Outline

Linear regression and correlation

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Association and correlation, their scientific relevance

- Discovering associations is fundamental in science
- Many scientific hypotheses are stated in terms of correlation or lack of correlation
- Although correlation does not imply causation, causation does imply correlation. That is, although a correlational study cannot definitely prove a causal hypothesis, it may rule one out
- Some variables simply cannot be manipulated for ethical reasons. Other variables, such as birth order, sex, and age are inherently correlational because they cannot be manipulated and, therefore, the scientific knowledge concerning them must be based on correlation evidence

Association and correlation, their scientific relevance

- Once correlation is known it can be used to make predictions
- When we know a score on one measure we can make a more accurate prediction of another measure that is highly related to it. The stronger the relationship between/among variables the more accurate the prediction
- Practical evidence from correlation studies can lead to testing that evidence under controlled experimental conditions
- Complex correlational statistics like multiple regression and partial correlation allow the correlation between two variables to be recalculated after the influence of other variables is removed

Kalama study

Kalama study

As part of an investigation into the physical development of children a health scientist measured the age (in months) and the height (in cm) of 12 children in the Kalama province in Egypt.

Research question: Is there a relationship between length and age?

Data

age	18	19	20	21	22	23	24	25	26	27	28	29
height	76.1	77.0	78.1	78.2	78.8	79.7	79.9	81.1	81.2	81.8	82.8	83.5

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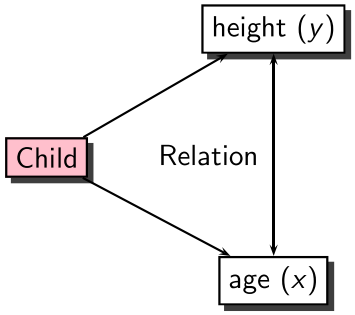
Research question: Is there a relationship between length and age?

Two variables measured for every child in the sample



- Strength of the association
- Is the relationship linear, quadratic, exponential?

Pearson correlation coefficient

Correlation coefficient

$$r_{xy}(x, y) = \frac{\text{cov}(x, y)}{\sqrt{s_x^2 s_y^2}}$$

- Range: $-1 \leq r_{xy} \leq 1$
- Perfect positive correlation between x and y: $r_{xy} = 1$
- No correlation between x en y: $r_{xy} = 0$
- Perfect negative correlation between x and y: $r_{xy} = -1$

Reading the data in R

```
> # Defining working directory
> setwd("C:\R-code-data")
>
> ## Reading the data
>
> kalama=read.table("kalama.txt", header=T)
> kalama
>
   age height
1   18   76.1
2   19   77.0
3   20   78.1
4   21   78.2
5   22   78.8
6   23   79.7
7   24   79.9
8   25   81.1
9   26   81.2
10  27   81.8
11  28   82.8
12  29   83.5
>
```

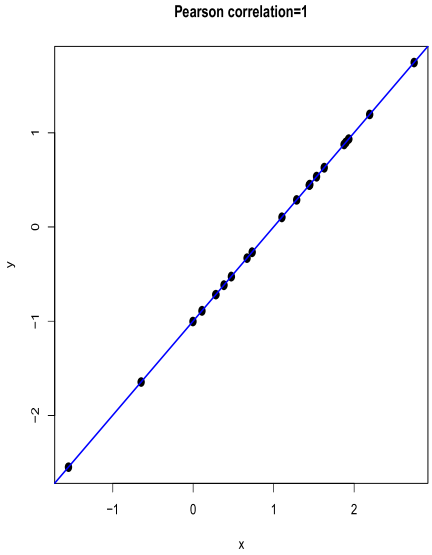
Descriptive statistics in R

```
> ## Descriptive Statistics
>
> options(digits=2)
> descrip.kalama<-stat.desc(kalama[,c("age","height")],basic=TRUE, desc=TRUE)
> descrip.kalama
>
                 age  height
nbr.val        12.00  12.000
min            18.00  76.100
max            29.00  83.500
range          11.00   7.400
sum           282.00 958.200
median         23.50  79.800
mean           23.50  79.850
SE.mean         1.04   0.665
CI.mean.0.95    2.29   1.463
var            13.00   5.301
std.dev         3.61   2.302
coef.var        0.15   0.029
>
```

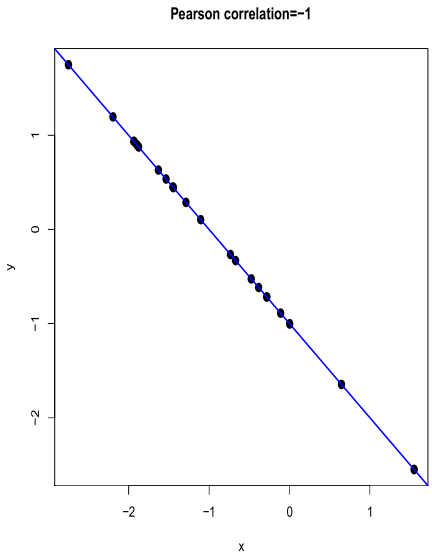

Estimating correlations in R

```
> ## Calculating the covariance and correlatio
> cov.age.height<-cov(kalama$age,kalama$height)
> corr.age.height<-cor(kalama$age,kalama$height)
> cov.age.height
[1] 8.3
> corr.age.height
[1] 0.99
> ## Testing if the population correlation is zero
> corr.age.height.test= cor.test(kalama$age, kalama$height,
+                       alternative="two.sided", method = "pearson")
> corr.age.height.test

        Pearson's product-moment correlation

data:  kalama$age and kalama$height
t = 30, df = 10, p-value = 4.428e-11
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 0.98 1.00
sample estimates:
 cor
0.99
>
```

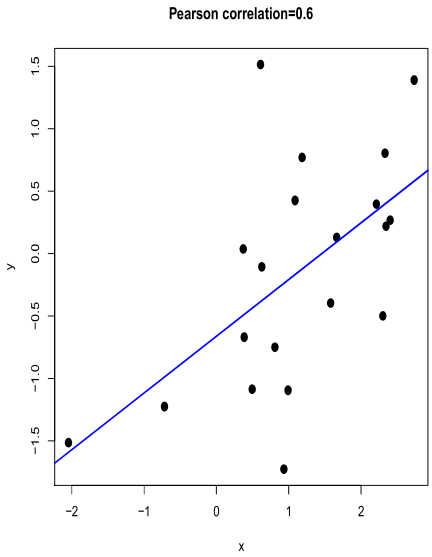
Pearson correlation coefficient



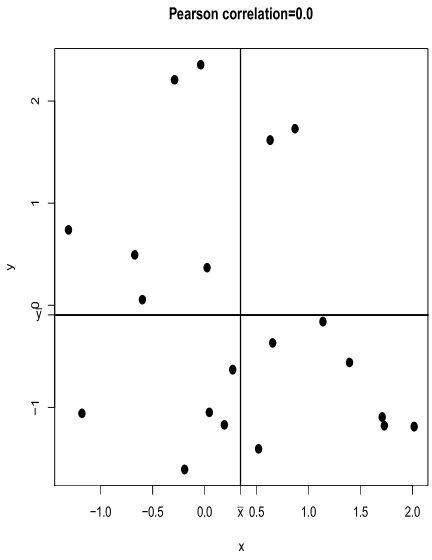
Pearson correlation coefficient



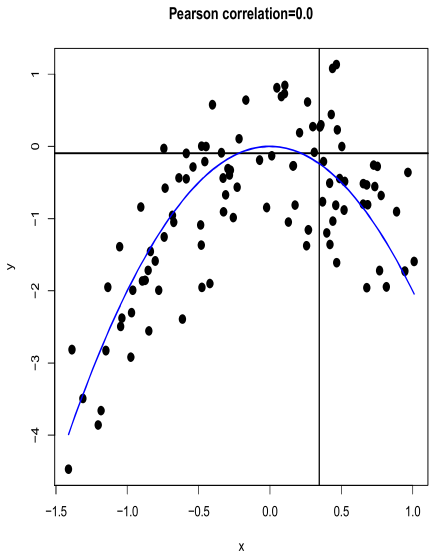
Pearson correlation coefficient



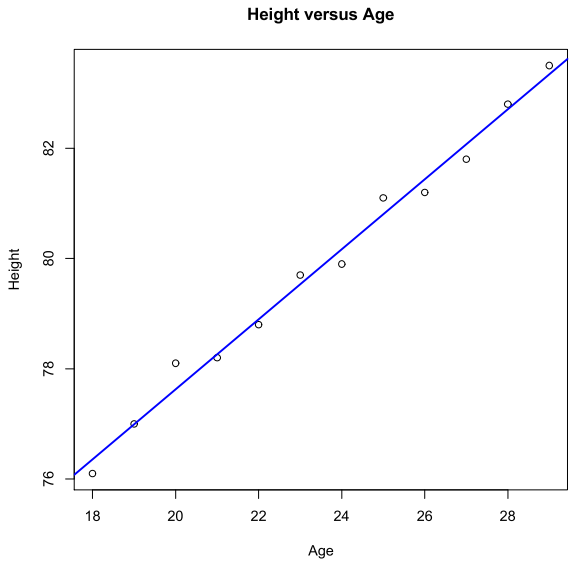
Pearson correlation coefficient



Pearson correlation coefficient



Kalama study ($r_K = 0.994$): Best line



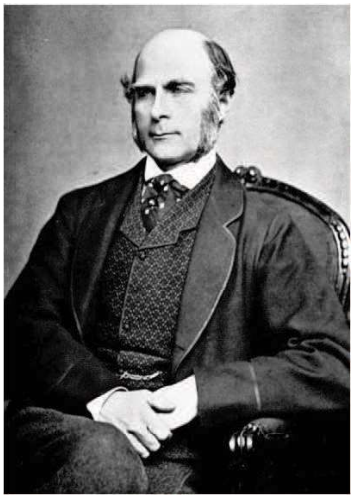
When to use Regression Analysis

- Regression analysis is used for explaining or modeling the relationship between a single variable Y, called the response output or dependent variable, and one or more predictor or explanatory variables, $\boldsymbol{X}^{'} = (X_1, \ldots, X_p)$
- When $p = 1$ it is called **simple** regression but when $p > 1$ it is called **multiple** regression
- When there is more than one Y, then it is called multivariate multiple regression which we wont be covering here
- The response must be a continuous variable but the explanatory variables can be continuous, discrete or categorical

Regression Analysis: Possible objectives

- Prediction of future observations
- Assessment of the effect of, or relationship between, explanatory variables on the response
- A general description of data structure
- Extensions exist to handle multivariate responses, binary responses (logistic regression analysis) and count responses (Poisson regression)

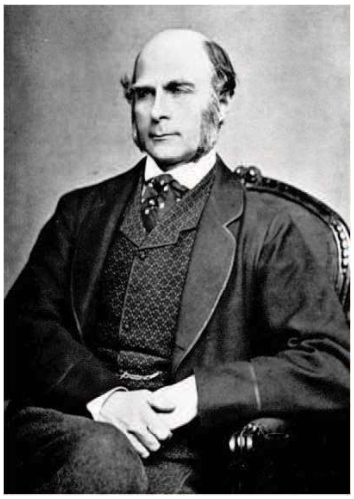
Francis Galton



- Cousin of Charles Darwin
- Regression and correlation
- The phenomenon of regression towards the mean

"Regression towards mediocrity in hereditary stature". Journal of the Anthropological Institute 15 (1886), 246-263.

Francis Galton

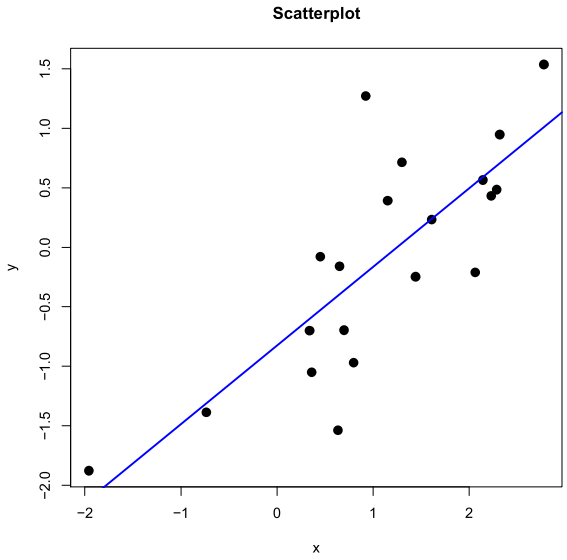


Francis Galton coined the term regression to mediocrity in 1875 in reference to the simple regression equation in the form

$$\frac{y-\bar{y}}{s_y} = r\left(\frac{x-\bar{x}}{s_x}\right).$$

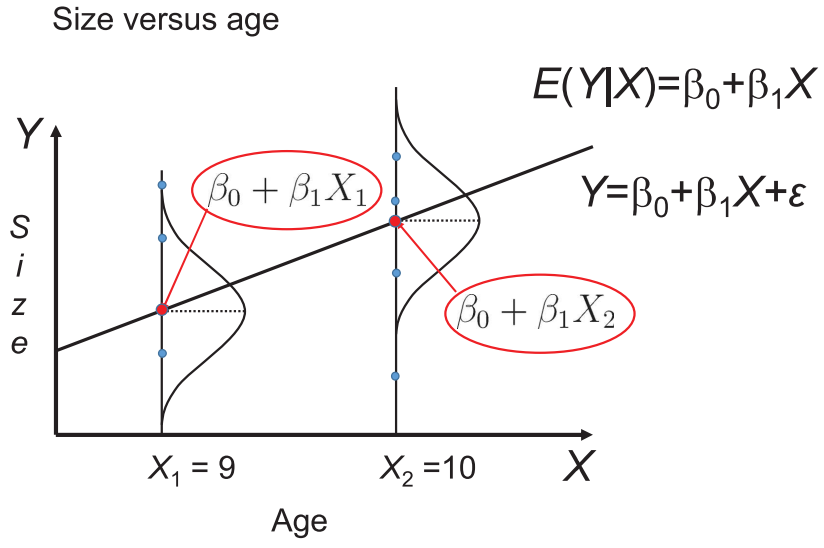
Sons of tall fathers tend to be tall but not as tall as their fathers while sons of short fathers tend to be short but not as short as their fathers. The **regression** effect.

Linear regression



$$Y = \beta_0 + \beta_1 X + \varepsilon$$

Linear regression



Formal Statement of the Model

For each unit $i = 1, \ldots, n$, the value of explanatory variable X_i and the response Y_i are recorded. *Simple Linear Regression* model.

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

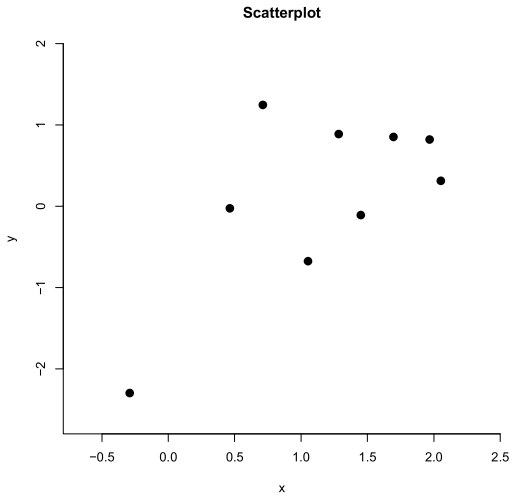
Assumptions

1. The value of X_i is precisely known.
2. Y_i is a continuous random variable.
3. β_0 and β_1 are parameters. That is, they are: unknown, constant and do not depend on the research unit.
4. ε_i is a random error term. It is not observable.

Formal Statement of the Model
Additional assumptions

5. For two different units, i and j, ε_i and ε_j are independent.
6. X_i and ε_i are independent.
7. $\varepsilon_i \sim N(0, \sigma^2)$ for all i, i.e., ε_i is normally distributed with $E(\varepsilon_i) = 0$, and $Var(\varepsilon_i) = \sigma^2$ for all i

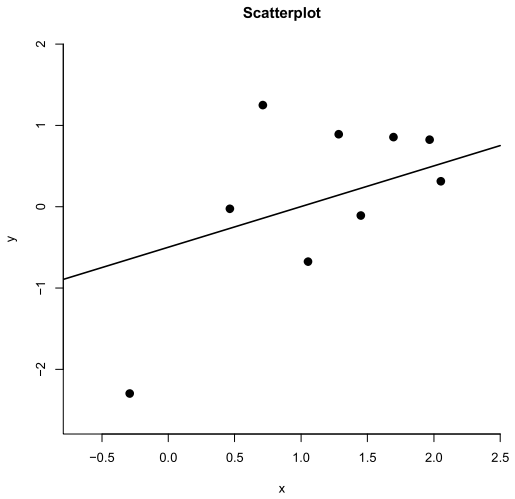
Least squares method



Which line fits the data best?

- $Y = \beta_0 + \beta_1 X + \varepsilon$

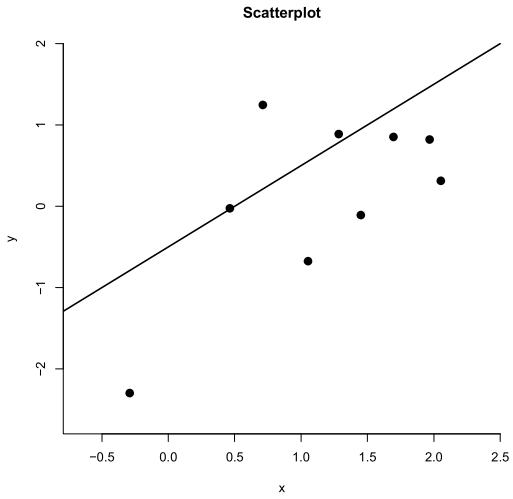
Least squares method



Which line fits the data best?

- $\hat{Y} = -0.5 + 0.5X$

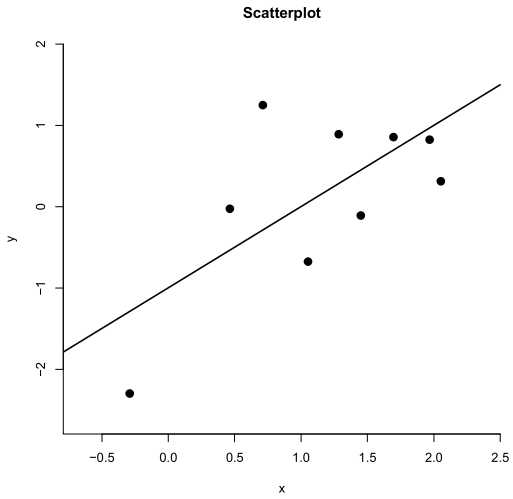
Least squares method



Which line fits the data best?

- $\hat{Y} = -0.5 + X$

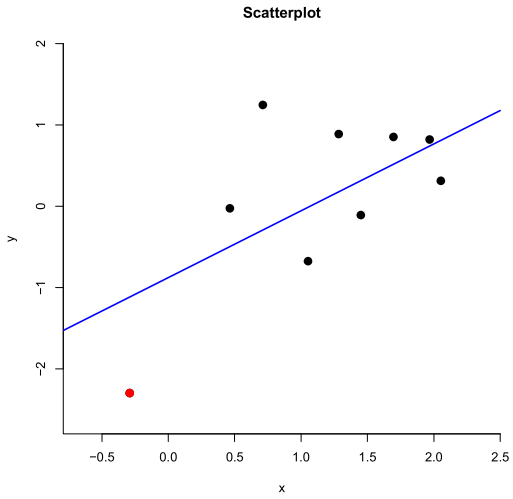
Least squares method



Which line fits the data best?

- $\hat{Y} = -0.26 + 0.45X$

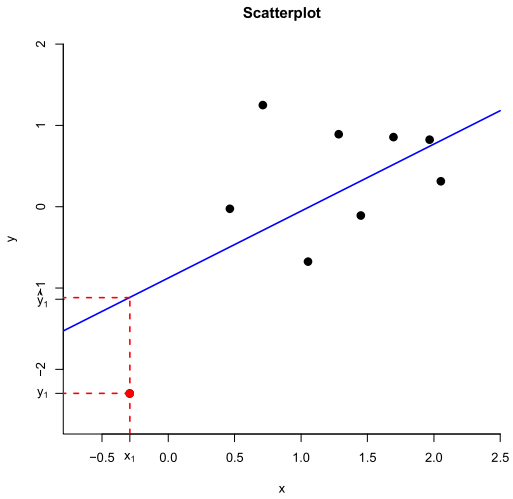
Least squares method



Which line fits the data best?

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

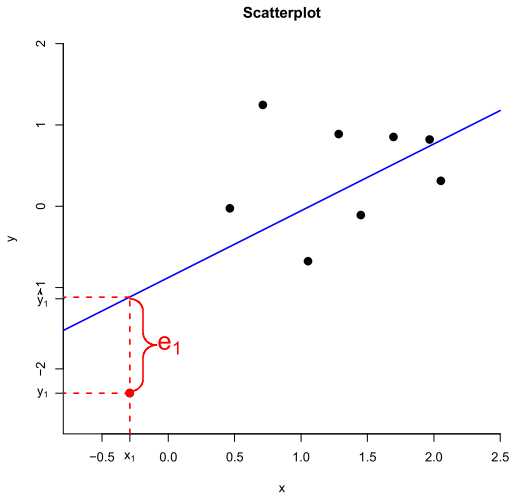
Least squares method



Which line fits the data best?

$$\hat{y}_1 = \hat{\beta}_0 + \hat{\beta}_1 x_1$$

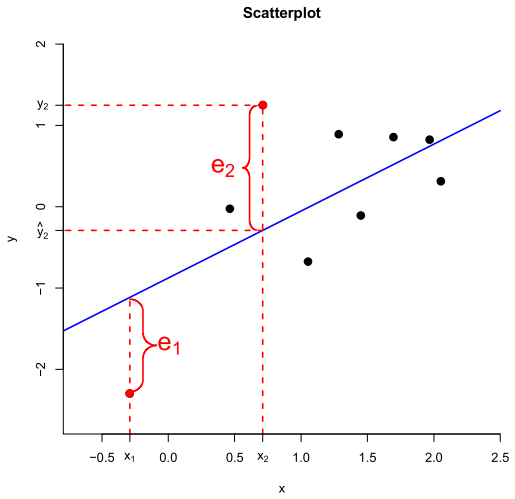
Least squares method



Which line fits the data best?

$$\hat{y}_1 = \hat{\beta}_0 + \hat{\beta}_1 x_1$$
$$y_1 = \hat{y}_1 + e_1$$
$$e_1 = y_1 - \hat{y}_1$$

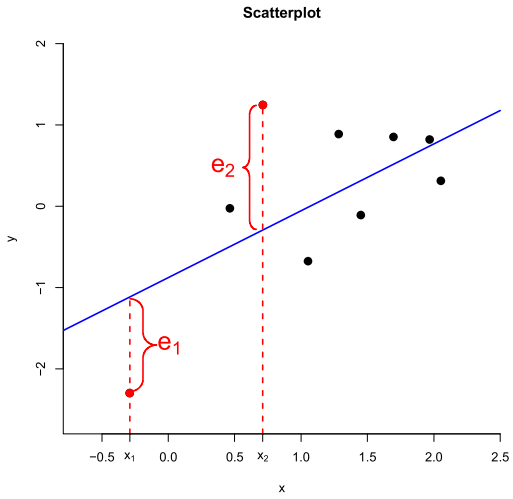
Least squares method



Which line fits the data best?

$$\hat{y}_2 = \hat{\beta}_0 + \hat{\beta}_1 x_2$$
$$y_2 = \hat{y}_2 + e_2$$
$$e_2 = y_2 - \hat{y}_2$$

Least squares method



Find the values of $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize

$$Q(\hat{\beta}_0, \hat{\beta}_1) = \sum_i e_i^2,$$

where

$$Q(\hat{\beta}_0, \hat{\beta}_1) = \sum_i (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

Estimation of the Regression Parameters

One needs to minimize

$$Q(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=n}^{n} e_i^2 = \sum_{i=n}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)^2$$

Taking partial derivates of $Q(\hat{\beta}_0, \hat{\beta}_1)$ w.r.t. $\hat{\beta}_0$ and $\hat{\beta}_1$ and setting the resulting expressions equal to zero leads to the so-called *Normal Equations*

$$\sum Y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum X_i$$

$$\sum X_i Y_i = \hat{\beta}_0 \sum X_i + \hat{\beta}_1 \sum X_i^2$$

Estimation of the Regression Parameters

A little algebra yields the ordinary least squares estimators for the parameters (OLS)

$$\hat{\beta}_1 = b_1 = \frac{\sum(X_i - \bar{X})(Y_i - \bar{Y})}{\sum(X_i - \bar{X})^2} = \frac{SS_{XY}}{SS_{XX}}$$

$$\hat{\beta}_0 = b_0 = \bar{Y} - b_1\bar{X}$$

where

$$SS_{XY} = \sum(X_i - \bar{X})(Y_i - \bar{Y}) \text{ and } SS_{XX} = \sum(X_i - \bar{X})^2$$

Estimation of the Regression Parameters

A little algebra yields the ordinary least squares estimators for the parameters (OLS)

Estimated model

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

$$\hat{\beta}_1 = b_1 = r_{xy}\frac{S_y}{S_x}$$

$$\hat{\beta}_0 = b_0 = \bar{Y} - b_1\bar{X}$$

where

$$S_x^2 = \frac{1}{n-1}\sum\left(X_i - \bar{X}\right)^2 \text{ and } S_y^2 = \frac{1}{n-1}\sum\left(Y_i - \bar{Y}\right)^2$$

Fitted Regression Line

With $\hat{\beta}_0$ and $\hat{\beta}_1$ one can compute the fitted model

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

The estimated model should be *close* to the true linear regression model. Thus, one can think of $\hat{Y}_i$ as the estimated mean response at $X = X_i$

What about σ^2?

Estimation of σ^2

The minimum value of $Q(\hat{\beta}_0, \hat{\beta}_1)$ is denoted as *SSE*

- It is the sum of squares deviations between the observations and the fitted line.
- It is a measure of how well the fitted line fits the data.

$$\begin{aligned} SSE = & Q(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)^2 \\ & = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} e_i^2 \end{aligned}$$

where e_i is called the *residual* for observation i.

Estimation of σ^2

Note

1. The residual $e_i = Y_i - \hat{Y}_i$ is the difference between observed and predicted values at X_i.
2. We can think of e_i as an estimator of the error ε_i.
3. The residuals are a fundamental tool to check the adequacy of the model.

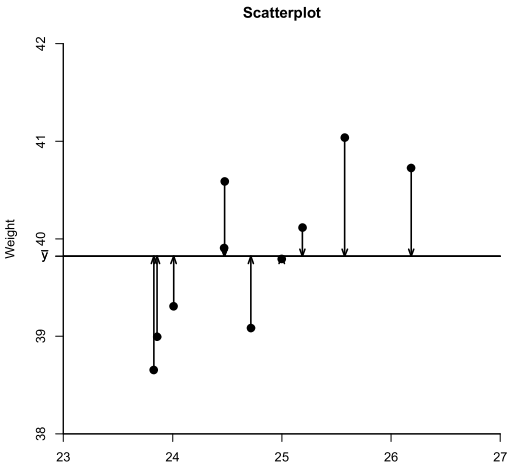
Estimation of σ^2

- Recall that σ^2 is the common variance for $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n$.
- Because $e_1, e_2, \ldots, e_n$ estimate the ε's, *SSE* should provide some information about the true variance σ^2.
- In fact,

$$s^2 = MSE = \frac{SSE}{n-2}$$

  is an *unbiased* estimator of σ^2.

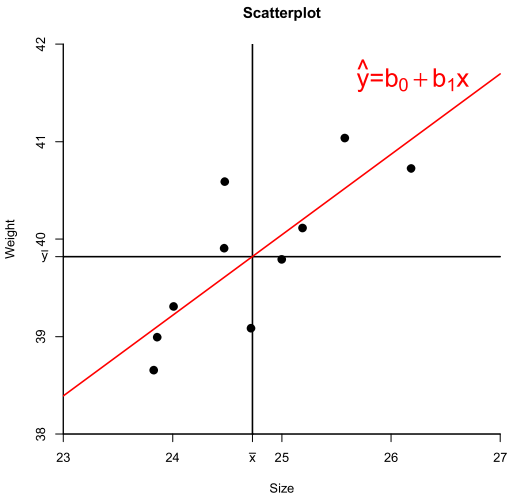
Sources of variation



Variation in Y

$$SSTO = \sum_i (y_i - \bar{y})^2$$

Sources of variation



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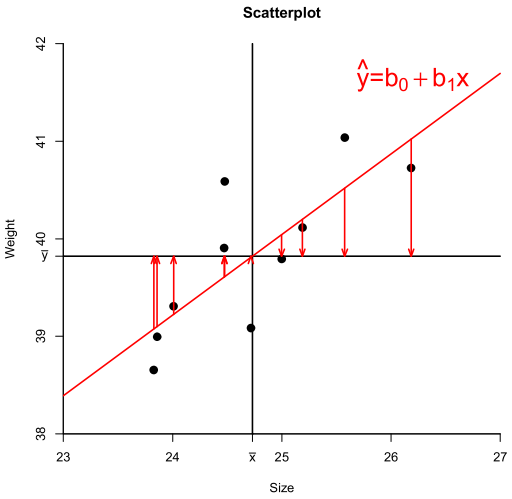
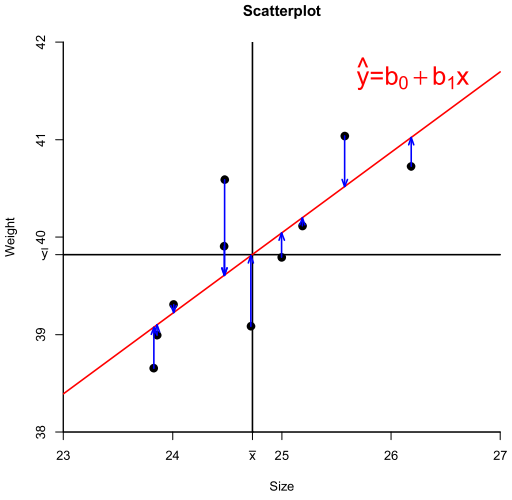


Variation in Y

$$SSTO = \sum_i (y_i - \bar{y})^2$$

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

Sources of variation



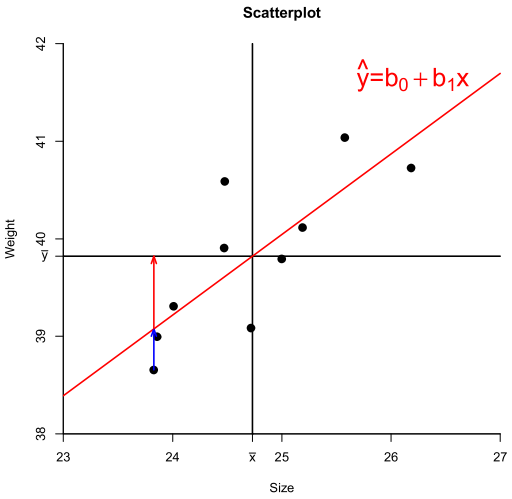
Variation in Y

$$SSTO = \sum_i (y_i - \bar{y})^2$$

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

$$SSE = \sum_i (y_i - \hat{y}_i)^2$$

Sources of variation



Variation in Y

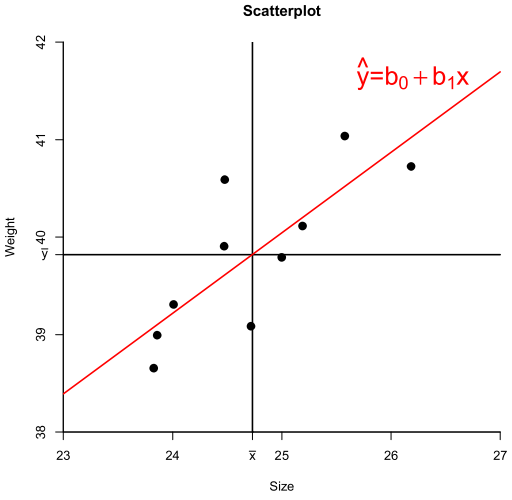
$$SSTO = \sum_i (y_i - \bar{y})^2$$

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

$$SSE = \sum_i (y_i - \hat{y}_i)^2$$

$$SSTO = SSR + SSE$$

Sources of variation



Variation in Y

$$SSTO = \sum_i (y_i - \bar{y})^2$$

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

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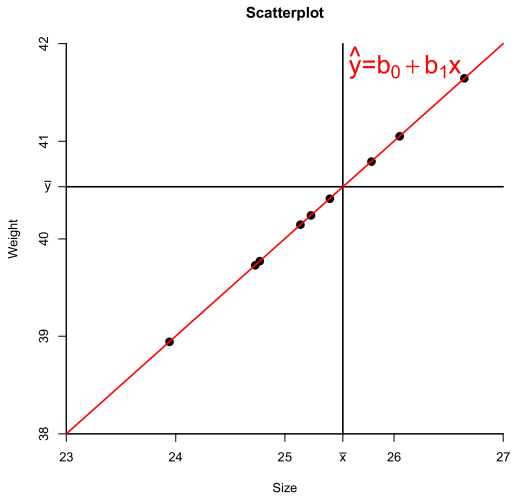


Variation in Y

$$SSTO = \sum_i (y_i - \bar{y})^2$$

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

$$SSE = 0$$

$$SSTO = SSR$$

The sum of the squares

$$SSTO = SSR + SSE$$

$SSTO$: Total variation in the response Y

SSE: The variation in Y not explained by the model

SSR: The variation in Y explained by the model

The sum of the squares

We can decompose the total sum of squares in two different sums of squares: the residual and regression sum of squares.

Coefficient of determination

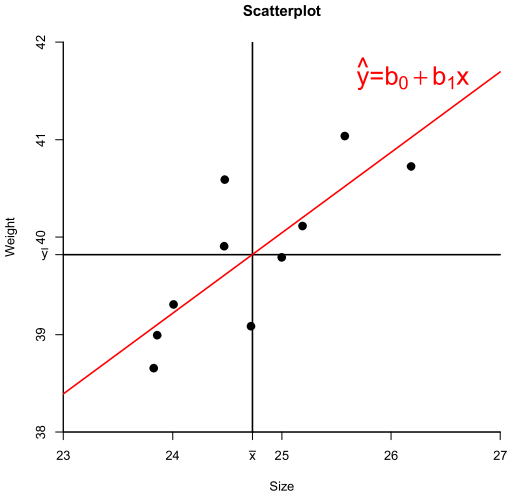
$$R^2 = \frac{SSR}{SSTO} = \frac{\sum_i (\hat{y}_i - \bar{y})^2}{\sum_i (y_i - \bar{y})^2}$$

Coefficient of determination

The coefficient of determination is a measure of the proportion of the total variation in the response that can be explained by the linear regression model.

- The coefficient of determination is always between 0 en 1

Sources of variation

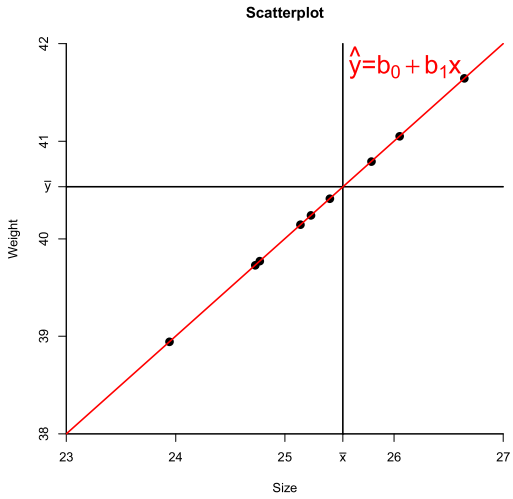


Variation van Y

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

- $0 \leq R^2 \leq 1$
- The larger the better

Sources of variation



Variation van Y

$$R^2 = \frac{SSR}{SSTO} = 1$$

Linear regression: R code and output

```
> ## Fitting the model
>
> res<-lm(height~age, data=kalama)
> kalama.anova<-anova(res)
> kalama.summary<-summary(res)
> kalama.anova
>
Analysis of Variance Table

Response: height
          Df Sum Sq Mean Sq F value    Pr(>F)
age        1 57.655  57.655  879.99 4.428e-11 ***
Residuals 10  0.655   0.066
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
```

Linear regression: R code and output

```
> kalama.summary
>
Call:
lm(formula = height ~ age, data = kalama)

Residuals:
     Min       1Q   Median       3Q      Max
-0.27238 -0.24248 -0.02762  0.16014  0.47238

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  64.9283     0.5084  127.71  < 2e-16 ***
age           0.6350     0.0214   29.66 4.43e-11 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.256 on 10 degrees of freedom
Multiple R-squared:  0.9888,    Adjusted R-squared:  0.9876
F-statistic:   880 on 1 and 10 DF,  p-value: 4.428e-11
>
```


Kalama Study: R Output

Anova

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Regression	1	57.65	57.65	879.99	0.0000
Residuals	10	0.66	0.07		
Total	11	58.31			

Coefficients

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	64.9283	0.5084	127.71	0.0000
age	0.6350	0.0214	29.66	0.0000

Kalama Study: R Output

Coefficients

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	64.9283	0.5084	127.71	0.0000
age	0.6350	0.0214	29.66	0.0000

- $y = \beta_0 + \beta_1 \cdot x + \epsilon$
- $b_0 = \bar{y} - b_1 \bar{x} = 64.928$
- $b_1 = r_{xy} \frac{s_y}{s_x} = 0.635$
- What does this p-value give?

Inference

$H_0 : \beta_1 = 0 \quad H_A : \beta_1 \neq 0$

Coefficients

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	64.9283	0.5084	127.71	0.0000
age	0.6350	0.0214	29.66	0.0000

Kalama Study

Anova

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Regression	1	57.65	57.65	879.99	0.0000
Residuals	10	0.66	0.07		
Total	11	58.31			

- $r_{xy}(x, y) = \frac{\text{cov}(x, y)}{\sqrt{s_x^2 s_y^2}} = 0.994$
- $R^2 = \frac{SSR}{SST} = \frac{57.65}{58.31} = 0.989$

$$r_{xy} = \sqrt{R^2}$$

Kalama Study

Anova

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Regression	1	57.65	57.65	879.99	0.0000
Residuals	10	0.66	0.07		
Total	11	58.31			

- $\hat{\sigma}^2 = MSE = \frac{SS_{Error}}{12 - 2} = \frac{0.66}{10} = 0.07$
- $R^2 = \frac{SSR}{SST} = \frac{57.65}{58.31} = 0.989$
- A substancial proportion of the variation in the outcome, 98.9%, is explained by the linear regression model.

Multiple linear regression

A multiple regression model is used to explain a dependent variable Y in terms of one or more independent variables $\boldsymbol{X}' = \left(1, X_1, \ldots, X_{p-1}\right)$.

If Y is a quantitative random variable and the elements in $\boldsymbol{X}$ can take both quantitative and qualitative values, then one can consider a *regression model*

$$Y = f(\boldsymbol{X}) + \epsilon,$$

with $\boldsymbol{X}$ and ϵ independent and $E(\epsilon) = 0$, $\text{Var}(\epsilon) = \sigma^2$. Often, it is also assumed that ϵ is normally distributed.

The previous model essentially describes the average behavior of Y as a function $f(\cdot)$ of $\boldsymbol{X}$, i.e., $E(Y) = f(\boldsymbol{X})$.

The regression model

Taylor's theorem states that if f is differentiable at certain point $\boldsymbol{a} \in \mathbb{R}^{p-1}$ then

$$f(\boldsymbol{X}) = f(\boldsymbol{a}) + (\boldsymbol{X} - \boldsymbol{a})'\beta_* + |\mathbf{X} - \mathbf{a}|h(\boldsymbol{X}), \qquad \lim_{\boldsymbol{X} \to \boldsymbol{a}} h(\boldsymbol{X}) = 0.$$

Therefore, at least locally (close to $\boldsymbol{a}$), $f(\cdot)$ can often be approximated by a *linear* model, i.e., $f(\boldsymbol{X}) = \boldsymbol{X}'\boldsymbol{\beta} = \beta_0 + \sum \beta_j X_j$.

$$\begin{aligned} Y &\approx \boldsymbol{X}'\boldsymbol{\beta} + \epsilon \\ &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1} + \epsilon \end{aligned}$$

The previous regression model is linear in the parameters and, hence, it is called a linear regression model.

Non-linear Regression Model: $Y = \beta_0 + \beta_1 X_1^{\beta_2} + \varepsilon$

General linear regression model

Model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1} + \epsilon$$

where

- $X_1, \ldots, X_{p-1}$ are known predictor variables.
- $\beta_0, \beta_1, \ldots, \beta_{p-1}$ are unknown parameters.
- ϵ is an error term. It is often assumed that $\epsilon \sim N(0, \sigma^2)$.

Interpretation of the parameters

$$E(Y|\boldsymbol{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1}$$

- This response function is a hyperplane, which is a plane in more than two dimensions.
- The parameter β_k indicates the change in the mean response $E(Y|\boldsymbol{X})$ with a unit increase in the predictor variable X_k, when all other predictor variables in the regression model are held constant.
- $E(Y|\boldsymbol{X} = \boldsymbol{0}) = \beta_0$. The intercept gives the average response when all covariates are zero. It may not be interpretable unless the covariates are centered.

Categorical covariates: Dummy variables

Example

- Y length in hospital stay
- X_1: patient's age
- X_2: gender coded as female (1) - male (0)
- Main effects model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$

Males	Females
$E(Y) = \beta_0 + \beta_1 X_1$	$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2$

Categorical covariates: Dummy variables

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- Y length in hospital stay
- X_1: patient's age
- X_2: gender coded as female (1) - male (0)
- Main effects model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$

Males	Females
$E(Y) = \beta_0 + \beta_1 X_1$	$E(Y) = (\beta_0 + \beta_2) + \beta_1 X_1$

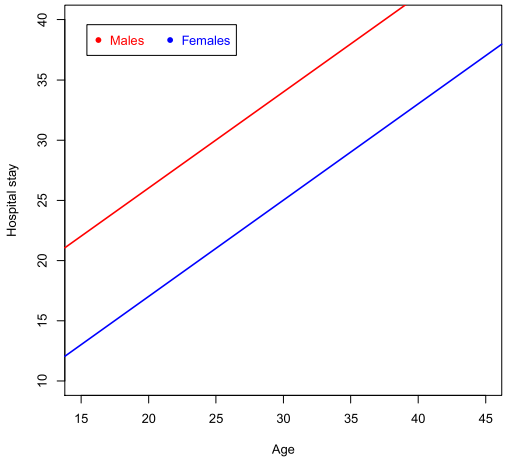
Main effects model: Parallel lines

Males

$$E(Y) = \beta_0 + \beta_1 X_1$$

Females

$$E(Y) = (\beta_0 + \beta_2) + \beta_1 X_1$$



Categorical covariates: Dummy variables

Example

- Y length in hospital stay
- X_1: patient's age
- X_2: gender coded as female (1) - male (0)
- Interaction model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \varepsilon$

Males

$$E(Y) = \beta_0 + \beta_1 X_1$$

Females

$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 + \beta_3 X_1$$

Categorical covariates: Dummy variables

Example

- Y length in hospital stay
- X_1: patient's age
- X_2: gender coded as female (1) - male (0)
- Interaction model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \varepsilon$

Males	Females
$E(Y) = \beta_0 + \beta_1 X_1$	$E(Y) = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X_1$

Categorical covariates: Dummy variables

Example

- Y length in hospital stay
- X_1: patient's age
- X_2: gender coded as female (1) - male (0)
- Interaction model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \varepsilon$

Males	Females
$E(Y) = \beta_0 + \beta_1 X_1$	$E(Y) = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X_1$

- It is still a linear model: $X_3 = X_1 X_2$

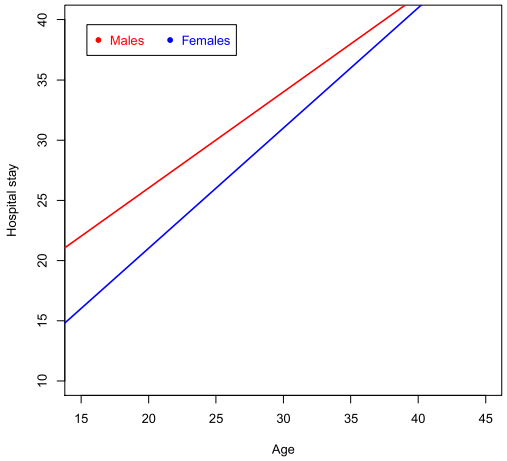
Interaction model: Non-parallel lines

Males

$$E(Y) = \beta_0 + \beta_1 X_1$$

Females

$$E(Y) = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X_1$$



Categorical covariates: Dummy variables

Example

- Y length in hospital stay
- X_1: patient's age
- X_2: female (1) - male (0)
- X disability status: 3 levels
  1. Not disabled
  2. Partially disabled
  3. Fully disabled

Categorical covariates: Dummy variables

For a factor with $r = 3$ levels, one needs to consider $(r-1) = 2$ indicator (dummy) variables as predictors:

$$x_3 = \begin{cases} 1 & \text{Not disabled} \\ 0 & \text{otherwise} \end{cases}$$

$$x_4 = \begin{cases} 1 & \text{Partially disabled} \\ 0 & \text{otherwise} \end{cases}$$

Main effects model

$$Y = \beta_0 + \beta_1 X_1 + \overbrace{\beta_2 X_2}^{\text{gender}} + \underbrace{\beta_3 X_3 + \beta_4 X_4}_{\text{disability status}} + \varepsilon$$

Categorical covariates: Dummy variables

For a factor with $r = 3$ levels, one needs to consider $(r-1) = 2$ indicator (dummy) variables as predictors:

$$x_3 = \begin{cases} 1 & \text{Not disabled} \\ 0 & \text{otherwise} \end{cases}$$

$$x_4 = \begin{cases} 1 & \text{Partially disabled} \\ 0 & \text{otherwise} \end{cases}$$

Interaction model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \underbrace{\beta_3 X_3 + \beta_4 X_4}_{\text{disability status}} + \underbrace{\beta_5 X_1 X_3 + \beta_6 X_1 X_4}_{\text{interaction: disability-age}} + \varepsilon$$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \varepsilon$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_3 + \varepsilon$, with $X_3 = X_1^2$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \varepsilon$
- Transformed variables:

$$\log(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \varepsilon$
- Transformed variables:

$$Y = e^{\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon_i}$$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \varepsilon$
- Transformed variables:

$$\log(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

- Transformed variables:

$$\frac{1}{Y} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

Great flexibility

- Polynomial regression: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \varepsilon$
- Transformed variables:

$$\log(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

- Transformed variables:

$$Y = \frac{1}{\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon}$$

Matrix formulation

Let us consider the following multiple regression model for the ith subject in the study, with $i = 1, 2, \ldots, n$

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_{p-1} X_{p-1\,i} + \varepsilon_i$$

Collecting all the information on all subjects into vectors and matrices, the previous model can be written as

$$\underbrace{\begin{pmatrix} Y_1 \\ . \\ . \\ . \\ Y_n \end{pmatrix}}_{\boldsymbol{Y}} = \underbrace{\begin{pmatrix} 1 & x_{11} & \ldots & x_{p-1\,1} \\ . & . & \ldots & . \\ . & . & \ldots & . \\ . & . & \ldots & . \\ 1 & x_{1n} & \ldots & x_{p-1\,n} \end{pmatrix}}_{\boldsymbol{X}} \cdot \underbrace{\begin{pmatrix} \beta_0 \\ . \\ . \\ . \\ \beta_{p-1} \end{pmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{pmatrix} \varepsilon_1 \\ . \\ . \\ \varepsilon_n \end{pmatrix}}_{\boldsymbol{\varepsilon}}$$

Matrix formulation

General linear regression model

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

- $\boldsymbol{Y}$ is the response vector.
- $\boldsymbol{\beta}$ is a vector of parameters.
- $\boldsymbol{X}$ is a matrix of known covariates with no measurement error.
- $\boldsymbol{\varepsilon}$ is a vector of errors with $E(\boldsymbol{\varepsilon}) = \mathbf{0}$ and $\text{Var}(\boldsymbol{\varepsilon}) = \sigma^2 \cdot \boldsymbol{I}$, where $\boldsymbol{I} = diag(1)$ is the so-called identity matrix.
- $\boldsymbol{\varepsilon}$ and $\boldsymbol{X}$ are assumed to be independent of each other.

Interpreting the the model: Y

- $\boldsymbol{Y}$ is called the regressand, response variable, criterion variable, or dependent variable.
- The decision as to which variable in a data set is modeled as the dependent variable and which are modeled as the independent variables may be based on a presumption that the value of one of the variables is caused by, or directly influenced by the other variables.
- Alternatively, there may be an operational reason, in which case there need be no presumption of causality.

Interpreting the the model: X

- $\boldsymbol{X}$: Its elements are called regressors, explanatory variables, covariates, input variables, predictor variables, or independent variables.
- Usually a constant is included as one of the regressors. The corresponding element of β is called the intercept.
- Many statistical inference procedures for linear models require an intercept to be present, so it is often included even if theoretical considerations suggest that its value should be zero.

Interpreting the the model: X

- Sometimes one of the regressors can be a non-linear function of another regressor, as in polynomial regression. The model remains linear as long as it is linear in the parameter vector β.
- The regressors may be viewed either as random variables, which one simply observes, or they can be considered as predetermined fixed values which one can choose.
- Both interpretations may be appropriate in different cases, and they generally lead to the same estimation procedures; however different approaches to asymptotic analysis are used in these two situations.

Interpreting the the model: β

- β is a p-dimensional parameter vector. Its elements are called effects, or regression coefficients.
- Statistical estimation and inference in linear regression focuses on β.
- The elements of this parameter vector are interpreted as the partial derivatives of the dependent variable with respect to the various independent variables.

Interpreting the the model: ε

- ε is called the error term, disturbance term, or noise.
- This variable captures all other factors which influence the dependent variable $\boldsymbol{Y}$ other than the regressors $\boldsymbol{X}$.
- The relationship between the error term and the regressors, for example whether they are correlated, is a crucial step in formulating a linear regression model, as it will determine the method to use for estimation.
- Typically, one assumes that $\boldsymbol{X}$ and ε are independent.

Estimating the model

Like before, the parameters can be estimated based on the ordinary least squares criterion (OLS)

$$\begin{aligned} Q &= \left(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}\right)' \left(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}\right) \\ &= \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{1i} - \cdots - \hat{\beta}_p X_{p-1\,i})^2 \end{aligned}$$

i.e., finding the values $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_{p-1}$ that minimize Q.

The solution to this optimization problem is given by the solution $\hat{\boldsymbol{\beta}}$ of the system of normal equations

$$\left(\boldsymbol{X}'\boldsymbol{X}\right)\hat{\boldsymbol{\beta}} = \boldsymbol{X}'\boldsymbol{Y} \qquad \Rightarrow \qquad \hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

Fitted values and residuals

- $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{1i} + \cdots + \hat{\beta}_{p-1} X_{p-1\,i}$
- Residuals $e_i = Y_i - \hat{Y}_i$
  - $\hat{\boldsymbol{Y}} = \boldsymbol{X}\hat{\beta}$
  - $\text{Var}(\hat{\beta}) = \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}$.
  - $\boldsymbol{e} = \boldsymbol{Y} - \hat{\boldsymbol{Y}} = \boldsymbol{Y} - \boldsymbol{X}\hat{\beta}$
  - $\hat{\boldsymbol{Y}} = \boldsymbol{H}\boldsymbol{Y} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{Y}$ with $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}$ (hat matrix)
  - $\boldsymbol{e} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{Y}$
  - $\text{Var}(\boldsymbol{e}) = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$

The sum of the squares

$$SST = \sum_i \left(Y_i - \bar{Y}\right)^2,\ SSR = \sum_i \left(\hat{Y}_i - \bar{Y}\right)^2,\ SSE = \sum_i \left(Y_i - \hat{Y}_i\right)^2$$

$$SST = SSR + SSE$$

SST: Total variation in the response

SSR: The variation explained by the model (covariates)

SSE: The variation not explained by the model (covariates)

- Coefficient of determination: $R^2 = \dfrac{SSR}{SST}$, interpretation idem
- $\hat{\sigma}^2 = MSE = \dfrac{SSE}{n-p}$

Inferences

$H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0 \quad H_A :$ not all β_k equal zero

Anova Table

Source of variation	SS	df	MS
Regression	SSR	$p-1$	$MSR = \dfrac{SSR}{p-1}$
Error	SSE	$n-p$	$MSE = \dfrac{SSE}{n-p}$
Total	$SSTO$	$n-1$	

- Under the null $F = \dfrac{MSR}{MSE} \sim F(p-1, n-p)$

Inferences

$H_0 : E(Y|\boldsymbol{X}) = \beta_0 \quad H_A : E(Y|\boldsymbol{X}) = \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1}$

Anova Table

Source of variation	SS	df	MS
Regression	SSR	$p-1$	$MSR = \dfrac{SSR}{p-1}$
Error	SSE	$n-p$	$MSE = \dfrac{SSE}{n-p}$
Total	$SSTO$	$n-1$	

- Under the null $F = \dfrac{MSR}{MSE} \sim F(p-1, n-p)$

Inferences: β_k

$$\mathrm{H}_0 : \beta_k = 0 \quad \mathrm{H}_A : \beta_k \neq 0$$

- Test statistics:
$$t = \frac{\hat{\beta}_k}{s\{\hat{\beta}_k\}} \sim t(1-\alpha/2; n-p)$$
- Confidence interval:
$$\hat{\beta}_k \pm t(1-\alpha/2; n-p) s\{\hat{\beta}_k\}$$

Comparing nested models

Likelihood ratio tests

- Null hypothesis of interest equals $H_0 : \boldsymbol{\beta} \in \Theta_{\boldsymbol{\beta},0}$, for some subspace $\Theta_{\boldsymbol{\beta},0}$ of the parameter space $\Theta_{\boldsymbol{\beta}}$
- For instance,
$$\mathrm{H}_0 : E(Y|\boldsymbol{X}) = \beta_0 + \beta_1 X_1 \quad \mathrm{H}_A : E(Y|\boldsymbol{X}) = \beta_0 + \beta_1 X_1 + \beta_3 X_3 + \beta_4 X_4$$

Comparing nested models

Likelihood ratio tests

- Null hypothesis of interest equals $H_0 : \boldsymbol{\beta} \in \Theta_{\boldsymbol{\beta},0}$, for some subspace $\Theta_{\boldsymbol{\beta},0}$ of the parameter space $\Theta_{\boldsymbol{\beta}}$
- For instance,

$$\mathrm{H}_0 : \beta_3 = \beta_4 = 0 \quad \mathrm{H}_A : \beta_3 \neq 0 \text{ and/or } \beta_4 \neq 0$$

- Notation:
  - L_{ML}: ML likelihood function
  - $\widehat{\boldsymbol{\beta}}_{ML,0}$: MLE under H_0
  - $\widehat{\boldsymbol{\beta}}_{ML}$: MLE under general model

Likelihood ratio tests

- Test statistic:

$$-2 \ln \lambda_N = -2 \ln \left[\frac{L_{ML}(\widehat{\boldsymbol{\beta}}_{ML,0})}{L_{ML}(\widehat{\boldsymbol{\beta}}_{ML})} \right]$$

- Asymptotic null distribution: χ^2 with d.f. equal to the difference in dimension of $\Theta_{\boldsymbol{\beta}}$ and $\Theta_{\boldsymbol{\beta},0}$.
- An equivalent F-test can also be used.

Patient satisfaction

Case study

A hospital administrator wanted to study the relation between patient satisfaction (Y) and patient's age (X_1, in years), severity of illness (X_2, an index), and anxiety level (X_3, an index).

The administrator randomly selected 46 patients and collected data on the previous variables. Larger values of Y, X_2, and X_3 are, respectively, associated with more satisfaction, increased severity of illness, and more anxiety.

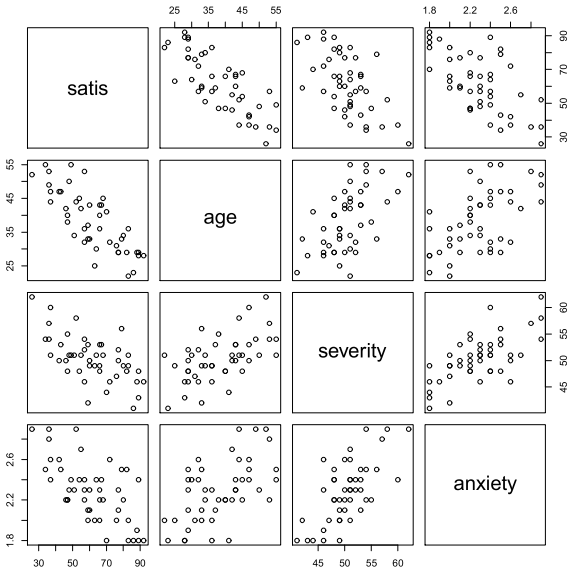
R code: Patient satisfaction

```
> ## Reading the data
>
> satisfaction=read.table("satisfaction.txt", header=T)
> head(satisfaction,10)
>
   satis age severity anxiety
1     48  50       51     2.3
2     57  36       46     2.3
3     66  40       48     2.2
4     70  41       44     1.8
5     89  28       43     1.8
6     36  49       54     2.9
7     46  42       50     2.2
8     54  45       48     2.4
9     26  52       62     2.9
10    77  29       50     2.1
>
```

R code: Patient satisfaction

```
> ## Exploring the data
>
> cor(satisfaction)
>
              satis        age   severity    anxiety
satis     1.0000000 -0.7867555 -0.6029417 -0.6445910
age      -0.7867555  1.0000000  0.5679505  0.5696775
severity -0.6029417  0.5679505  1.0000000  0.6705287
anxiety  -0.6445910  0.5696775  0.6705287  1.0000000
>
> options(digits=2)
> descrip.satisfaction<-stat.desc(satisfaction,basic=TRUE, desc=TRUE)
> descrip.satisfaction
>
               satis     age severity anxiety
nbr.val        46.00   46.00  4.6e+01  46.000
min            26.00   22.00  4.1e+01   1.800
max            92.00   55.00  6.2e+01   2.900
range          66.00   33.00  2.1e+01   1.100
median         60.00   37.50  5.0e+01   2.300
mean           61.57   38.39  5.0e+01   2.287
SE.mean         2.54    1.31  6.4e-01   0.044
var           297.10   79.53  1.9e+01   0.090
std.dev        17.24    8.92  4.3e+00   0.299
coef.var        0.28    0.23  8.6e-02   0.131
>
> plot(satisfaction)
>
```


R code: Patient satisfaction



R code: Patient satisfaction

```
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>
> satis = β0 + β1 age + β2 severity + β3 anxiety + ϵ
> satisfaction.lm<-lm(satis~age+severity+anxiety, data=satisfaction)
> satisfaction.summary<-summary(satisfaction.lm)
> satisfaction.summary

Call:
lm(formula = satis ~ age + severity + anxiety, data = satisfaction)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.491     18.126    8.74  5.3e-11 ***
age           -1.142      0.215   -5.31  3.8e-06 ***
severity      -0.442      0.492   -0.90    0.374
anxiety      -13.470      7.100   -1.90    0.065 .
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 10 on 42 degrees of freedom
Multiple R-squared:  0.682,     Adjusted R-squared:  0.659
F-statistic: 30.1 on 3 and 42 DF,  p-value: 1.54e-10
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Call:
lm(formula = satis ~ age + severity + anxiety, data = satisfaction)

Coefficients:
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(Intercept)  158.491     18.126    8.74  5.3e-11 ***
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severity      -0.442      0.492   -0.90    0.374
anxiety      -13.470      7.100   -1.90    0.065 .
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 10 on 42 degrees of freedom  √MSE = 10
Multiple R-squared:  0.682,     Adjusted R-squared:  0.659
F-statistic: 30.1 on 3 and 42 DF,  p-value: 1.54e-10
>
```


R code: Patient satisfaction

```
> ## Likelihood ratio test null model versus full model
>
> satis = β0 + ε  ⇔ satis = β0 + β1 age + β2 severity + β3 anxiety + ε
> satisfaction.lm.int<-lm(satis~1, data=satisfaction) # Null model
> anova(satisfaction.lm.int,satisfaction.lm)          # Null versus full
>
Analysis of Variance Table

Model 1: satis ~ 1
Model 2: satis ~ age + severity + anxiety
  Res.Df   RSS Df Sum of Sq    F  Pr(>F)
1     45 13369
2     42  4249  3      9120 30.1 1.5e-10 ***   H0 : β1 = β2 = β3 = 0
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
> ## Previous analysis with summary function

Multiple R-squared:  0.682,     Adjusted R-squared:  0.659
F-statistic: 30.1 on 3 and 42 DF,  p-value: 1.54e-10 H0 : β1 = β2 = β3 = 0
>
```

R code: Patient satisfaction

```
> ## Sequential building of the model
>
> satisfaction.anova<-anova(satisfaction.lm)
> satisfaction.anova
>
Analysis of Variance Table

Response: satis
          Df Sum Sq Mean Sq F value  Pr(>F)
age        1   8275    8275   81.80 2.1e-11 ***
severity   1    481     481    4.75   0.035 *
anxiety    1    364     364    3.60   0.065 .
Residuals 42   4249     101
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
> ## Previous analysis with summary function
>
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.491     18.126    8.74  5.3e-11 ***
age           -1.142      0.215   -5.31  3.8e-06 ***
severity      -0.442      0.492   -0.90    0.374
anxiety      -13.470      7.100   -1.90    0.065 .   # Same p-value as before (-1.9)^2=3.6
>
```


R code: Patient satisfaction

```
> ## Sequential building of the model
>
> satisfaction.lm2<-lm(satis~age+anxiety+severity, data=satisfaction)
> satisfaction.anova2<-anova(satisfaction.lm2)
> satisfaction.anova2
>
Analysis of Variance Table

Response: satis
          Df Sum Sq Mean Sq F value  Pr(>F)
age        1   8275    8275   81.80 2.1e-11 ***
anxiety    1    763     763    7.55  0.0088 **
severity   1     82      82    0.81  0.3741
Residuals 42   4249     101
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
>
> ## Previous analysis with summary function
>
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  158.491     18.126    8.74  5.3e-11 ***
age           -1.142      0.215   -5.31  3.8e-06 ***
severity      -0.442      0.492   -0.90    0.374     # Same p-value as before (-0.9)^2=0.81
anxiety      -13.470      7.100   -1.90    0.065 .
>
```

R code: Patient satisfaction

```
> ## Sequential building of the model
>
> satisfaction.anova<-anova(satisfaction.lm)
> satisfaction.anova
>
Analysis of Variance Table

Response: satis
          Df Sum Sq Mean Sq F value  Pr(>F)
age        1   8275    8275   81.80 2.1e-11 ***
severity   1    481     481    4.75   0.035 *
anxiety    1    364     364    3.60   0.065 .
Residuals 42   4249     101
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
```

$H_0:$ $satis = \beta_0 + \epsilon$ $H_1: satis = \beta_0 + \beta_1 age + \epsilon$

$H_0:$ $satis = \beta_0 + \beta_1 age + \epsilon$ $H_1: satis = \beta_0 + \beta_1 age + \beta_2 severity + \epsilon$

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Final model

Final model:

$$Y_i = 145.941 - 1.2X_{1i} - 16.742X_{3i} + \varepsilon_i$$

```
> ## Final model
>
> satisfaction.lm.final<-lm(satis~age+anxiety, data=satisfaction)
> satisfaction.final.summary<-summary(satisfaction.lm.final)
> satisfaction.final.summary
>
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  145.941     11.525   12.66  4.2e-16 ***
age           -1.200      0.204   -5.88  5.4e-07 ***
anxiety      -16.742      6.081   -2.75   0.0086 **
---
>
```

Inference for mean response

- In many applications one wants to estimate and/or make inferences about the mean of the response Y for a given value of the predictors $\boldsymbol{X}_h$

$$Y_h = E(Y|\boldsymbol{X}_h) = \boldsymbol{X}_h'\beta$$

- Point estimate: $\hat{Y}_h = \boldsymbol{X}_h'\hat{\beta}$.
- Confidence intervals are used for inferences.

Inference for mean response

- $E(Y_h) = \boldsymbol{X}_h'\beta$
- $\hat{Y}_h = \boldsymbol{X}_h'\hat{\beta}$
- $s^2\left(\hat{Y}_h\right) = \boldsymbol{X}_h'\text{Var}(\hat{\beta})\boldsymbol{X}_h$
- $s^2(\hat{Y}_h) = MSE(\boldsymbol{X}_h'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}_h)$
- Hence $1-\alpha$ confidence limits are

$$\hat{Y}_h \pm t(1-\alpha/2; n-p) \cdot s(\hat{Y}_h)$$

Prediction of a new observation

- Let now assume that one wants to predict a new observation $Y_{h,new}$ corresponding to a given level of the predictor variable $\boldsymbol{X} = \boldsymbol{X}_h$.
- This is typically done by constructing a $1 - \alpha$ prediction interval, i.e., by finding values $Y_{h,low}$ and $Y_{h,up}$ so that

$$P(Y_{h,low} \leq Y_{h,new} \leq Y_{h,up} | \boldsymbol{X} = \boldsymbol{X}_h) = 1 - \alpha$$

- The prediction interval is given by

$$\hat{Y}_h \pm t(1 - \alpha/2; n - p) s\{pred\}$$

where $s^2\{pred\} = MSE + s^2(\hat{Y}_h)$

R code: Predicting a new observation

```
> ## Predicting a new observation
>
> newdata = data.frame(age=43, anxiety=2.7)
> pred.w.plim <- predict(satisfaction.lm.final, newdata, interval="predict")
> pred.w.clim <- predict(satisfaction.lm.final, newdata, interval = "confidence")
> pred.w.plim
>
  fit lwr upr
1  49  28  70
>
> pred.w.clim
>
  fit lwr upr
1  49  44  54
>
```

$\hat{Y}_h = \boldsymbol{X}_h' \hat{\boldsymbol{\beta}}$