Model validation

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Outline

- Normal distribution
- Linear models ...

Recap

Recall:

$$y_i = \alpha + \mathbf{x}_i\boldsymbol{\beta} + \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- the systematic component: the regression line
- the random component: leftover stuff

Models make assumptions

Our models make assumptions. Sometimes, these are realistic.

All models are wrong, but some are useful

Is is important to:

- Know which assumptions your model makes
- Assess if they are realistic
- Determine if they are violated

Tests make assumptions too

But more on that later

Linear regression assumptions

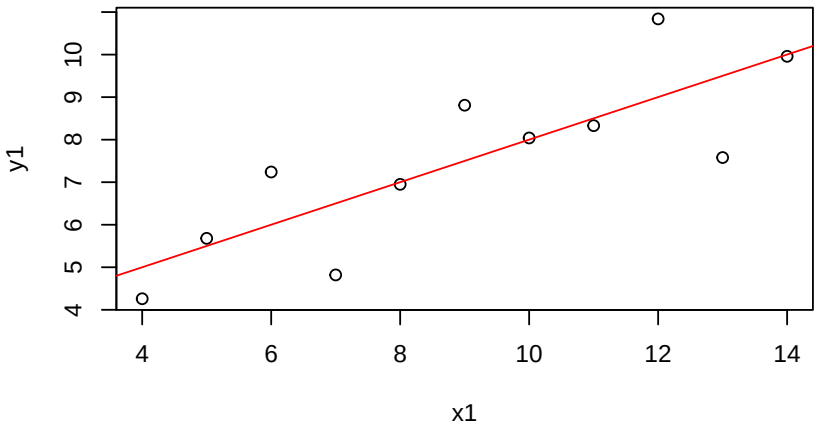
$$y_i = \alpha + \sum_{k=1}^{p} x_{ik}\beta_k + \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

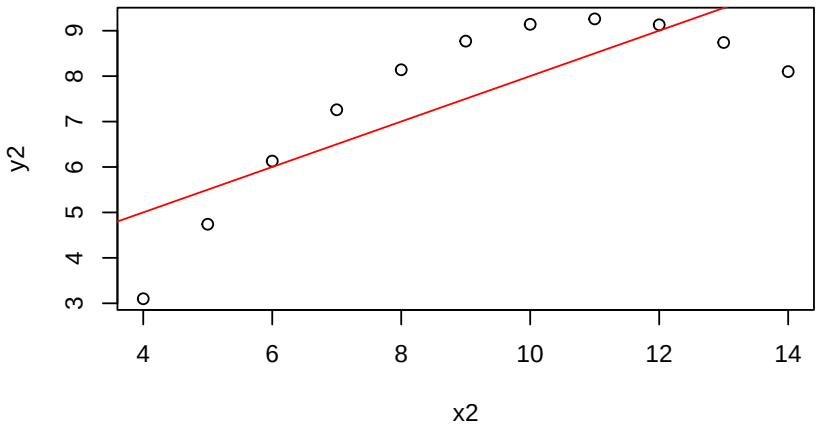
- Linearity
- Normality: normally distributed errors
- Homoscedastcity: same variance for all errors
- Independence of errors
- Lack of perfect multicollinearity ($\mathbf{x}_1 \neq \mathbf{x}_2$)
- No outliers
- No error in the explanatory variables

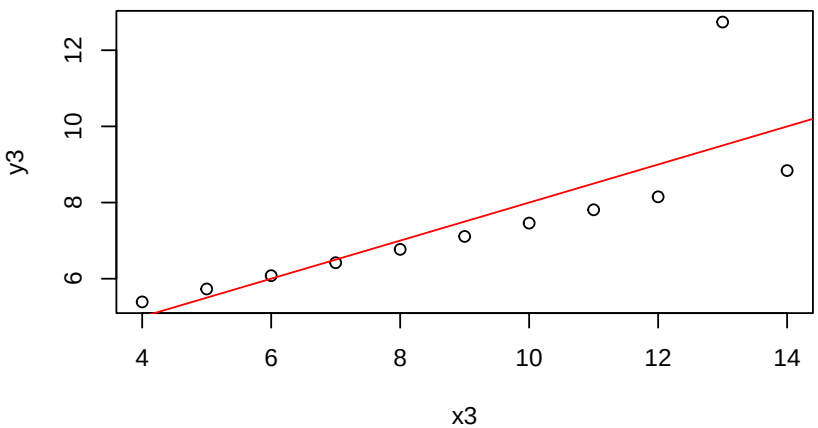
Violating assumptions

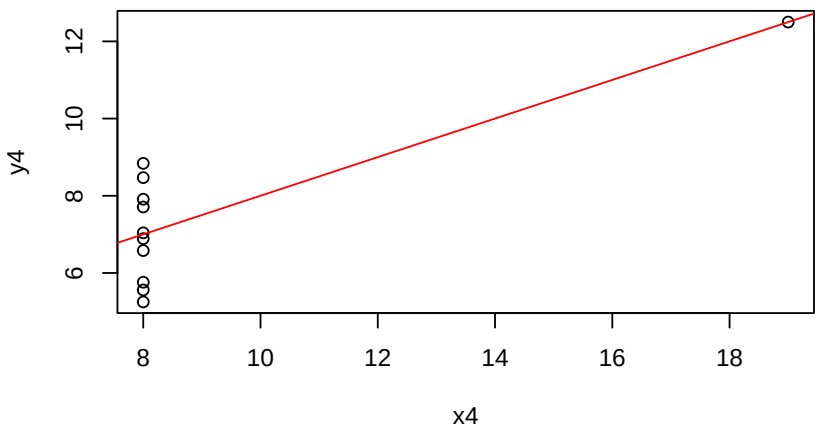
- Linearity: Eek
- Normality: cannot trust tests and confidence intervals
- Homoscedasticity: cannot trust tests and confidence intervals
- Independence of errors: Eek
- Lack of perfect multicollinearity
- No outliers: biased parameter estimates

Anscombe's quartet









All of these regressions have the same parameter estimates

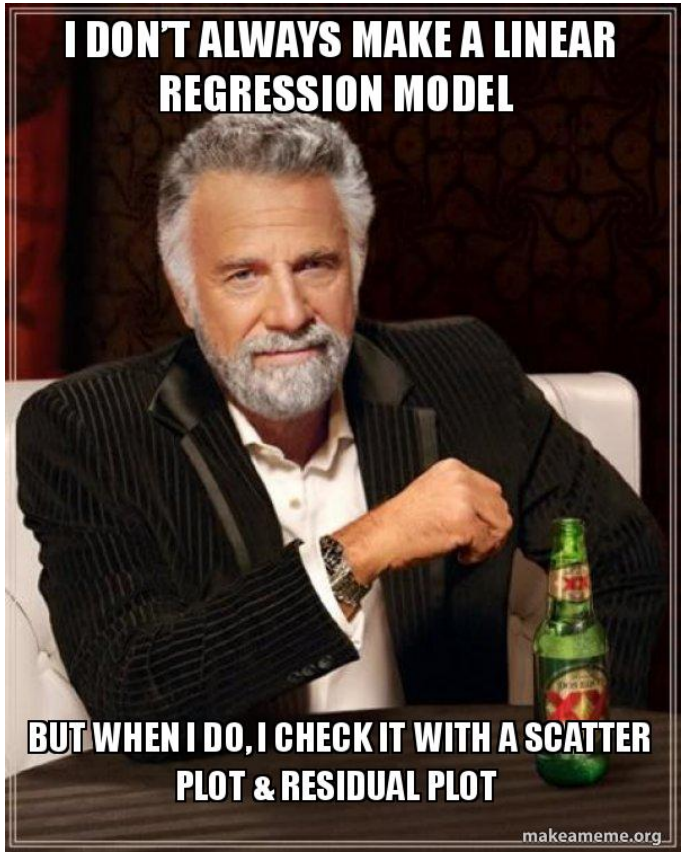
Assumption checking: methods

Tests:

- Score test for non-constant error variance `car::ncvTest`
- Durbin-Watson test for Autocorrelated errors `car::durbinWatsonTest`
- Bonferroni outlier test `car::outlierTest`
- Shapiro-Wilk normality test `shapiro.est`

Rather: **Residual plots**

- `plot(model)`
- Various packages (e.g., `car` or `DHARMa`)



Errors vs. Residuals

The true model:

$$y_i = \alpha + \sum_{k=1}^{p} x_{ik}\beta_k + \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

The fitted model:

$$y_i = \hat{\alpha} + \sum_{k=1}^{p} x_{ik}\hat{\beta}_k + \hat{\epsilon}_i$$

- $\epsilon_i = y_i - \alpha - \sum_{i=1}^{n} x_{ik}\beta$
- $\hat{\epsilon}_i = y_i - \hat{\alpha} - \sum_{i=1}^{n} x_{ik}\hat{\beta}$

Residuals are the **observed** deviation from the regression line.

In R

```
model <- lm(y~x)
residuals(model) # estimated random part
fitted(model) # estimated systematic part
```

Standardised residuals

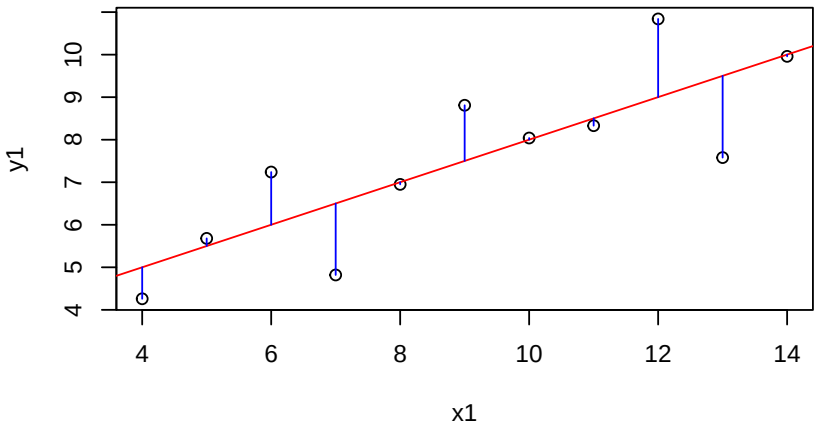
$$\frac{\widehat{\epsilon}_i}{s\sqrt{1-h_i}}, \qquad \text{where } h_i \text{ is "influence"} \tag{1}$$

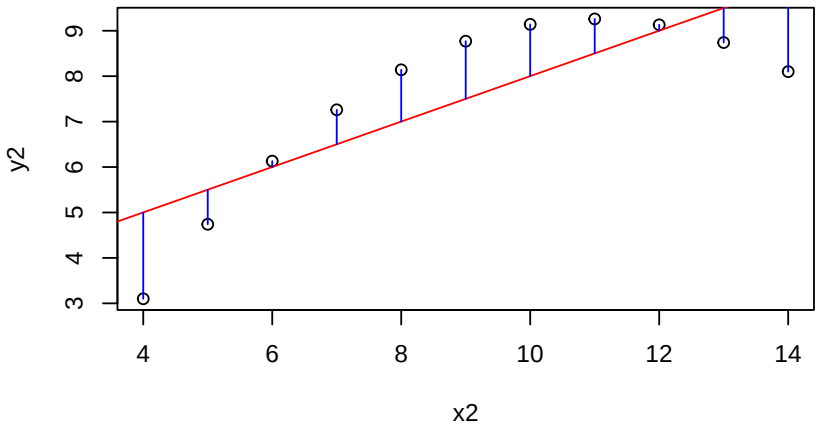
Studentized residuals

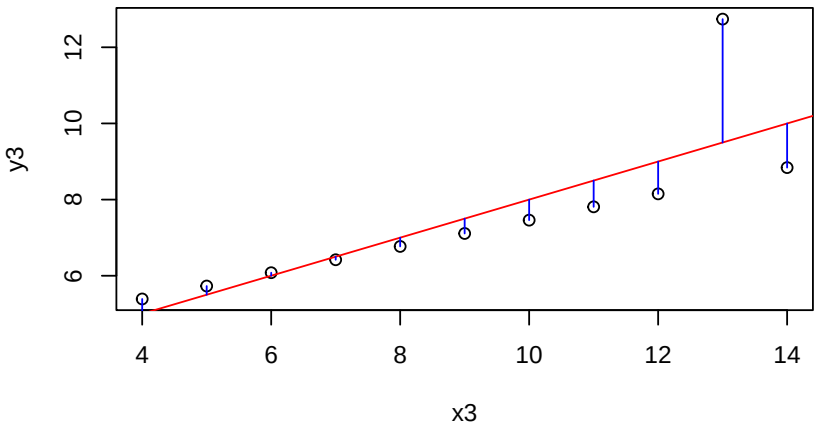
- omit observation i
- re-compute residual variance
- calculate standardised residual (with hat matrix)

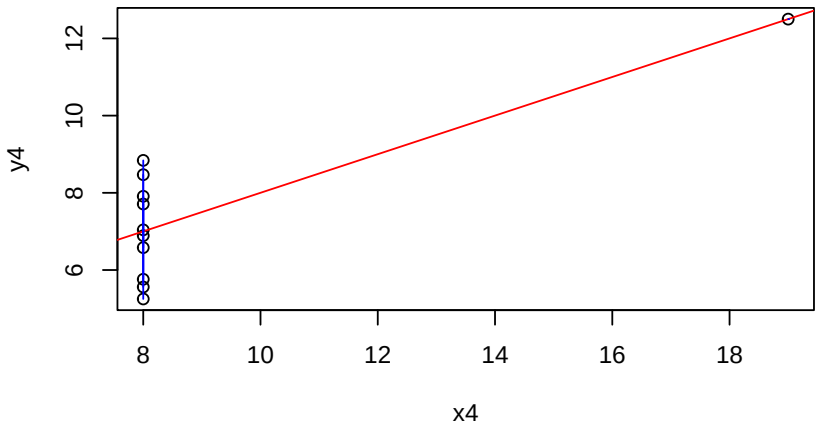
`rstand` or `rstudent`

Anscombe's quartet









Residual plots

Residual plots should have no discernible patterns.

- No curvature
- No shapes whatsoever
- No outliers
- No change in variance

This can be difficult with few observations.

Our toolbox

- Residuals versus fitted: $\hat{\epsilon}_i \; vs. \; \hat{\mu}_i$
- Observed versus theoretical quantiles: $Pr(X \leq y_i) \; vs. \; Pr(X \leq x)$
- Cook's distance plot: $\hat{\epsilon}_i \; vs. \; \hat{\mu}_i$
- Standardized residuals vs. fitted (Scale-location)
- Leverage and influence

Leverage: hat matrix

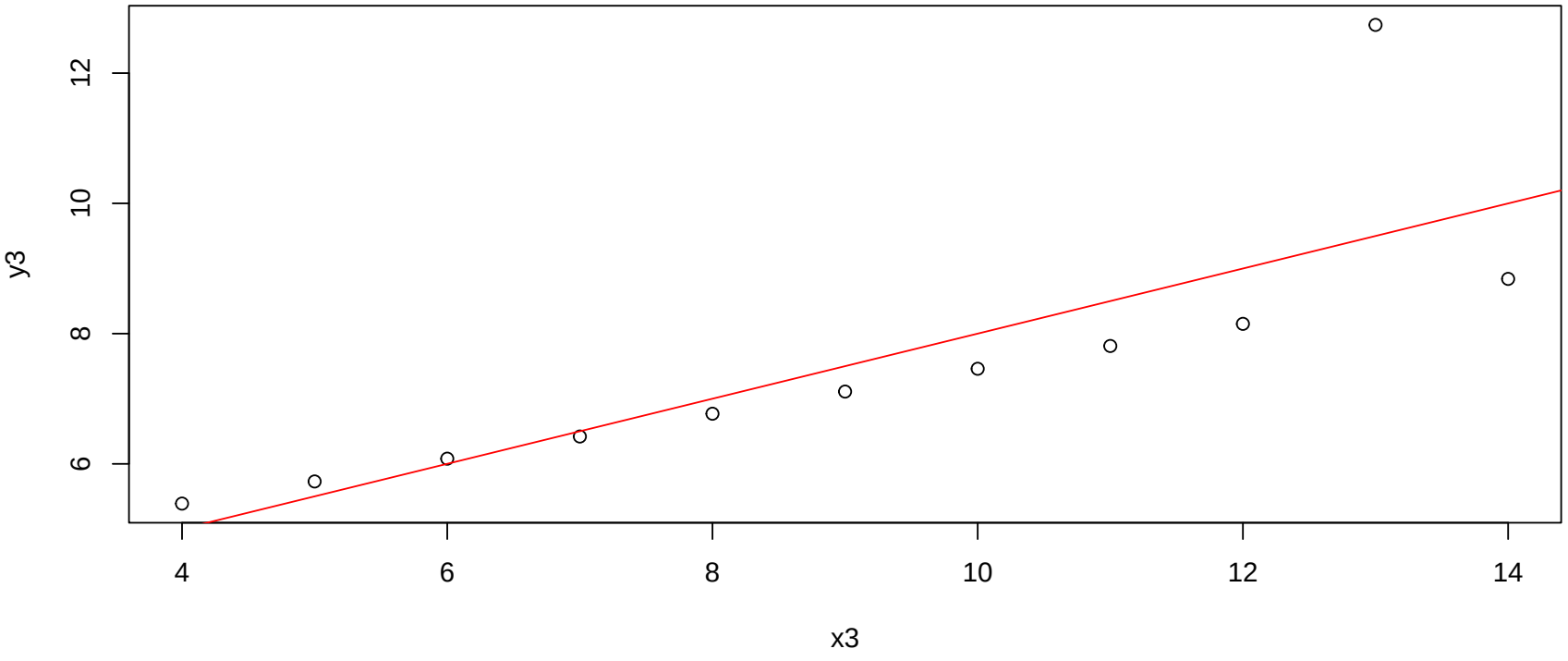
$$\hat{\mu}_i = \hat{\alpha} - \sum_{i=1}^{n} x_{ik}\hat{\beta}$$

but we can also write:

$\hat{\mu} = \mathbf{Hy}$

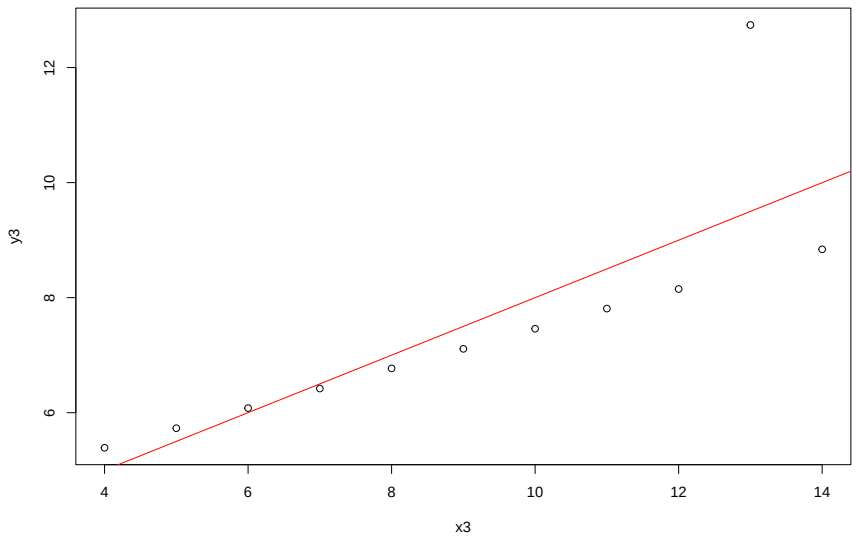
- $\mathbf{H}$ is the "hat" matrix
- $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$
- Its diagonal gives "leverage" and is between 0 and 1
- Leverage: observation that is far from others on the explanatory variable

Influence



An observation that has undue impact on the regression line.

Outliers



- Outliers are observations far away from the regression line
- Can be erroneous
- Might be real data
- Remove with caution
- Better: sensitivity analysis

Cook's distance

Cook's distance: how much the fitted values change if we remove an observation

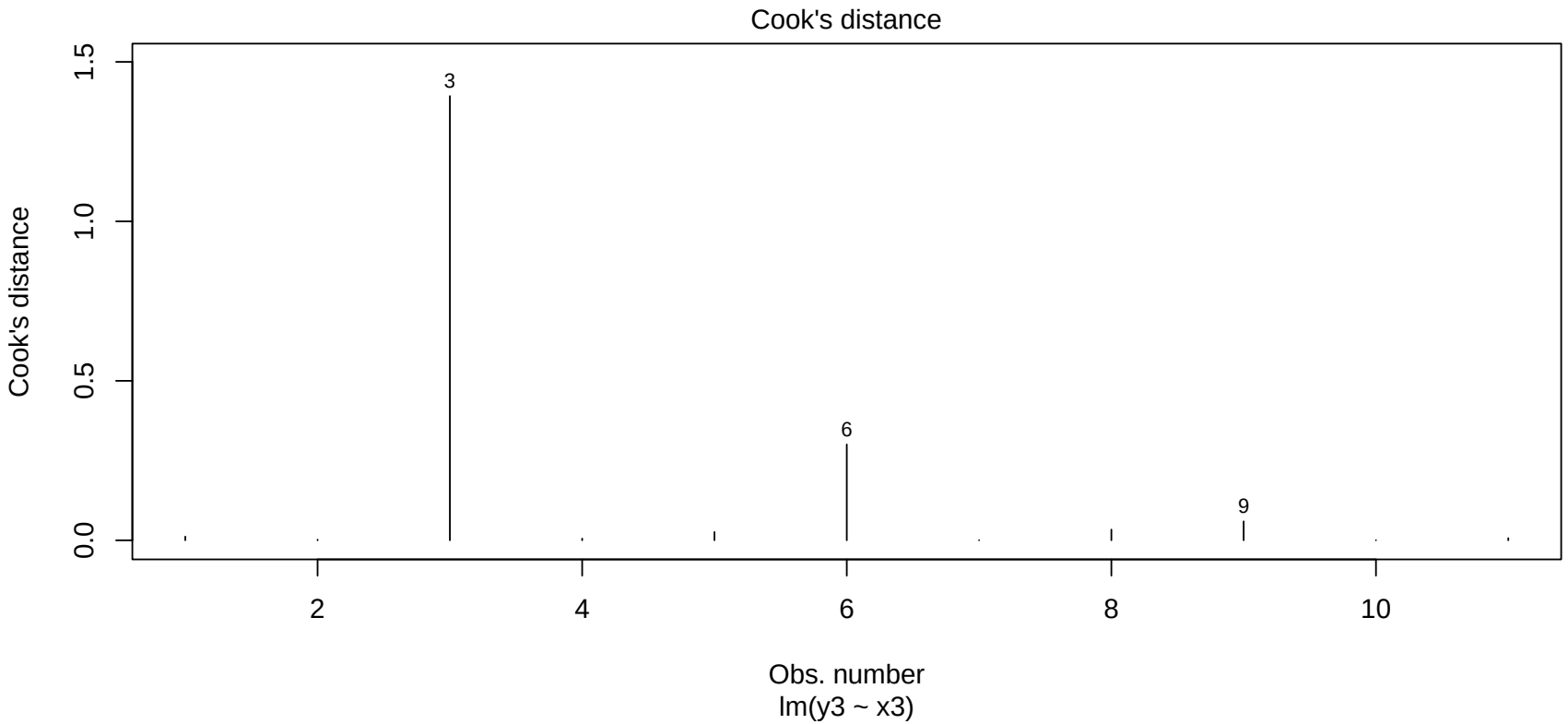
$$D_j = \frac{\sum_{i=1}^{n} (\hat{y}_i - \hat{y}_{i(-j)})^2}{\sigma^2}$$

- $\hat{y}_i$ - prediction
- $\hat{y}_{i(-j)}$ - prediction for model with data point j removed
- σ^2 - residual variance

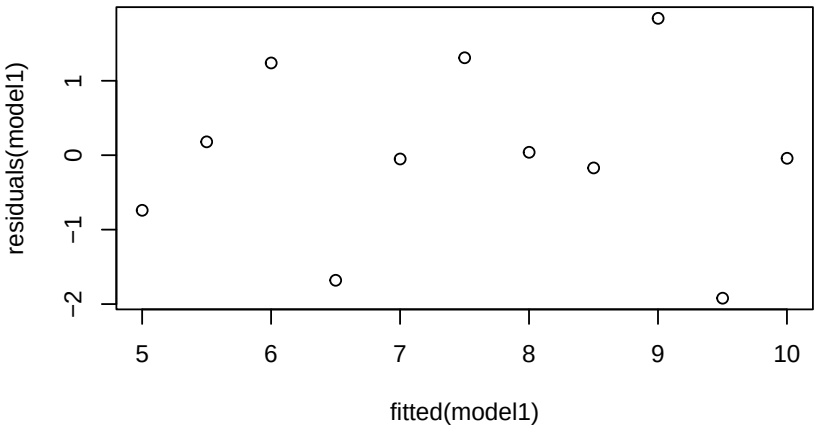
What is influential?

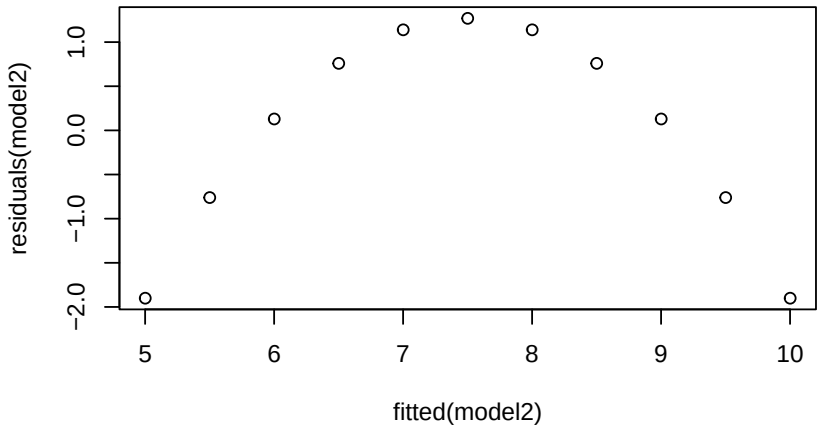
Large values of D_i mean a large influence

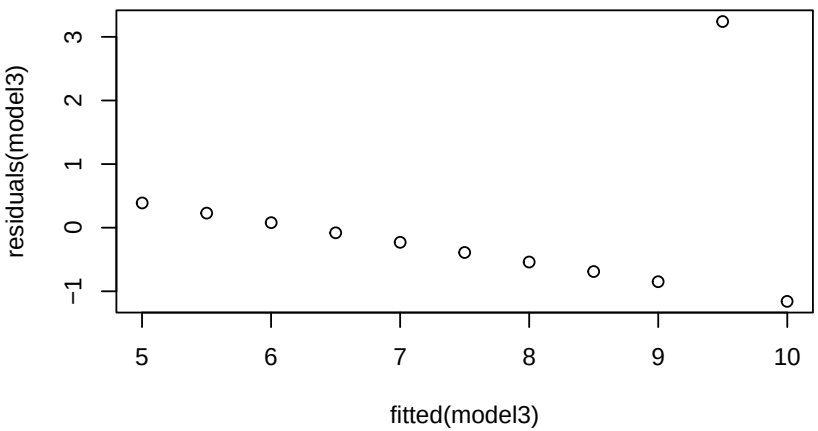
Usually $D_i > 1$, or $4/n$

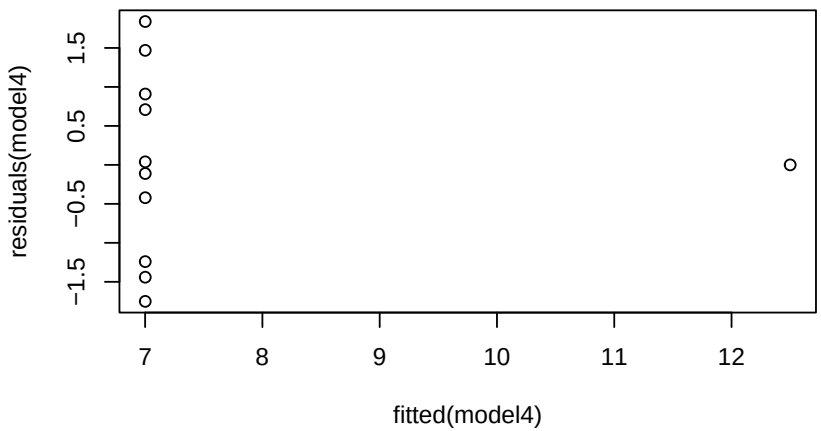


Anscombe's quartet: residuals



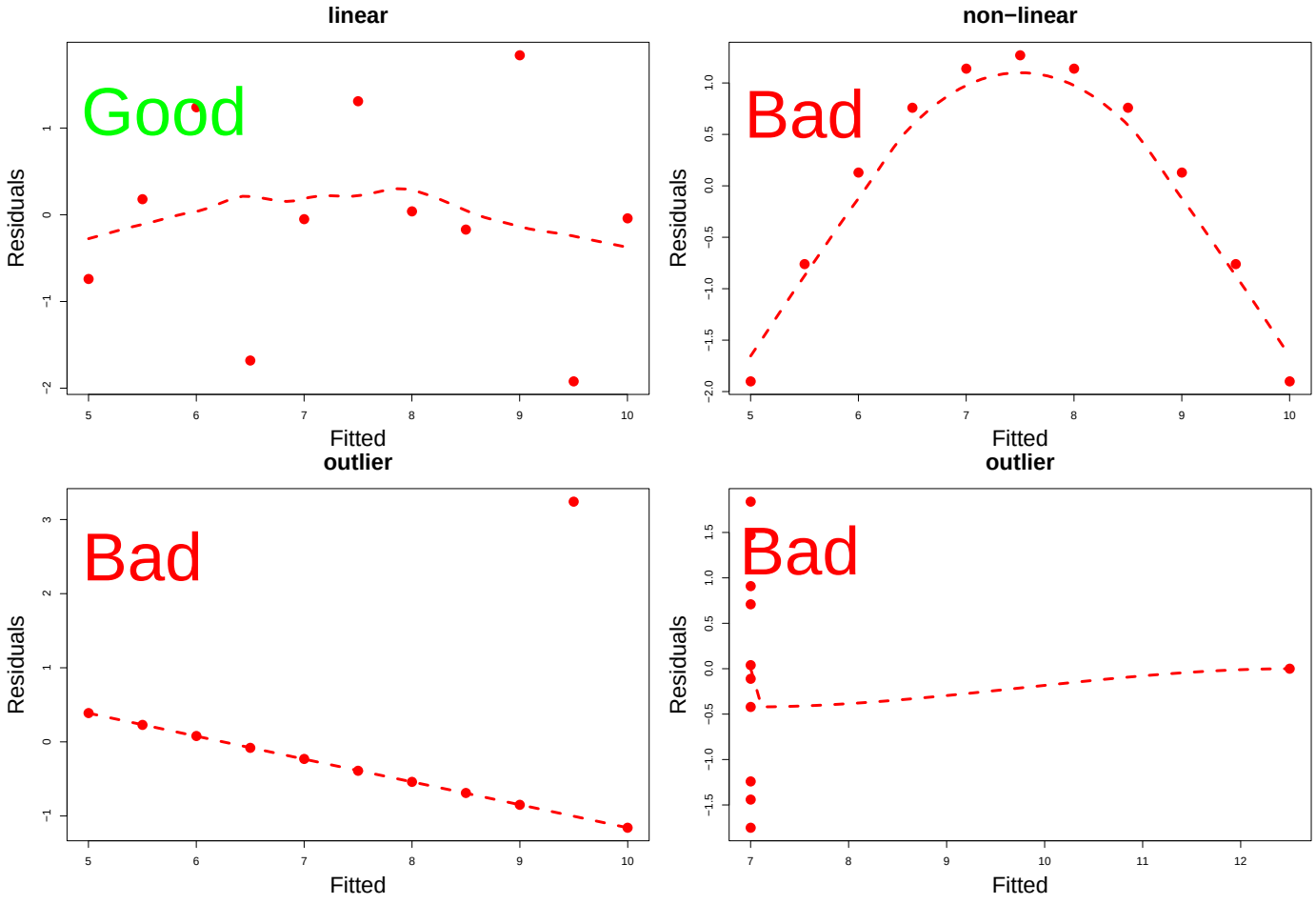




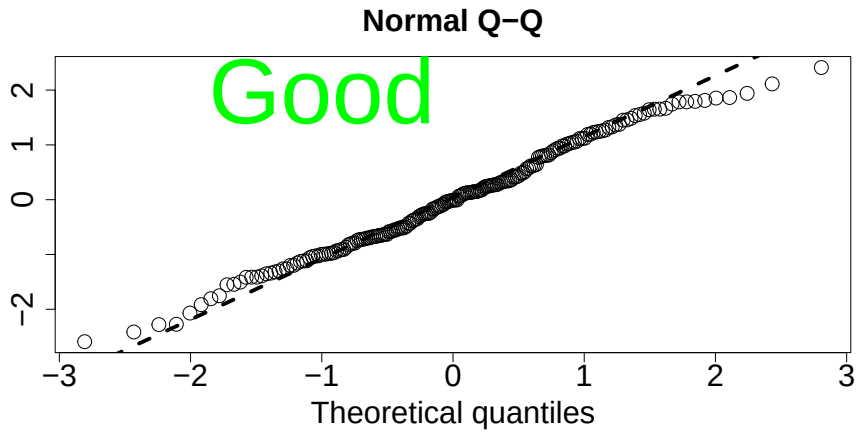


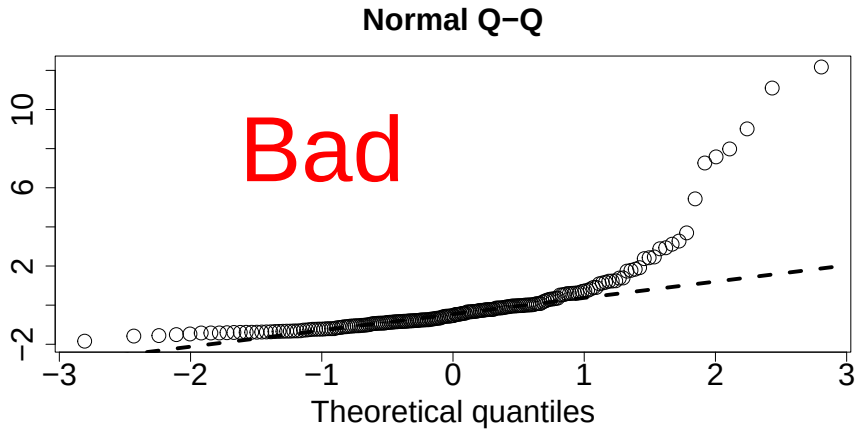
What do you see?

Residual diagnostics: residuals vs. fitted



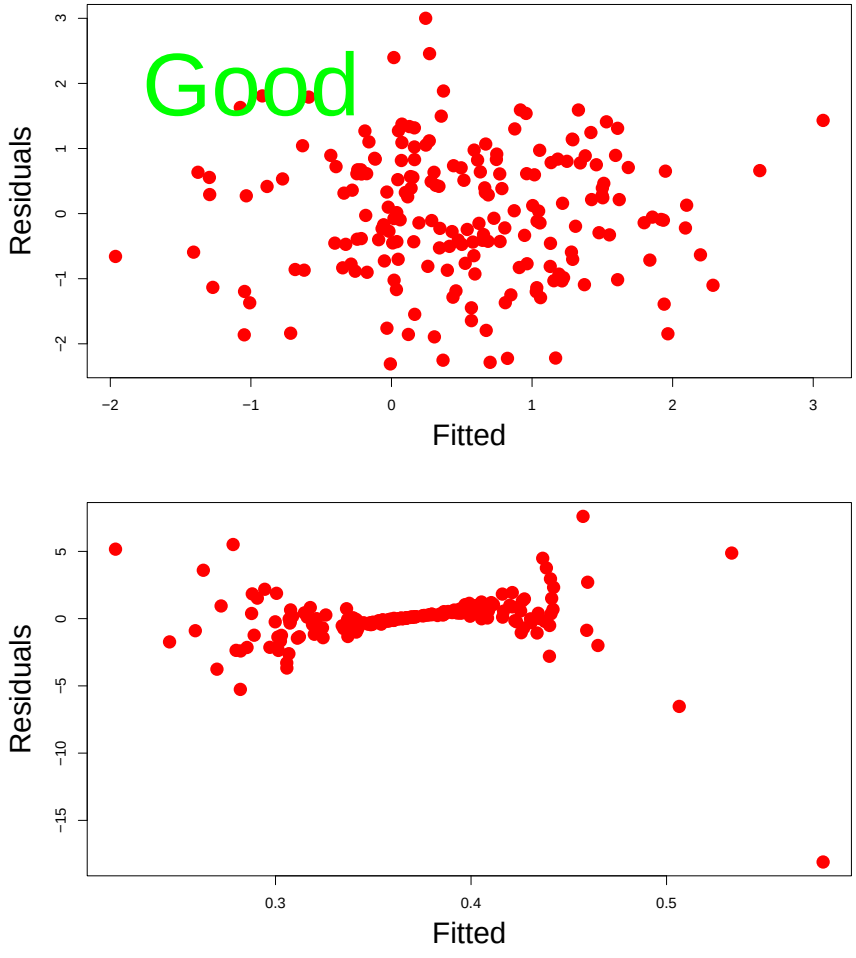
Residual diagnostics: normality with QQ-plot





1. compare residuals to theoretical quantiles
2. points should follow the line

Residual diagnostics: constant variance



1. compare residuals to fitted
2. points should be randomly distributed

Addressing assumption violations

- Curvature? Add quadratic term
- Outlier? Sensitivity analysis (if not error)
- Normality? GLM
- Constant variance? GLM

Alternative: data transformation

Data transformation

$$\mathbb{E}\{\mathsf{h}(y_i)|x_i\} = \alpha + \beta x_i \tag{2}$$

- $\mathsf{h}(\cdot)$ data transformation (e.g. $\sqrt{(\cdot)}$ or $\log(\cdot)$)
- To stabilize variance
- To normalize residuals

Use a Generalised linear model instead

Summary

Now we have a valid model, we can check **how** good it is (more on that tomorrow)