Kursus 02403 Introduktion til Matematisk Statistik

Forelæsning 8: Simpel lineær regression

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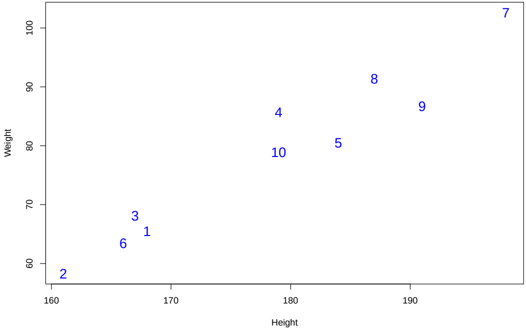
Oversigt

Oversigt

Heights (x_i)	168	161	167	179	184	166	198	187	191	179
Weights (y_i)	65.5	58.3	68.1	85.7	80.5	63.4	102.6	91.4	86.7	78.9



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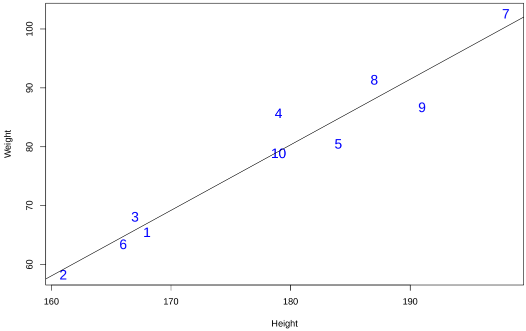

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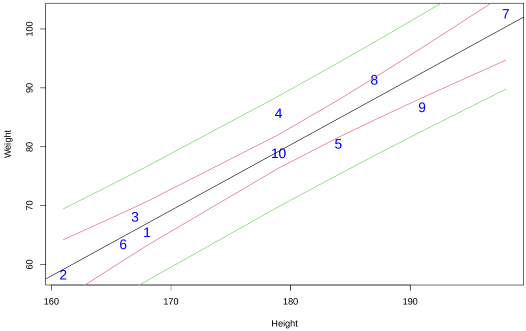
```
##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -5.876 -1.451 -0.608  2.234  6.477
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -119.958     18.897   -6.35  0.00022 ***
## x              1.113      0.106   10.50  5.9e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.88 on 8 degrees of freedom
## Multiple R-squared:  0.932,Adjusted R-squared:  0.924
## F-statistic:  110 on 1 and 8 DF,  p-value: 5.87e-06
```

Heights (x_i)	168	161	167	179	184	166	198	187	191	179
Weights (y_i)	65.5	58.3	68.1	85.7	80.5	63.4	102.6	91.4	86.7	78.9



Oversigt

Opstil en lineær regressionsmodel

- Opstil den *lineære regressionsmodel*

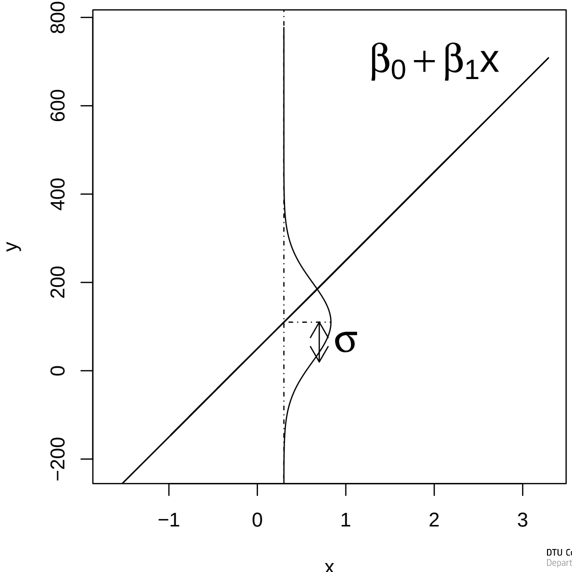
$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

- Y_i er den *afhængige variabel* (dependent variable). En stokastisk variabel.
- x_i er en *forklarende variabel* (explanatory variable)
- ε_i er afvigelsen (error). En stokastisk variabel.

og vi antager

ε_i er independent and identically distributed (i.i.d.) og $N(0, \sigma^2)$

Model-illustration



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Mindste kvadraters metode

- Minimer variansen σ^2 på afvigelsen. Det er på næsten alle måder det bedste valg i dette setup.
- Formelt: Minimer summen af de kvadrerede afvigelser (Residual Sum of Squares (RSS))

$$RSS(\beta_0, \beta_1) = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

$\hat{\beta}_0$ og $\hat{\beta}_1$ minimerer RSS

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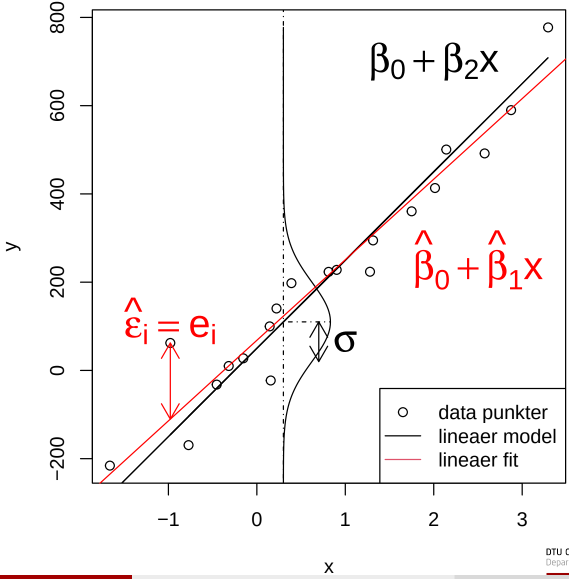
Illustration af model, data og fit



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Least squares estimator

Theorem 5.4 (her for estimatorer som i eNoten)

The least squares estimators of β_0 and β_1 are given by

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(x_i - \bar{x})}{S_{xx}}$$

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x}$$

where $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2$.

Least squares estimater

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where $S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2$.

Oversigt

- Hvordan er parameter estimaterne i en lineær regressionsmodel fordelt (givet normalfordelte afvigelser)?

  De er normalfordelte og deres varians kan estimeres:

Theorem 5.8 (første del)

$$
\begin{aligned}
V[\hat{\beta}_0] &= \frac{\sigma^2}{n} + \frac{\bar{x}^2\sigma^2}{S_{xx}} \\
V[\hat{\beta}_1] &= \frac{\sigma^2}{S_{xx}} \\
Cov[\hat{\beta}_0, \hat{\beta}_1] &= -\frac{\bar{x}\sigma^2}{S_{xx}}
\end{aligned}
$$

Estimater af standard afvigelserne på $\hat{\beta}_0$ og $\hat{\beta}_1$

Theorem 5.8 (anden del)

Where σ^2 is usually replaced by its estimate ($\hat{\sigma}^2$). The central estimator for σ^2 is

$$\hat{\sigma}^2 = \frac{RSS(\hat{\beta}_0, \hat{\beta}_1)}{n-2} = \frac{\sum_{i=1}^n e_i^2}{n-2}.$$

When the estimate of σ^2 is used the variances also become estimates and we'll refer to them as $\hat{\sigma}^2_{\beta_0}$ and $\hat{\sigma}^2_{\beta_1}$.

Estimat af standard afvigelserne for $\hat{\beta}_0$ og $\hat{\beta}_1$ (ligningerne (5-73))

$$\hat{\sigma}_{\beta_0} = \hat{\sigma}\sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}; \quad \hat{\sigma}_{\beta_1} = \hat{\sigma}\sqrt{\frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2}}$$

Oversigt

Hypotesetests for parameter estimaterne

- Vi kan altså udføre hypotesetests for parameter estimater i en lineær regressionsmodel:

$$\begin{aligned} H_{0,i}: &\quad \beta_i = \beta_{0,i} \\ H_{1,i}: &\quad \beta_i \neq \beta_{0,i} \end{aligned}$$

- Vi bruger de t-fordelte test størrelser:

Theorem 5.12

Under the null-hypothesis ($\beta_0 = \beta_{0,0}$ and $\beta_1 = \beta_{0,1}$) the statistics

$$T_{\beta_0} = \frac{\hat{\beta}_0 - \beta_{0,0}}{\hat{\sigma}_{\beta_0}}; \quad T_{\beta_1} = \frac{\hat{\beta}_1 - \beta_{0,1}}{\hat{\sigma}_{\beta_1}},$$

are t-distributed with $n-2$ degrees of freedom, and inference should be based on this distribution.

Konfidensintervaller for parametrene

Method 5.15

$(1-\alpha)$ confidence intervals for β_0 and β_1 are given by

$$\hat{\beta}_0 \pm t_{1-\alpha/2}\,\hat{\sigma}_{\beta_0}$$
$$\hat{\beta}_1 \pm t_{1-\alpha/2}\,\hat{\sigma}_{\beta_1}$$

where $t_{1-\alpha/2}$ is the $(1-\alpha/2)$-quantile of a t-distribution with $n-2$ degrees of freedom.

- husk at $\hat{\sigma}_{\beta_0}$ og $\hat{\sigma}_{\beta_1}$ findes ved ligningerne (5-74)
- i R kan $\hat{\sigma}_{\beta_0}$ og $\hat{\sigma}_{\beta_1}$ aflæses ved "Std. Error" ved "summary(fit)"

Oversigt

Method 5.18: Konfidensinterval for $\beta_0 + \beta_1 x_0$

- Konfidensinterval for $\beta_0 + \beta_1 x_0$ svarer til et konfidensinterval for linien i punktet x_0
- Beregnes med

$$(\hat{\beta}_0 + \hat{\beta}_1 x_0) \pm t_{\alpha/2} \cdot \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}}$$

- Konfidensintervallet vil i $100(1-\alpha)\%$ af gangene indeholde den rigtige linie, altså $\beta_0 + \beta_1 x_0$

Method 5.18: Prædiktionsinterval for $\beta_0 + \beta_1 x_0 + \varepsilon_0$

- Prædiktionsintervallet (prediction interval) for Y_0 beregnes med en værdi x_0
- Dette gøres *før* Y_0 observeres med

$$(\hat{\beta}_0 + \hat{\beta}_1 x_0) \pm t_{\alpha/2} \cdot \hat{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}}$$

- Prædiktionsintervallet vil $100(1 - \alpha)$% af gangene indeholde den observerede y_0
- Et prædiktionsinterval bliver altså større end et konfidensinterval for fastholdt α

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Eksempel med konfidensinterval for linien

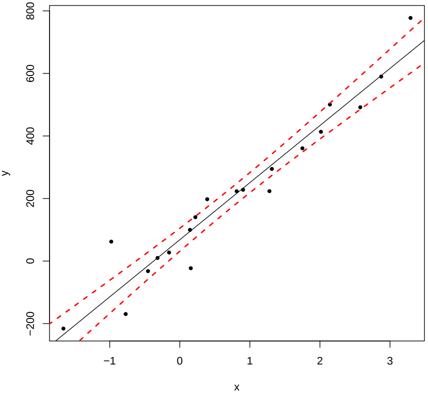
```r
## Eksempel med konfidensinterval for linien

## Lav en sekvens af x værdier
xval <- seq(from=-2, to=6, length.out=100)

## Brug predict funktionen
CI <- predict(fit, newdata=data.frame(x=xval),
interval="confidence",
level=.95)

## Se lige hvad der kom
head(CI)

## Plot data, model og intervaller
plot(x, y, pch=20)
abline(fit)
lines(xval, CI[, "lwr"], lty=2, col="red", lwd=2)
lines(xval, CI[, "upr"], lty=2, col="red", lwd=2)
```



Eksempel med prædiktionsinterval

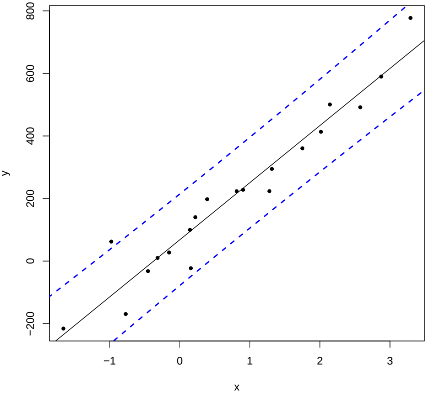
```r
## Eksempel med prædiktionsinterval

## Lav en sekvens a x værdier
xval <- seq(from=-2, to=6, length.out=100)

## Beregn interval for hvert x
PI <- predict(fit, newdata=data.frame(x=xval),
interval="prediction",
level=.95)

## Se lige hvad der kom tilbage
head(PI)

## Plot data, model og intervaller
plot(x, y, pch=20)
abline(fit)
lines(xval, PI[, "lwr"], lty=2, col="blue", lwd=2)
lines(xval, PI[, "upr"], lty=2, col="blue", lwd=2)
```



Oversigt

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Matrix formulering

The simple linear regression problem can be formulated in vector-matrix notation as

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \qquad \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

or

$$\begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}; \qquad \epsilon_i \sim N(0, \sigma^2)$$

RSS in matrix-vector notation

$$RSS = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} = (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})$$

Matrix formulering: Parameter estimater

The estimators of the parameters in the simple linear regression model are given by

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y} \tag{1}$$

and the covariance matrix of the estimates is

$$V[\hat{\boldsymbol{\beta}}] = \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1} \tag{2}$$

and central estimate for the residual variance is

$$\hat{\sigma}^2 = \frac{RSS}{n-2} \tag{3}$$

Oversigt

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Hvad bliver mere skrevet ud af summary?

```
summary(fit)


##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -119.70  -23.74   -4.15   22.44  172.64
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)     68.2       17.5     3.9    0.001 **
## x              182.6       11.4    16.0  4.2e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 67.4 on 18 degrees of freedom
## Multiple R-squared:  0.935,Adjusted R-squared:  0.931
## F-statistic:  257 on 1 and 18 DF,  p-value: 4.17e-12
```

summary(lm(y∼x)) wrap up

- `Residuals: Min 1Q Median 3Q Max:`
  Residualernes: Minimum, 1. kvartil, Median, 3. kvartil, Maximum

- `Coefficients:`
  `Estimate Std. Error t value Pr(>|t|) "stjerner"`
  Koefficienternes:
  Estimat $\hat{\sigma}_{\beta_i}$ t_{obs} p-værdi
  - Testen er $H_{0,i} : \beta_i = 0$ vs. $H_{1,i} : \beta_i \neq 0$

- `Residual standard error: XXX on XXX degrees of freedom`
  $\varepsilon_i \sim N(0, \sigma^2)$ udskrevet er $\hat{\sigma}$ og ν frihedsgrader (brug til hypotesetesten)

- `Multiple R-squared: XXX`
  Forklaret varians r^2

- Resten bruger vi ikke i det her kursus

Forklaret varians og korrelation

- Forklaret varians af en model er r^2, i summary "Multiple R-squared"
- Beregnes med

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

hvor $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$

- Andel af den totale varians der er forklaret med modellen

Forklaret varians og korrelation

- Korrelationen ρ er et mål for *lineær sammenhæng* mellem to stokastiske variable

- Estimeret (i.e. empirisk) korrelation

$$\hat{\rho} = r = \sqrt{r^2}\, sgn(\hat{\beta}_1)$$

hvor $sgn(\hat{\beta}_1)$ er: -1 for $\hat{\beta}_1 \leq 0$ og 1 for $\hat{\beta}_1 > 0$

- Altså:
  - Positiv korrelation ved positiv hældning
  - Negativ korrelation ved negativ hældning

Test for signifikant korrelation

- Test for signifikant korrelation (lineær sammenhæng) mellem to variable

$$H_0 : \rho = 0$$
$$H_1 : \rho \neq 0$$

er ækvivalent med

$$H_0 : \beta_1 = 0$$
$$H_1 : \beta_1 \neq 0$$

hvor $\hat{\beta}_1$ er estimatet af hældningen i simpel lineær regressionsmodel

Oversigt

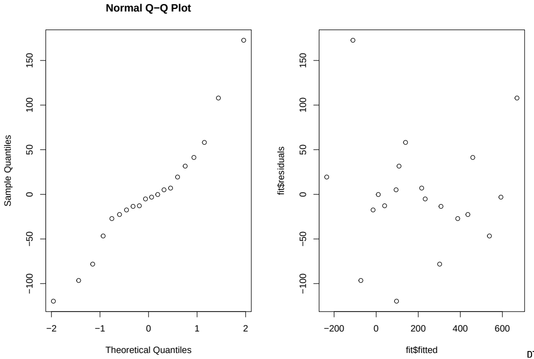
Residual Analysis

Method 5.28

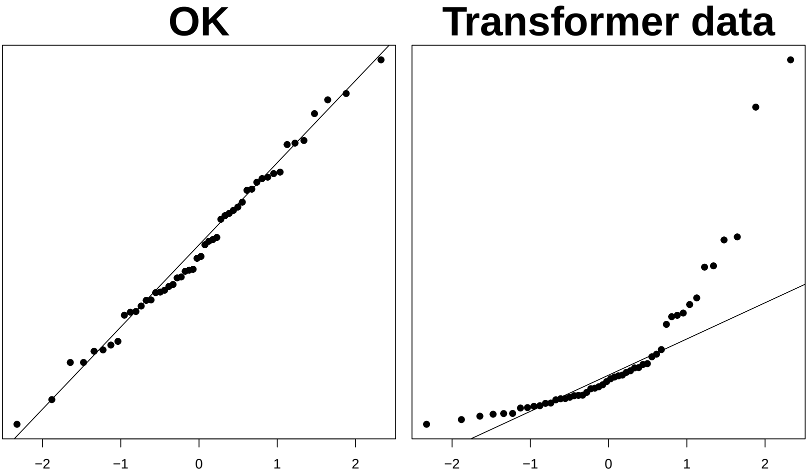
- Check normality assumption with qq-plot.
- Check (non)systematic behavior by plotting the residuals e_i as a function of fitted values $\hat{y}_i$

Residual Analysis in R

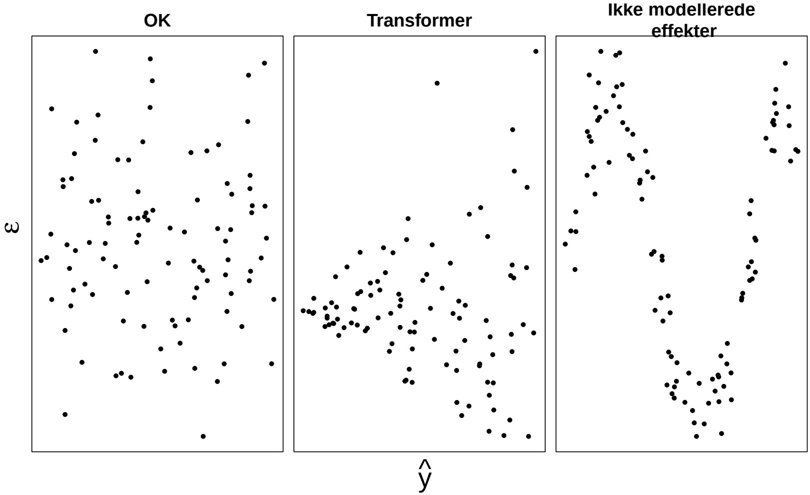
```
fit <- lm(y ~ x)
par(mfrow = c(1, 2))
qqnorm(fit$residuals)
plot(fit$fitted, fit$residuals)
```



Residual Analyse - Normal antagelsen



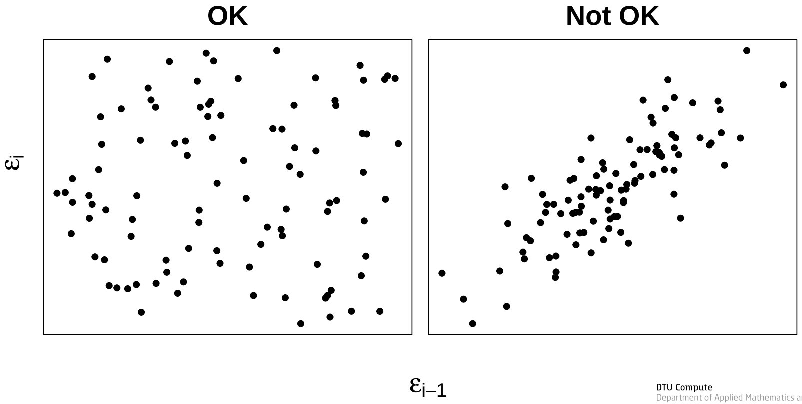
Residual Analyse - Systematiske effekter



Residual Analyse - uafhængighedsantagelsen

For tidsrække data bør uafhængigheds antagelsen også tjekkes, to simple tjek er

- Plot ϵ_i vs. ϵ_{i-1}
- Udregn $cor(\epsilon_i, \epsilon_{i-1})$



Oversigt

Modellering af phytoplankton

Formuler en lineær model for phytoplankton i Skive fjord, estimer modellens parametre og foretag modelkontrol.

Outline