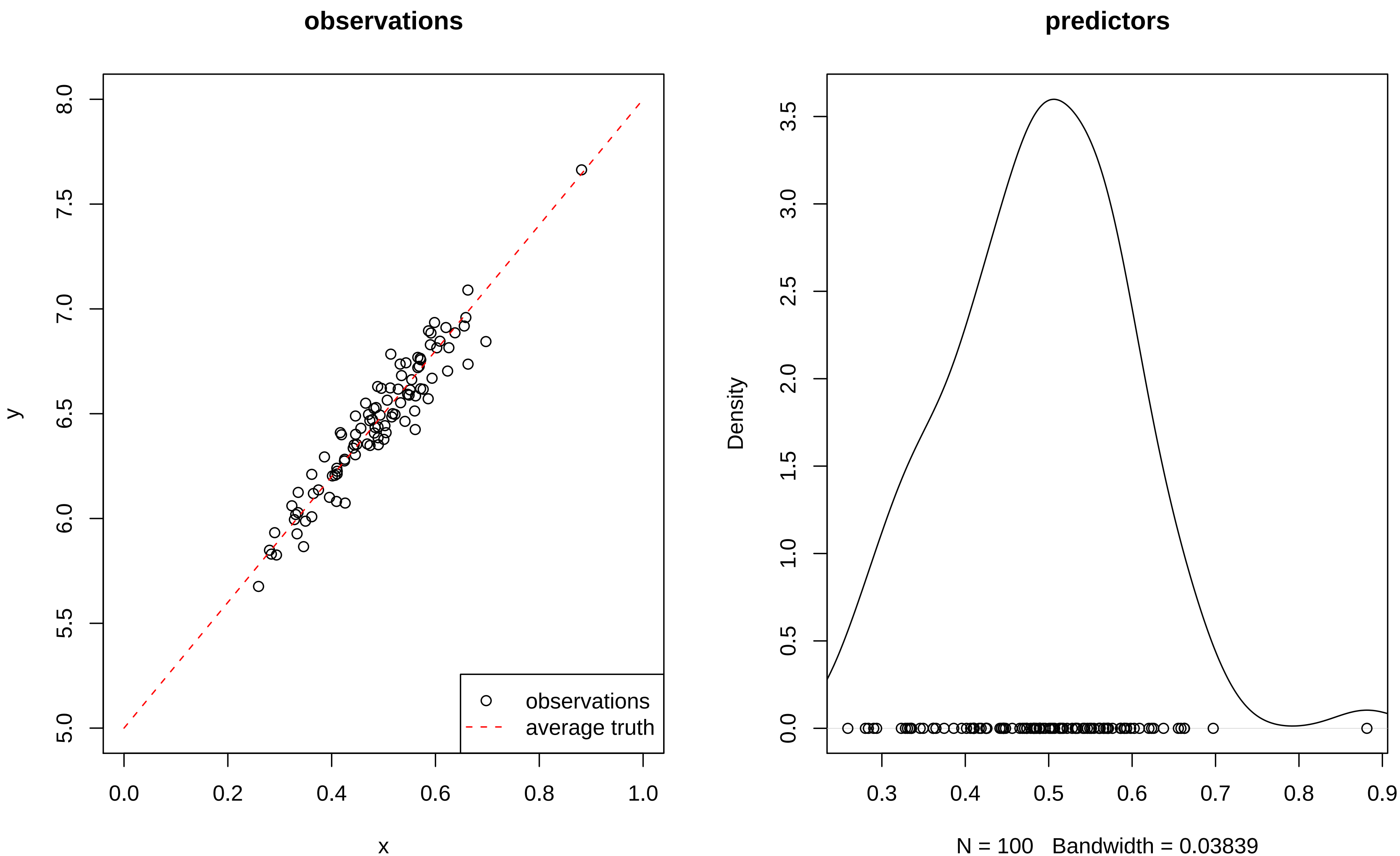

. . . errors do depend on predictors (heteroscedastic).

# Simple Examples: Distribution of Predictors (1/2)




Predictors are uniformly distributed vs. . . .

# Simple Examples: Distribution of Predictors (2/2)




. . . predictors are normally distributed.

## Simple Linear Regression Model

Make it simple:

- the predictor $X$ is simple, i.e., one-dimensional ($X = X_1$).
- $r(x)$ is assumed to be linear:

$$r(x) = \beta_0 + \beta_1 x$$

- assume that the variance does not depend on $X$:

$$Y = \beta_0 + \beta_1 X + \epsilon, \quad E(\epsilon|X) = 0, V(\epsilon|X) = \sigma^2$$

- 3 parameters:

  $\beta_0$ **intercept** (sometimes also called bias)
  $\beta_1$ **slope**
  $\sigma^2$ **variance**

# Simple Linear Regression Model

**parameter estimates**

$$\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2$$

**fitted line**

$$\hat{r}(x) := \hat{\beta}_0 + \hat{\beta}_1 x$$

**predicted / fitted values**

$$\hat{y}_i := \hat{r}(x_i)$$

**residuals**

$$\hat{\epsilon}_i := y_i - \hat{y}_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)$$

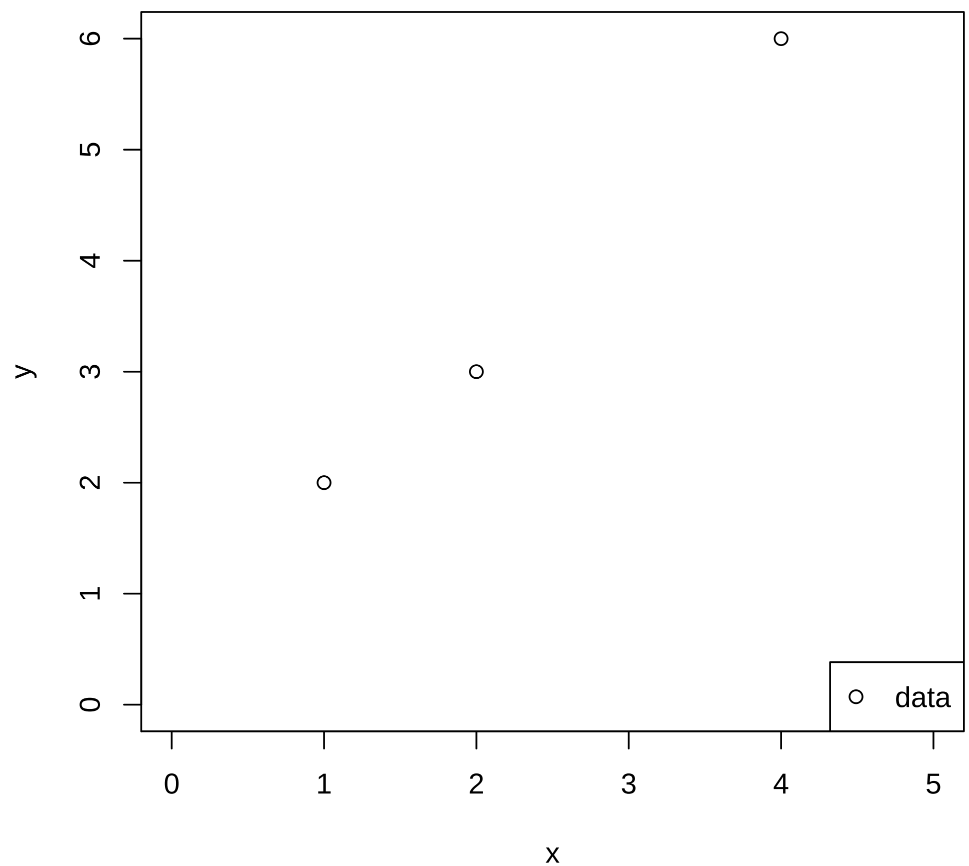
**residual sums of squares (RSS) / square loss / L2 loss**

$$\text{RSS} = \sum_{i=1}^{n} \hat{\epsilon}_i^2$$

# How to estimate the parameters?

Example:

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.



# How to estimate the parameters?

Example:

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.

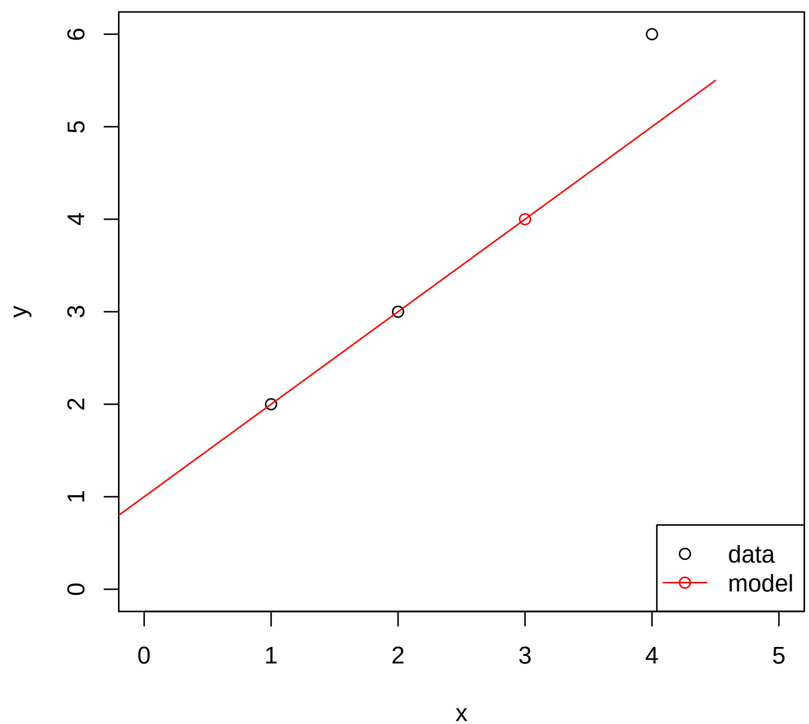
Line through first two points:

$$\hat{\beta}_1 = \frac{y_2 - y_1}{x_2 - x_1} = 1$$
$$\hat{\beta}_0 = y_1 - \hat{\beta}_1 x_1 = 1$$

RSS:

| $i$ | $y_i$ | $\hat{y}_i$ | $(y_i - \hat{y}_i)^2$ |
|---|---|---|---|
| 1 | 2 | 2 | 0 |
| 2 | 3 | 3 | 0 |
| 3 | 6 | 5 | 1 |
| $\sum$ | | | 1 |

$\hat{r}(3) = 4$



## How to estimate the parameters?

Example:

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.

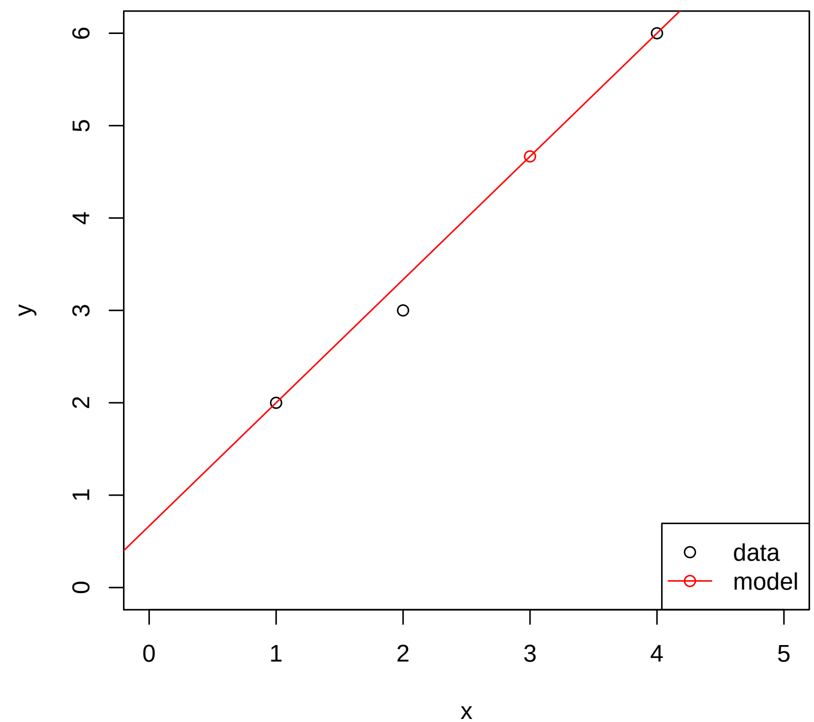
Line through first and last point:

$$\hat{\beta}_1 = \frac{y_3 - y_1}{x_3 - x_1} = 4/3 = 1.333$$
$$\hat{\beta}_0 = y_1 - \hat{\beta}_1 x_1 = 2/3 = 0.667$$

RSS:

| $i$ | $y_i$ | $\hat{y}_i$ | $(y_i - \hat{y}_i)^2$ |
|---|---|---|---|
| 1 | 2 | 2 | 0 |
| 2 | 3 | 3.333 | 0.111 |
| 3 | 6 | 6 | 0 |
| $\sum$ | | | 0.111 |

$\hat{r}(3) = 4.667$



## Least Squares Estimates / Definition

In principle, there are many different methods to estimate the parameters $\hat{\beta}_0, \hat{\beta}_1$ and $\hat{\sigma}^2$ from data — depending on the properties the solution should have.

The **least squares estimates** are those parameters that minimize

$$\text{RSS} = \sum_{i=1}^{n} \hat{\epsilon}_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$$

They can be written in closed form as follows:

$$\begin{aligned}
\hat{\beta}_1 &= \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \\
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
\hat{\sigma}^2 &= \frac{1}{n-2} \sum_{i=1}^{n} \hat{\epsilon}_i^2
\end{aligned}$$

# Least Squares Estimates / Proof

Proof (1/2):

$$\text{RSS} = \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2$$

$$\frac{\partial\, \text{RSS}}{\partial \hat{\beta}_0} = \sum_{i=1}^{n} 2(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))(-1) \stackrel{!}{=} 0$$

$$\Longrightarrow \quad n\hat{\beta}_0 = \sum_{i=1}^{n} (y_i - \hat{\beta}_1 x_i)$$

## Least Squares Estimates / Proof

Proof (2/2):

$$
\begin{aligned}
\text{RSS} &= \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2 \\
&= \sum_{i=1}^{n} (y_i - (\bar{y} - \hat{\beta}_1 \bar{x}) - \hat{\beta}_1 x_i)^2 \\
&= \sum_{i=1}^{n} (y_i - \bar{y} - \hat{\beta}_1 (x_i - \bar{x}))^2 \\
\frac{\partial\, \text{RSS}}{\partial \hat{\beta}_1} &= \sum_{i=1}^{n} 2(y_i - \bar{y} - \hat{\beta}_1 (x_i - \bar{x}))(-1)(x_i - \bar{x}) \stackrel{!}{=} 0 \\
\implies \quad \hat{\beta}_1 &= \frac{\sum_{i=1}^{n} (y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}
\end{aligned}
$$

## Least Squares Estimates / Example

Example:

Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.

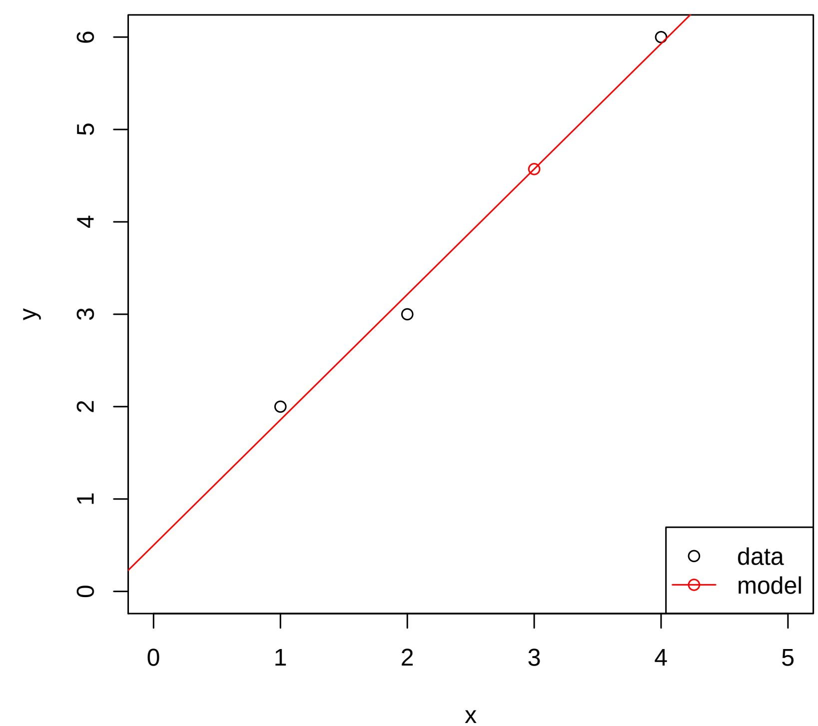
Assume simple linear model.

$\bar{x} = 7/3$, $\bar{y} = 11/3$.

| $i$ | $x_i - \bar{x}$ | $y_i - \bar{y}$ | $(x_i - \bar{x})^2$ | $(x_i - \bar{x})(y_i - \bar{y})$ |
|---|---|---|---|---|
| 1 | $-4/3$ | $-5/3$ | $16/9$ | $20/9$ |
| 2 | $-1/3$ | $-2/3$ | $1/9$ | $2/9$ |
| 3 | $5/3$ | $7/3$ | $25/9$ | $35/9$ |
| $\sum$ | | | $42/9$ | $57/9$ |

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = 57/42 = 1.357$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = \frac{11}{3} - \frac{57}{42} \cdot \frac{7}{3} = \frac{63}{126} = 0.5$$



## Least Squares Estimates / Example

Example:
Given the data $\mathcal{D} := \{(1,2),(2,3),(4,6)\}$, predict a value for $x = 3$.
Assume simple linear model.

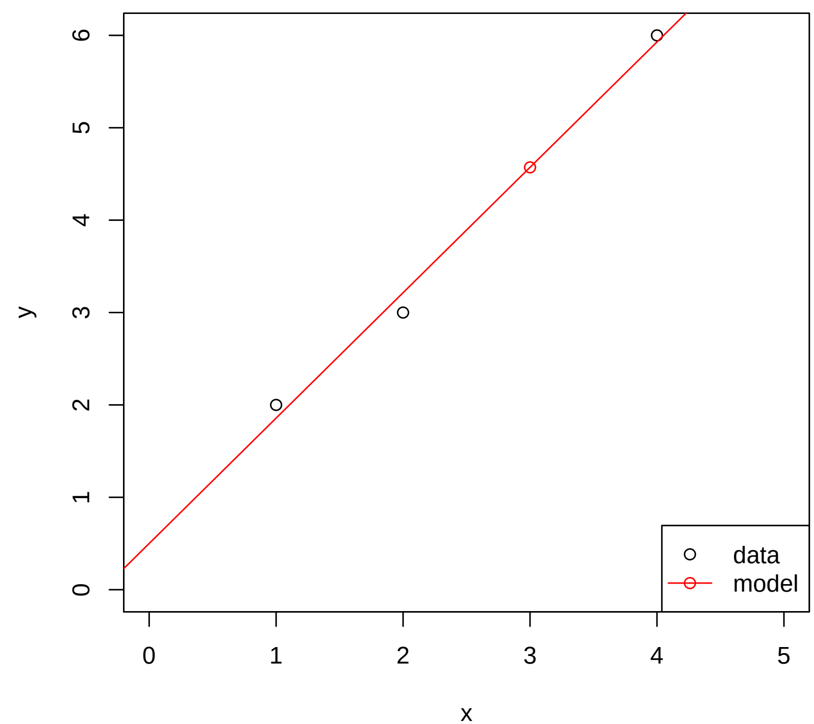
$$\hat\beta_1 = \frac{\sum_{i=1}^n (x_i - \bar x)(y_i - \bar y)}{\sum_{i=1}^n (x_i - \bar x)^2} = 57/42 = 1.357$$

$$\hat\beta_0 = \bar y - \hat\beta_1 \bar x = \frac{11}{3} - \frac{57}{42} \cdot \frac{7}{3} = \frac{63}{126} = 0.5$$

RSS:

| $i$ | $y_i$ | $\hat y_i$ | $(y_i - \hat y_i)^2$ |
|---|---|---|---|
| 1 | 2 | 1.857 | 0.020 |
| 2 | 3 | 3.214 | 0.046 |
| 3 | 6 | 5.929 | 0.005 |
| $\sum$ | | | 0.071 |

$\hat r(3) = 4.571$



# A Generative Model

So far we assumed the model

$$Y = \beta_0 + \beta_1 X + \epsilon, \quad E(\epsilon|X) = 0, V(\epsilon|X) = \sigma^2$$

where we required some properties of the errors,
but not its exact distribution.

If we make assumptions about its distribution, e.g.,

$$\epsilon|X \sim \mathcal{N}(0, \sigma^2)$$

and thus

$$Y|X = x \sim \mathcal{N}(\beta_0 + \beta_1 x, \sigma^2)$$

we can sample from this model.

## Maximum Likelihood Estimates (MLE)

Let $p(X, Y \mid \theta)$ be a joint probability density function for $X$ and $Y$ with parameters $\theta$.

Likelihood:

$$L_{\mathcal{D}}(\theta) := \prod_{i=1}^{n} p(x_i, y_i \mid \theta)$$

The likelihood describes the probability of the data.

The **maximum likelihood estimates (MLE)** are those parameters that maximize the likelihood.

# Least Squares Estimates and Maximum Likelihood Estimates

Likelihood:

$$L_{\mathcal{D}}(\hat\beta_0, \hat\beta_1, \hat\sigma^2) := \prod_{i=1}^n \hat p(x_i, y_i) = \prod_{i=1}^n \hat p(y_i \mid x_i) p(x_i) = \prod_{i=1}^n \hat p(y_i \mid x_i) \prod_{i=1}^n p(x_i)$$

Conditional likelihood:

$$L_{\mathcal{D}}^{\text{cond}}(\hat\beta_0, \hat\beta_1, \hat\sigma^2) := \prod_{i=1}^n \hat p(y_i \mid x_i) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\hat\sigma} e^{-\frac{(y_i-\hat y_i)^2}{2\hat\sigma^2}} = \frac{1}{\sqrt{2\pi}^n \hat\sigma^n} e^{\frac{1}{-2\hat\sigma^2}\sum_{i=1}^n (y_i-\hat y_i)^2}$$

Conditional log-likelihood:

$$\log L_{\mathcal{D}}^{\text{cond}}(\hat\beta_0, \hat\beta_1, \hat\sigma^2) \propto -n \log \hat\sigma - \frac{1}{2\hat\sigma^2} \sum_{i=1}^n (y_i - \hat y_i)^2$$

$\Longrightarrow$ if we assume normality, the maximum likelihood estimates are just the least squares estimates.

# Implementation Details

simple-regression$(\mathcal{D})$ :
$\text{sx} := 0, \text{sy} := 0$
**for** $i = 1, \ldots, n$ **do**
    $\text{sx} := \text{sx} + x_i$
    $\text{sy} := \text{sy} + y_i$
**od**
$\bar{x} := \text{sx}/n, \bar{y} := \text{sy}/n$
$a := 0, b := 0$
**for** $i = 1, \ldots, n$ **do**
    $a := a + (x_i - \bar{x})(y_i - \bar{y})$
    $b := b + (x_i - \bar{x})^2$
**od**
$\beta_1 := a/b$
$\beta_0 := \bar{y} - \beta_1 \bar{x}$
**return** $(\beta_0, \beta_1)$

# Implementation Details

## naive:

simple-regression($\mathcal{D}$) :
$\text{sx} := 0, \text{sy} := 0$
for $i = 1, \ldots, n$ do
  $\text{sx} := \text{sx} + x_i$
  $\text{sy} := \text{sy} + y_i$
od
$\bar{x} := \text{sx}/n, \bar{y} := \text{sy}/n$
$a := 0, b := 0$
for $i = 1, \ldots, n$ do
  $a := a + (x_i - \bar{x})(y_i - \bar{y})$
  $b := b + (x_i - \bar{x})^2$
od
$\beta_1 := a/b$
$\beta_0 := \bar{y} - \beta_1 \bar{x}$
return $(\beta_0, \beta_1)$

## single loop:

simple-regression($\mathcal{D}$) :
$\text{sx} := 0, \text{sy} := 0, \text{sxx} := 0, \text{syy} := 0, \text{sxy} := 0$
**for** $i = 1, \ldots, n$ **do**
  $\text{sx} := \text{sx} + x_i$
  $\text{sy} := \text{sy} + y_i$
  $\text{sxx} := \text{sxx} + x_i^2$
  $\text{syy} := \text{syy} + y_i^2$
  $\text{sxy} := \text{sxy} + x_i y_i$
**od**
$\beta_1 := (n \cdot \text{sxy} - \text{sx} \cdot \text{sy})/(n \cdot \text{sxx} - \text{sx} \cdot \text{sx})$
$\beta_0 := (\text{sy} - \beta_1 \cdot \text{sx})/n$
**return** $(\beta_0, \beta_1)$

## Summary

- Simple regression model: $\hat{y}(x) = \beta_0 + \beta_1 x$
- The best parameters with respect to minimal RSS are:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- Minimal RSS (least squares) corresponds to Maximum Likelihood assuming normal distributed error.

## Several predictors

Several predictor variables $X_1, X_2, \ldots, X_p$:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots \beta_P X_P + \epsilon$$
$$= \beta_0 + \sum_{i=1}^{p} \beta_i X_i + \epsilon$$

with $p+1$ parameters $\beta_0, \beta_1, \ldots, \beta_p$.

## Linear form

Several predictor variables $X_1, X_2, \ldots, X_p$:

$$\begin{aligned} Y =& \beta_0 + \sum_{i=1}^{p} \beta_i X_i + \epsilon \\ =& \langle \beta, X \rangle + \epsilon \end{aligned}$$

where

$$\beta := \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}, \quad X := \begin{pmatrix} 1 \\ X_1 \\ \vdots \\ X_p \end{pmatrix},$$

Thus, the intercept is handled like any other parameter, for the artificial constant variable $X_0 \equiv 1$.

## Simultaneous equations for the whole dataset

For the whole dataset $(x_1, y_1), \ldots, (x_n, y_n)$:

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

where

$$\mathbf{Y} := \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad \mathbf{X} := \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & \ldots & x_{1,p} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n,1} & x_{n,2} & \ldots & x_{n,p} \end{pmatrix}, \quad \epsilon := \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix},$$

## Least squares estimates

**Least squares estimates** $\hat{\beta}$ minimize

$$||\mathbf{Y} - \hat{\mathbf{Y}}||^2 = ||\mathbf{Y} - \mathbf{X}\hat{\beta}||^2$$

The least squares estimates $\hat{\beta}$ are computed via

$$\mathbf{X}^T\mathbf{X}\hat{\beta} = \mathbf{X}^T\mathbf{Y}$$

Proof:

$$||\mathbf{Y} - \mathbf{X}\hat{\beta}||^2 = \langle \mathbf{Y} - \mathbf{X}\hat{\beta}, \mathbf{Y} - \mathbf{X}\hat{\beta} \rangle$$

$$\frac{\partial(\ldots)}{\partial\hat{\beta}} = 2\langle -\mathbf{X}, \mathbf{Y} - \mathbf{X}\hat{\beta} \rangle = -2(\mathbf{X}^T\mathbf{Y} - \mathbf{X}^T\mathbf{X}\hat{\beta}) \stackrel{!}{=} 0$$

# How to compute least squares estimates $\hat{\beta}$

Solve the $p \times p$ system of linear equations

$$\mathbf{X}^T\mathbf{X}\hat{\beta} = \mathbf{X}^T\mathbf{Y}$$

i.e., $Ax = b$ (with $A := \mathbf{X}^T\mathbf{X}, b = \mathbf{X}^T\mathbf{Y}, x = \hat{\beta}$).

There are several numerical methods available:

1. Gaussian elimination

2. Cholesky decomposition

3. QR decomposition

## How to compute least squares estimates $\hat{\beta}$ / Example

Given is the following data:

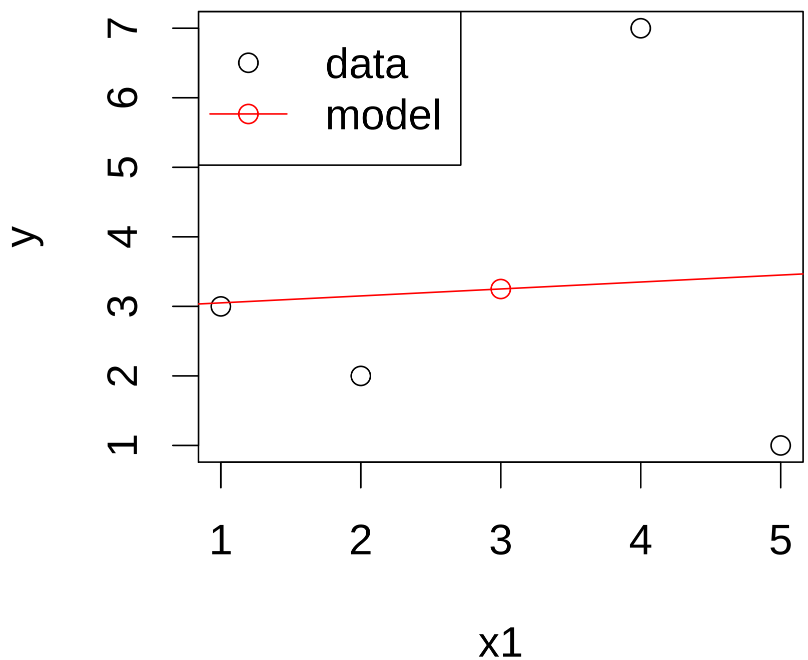
| $x_1$ | $x_2$ | $y$ |
|---|---|---|
| 1 | 2 | 3 |
| 2 | 3 | 2 |
| 4 | 1 | 7 |
| 5 | 5 | 1 |

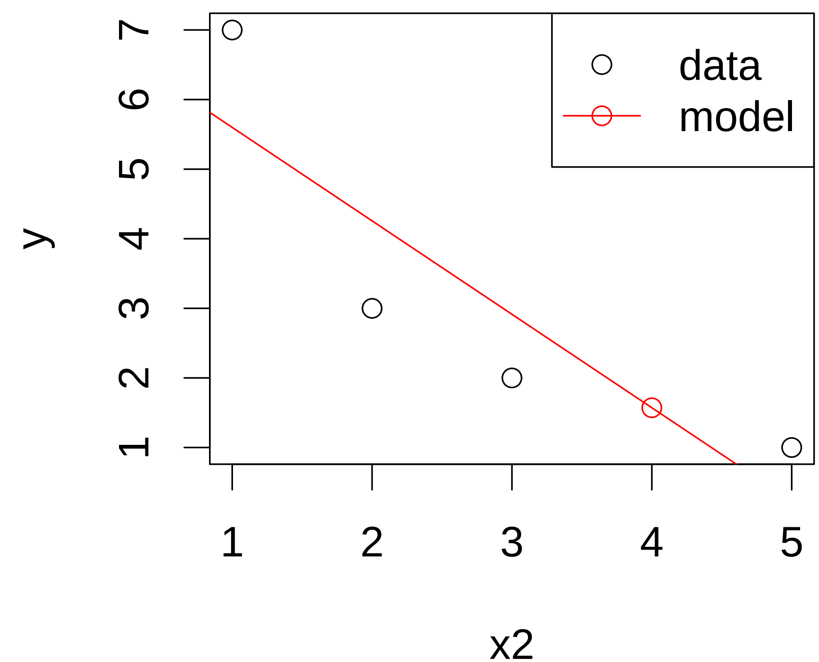
Predict a y value for $x_1 = 3, x_2 = 4$.

# How to compute least squares estimates $\hat{\beta}$ / Example

$$\begin{aligned} Y =& \beta_0 + \beta_1 X_1 + \epsilon \\ =& 2.95 + 0.1 X_1 + \epsilon \end{aligned}$$

$$\begin{aligned} Y =& \beta_0 + \beta_2 X_2 + \epsilon \\ =& 6.943 - 1.343 X_2 + \epsilon \end{aligned}$$




$$\hat{y}(x_1 = 3) = 3.25$$

$$\hat{y}(x_2 = 4) = 1.571$$

# How to compute least squares estimates $\hat{\beta}$ / Example

Now fit

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

to the data:

| $x_1$ | $x_2$ | $y$ |
|---|---|---|
| 1 | 2 | 3 |
| 2 | 3 | 2 |
| 4 | 1 | 7 |
| 5 | 5 | 1 |

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 3 \\ 1 & 4 & 1 \\ 1 & 5 & 5 \end{pmatrix}, \quad \mathbf{Y} = \begin{pmatrix} 3 \\ 2 \\ 7 \\ 1 \end{pmatrix}$$

$$\mathbf{X}^T\mathbf{X} = \begin{pmatrix} 4 & 12 & 11 \\ 12 & 46 & 37 \\ 11 & 37 & 39 \end{pmatrix}, \quad \mathbf{X}^T\mathbf{Y} = \begin{pmatrix} 13 \\ 40 \\ 24 \end{pmatrix}$$

## How to compute least squares estimates $\hat{\beta}$ / Example

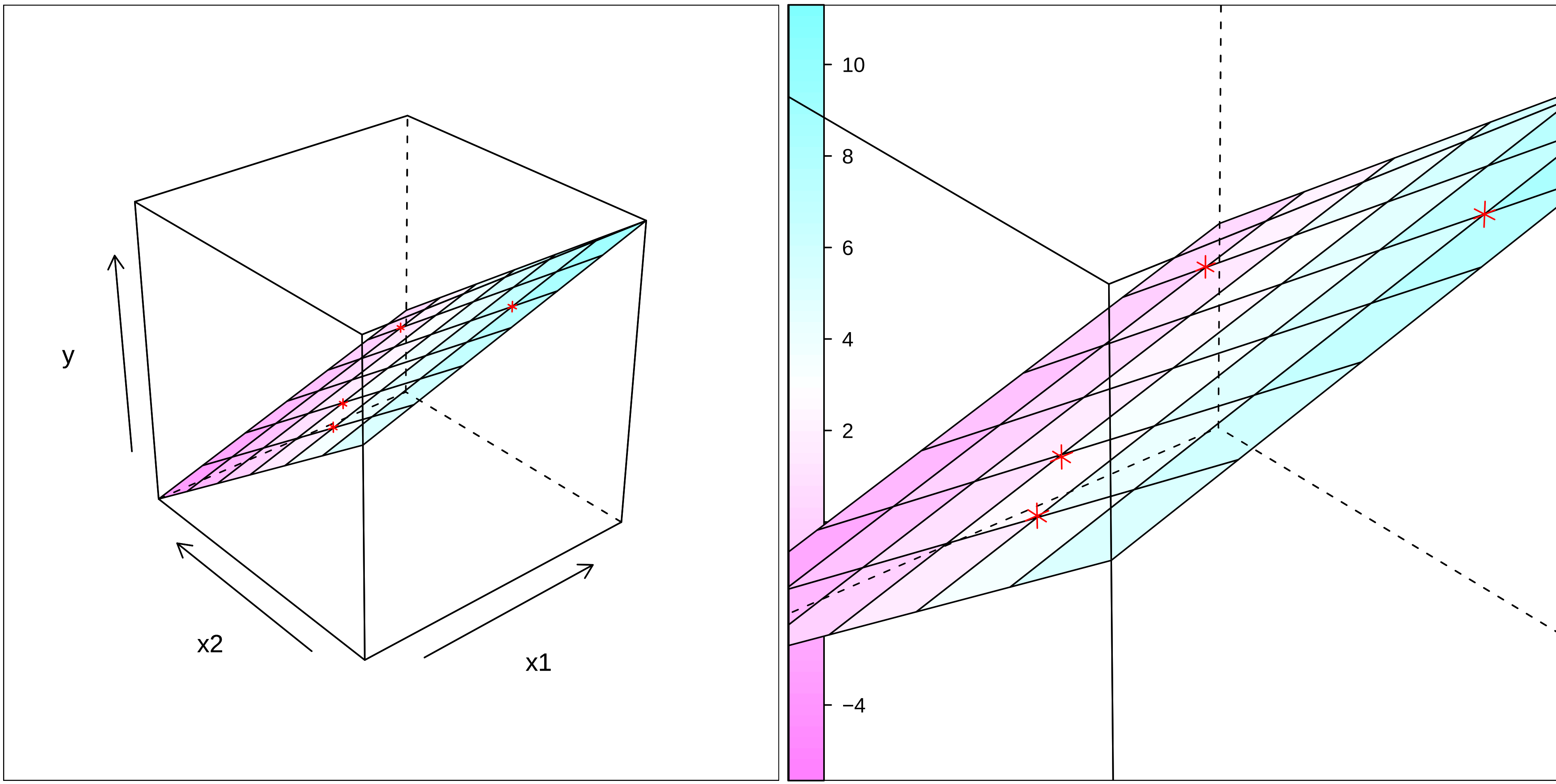
$$\left(\begin{array}{ccc|c} 4 & 12 & 11 & 13 \\ 12 & 46 & 37 & 40 \\ 11 & 37 & 39 & 24 \end{array}\right) \sim \left(\begin{array}{ccc|c} 4 & 12 & 11 & 13 \\ 0 & 10 & 4 & 1 \\ 0 & 16 & 35 & -47 \end{array}\right) \sim \left(\begin{array}{ccc|c} 4 & 12 & 11 & 13 \\ 0 & 10 & 4 & 1 \\ 0 & 0 & 143 & -243 \end{array}\right)$$

$$\sim \left(\begin{array}{ccc|c} 4 & 12 & 11 & 13 \\ 0 & 1430 & 0 & 1115 \\ 0 & 0 & 143 & -243 \end{array}\right) \sim \left(\begin{array}{ccc|c} 286 & 0 & 0 & 1597 \\ 0 & 1430 & 0 & 1115 \\ 0 & 0 & 143 & -243 \end{array}\right)$$

i.e.,

$$\hat{\beta} = \begin{pmatrix} 1597/286 \\ 1115/1430 \\ -243/143 \end{pmatrix} \approx \begin{pmatrix} 5.583 \\ 0.779 \\ -1.699 \end{pmatrix}$$

# How to compute least squares estimates $\hat{\beta}$ / Example

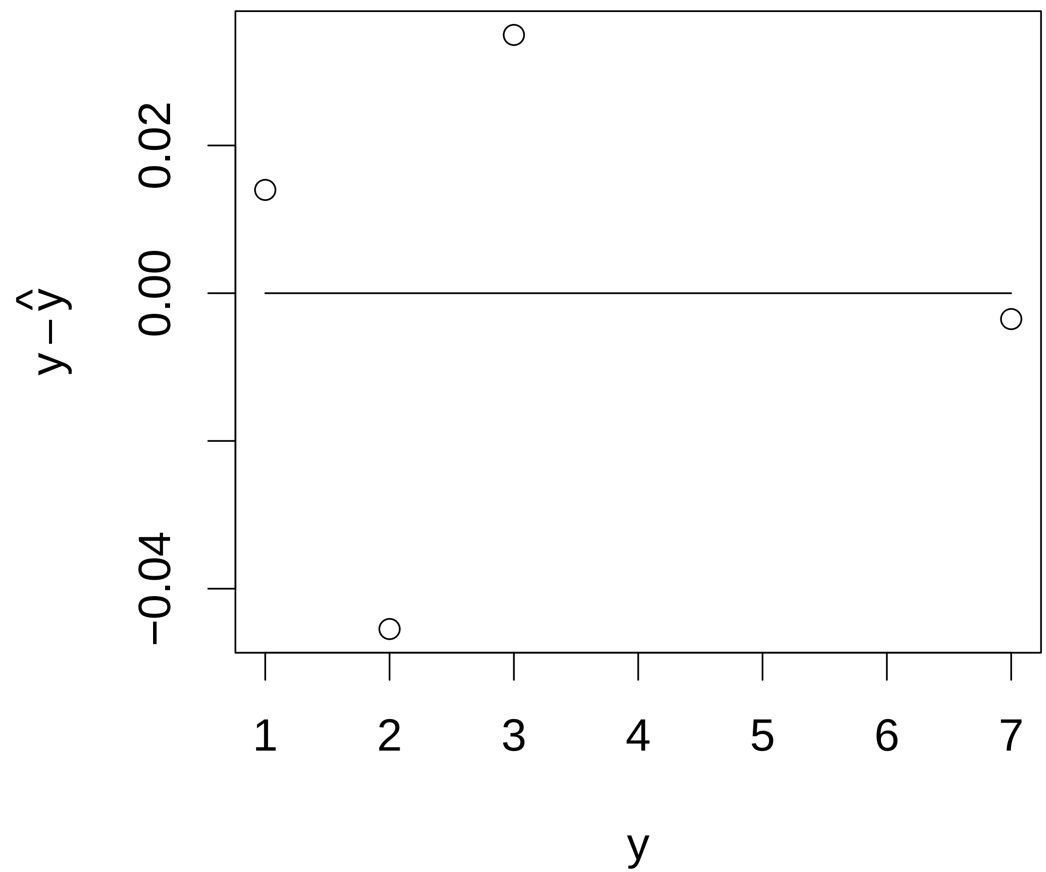


## How to compute least squares estimates $\hat{\beta}$ / Example

To visually assess the model fit, a plot

$$\text{residuals } \hat{\epsilon} = y - \hat{y} \text{ vs. true values } y$$

can be plotted:



# The Normal Distribution (also Gaussian)

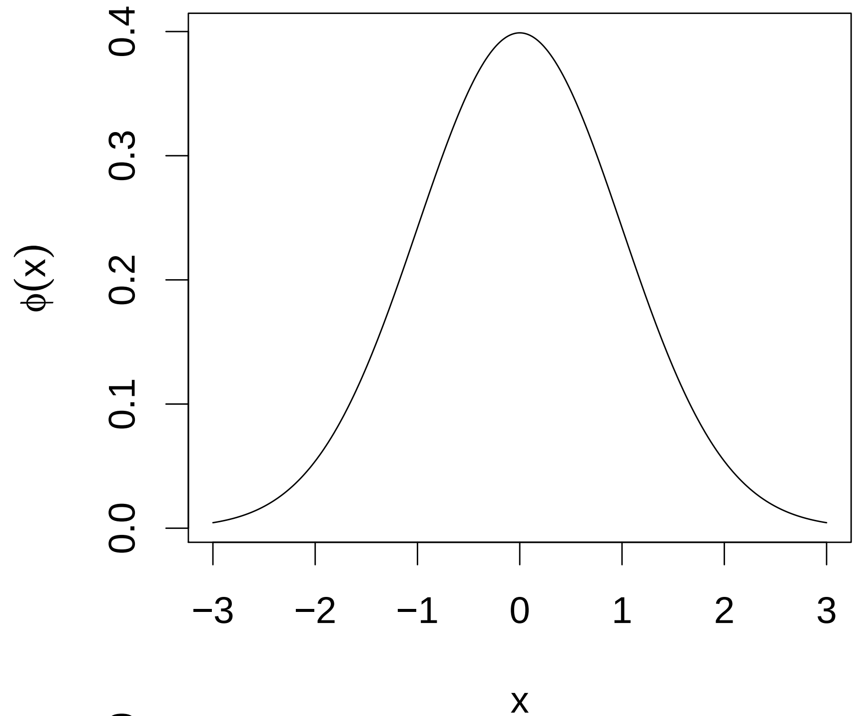
written as:

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

with parameters:
$\mu$ mean,
$\sigma$ standard deviance.

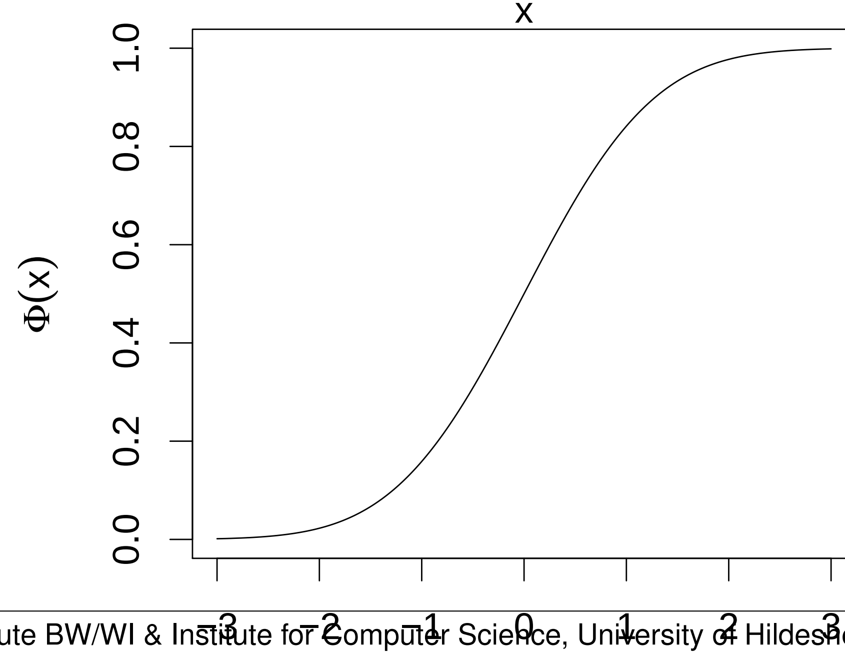
**probability density function (pdf)**:

$$\phi(x) := \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$




**cumulative distribution function (cdf)**:

$$\Phi(x) := \int_{-\infty}^{x} \phi(t)dt$$




$\Phi^{-1}$ is called **quantile function**.

$\Phi$ and $\Phi^{-1}$ have no analytical form, but have to be computed numerically.

# The $t$ Distribution

written as:

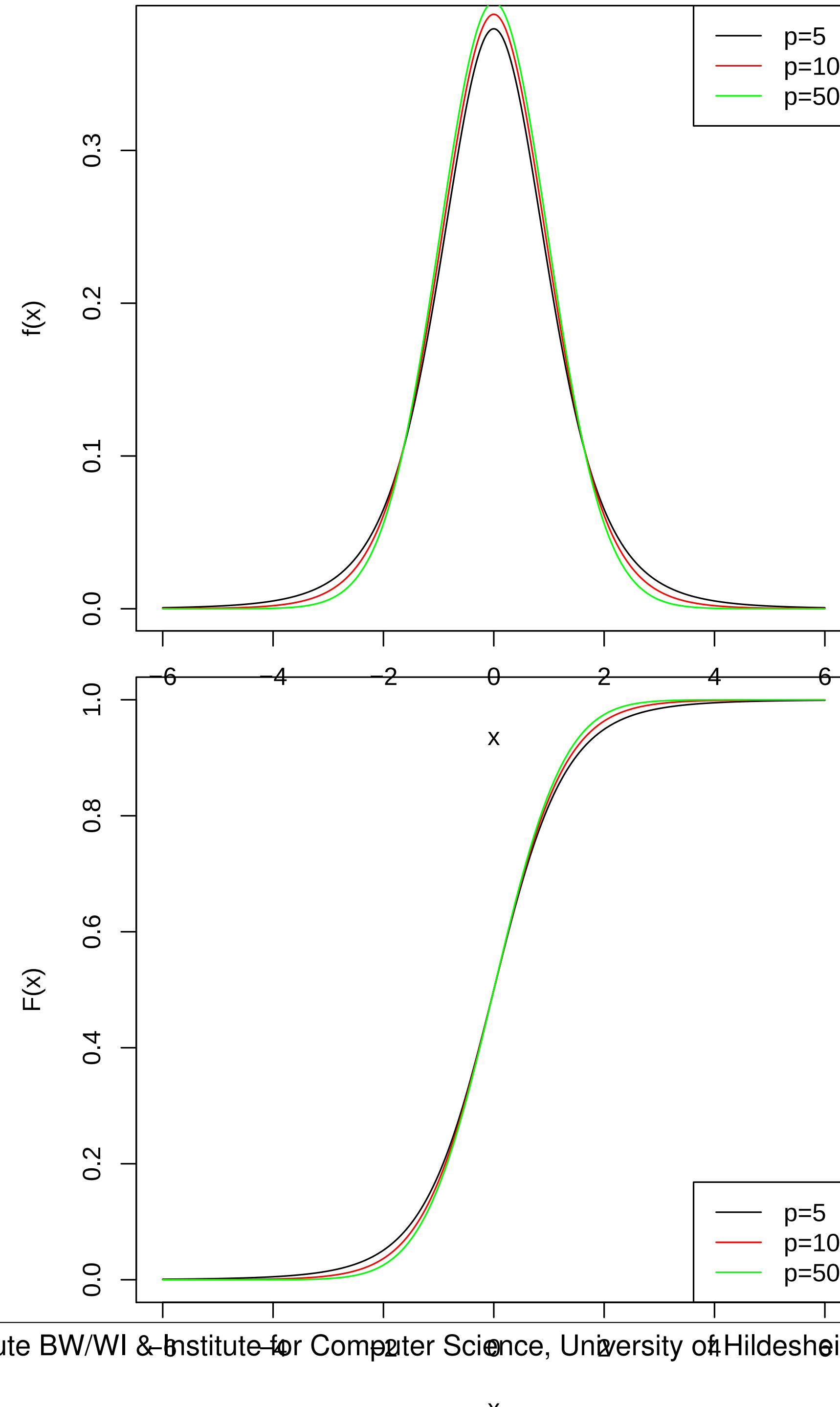
$$X \sim t_p$$

with parameter:
$p$ degrees of freedom.

**probability density function (pdf)**:

$$p(x) := \frac{\Gamma(\frac{p+1}{2})}{\sqrt{p\,\pi}\,\Gamma(\frac{p}{2})}(1+\frac{x^2}{p})^{-\frac{p+1}{2}}$$

$$t_p \xrightarrow{p\to\infty} \mathcal{N}(0,1)$$



# The $\chi^2$ Distribution

written as:

$$X \sim \chi^2_p$$

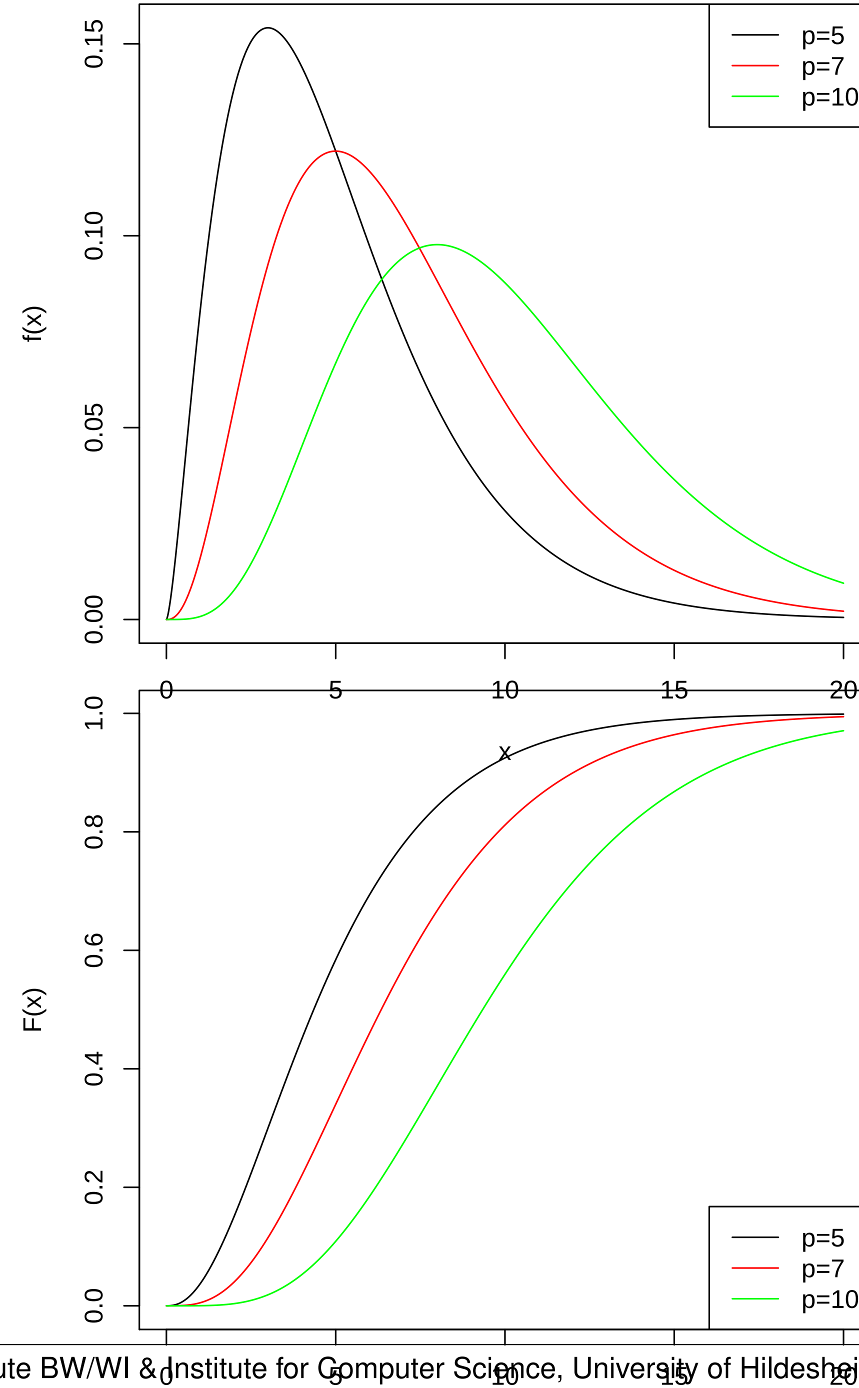
with parameter:
$p$ degrees of freedom.

**probability density function (pdf)**:

$$p(x) := \frac{1}{\Gamma(p/2)2^{p/2}} x^{\frac{p}{2}-1} e^{-\frac{x}{2}}, \quad x \geq 0$$

If $X_1, \ldots, X_p \sim \mathcal{N}(0,1)$, then

$$Y := \sum_{i=1}^{p} X_i^2 \sim \chi^2_p$$



# Parameter Variance

$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ is an unbiased estimator for $\beta$ (i.e., $E(\hat{\beta}) = \beta$).
Its variance is

$$V(\hat{\beta}) = (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2$$

proof:

$$\hat{\beta} =(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}\beta + \epsilon) = \beta + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

As $E(\epsilon) = 0$: $E(\hat{\beta}) = \beta$

$$\begin{aligned} V(\hat{\beta}) =& E((\hat{\beta} - E(\hat{\beta}))(\hat{\beta} - E(\hat{\beta}))^T) \\ =& E((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon\epsilon^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}) \\ =& (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2 \end{aligned}$$

## Parameter Variance

An unbiased estimator for $\sigma^2$ is

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

If $\epsilon \sim \mathcal{N}(0, \sigma^2)$, then

$$\hat{\beta} \sim \mathcal{N}(\beta, (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2)$$

Furthermore

$$(n-p)\hat{\sigma}^2 \sim \sigma^2\chi^2_{n-p}$$

## Parameter Variance / Standardized coefficient

standardized coefficient ("z-score"):

$$z_i := \frac{\hat{\beta}_i}{\widehat{\text{se}}(\hat{\beta}_i)}, \quad \text{with } \widehat{\text{se}}^2(\hat{\beta}_i) \text{ the } i\text{-th diagonal element of } (\mathbf{X}^T\mathbf{X})^{-1}\hat{\sigma}^2$$

$z_i$ would be $z_i \sim \mathcal{N}(0,1)$ if $\sigma$ is known (under $H_0 : \beta_i = 0$).
With estimated $\hat{\sigma}$ it is $z_i \sim t_{n-p}$.

The Wald test for $H_0 : \beta_i = 0$ with size $\alpha$ is:

$$\text{reject } H_0 \text{ if } |z_i| = |\frac{\hat{\beta}_i}{\widehat{\text{se}}(\hat{\beta}_i)}| > F^{-1}_{t_{n-p}}(1 - \frac{\alpha}{2})$$

i.e., its $p$-value is

$$p\text{-value}(H_0 : \beta_i = 0) = 2(1 - F_{t_{n-p}}(|z_i|)) = 2(1 - F_{t_{n-p}}(|\frac{\hat{\beta}_i}{\widehat{\text{se}}(\hat{\beta}_i)}|))$$

and small $p$-values such as $0.01$ and $0.05$ are good.

## Parameter Variance / Confidence interval

The $1 - \alpha$ confidence interval for $\beta_i$:

$$\beta_i \pm F_{t_{n-p}}^{-1}(1 - \frac{\alpha}{2})\widehat{\mathsf{se}}(\hat{\beta}_i)$$

For large $n$, $F_{t_{n-p}}$ converges to the standard normal cdf $\Phi$.

As $\Phi^{-1}(1 - \frac{0.05}{2}) \approx 1.95996 \approx 2$, the rule-of-thumb for a 5% confidence interval is

$$\beta_i \pm 2\widehat{\mathsf{se}}(\hat{\beta}_i)$$

## Parameter Variance / Example

We have already fitted

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2$$
$$= 5.583 + 0.779 X_1 - 1.699 X_2$$

to the data:

| $x_1$ | $x_2$ | $y$ | $\hat{y}$ | $\hat{\epsilon}^2 = (y-\hat{y})^2$ |
|---|---|---|---|---|
| 1 | 2 | 3 | 2.965 | 0.00122 |
| 2 | 3 | 2 | 2.045 | 0.00207 |
| 4 | 1 | 7 | 7.003 | 0.0000122 |
| 5 | 5 | 1 | 0.986 | 0.000196 |
| RSS | | | | 0.00350 |

$$\hat{\sigma}^2 = \frac{1}{n-p}\sum_{i=1}^{n} \hat{\epsilon}_i^2 = \frac{1}{4-3} 0.00350 = 0.00350$$

$$(X^T X)^{-1}\hat{\sigma}^2 = \begin{pmatrix} 0.00520 & -0.00075 & -0.00076 \\ -0.00075 & 0.00043 & -0.00020 \\ -0.00076 & -0.00020 & 0.00049 \end{pmatrix}$$

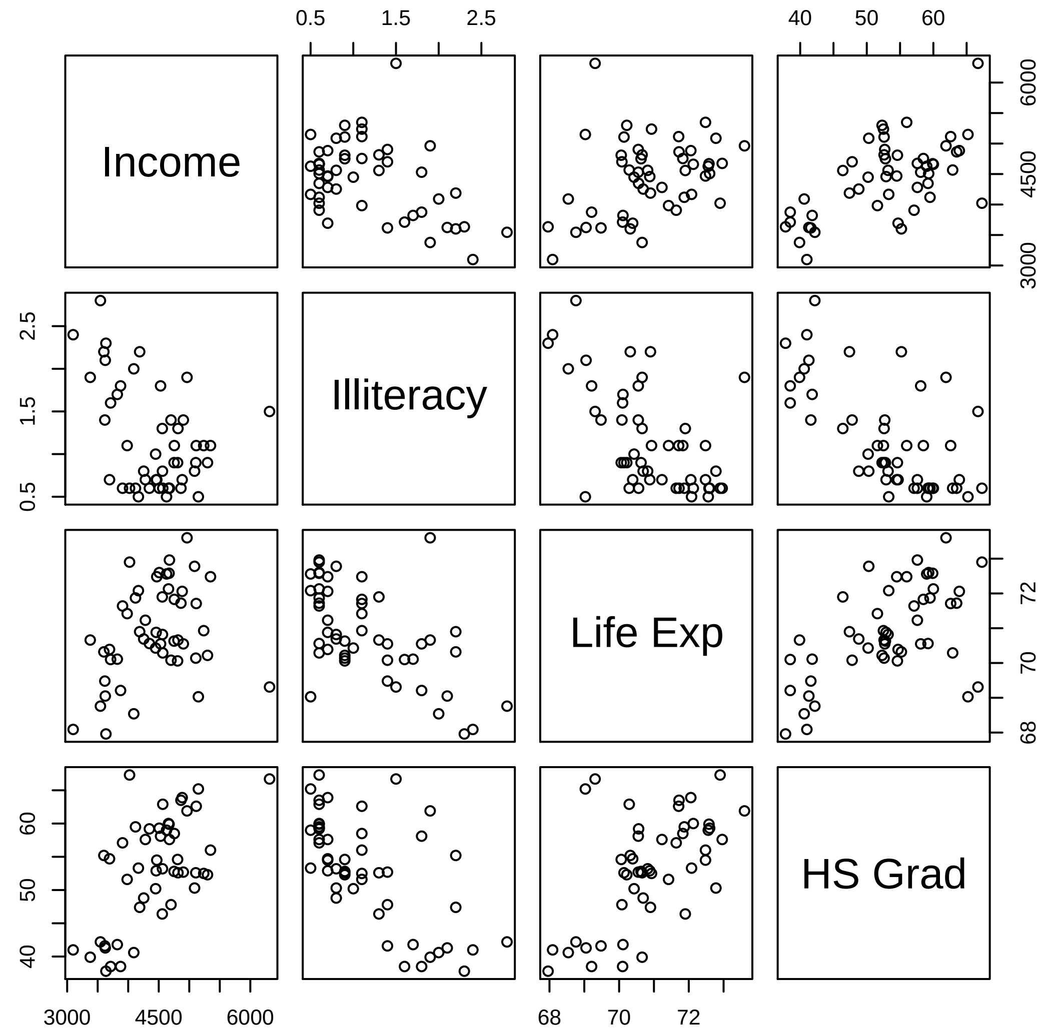
| covariate | $\hat{\beta}_i$ | $\widehat{\text{se}}(\hat{\beta}_i)$ | z-score | p-value |
|---|---|---|---|---|
| (intercept) | 5.583 | 0.0721 | 77.5 | 0.0082 |
| $X_1$ | 0.779 | 0.0207 | 37.7 | 0.0169 |
| $X_2$ | −1.699 | 0.0221 | −76.8 | 0.0083 |

# Parameter Variance / Example 2

Example: sociographic data of the 50 US states in 1977.

state dataset:

- income (per capita, 1974),
- illiteracy (percent of population, 1970),
- life expectancy (in years, 1969–71),
- percent high-school graduates (1970).
- population (July 1, 1975)
- murder rate per 100,000 population (1976)
- mean number of days with minimum temperature below freezing (1931–1960) in capital or large city
- land area in square miles



## Parameter Variance / Example 2

$$\begin{aligned}\text{Murder} =& \beta_0 + \beta_1 \text{Population} + \beta_2 \text{Income} + \beta_3 \text{Illiteracy} \\ &+ \beta_4 \text{LifeExp} + \beta_5 \text{HSGrad} + \beta_6 \text{Frost} + \beta_7 \text{Area}\end{aligned}$$

$n = 50$ states, $p = 8$ parameters, $n - p = 42$ degrees of freedom.

Least squares estimators:

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.222e+02  1.789e+01   6.831 2.54e-08 ***
Population   1.880e-04  6.474e-05   2.905  0.00584 **
Income      -1.592e-04  5.725e-04  -0.278  0.78232
Illiteracy   1.373e+00  8.322e-01   1.650  0.10641
`Life Exp`  -1.655e+00  2.562e-01  -6.459 8.68e-08 ***
`HS Grad`    3.234e-02  5.725e-02   0.565  0.57519
Frost       -1.288e-02  7.392e-03  -1.743  0.08867 .
Area         5.967e-06  3.801e-06   1.570  0.12391
```

## Summary

- Regression model: $\hat{\mathbf{Y}} = \mathbf{X}\,\beta$
- The best parameters with respect to minimal least square is the solution of the following system of linear equations:

$$\mathbf{X}^{\mathbf{T}}\,\mathbf{X}\,\beta = \mathbf{X}^{\mathbf{T}}\,\mathbf{Y}$$

- With the variance $\sigma_i$ we can test if a parameter $\beta_i$ is meaningful.

# Need for higher orders

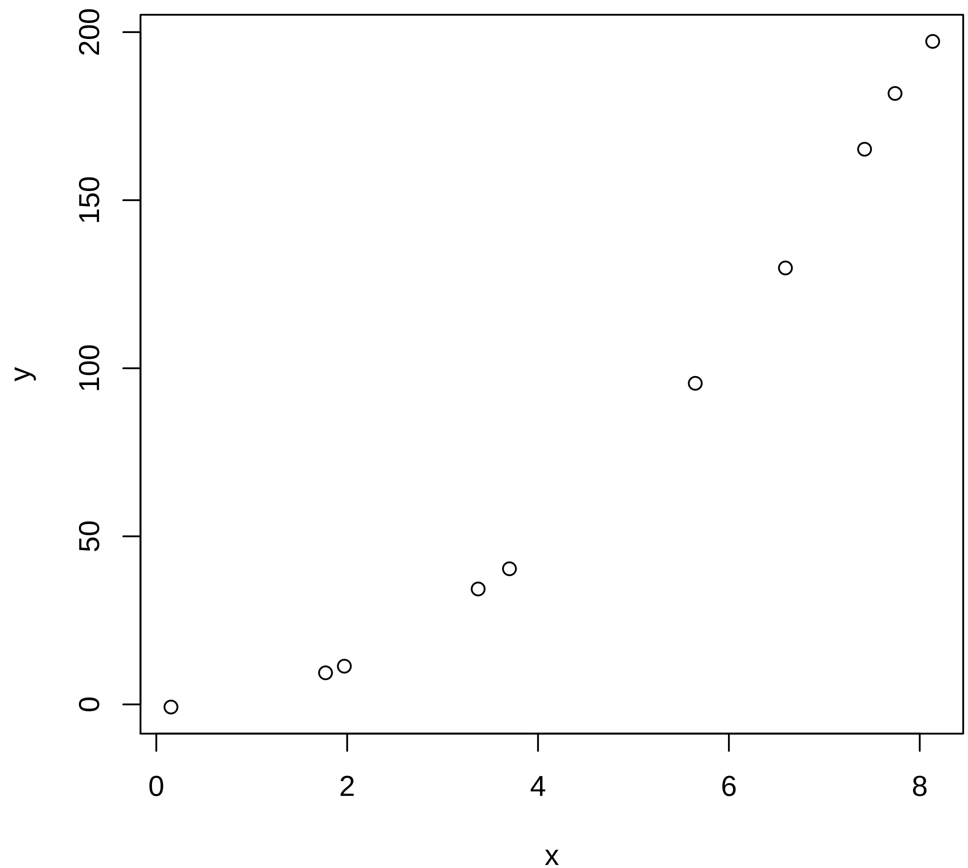
Assume a target variable does not depend linearly on a predictor variable, but say quadratic.

Example: way length vs. duration of a moving object with constant acceleration $a$.

$$s(t) = \frac{1}{2}at^2 + \epsilon$$

Can we catch such a dependency?

Can we catch it with a linear model?



## Need for general transformations

To describe many phenomena, even more complex functions of the input variables are needed.

Example: the number of cells $n$ vs. duration of growth $t$:

$$n = \beta e^{\alpha t} + \epsilon$$

$n$ does not depend on $t$ directly, but on $e^{\alpha t}$ (with a known $\alpha$).

## Need for variable interactions

In a linear model with two predictors

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

$Y$ depends on both, $X_1$ and $X_2$.

But changes in $X_1$ will affect $Y$ the same way, regardless of $X_2$.

There are problems where $X_2$ mediates or influences the way $X_1$ affects $Y$, e.g. : the way length $s$ of a moving object vs. its constant velocity $v$ and duration $t$:

$$s = vt + \epsilon$$

Then an additional $1s$ duration will increase the way length not in a uniform way (regardless of the velocity), but a little for small velocities and a lot for large velocities.

$v$ and $t$ are said to interact: $y$ does not depend only on each predictor separately, but also on their product.

## Derived variables

All these cases can be handled by looking at **derived variables**, i.e., instead of

$$
\begin{aligned}
Y =& \beta_0 + \beta_1 X_1^2 + \epsilon \\
Y =& \beta_0 + \beta_1 e^{\alpha X_1} + \epsilon \\
Y =& \beta_0 + \beta_1 X_1 \cdot X_2 + \epsilon
\end{aligned}
$$

one looks at

$$Y = \beta_0 + \beta_1 X_1' + \epsilon$$

with

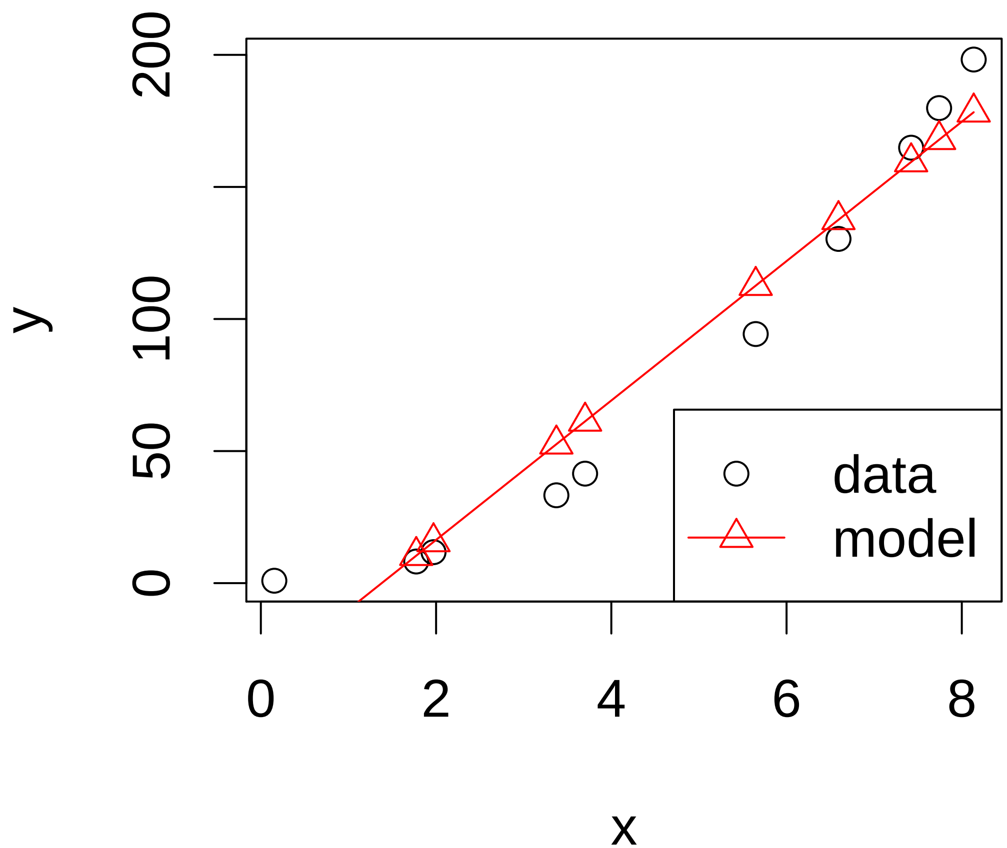
$$
\begin{aligned}
X_1' :=& X_1^2 \\
X_1' :=& e^{\alpha X_1} \\
X_1' :=& X_1 \cdot X_2
\end{aligned}
$$

Derived variables are computed before the fitting process and taken into account either additional to the original variables or instead of.

## Summary

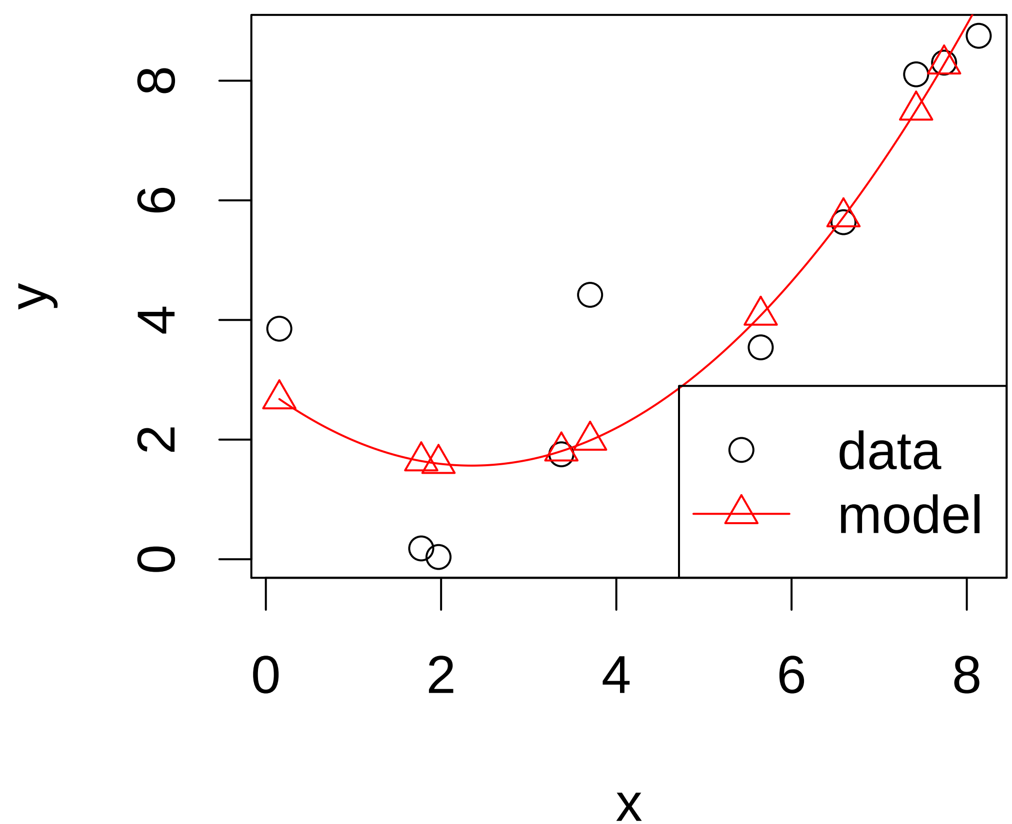
- By deriving new variables (e.g. squares, exponentials, interactions) more complex problems can be solved.
- On the new dataset (with derived variables), standard linear regression can be applied.
- The solution is linear in the derived variables but nonlinear in the original variables.

# Underfitting

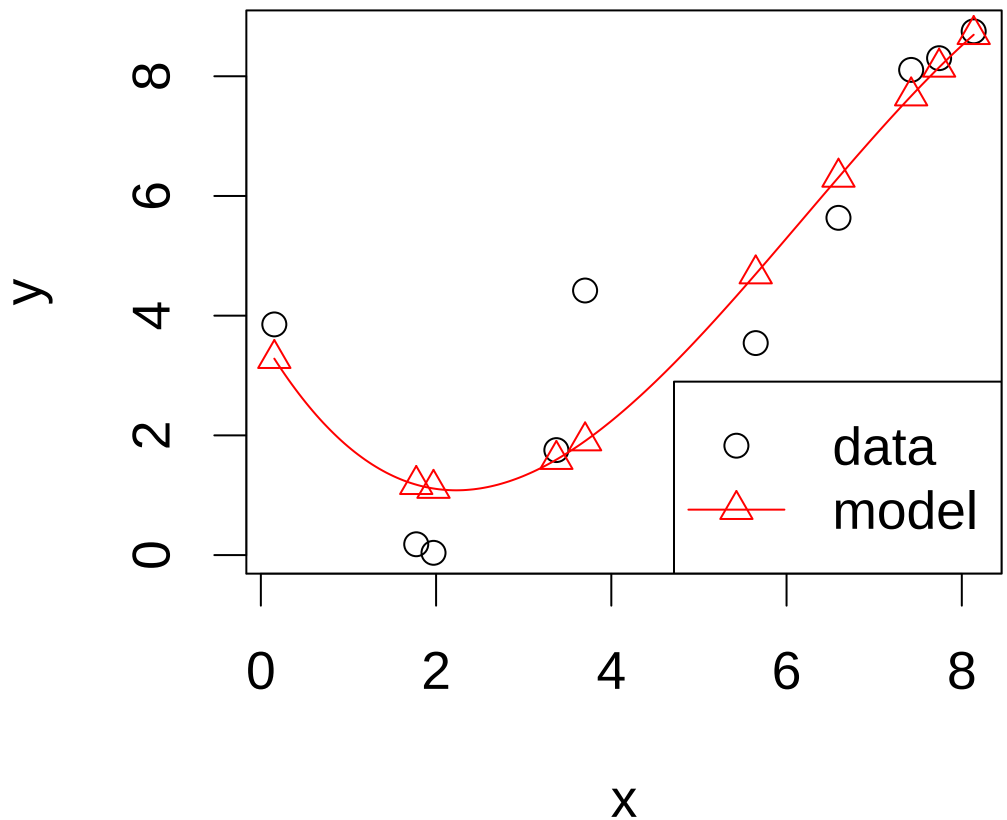



If a model does not well explain the data,
e.g., if the true model is quadratic, but we try to fit a linear model,
one says, the model **underfits**.

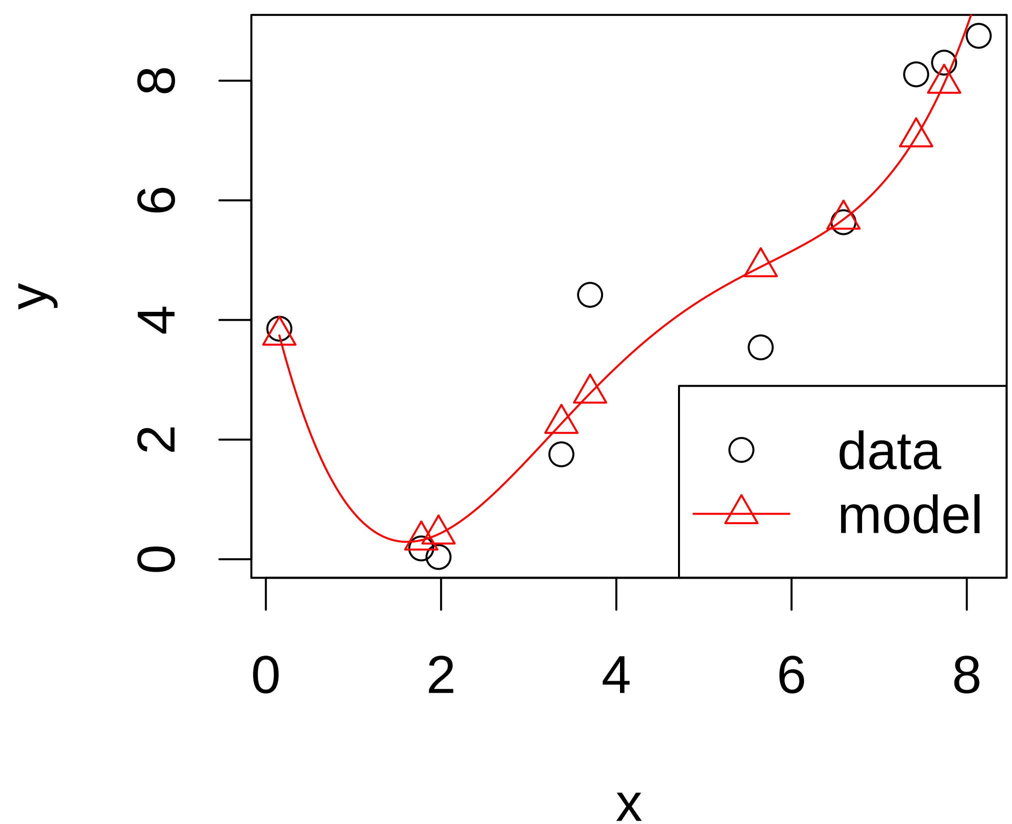
# Overfitting / Fitting Polynomials of High Degree



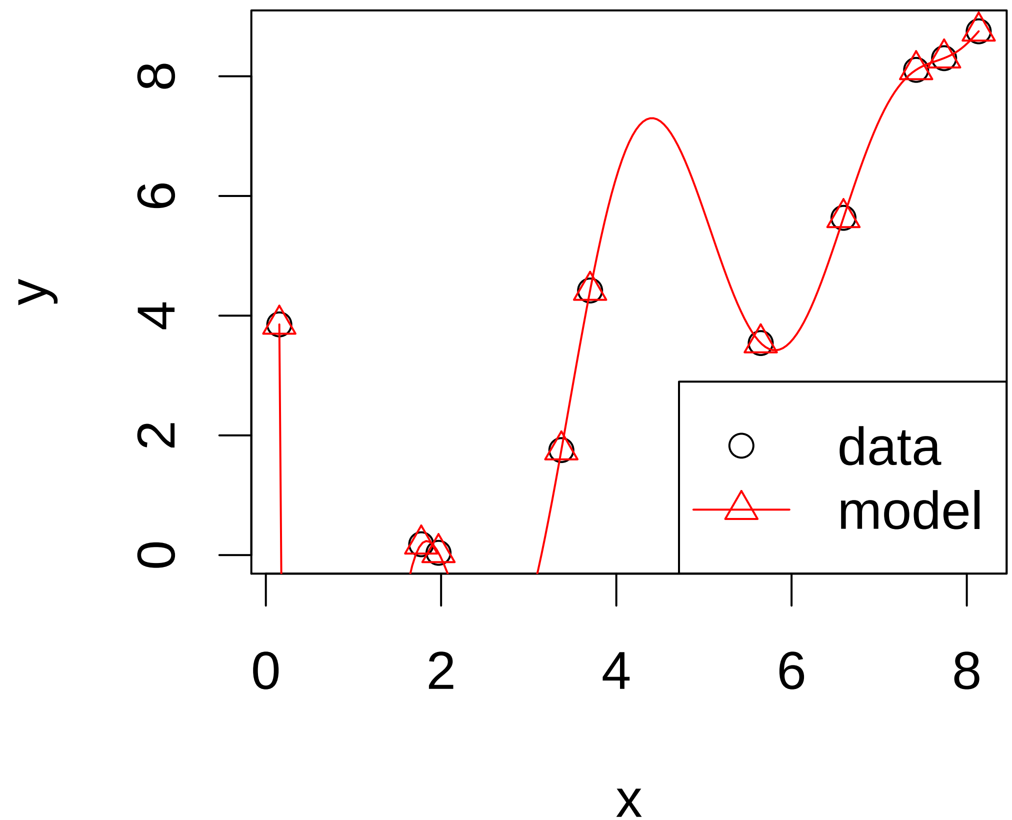
# Overfitting / Fitting Polynomials of High Degree



## Overfitting / Fitting Polynomials of High Degree



## Overfitting / Fitting Polynomials of High Degree



## Overfitting / Fitting Polynomials of High Degree

If to data

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

consisting of $n$ points we fit

$$X = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{n-1} X_{n-1}$$

i.e., a polynomial with degree $n-1$, then this results in an interpolation of the data points
(if there are no repeated measurements, i.e., points with the same $X_1$.)

As the polynomial

$$r(X) = \sum_{i=1}^{n} y_i \prod_{j \neq i} \frac{X - x_j}{x_i - x_j}$$

is of this type, and has minimal RSS $= 0$.

## Model Selection Measures

Model selection means: we have a set of models, e.g.,

$$Y = \sum_{i=0}^{p-1} \beta_i X_i$$

indexed by $p$ (i.e., one model for each value of $p$),
make a choice which model **describes** the data best.

If we just look at **losses** / **fit measures** such as RSS, then

the larger $p$, the better the fit

or equivalently

the larger $p$, the lower the loss

as the model with $p$ parameters can be **reparametrized** in a model with $p' > p$ parameters by setting

$$\beta'_i = \begin{cases} \beta_i, & \text{for } i \leq p \\ 0, & \text{for } i > p \end{cases}$$

## Model Selection Measures

One uses **model selection measures** of type

$$\text{model selection measure} = \text{fit} - \text{complexity}$$

or equivalently

$$\text{model selection measure} = \text{loss} + \text{complexity}$$

The smaller the loss (= lack of fit), the better the model.

The smaller the complexity, the simpler and thus better the model.

The model selection measure tries to find a trade-off between fit/loss and complexity.

# Model Selection Measures

**Akaike Information Criterion (AIC):** (maximize)

$$\text{AIC} := \log L - p$$

or (minimize)

$$\text{AIC} := -2 \log L + 2p = -2n \log(\text{RSS}/n) + 2p$$

**Bayes Information Criterion (BIC) /**
**Bayes-Schwarz Information Criterion:** (maximize)

$$\text{BIC} := \log L - \frac{p}{2} \log n$$

# Variable Backward Selection

{ A, F, H, I, J, L, P }
AIC = 63.01

# Variable Backward Selection

{ A, F, H, I, J, L, P }
AIC = 63.01

{ ~~A~~, F, H, I, J, L, P }
AIC = 63.87

...

{ A, F, H, ~~I~~, J, L, P }
AIC = 61.11

...

{ A, F, H, I, J, L, ~~P~~ }
AIC = 70.17

# Variable Backward Selection

{ A, F, H, I, J, L, P }
AIC = 63.01

{ ~~A~~, F, H, I, J, L, P } AIC = 63.87 ... { A, F, H, ~~I~~, J, L, P } AIC = 61.11 ... { A, F, H, I, J, L, ~~P~~ } AIC = 70.17

{ ~~A~~, F, H, ~~I~~, J, L, P } AIC = 61.88 ... { A, F, ~~H~~, ~~I~~, J, L, P } AIC = 59.40 ... { A, F, H, ~~I~~, J, L, ~~P~~ } AIC = 68.70

# Variable Backward Selection

{ A, F, H, I, J, L, P }
AIC = 63.01

{ ~~A~~, F, H, I, J, L, P } AIC = 63.87 ... { A, F, H, ~~I~~, J, L, P } AIC = 61.11 ... { A, F, H, I, J, L, ~~P~~ } AIC = 70.17

{ ~~A~~, F, H, ~~I~~, J, L, P } AIC = 61.88 ... { A, F, ~~H~~, ~~I~~, J, L, P } AIC = 59.40 ... { A, F, H, ~~I~~, J, L, ~~P~~ } AIC = 68.70

{ ~~A~~, F, ~~H~~, ~~I~~, J, L, P } AIC = 63.23 { A, ~~F~~, ~~H~~, ~~I~~, J, L, P } AIC = 61.50 ... { A, F, ~~H~~, ~~I~~, J, L, ~~P~~ } AIC = 66.71

X removed variable

# Variable Backward Selection

full model:

| | Estimate | Std. Error | t value | Pr(>\|t\|) | |
|---|---|---|---|---|---|
| (Intercept) | 1.222e+02 | 1.789e+01 | 6.831 | 2.54e-08 | *** |
| Population | 1.880e-04 | 6.474e-05 | 2.905 | 0.00584 | ** |
| Income | -1.592e-04 | 5.725e-04 | -0.278 | 0.78232 | |
| Illiteracy | 1.373e+00 | 8.322e-01 | 1.650 | 0.10641 | |
| \`Life Exp\` | -1.655e+00 | 2.562e-01 | -6.459 | 8.68e-08 | *** |
| \`HS Grad\` | 3.234e-02 | 5.725e-02 | 0.565 | 0.57519 | |
| Frost | -1.288e-02 | 7.392e-03 | -1.743 | 0.08867 | . |
| Area | 5.967e-06 | 3.801e-06 | 1.570 | 0.12391 | |

AIC optimal model by backward selection:

| | Estimate | Std. Error | t value | Pr(>\|t\|) | |
|---|---|---|---|---|---|
| (Intercept) | 1.202e+02 | 1.718e+01 | 6.994 | 1.17e-08 | *** |
| Population | 1.780e-04 | 5.930e-05 | 3.001 | 0.00442 | ** |
| Illiteracy | 1.173e+00 | 6.801e-01 | 1.725 | 0.09161 | . |
| \`Life Exp\` | -1.608e+00 | 2.324e-01 | -6.919 | 1.50e-08 | *** |
| Frost | -1.373e-02 | 7.080e-03 | -1.939 | 0.05888 | . |
| Area | 6.804e-06 | 2.919e-06 | 2.331 | 0.02439 | * |

# How to do it in R

```
library(datasets);
library(MASS);
st = as.data.frame(state.x77);

mod.full = lm(Murder ~ ., data=st);
summary(mod.full);

mod.opt = stepAIC(mod.full);
summary(mod.opt);
```

## Shrinkage

Model selection operates by

- fitting models for a set of models with varying complexity and then picking the “best one” ex post,
- omitting some parameters completely (i.e., forcing them to be 0)

**shrinkage** operates by

- including a penalty term directly in the model equation and
- favoring small parameter values in general.

## Shrinkage / Ridge Regression

**Ridge regression**: minimize

$$
\begin{aligned}
\text{RSS}_\lambda(\hat{\beta}) =& \text{RSS}(\hat{\beta}) + \lambda \sum_{j=1}^{p} \hat{\beta}_j^2 \\
=& \langle \mathbf{y} - \mathbf{X}\hat{\beta}, \mathbf{y} - \mathbf{X}\hat{\beta} \rangle + \lambda \sum_{j=1}^{p} \hat{\beta}_j^2 \\
\Rightarrow \hat{\beta} =& (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}
\end{aligned}
$$

with $\lambda \geq 0$ a **complexity parameter / regularization parameter**.

As

- solutions of ridge regression are not equivariant under scaling of the predictors, and as
- it does not make sense to include a constraint for the parameter of the intercept

data is normalized before ridge regression:

$$x'_{i,j} := \frac{x_{i,j} - \bar{x}_{.,j}}{\hat{\sigma}(x_{.,j})}$$

# Shrinkage / Ridge Regression (2/3)

Ridge regression is a combination of

$$\underbrace{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}_{} + \lambda \underbrace{\sum_{j=1}^{p}\beta_j^2}_{}$$

$$= \text{L2 loss} \quad + \lambda \text{ L2 regularization}$$

# How to compute ridge regression / Example

Fit

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

to the data:

| $x_1$ | $x_2$ | $y$ |
|---|---|---|
| 1 | 2 | 3 |
| 2 | 3 | 2 |
| 4 | 1 | 7 |
| 5 | 5 | 1 |

$$X = \begin{pmatrix} 1 & 1 & 2 \\ 1 & 2 & 3 \\ 1 & 4 & 1 \\ 1 & 5 & 5 \end{pmatrix}, \quad Y = \begin{pmatrix} 3 \\ 2 \\ 7 \\ 1 \end{pmatrix}, \quad I := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$X^T X = \begin{pmatrix} 4 & 12 & 11 \\ 12 & 46 & 37 \\ 11 & 37 & 39 \end{pmatrix}, \quad X^T X + 5I = \begin{pmatrix} 9 & 12 & 11 \\ 12 & 51 & 37 \\ 11 & 37 & 44 \end{pmatrix}, \quad X^T Y = \begin{pmatrix} 13 \\ 40 \\ 24 \end{pmatrix}$$

## Shrinkage / Ridge Regression (3/3) / Tikhonov Regularization (1/2)

**L2 regularization** / **Tikhonov regularization** can be derived for linear regression as follows:

Treat the true parameters $\theta_j$ as random variables $\Theta_j$ with the following distribution (**prior**):

$$\Theta_j \sim \mathcal{N}(0, \sigma_\Theta), \quad j = 1, \ldots, p$$

Then the **joint likelihood of the data and the parameters** is

$$L_{\mathcal{D},\Theta}(\theta) := \left( \prod_{i=1}^{n} p(x_i, y_i \,|\, \theta) \right) \prod_{j=1}^{p} p(\Theta_j = \theta_j)$$

and the conditional joint log likelihood of the data and the parameters accordingly

$$\log L^{\text{cond}}_{\mathcal{D},\Theta}(\theta) := \left( \sum_{i=1}^{n} \log p(y_i \,|\, x_i, \theta) \right) + \sum_{j=1}^{p} \log p(\Theta_j = \theta_j)$$

and

$$\log p(\Theta_j = \theta_j) = \log \frac{1}{\sqrt{2\pi}\sigma_\Theta} e^{-\frac{\theta_j^2}{2\sigma_\Theta^2}} = -\log(\sqrt{2\pi}\sigma_\Theta) - \frac{\theta_j^2}{2\sigma_\Theta^2}$$

## Shrinkage / Ridge Regression (3/3) / Tikhonov Regularization (2/2)

Dropping the terms that do not depend on $\theta_j$ yields:

$$\log L^{\text{cond}}_{\mathcal{D},\Theta}(\theta) := \left(\sum_{i=1}^{n} \log p(y_i \,|\, x_i, \theta)\right) + \sum_{j=1}^{p} \log p(\Theta_j = \theta_j)$$
$$\propto \left(\sum_{i=1}^{n} \log p(y_i \,|\, x_i, \theta)\right) - \frac{1}{2\sigma^2_\Theta} \sum_{j=1}^{p} \theta_j^2$$

This also gives a semantics to the complexity / regularization parameter $\lambda$:

$$\lambda = \frac{1}{2\sigma^2_\Theta}$$

but $\sigma^2_\Theta$ is unknown. (We will see methods to estimate $\lambda$ later on.)

The parameters $\theta$ that maximize the joint likelihood of the data and the parameters are called **Maximum Aposteriori Estimators (MAP estimators)**.

Putting a prior on the parameters is called **Bayesian approach.**

# Summary

- Complex models (e.g. with many derived variables) can fit to any training data (overfit). But we are interested in good prediction for unseen data (generalization).
- There is a tradeoff between model complexity and fit.
- With BIC/ AIC unimportant variables can be removed.
- Ridge regression favors solutions with small parameter values. It is equivalent to the MAP estimator with Gaussian priors on the parameters.

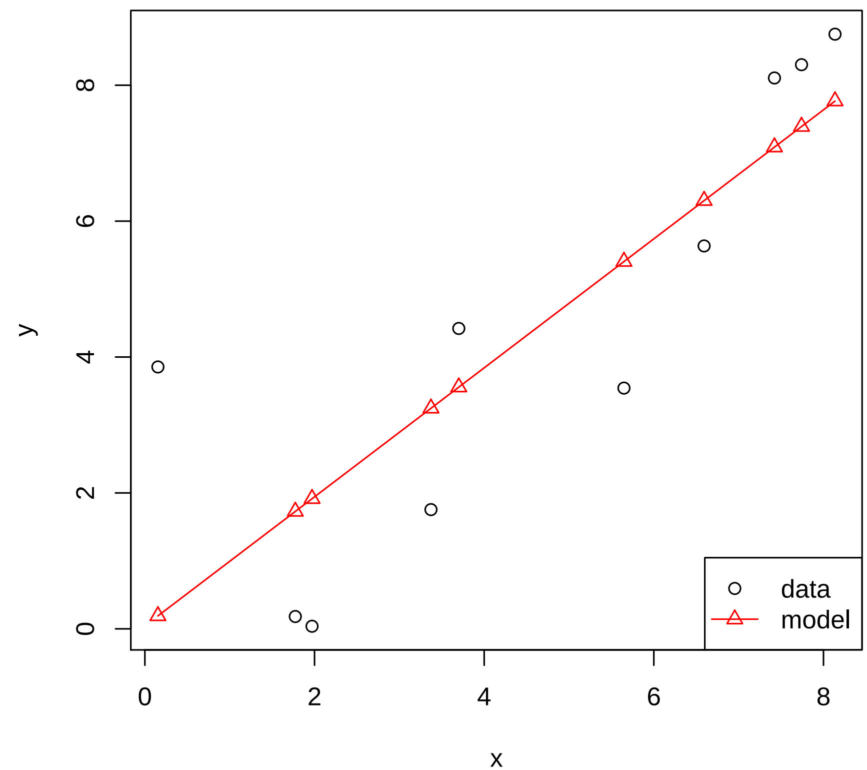
## Cases of Different Importance

Sometimes different cases are of different importance, e.g., if their measurements are of different accurracy or reliability.

Example: assume the left most point is known to be measured with lower reliability.

Thus, the model does not need to fit to this point equally as well as it needs to do to the other points.

I.e., residuals of this point should get lower weight than the others.



# Case Weights

In such situations, each case $(x_i, y_i)$ is assigned a **case weight** $w_i \geq 0$:

- the higher the weight, the more important the case.
- cases with weight $0$ should be treated as if they have been discarded from the data set.

Case weights can be managed as an additional pseudo-variable $w$ in applications.

# Weighted Least Squares Estimates

Formally, one tries to minimize the **weighted residual sum of squares**

$$\sum_{i=1}^{n} w_i (y_i - \hat{y}_i)^2 = ||\mathbf{W}^{\frac{1}{2}}(\mathbf{y} - \hat{\mathbf{y}})||^2$$

with

$$\mathbf{W} := \begin{pmatrix} w_1 & & & 0 \\ & w_2 & & \\ & & \ddots & \\ 0 & & & w_n \end{pmatrix}$$

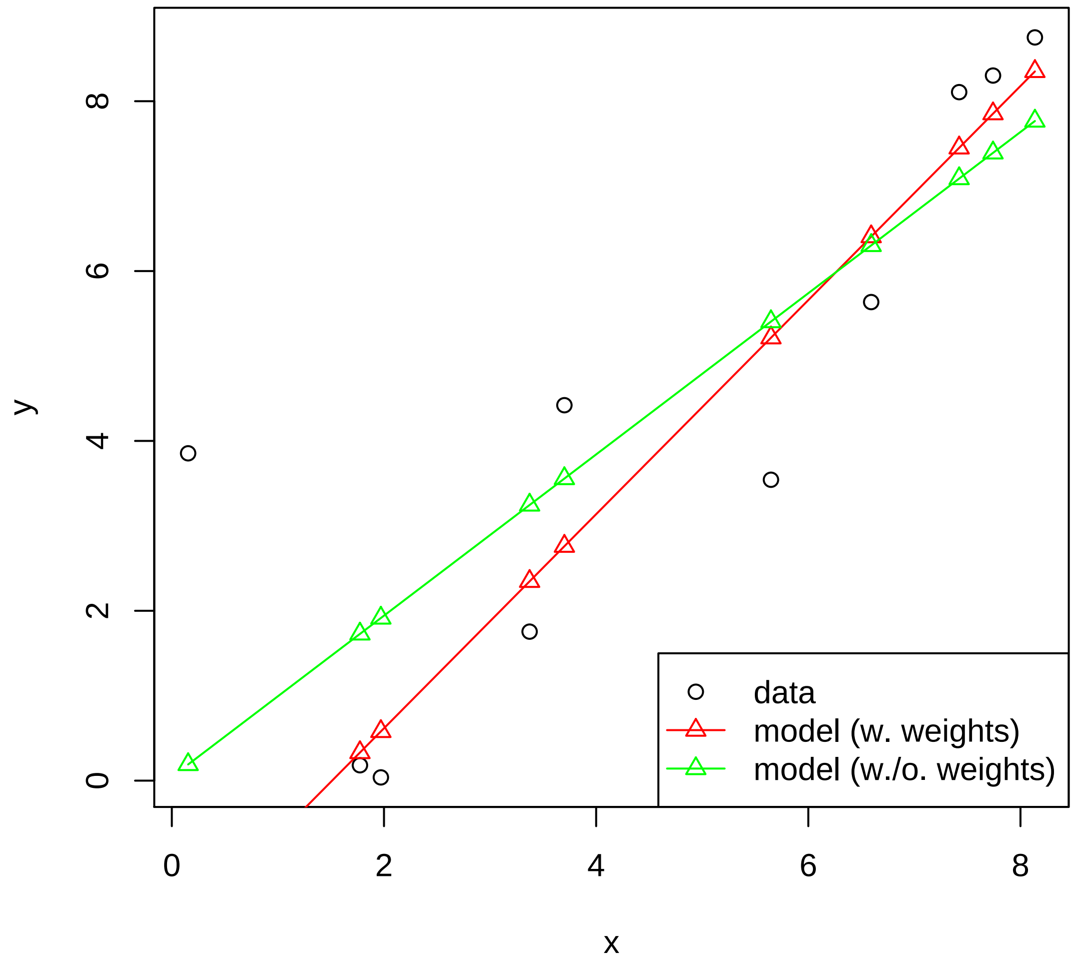
The same argument as for the unweighted case results in the **weighted least squares estimates**

$$\mathbf{X}^T \mathbf{W} \mathbf{X} \hat{\beta} = \mathbf{X}^T \mathbf{W} \mathbf{y}$$

# Weighted Least Squares Estimates / Example

Do downweight the left most point, we assign case weights as follows:

| $w$ | $x$ | $y$ |
|---|---|---|
| 1 | 5.65 | 3.54 |
| 1 | 3.37 | 1.75 |
| 1 | 1.97 | 0.04 |
| 1 | 3.70 | 4.42 |
| 0.1 | 0.15 | 3.85 |
| 1 | 8.14 | 8.75 |
| 1 | 7.42 | 8.11 |
| 1 | 6.59 | 5.64 |
| 1 | 1.77 | 0.18 |
| 1 | 7.74 | 8.30 |



## Summary

- For regression, **linear models** of type $Y = \langle X, \beta \rangle + \epsilon$ can be used to predict a quantitative $Y$ based on several (quantitative) $X$.
- The **ordinary least squares estimates (OLS)** are the parameters with minimal residual sum of squares (RSS). They coincide with the **maximum likelihood estimates (MLE)**.
- OLS estimates can be computed by solving the **system of linear equations** $\mathbf{X}^T\mathbf{X}\hat{\beta} = \mathbf{X}^T\mathbf{Y}$.
- The **variance of the OLS estimates** can be computed likewise ($(\mathbf{X}^T\mathbf{X})^{-1}\hat{\sigma}^2$).
- For deciding about inclusion of predictors as well as of powers and interactions of predictors in a model, **model selection measures** (AIC, BIC) and different search strategies such as forward and backward search are available.