Linear models

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LECTURE OUTLINE

Topics:

- What is a linear model?
  - Regression
  - ANOVA
  - Multiple explanatory variables (ANCOVA)
- Fitting linear models to your data
- Is the fitted linear model appropriate for the data?
- How well does a fitted linear model explain the data?

Concepts:

- Types of variable: continuous versus categorical
- Terms and coefficients of a model
- Model fitting and model residuals
- Significance testing and p-values

WHAT PREDICTS THE WEIGHTS (w) OF LECTURERS?

Use *intuition* and *prior knowledge* to identify the *variables* to collect...

- Height (h) in metres
- Exercise per week (e) in hours
- Gender (g)
- Distance from home to nearest Greggs bakery (d) in metres
- Ownership of a games console (c)

. . . and build a mathematical model:

Lecturer weight (w) = *Combination* of *Independent Variables* (that determine w)

$$w = \beta_1 + \beta_2 h + \beta_3 e + \beta_4 g_m + \beta_5 d + \beta_6 c_s + \beta_7 c_a + \varepsilon$$

A combination of four components:

Response variable

Explanatory variables

$$w = \beta_1 + \beta_2\, h + \beta_3\, e + \beta_4\, g_m + \beta_5\, d + \beta_6\, c_s + \beta_7\, c_a + \varepsilon$$

Coefficients

Residuals

- A response variable (w)
- A set of explanatory variables (h, e, g, d, c)
- A set of coefficients ($\beta_1 - \beta_7$)
- A set of residuals (ε)

The Variables

Continuous variables

$$w = \beta_1 + \beta_2 h + \beta_3 e + \beta_4 g_m + \beta_5 d + \beta_6 c_s + \beta_7 c_a + \varepsilon$$

Categorical variables

- The response variable is always continuous.
- The explanatory variables can be a mix of:
  - Continuous variables: height, exercise and distance.
  - Categorical variables: gender and console ownership.
- Categorical variables or *factors* have a number of *levels*:
  - Gender has two levels (Male / Female)
  - Console has three levels (None / Sofa-based / Active)

The Terms and Coefficients

$$w = \beta_1 + \beta_2 \underbrace{h}_{\text{Height}} + \beta_3 \underbrace{e}_{\text{Exercise}} + \beta_4 \overbrace{g_m}^{\text{Gender}} + \beta_5 \underbrace{d}_{\text{Distance}} + \beta_6 \overbrace{c_s + \beta_7 c_a}^{\text{Console}} + \varepsilon$$

- Each explanatory variable is a *term* in the model
- Each term has at least one coefficient
- Continuous terms always have one coefficient
- Categorical Factors have $N - 1$ coefficients, where N is the number of levels (*where are the missing coefficients??*)

Wait! Why $N-1$ Coefficients? What is β_1?

$$w = \boxed{\beta_1} + \boxed{\beta_2\ h} + \boxed{\beta_3\ e} + \boxed{\beta_4\ g_m} + \boxed{\beta_5\ d} + \boxed{\beta_6\ c_s} + \boxed{\beta_7\ c_a} + \varepsilon$$

- Two ways of thinking about β_1:
  - Continuous variables: the *y intercept*
  - Factors: the baseline or *reference* value
- This baseline is the value for the *first levels* of each factor
- All response values start at this baseline
- All the other coefficients measure *differences* from β_1:
  - along a continuous slope
  - as an offset to a different level

So, to put it simply,

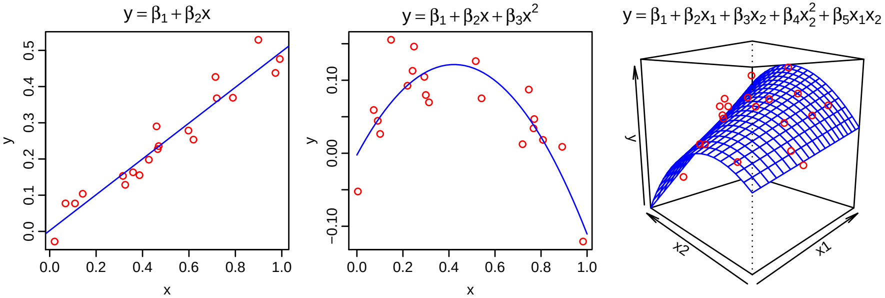
Linear models are just a sum of terms that are *linear* in the coefficients:

$$w = \beta_1 \mathbf{+} \beta_2\, h \mathbf{+} \beta_3\, e \mathbf{+} \beta_4\, g_m \mathbf{+} \beta_5\, d \mathbf{+} \beta_6\, c_s \mathbf{+} \beta_7\, c_a \mathbf{+} \varepsilon$$

What our example linear model means (literally):

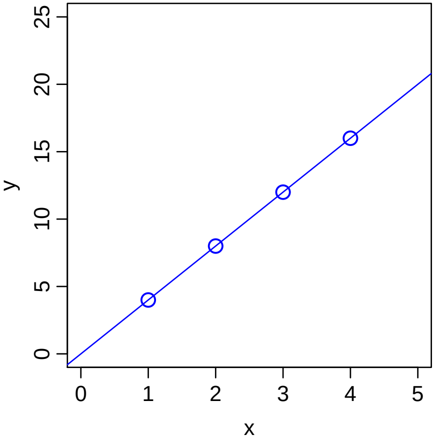
- β_1 is the baseline value of *weight* for *women* with *no games console*
- The model tells us how much to add to this baseline weight ...
  - for a height of 1.82 metres?
  - for doing 150 minutes of exercise a week?
  - for being male?
  - for living 2416 metres from a Greggs?
  - for owning an Xbox?

Examples of Linear Models



- These are *all* linear models (fitted to data)
- Each model a *sum* of *terms* that are *linear in coefficients*
- *Linear models can include curved relationships (e.g. polynomials) — this is a common point of confusion!*

Linear model with one continuous variable

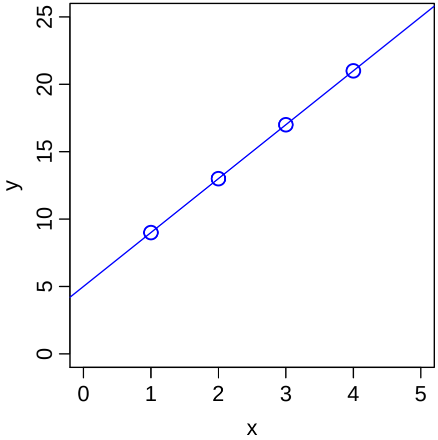


$$y = \beta_1 x$$

$$4 = 4 \times 1$$
$$8 = 4 \times 2$$
$$12 = 4 \times 3$$
$$16 = 4 \times 4$$

$$\beta_1 = 4$$

Regression with *known baseline value (intercept)*



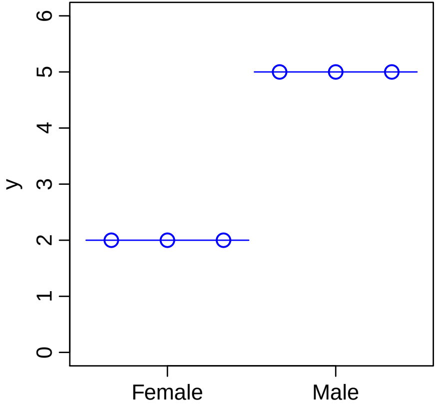
$$y = \beta_1 + \beta_2 x$$

$$9 = 5 + 4 \times 1$$
$$13 = 5 + 4 \times 2$$
$$17 = 5 + 4 \times 3$$
$$21 = 5 + 4 \times 4$$

$$\beta_1 = 5; \beta_2 = 4$$

Regression with *unknown baseline value (intercept)*

Linear model with one factor (categorical variable)



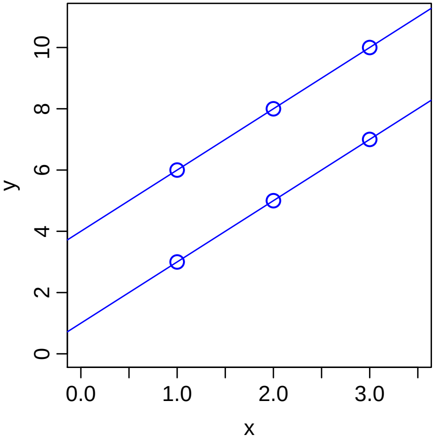
$$y = \beta_1 + \beta_2 g_m$$

$$2 = 2 + 3 \times 0$$
$$2 = 2 + 3 \times 0$$
$$2 = 2 + 3 \times 0$$
$$5 = 2 + 3 \times 1$$
$$5 = 2 + 3 \times 1$$
$$5 = 2 + 3 \times 1$$

$$\beta_1 = 2; \beta_2 = 3$$

Analysis of Variance (**ANOVA**)

Linear model with one continuous variable and one factor



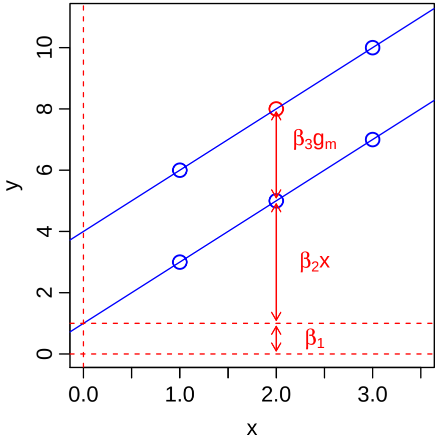
$$y = \beta_1 + \beta_2 x + \beta_3 g_m$$

$$3 = 1 + 2 \times 1 + 3 \times 0$$
$$5 = 1 + 2 \times 2 + 3 \times 0$$
$$7 = 1 + 2 \times 3 + 3 \times 0$$
$$6 = 1 + 2 \times 1 + 3 \times 1$$
$$8 = 1 + 2 \times 2 + 3 \times 1$$
$$10 = 1 + 2 \times 3 + 3 \times 1$$

$$\beta_1 = 1; \beta_2 = 2; \beta_3 = 3$$

Multiple Expanatory variables, Analysis of Covariance (**ANCOVA**)

Closer look at the ANCOVA example

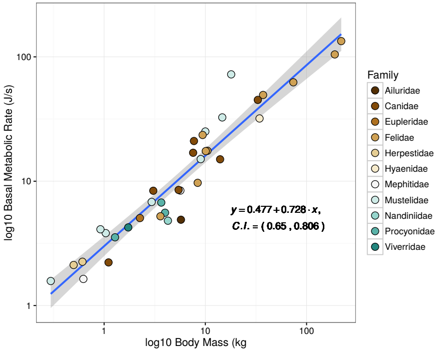


$$y = \beta_1 + \beta_2 x + \beta_3 g_m$$

$$3 = 1 + 2 \times 1 + 3 \times 0$$
$$5 = 1 + 2 \times 2 + 3 \times 0$$
$$7 = 1 + 2 \times 3 + 3 \times 0$$
$$6 = 1 + 2 \times 1 + 3 \times 1$$
$$8 = 1 + 2 \times 2 + 3 \times 1$$
$$10 = 1 + 2 \times 3 + 3 \times 1$$

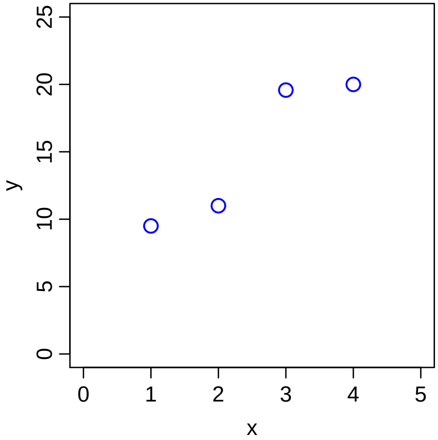
$$\beta_1 = 1; \beta_2 = 2; \beta_3 = 3$$

"FITTING" A LINEAR MODEL TO DATA



Rizzuto et al. 2017, Nat Ecol Evol

- Data always shows variation from a perfect model (deviations)
    - Missing variables (age, lab vs. field biology, time of day)
    - Measurement error
    - Stochastic variation

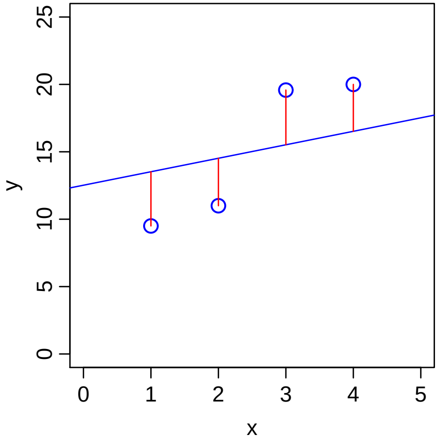


What line best passes through (describes) these data?

$$y = \beta_1 + \beta_2 x$$

$$9.50 = ? + ? \times 1$$
$$11.00 = ? + ? \times 2$$
$$19.58 = ? + ? \times 3$$
$$20.00 = ? + ? \times 4$$

Fitting a Linear Model to Data: Guess

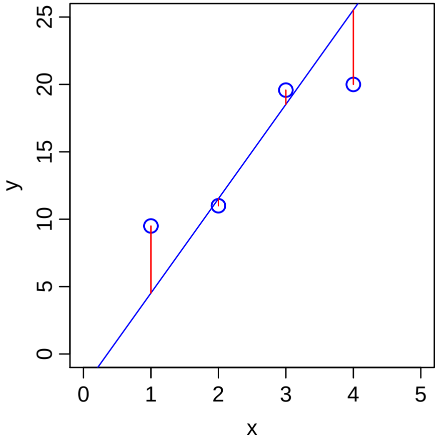


$$y = \beta_1 + \beta_2 x + \varepsilon$$

$$9.50 = 12.52 + 1 \times 1 - 4.02$$
$$11.00 = 12.52 + 1 \times 2 - 3.52$$
$$19.58 = 12.52 + 1 \times 3 + 4.06$$
$$20.00 = 12.52 + 1 \times 4 + 3.48$$

$$\beta_1 = 12.52; \beta_2 = 1$$

Fitting a Linear Model to Data: Guess again!



$$y = \beta_1 + \beta_2 x + \varepsilon$$

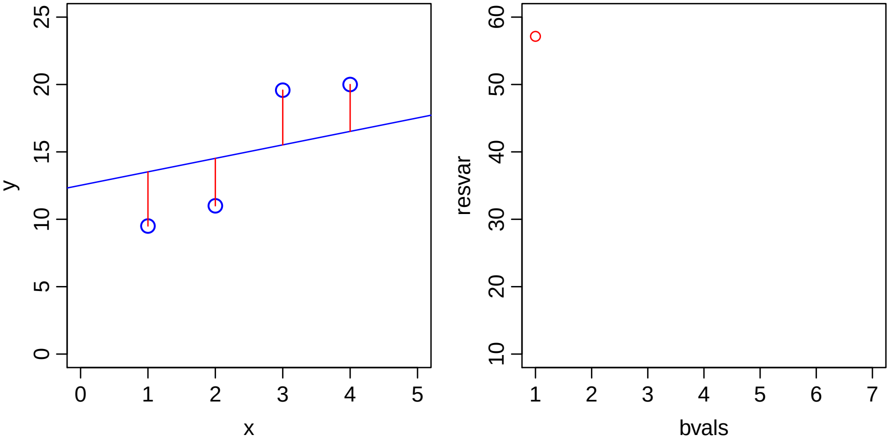
$$9.50 = -2.48 + 7 \times 1 + 4.98$$
$$11.00 = -2.48 + 7 \times 2 - 0.52$$
$$19.58 = -2.48 + 7 \times 3 + 1.06$$
$$20.00 = -2.48 + 7 \times 4 - 5.52$$

$$\beta_1 = -2.48; \beta_2 = 7$$

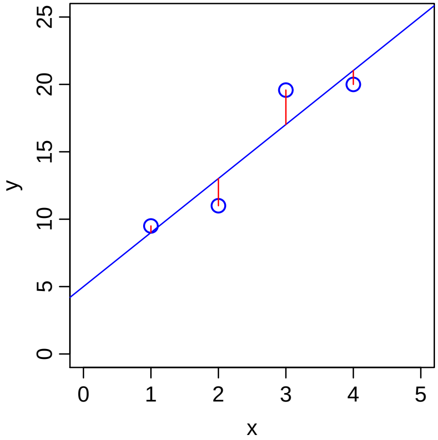
There must be a better way to do this!

Fitting a Linear Model: Least squares solution

Minimize the *sum* of the *squared residuals:*



The (Ordinary) Least Squares fitting solution



$$y = \beta_1 + \beta_2 x + \varepsilon$$

$$9.50 = 5 + 4 \times 1 + 0.50$$
$$11.00 = 5 + 4 \times 2 - 2.00$$
$$19.58 = 5 + 4 \times 3 + 2.58$$
$$20.00 = 5 + 4 \times 4 - 1.00$$

$$\beta_1 = 5; \beta_2 = 4$$

THE MATHS MAGIC UNDER THE HOOD

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

Observed values

Coefficients

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_{\text{Observed values}} = \underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix}}_{\text{Model matrix}} \underbrace{\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}}_{\text{Coefficients}} + \underbrace{\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}}_{\text{Residuals}}$$

Model matrix

Residuals

THE MATHS MAGIC UNDER THE HOOD

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

Obser | Given these ... | Co | ...find the set of these...

$$\begin{bmatrix} 9.50 \\ 11.00 \\ 19.58 \\ 20.00 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ 4 \end{bmatrix} + \begin{bmatrix} 0.50 \\ -2.00 \\ 2.58 \\ -1.00 \end{bmatrix}$$

...that minimize the sum of the squares of these.

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

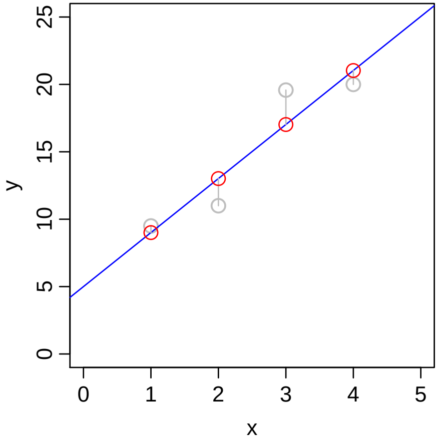
Predicted or fitted values

Coefficients

$$\begin{bmatrix} 9 \\ 13 \\ 17 \\ 21 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

Model matrix

Predicted values and Residuals



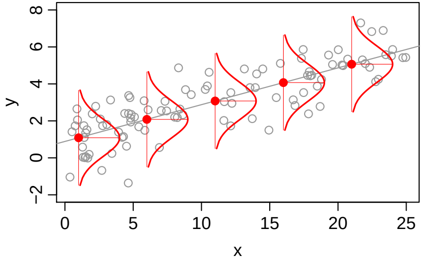
$$\hat{y} = \beta_1 + \beta_2 x$$

$$9 = 5 + 4 \times 1$$
$$13 = 5 + 4 \times 2$$
$$17 = 5 + 4 \times 3$$
$$21 = 5 + 4 \times 4$$

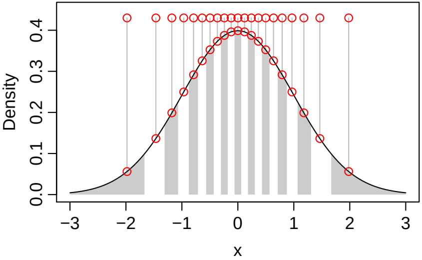
FITTING A LINEAR MODEL: ASSUMPTIONS

- Linear models are fitted with the following assumptions:
  - No measurement error in explanatory variables
  - The explanatory variables are not very highly (inter-) correlated
  - The model has constant normal variance
- **If these assumptions are not met, the model can be very wrong**
- The first two you will should consider *before* even fitting a linear model
- The last one needs can be tested *after* fitting a linear model

‘THE MODEL HAS CONSTANT NORMAL VARIANCE’

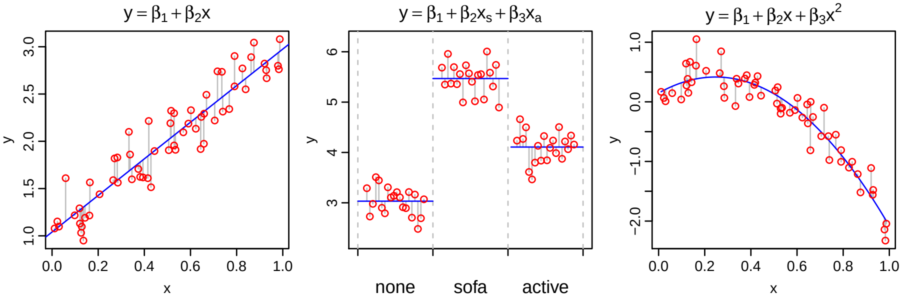


- The data have a similar spread around any predicted point in the model



- Overall, the residuals are *normally distributed*: mostly small but a few larger values
- Points *should* be spaced so as to to best capture the normal (gaussian) curve

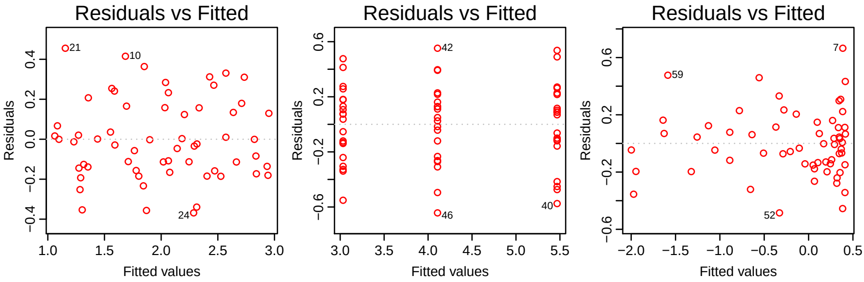
Checking if the linear model is appropriate



- All these three linear model fits appropriate for the data? Are assumptions of the linear model fit satisfied?
  - The spread of the real data around the fitted line (fitted values) is about the same across the x-axis – good
  - But are the residuals normally distributed?

DIAGNOSTICS FOR A FITTED LINEAR MODEL

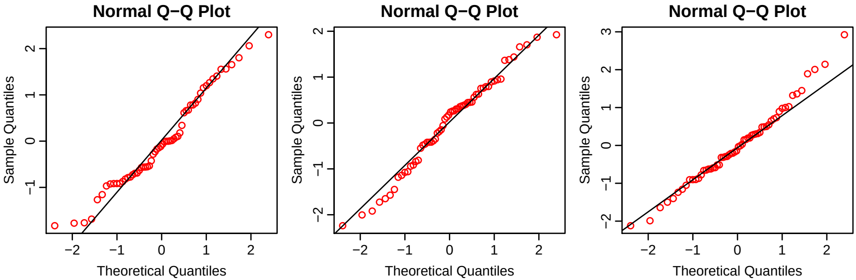
- *The spread of the real data around the fitted line (fitted values) is about the same across the x-axis*



- That is, the residuals have about the same spread irrespective of the fitted values
- The three numbered points in each plot are the three most 'badly behaved' data points.
  - Each number is the datum's row number in the R data frame

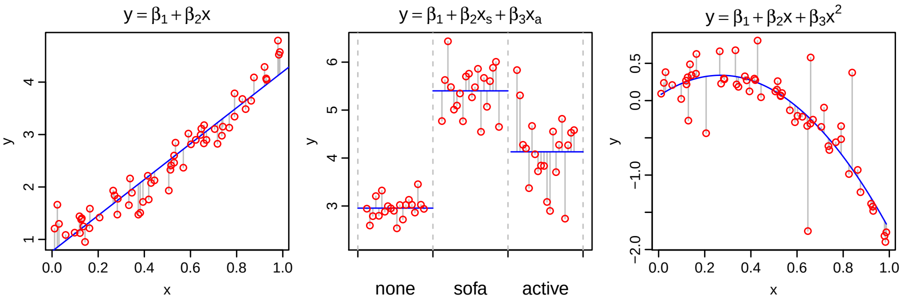
Diagnostics for a fitted linear model

- *Are the residuals normally distributed?*



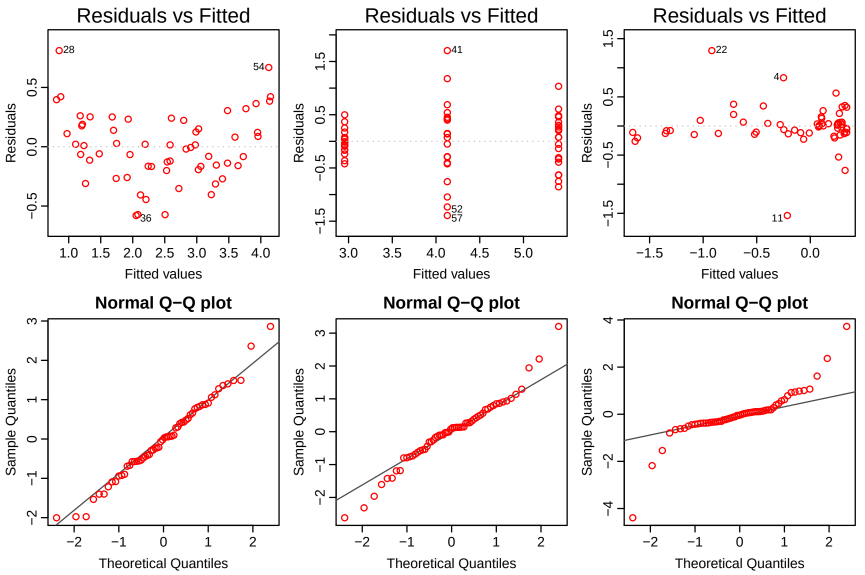
- Residuals from the first (simple regression) and third (polynomial) model's fits show some deviations from normality at the ends (high and low ends of their distributions), but it's acceptable

Three bad linear model fits



- These are three bad linear model fits
  - The data spread is not the same for all fitted values
  - The first model clearly spread is not the same for all fitted values
  - Are the residuals normally distributed?

Diagnostics for a (badly) fitted linear model



Is a linear model appropriate?

Plot the data!
Plot the residuals!

HOW EXPLANATORY IS THE FITTED LINEAR MODEL?

- The role of F and t tests in Linear Model fitting

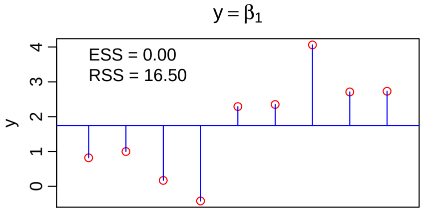
- Significance of *Terms*: F test
  - Does the model explain enough variation?
  - Does each term explain enough variation?

- Significance of *Coefficients*: t tests
  - Are the coefficients different from zero?

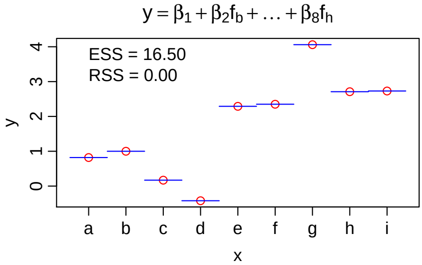
IS THE FITTED LINEAR MODEL SIGNIFICANT?: F TEST

- **Total sum of squares** (TSS): Sum of the squared difference between the observed dependent variable (y) and the mean of y ($\bar{y}$), or, TSS = $\sum_{i=1}^{n}(y_i - \bar{y})^2$
  TSS tells us how much variation there is in the dependent variable
- **Explained sum of squares** (ESS): Sum of the squared differences between the predicted y ($\hat{y}$) and $\bar{y}$, or, ESS = $\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$
  ESS tells us how much of the variation in the dependent variable our model was able to explain
- **Residual sum of squares** (RSS): Sum of the squared differences between the observed y and the predicted $\hat{y}$ (residuals), or, RSS = $\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$
  RSS tells us how much of the variation in the dependent variable our model could not explain
- Of course, TSS = ESS + RSS

Null vs. over-specified models: two endpoints

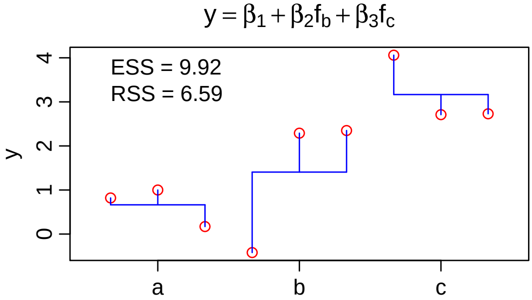


- The null model (H_0)
- Nothing is going on
- Biggest possible residuals
- Residual sum of squares (RSS) is as big as it can be



- The saturated model
- One coefficient per data point
- RSS is zero - all the sums of squares are now explained (ESS)

THE 'RIGHT' (INTERESTING) MODEL



- Added a term with three levels
- Some but not all of the residual sums of squares are explained
- Is this enough to be interesting?

Large ESS is good

Fewer coefficients is better

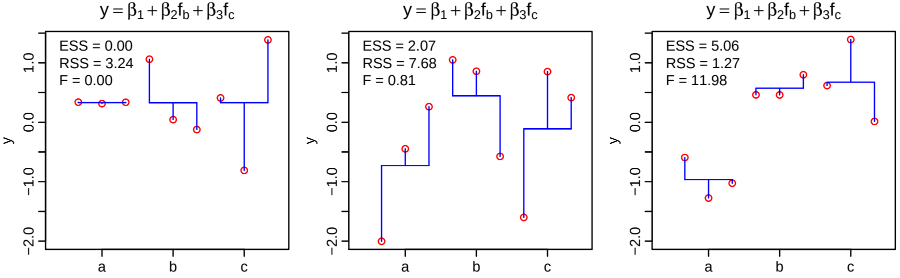
$$F = \frac{\text{ESS} \;/\; N_c}{\text{RSS} \;/\; N_r} = \frac{9.92 \;/\; 2}{6.59 \;/\; 6} = 4.52$$

Small RSS is good

Residual degrees of freedom: larger sample size is better

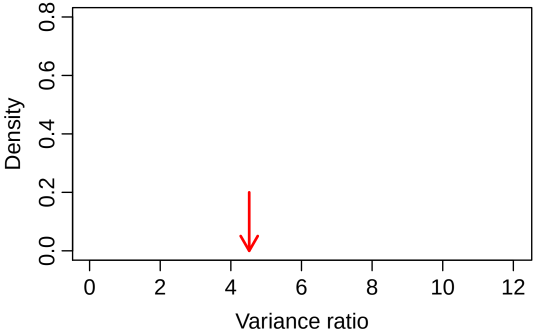
WHAT IT REALLY MEANS: F VALUE BY CHANCE?

What would be the distribution of F if nothing is going on?



- Simulate 10,000 datasets where nothing is going on (H_0 is true)
- Calculate F for each random dataset under H_1
- H_1 typically has a low F – but sometimes it is high *by chance*

What it really means: F value by chance?



- In our possibly interesting model, $F = 4.52$
- 95% of the random data sets have $F \leq 5.5$
- A model this good would be found by chance 1 in 16 times (p$=$ 0.063)
- Close, but not quite interesting (significant) enough!

ARE THE COEFFICIENTS DIFFERENT FROM ZERO?

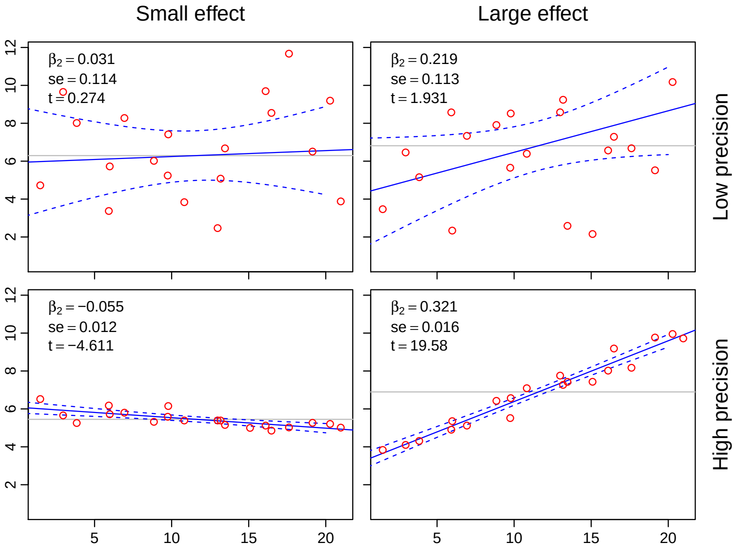
Large is good: bigger changes

$$t = \frac{\text{Effect size}}{\text{Precision}} = \frac{\text{Coefficient value}}{\text{Standard error}}$$

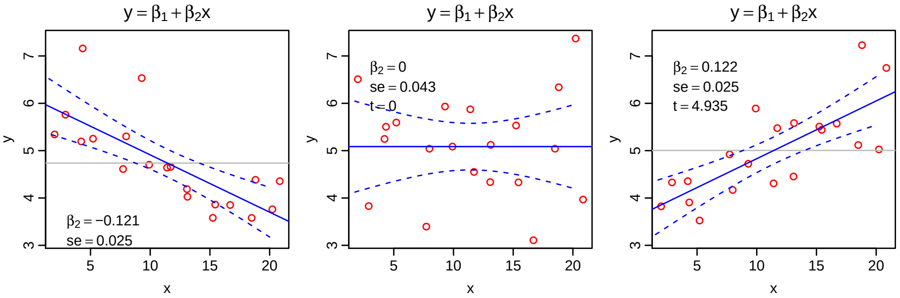
Small is good: known more precisely

- The value of a coefficient in a model is an *effect size*
- How much does changing that predictor variable change the response variable?
- The *standard error* estimates how precisely we know the value

Variation in effect size and precision

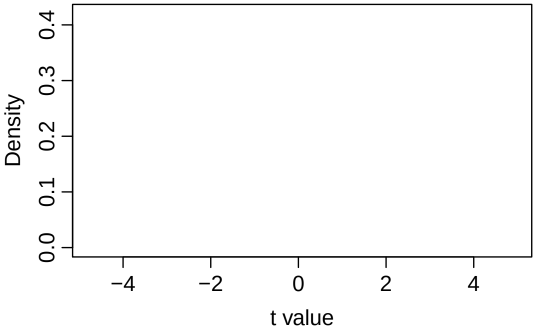


What is the distribution of t if nothing is going on?



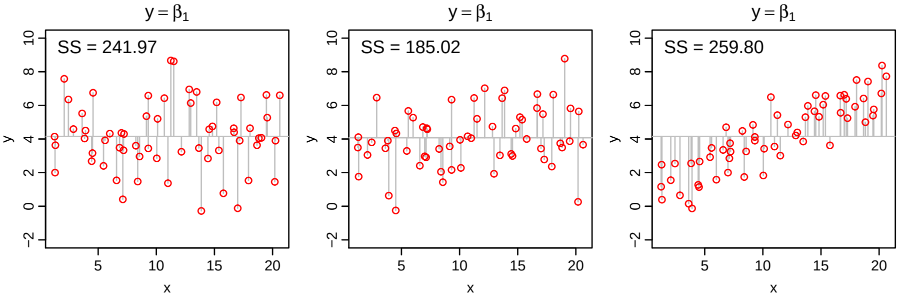
- Simulate 10,000 datasets where nothing is going on (H_0 is true)
- Calculate t for each random dataset under H_1
- H_1 typically has a t near zero but can be strongly positive or negative *by chance*

Distribution of t



- 95% of the random data sets have $t \leq \pm 2.09$
- Only the two higher precision models are expected to occur less than 1 time in 20 by chance.

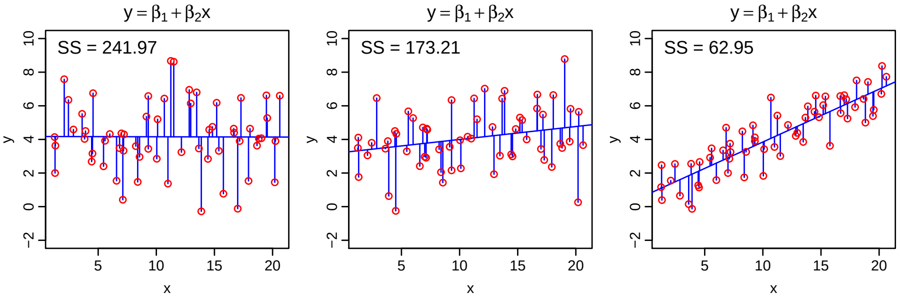
Some more examples of linear model fitting



- The null hypothesis (H_0): Nothing is going on (model is just β_1!)
- The residuals (and therefore, RSS) will get *smaller* as we include more terms to the model
- *How much smaller is enough?*

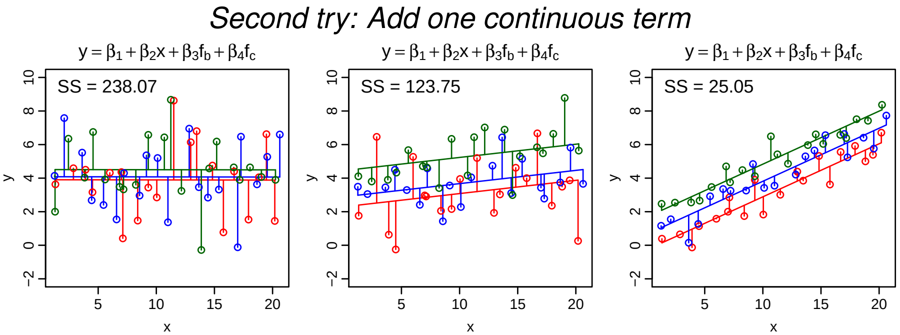
Some more examples of linear model fitting

First try: Add one continuous term



- Fitted an *alternative* model (H_1) using a predictor variable x
- i.e., Added one term (x) to the model to give (H_1)
- Do we reject H_0 and accept this new model?

Some more examples of linear model fitting



- Fitted another model (H_2) with continuous predictor x and factor f
- The RSS gets still smaller
- Is this *even* better than H_1?

Compare the three models

		Model A	Model B	Model C
H_0	Unexplained SS	241.97	185.02	259.80
	Explained SS	0	0	0
H_1	Unexplained SS	241.97	173.21	62.95
	Explained SS	0.00	11.81	196.85
H_2	Unexplained SS	238.07	123.75	25.05
	Explained SS	3.9	61.27	234.75

- Which model would you choose between H_1 and H_2?
- Every alternative model is an *alternative hypothesis*

Linear Models: Summary

- Linear models predict a continuous response variable
- A LM is a sum of terms that are linear in the coefficients capturing the effect sizes of explanatory variables
- LMs are fitted using (ordinary) least squares — minimizes sum of squared residuals
- Need to check if the fitted LM is appropriate
- Then check if the LM is explanatory
- Fitting alternative LMs = Testing alternative hypotheses