# 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 $w$)

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

# THE LINEAR MODEL

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 ($\varepsilon$)

# The Variables

$$\overbrace{w}^{\text{Continuous variables}} = \beta_1 + \beta_2\, h + \beta_3\, e + \beta_4\, g_m + \beta_5\, d + \beta_6\, c_s + \beta_7\, c_a + \varepsilon$$

Continuous variables: $w$, $h$, $e$, $d$

Categorical variables: $g_m$, $c_s$, $c_a$

- 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

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

- 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 $\beta_1$?

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

- Two ways of thinking about $\beta_1$:
    - 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 $\beta_1$:
    - along a continuous slope
    - as an offset to a different level

## So, to put it simply,

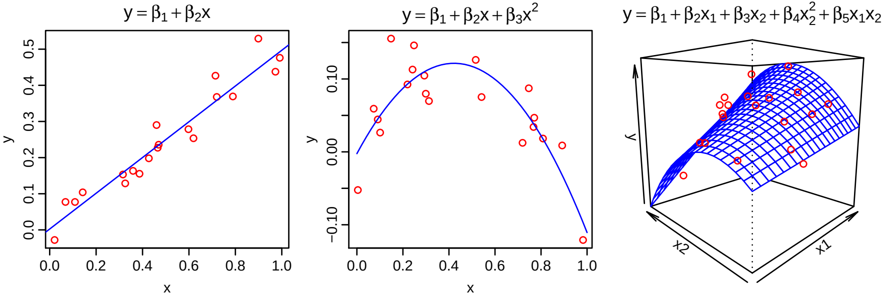
Linear models are just a sum of terms that are *linear* in the coefficients:

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

What our example linear model means (literally):

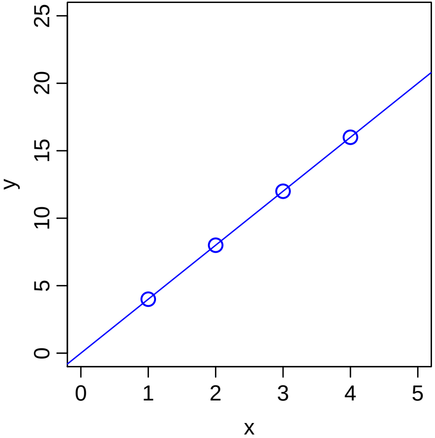
- $\beta_1$ is the baseline value of *weight* for *women* with *no games console*
- The model tells us how much to add to this baseline weight . . .
  - for a height of 1.82 metres?
  - for doing 150 minutes of exercise a week?
  - for being male?
  - for living 2416 metres from a Greggs?
  - for owning 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



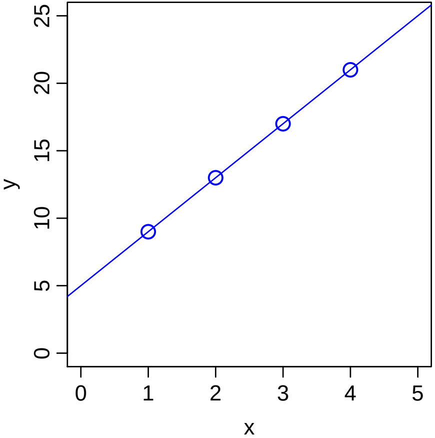

$$y = \beta_1 x$$

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

$$\beta_1 = 4$$

**Regression** with *known baseline value (intercept)*

# Linear model with one continuous variable



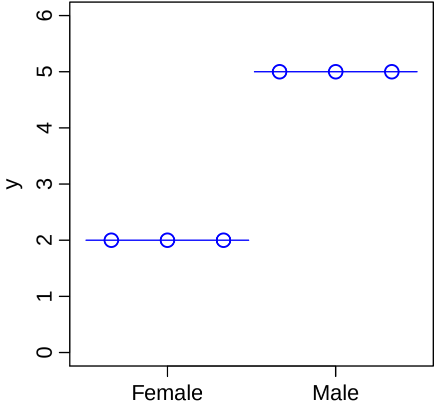

$$y = \beta_1 + \beta_2 x$$

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

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

**Regression** with *unknown baseline value (intercept)*

# Linear model with one factor (categorical variable)



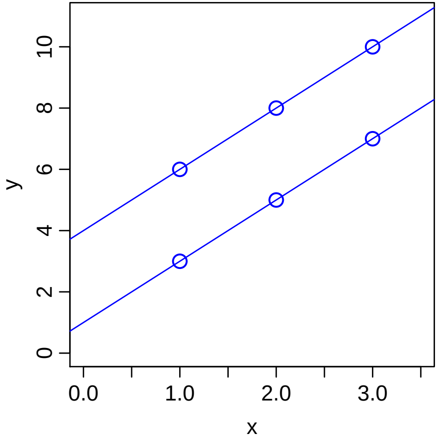

$$y = \beta_1 + \beta_2 g_m$$

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

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

*Analysis of Variance* (**ANOVA**)

# LINEAR MODEL WITH ONE CONTINUOUS VARIABLE AND ONE FACTOR

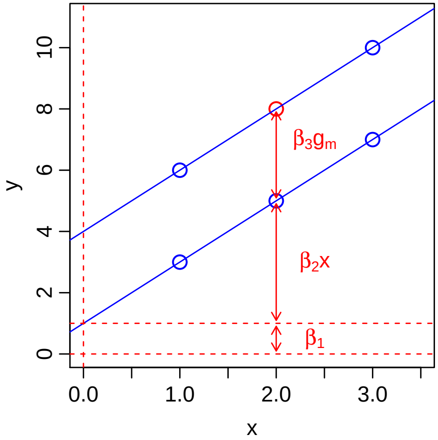



$$y = \beta_1 + \beta_2 x + \beta_3 g_m$$

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

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

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

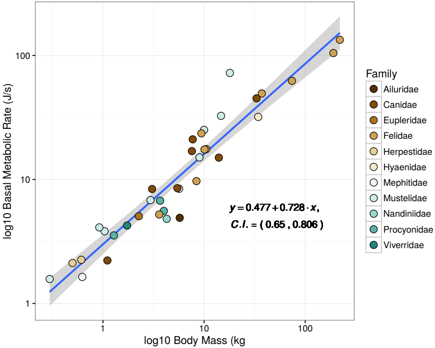



$$y = \beta_1 + \beta_2 x + \beta_3 g_m$$

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

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

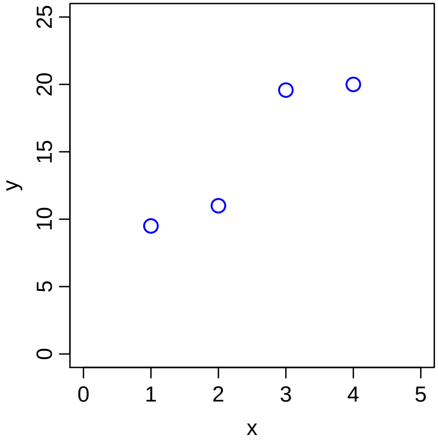
# "Fitting" a linear model to data




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

# Fitting a Linear Model to Data

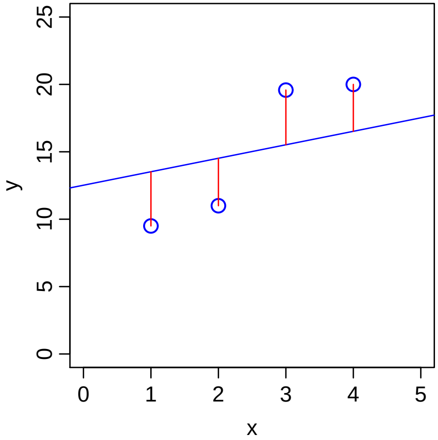



*What line best passes through (describes) these data?*

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

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

# Fitting a Linear Model to Data: Guess

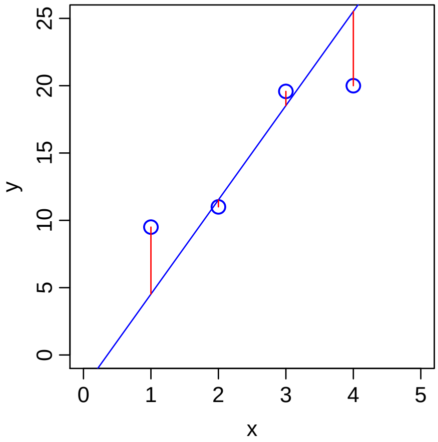



$$y = \beta_1 + \beta_2 x + \varepsilon$$

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

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

# Fitting a Linear Model to Data: Guess again!




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

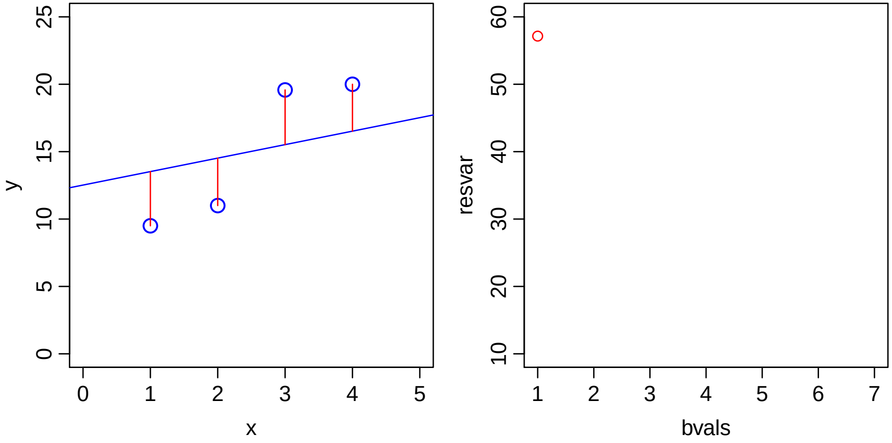
$$\begin{aligned}
9.50 &= -2.48 + 7 \times 1 + 4.98 \\
11.00 &= -2.48 + 7 \times 2 - 0.52 \\
19.58 &= -2.48 + 7 \times 3 + 1.06 \\
20.00 &= -2.48 + 7 \times 4 - 5.52
\end{aligned}$$

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

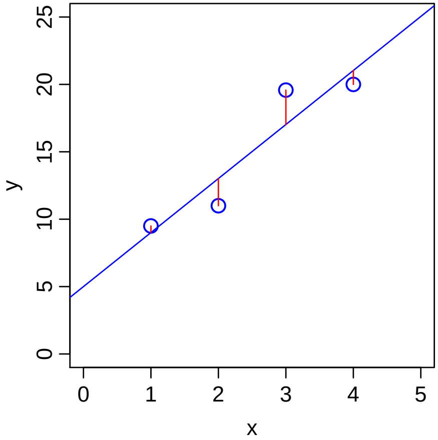
*There must be a better way to do this!*

# FITTING A LINEAR MODEL: LEAST SQUARES SOLUTION

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



# The (Ordinary) Least Squares fitting solution




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

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

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

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

Observed values

Coefficients

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}$$

Model matrix

Residuals

# The maths magic under the hood

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

Obser

Given these . . .

Co

. . . find the set of these. . .

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

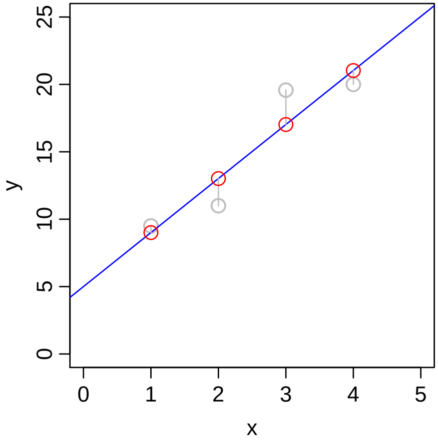
. . . that minimize the sum of the squares of these.

# The maths magic under the hood

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

$$\underbrace{\begin{bmatrix} 9 \\ 13 \\ 17 \\ 21 \end{bmatrix}}_{\text{Predicted or fitted values}} = \underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}}_{\text{Model matrix}} \underbrace{\begin{bmatrix} 5 \\ 4 \end{bmatrix}}_{\text{Coefficients}}$$

# PREDICTED VALUES AND RESIDUALS




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

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

# FITTING A LINEAR MODEL: ASSUMPTIONS

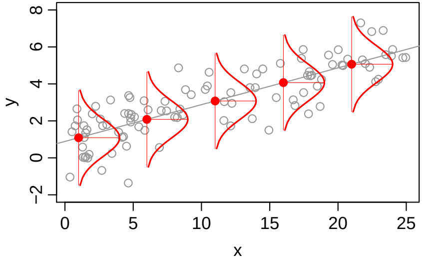
- Linear models are fitted with the following assumptions:
  - No measurement error in explanatory variables
  - The explanatory variables are not very highly (inter-) correlated
  - The model has constant normal variance

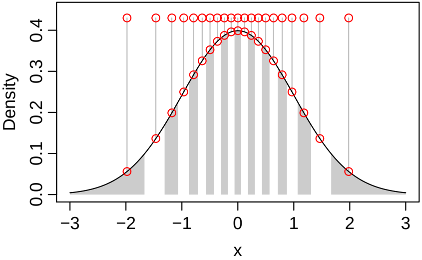
- **If these assumptions are not met, the model can be very wrong**

- 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'

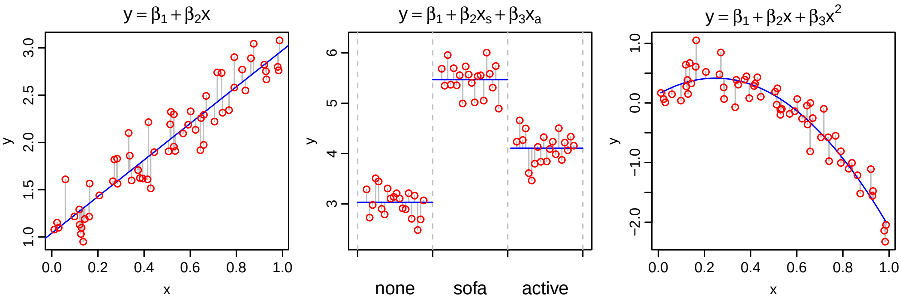



- The data have a similar spread around any predicted point in the model

- 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

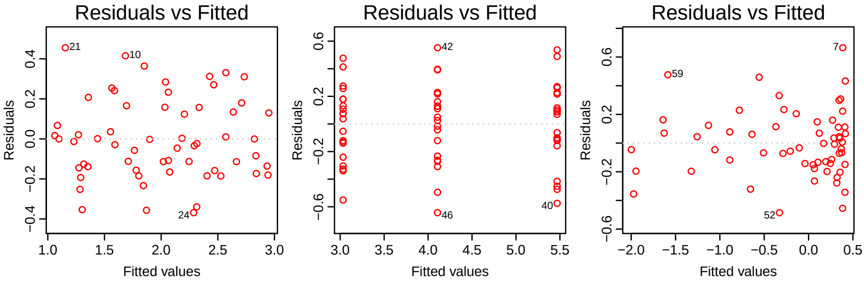
# Checking if the linear model is appropriate




- 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

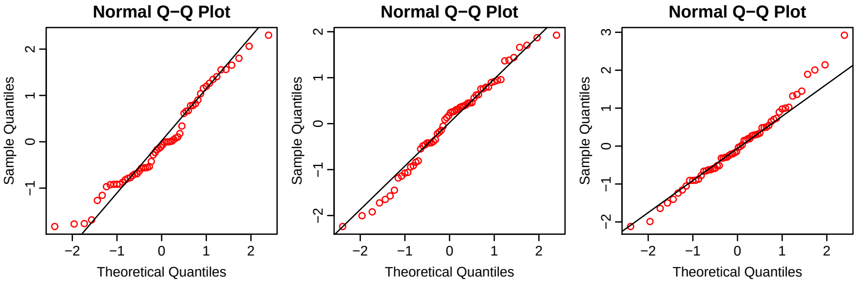
- *The spread of the real data around the fitted line (fitted values) is about the same across the x-axis*




- 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

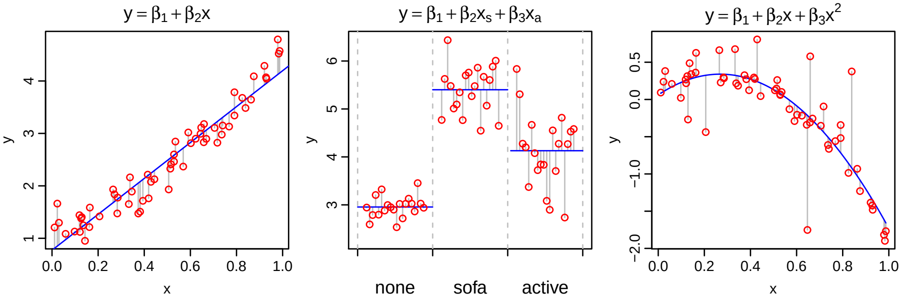
# Diagnostics for a fitted linear model

- *Are the residuals normally distributed?*



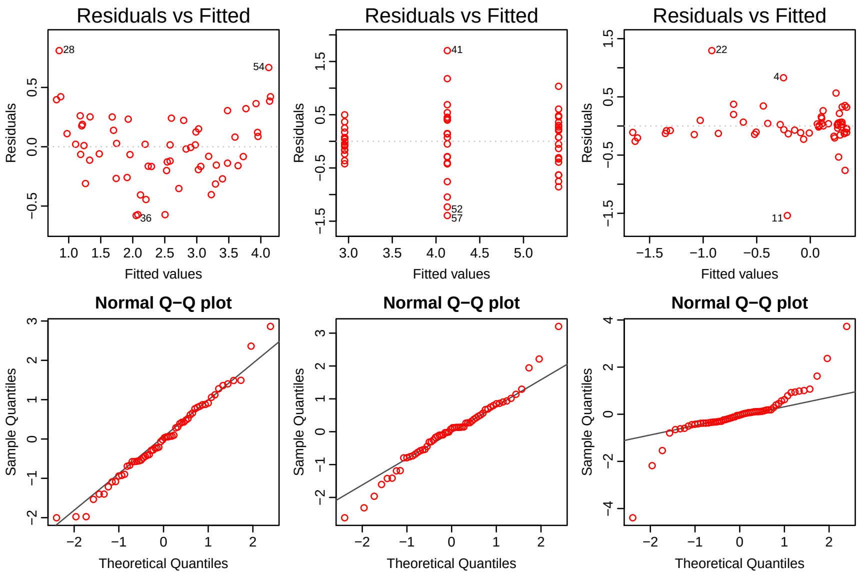

- Residuals from the first (simple regression) and third (polynomial) model's fits show some deviations from normality at the ends (high and low ends of their distributions), but it's acceptable

# 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!

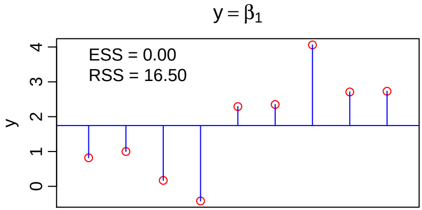
# How explanatory is the fitted linear model?

- 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?

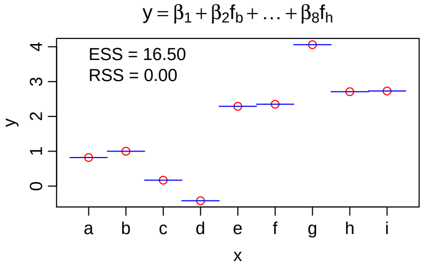
## IS THE FITTED LINEAR MODEL SIGNIFICANT?: $F$ TEST

- **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

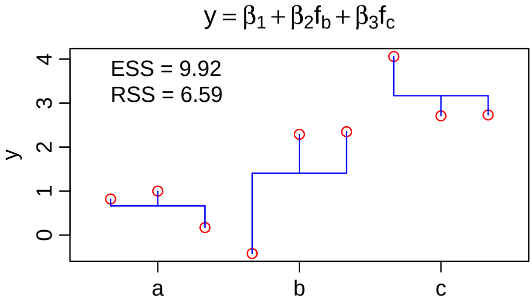



- The null model ($H_0$)
- Nothing is going on
- Biggest possible residuals
- Residual sum of squares (RSS) is as big as it can be




- 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?

# $F$ statistic of the fitted Linear Model

Large ESS is good

Fewer coefficients is better

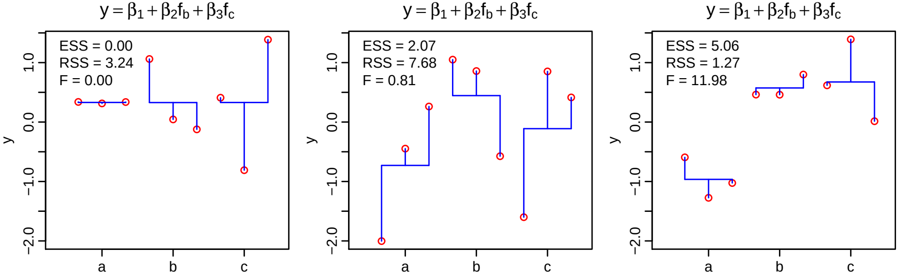
$$F = \frac{\text{ESS} \;/\; N_c}{\text{RSS} \;/\; N_r} = \frac{9.92 \;/\; 2}{6.59 \;/\; 6} = 4.52$$

Small RSS is good

Residual degrees of freedom: larger sample size is better

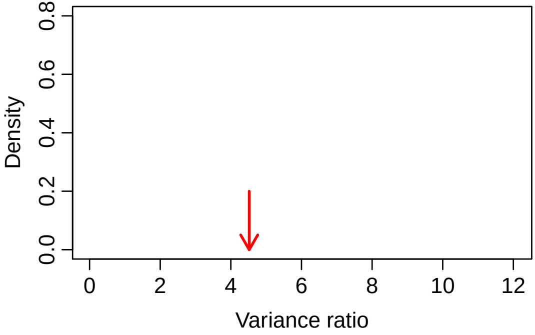
# What it really means: $F$ value by chance?

*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?

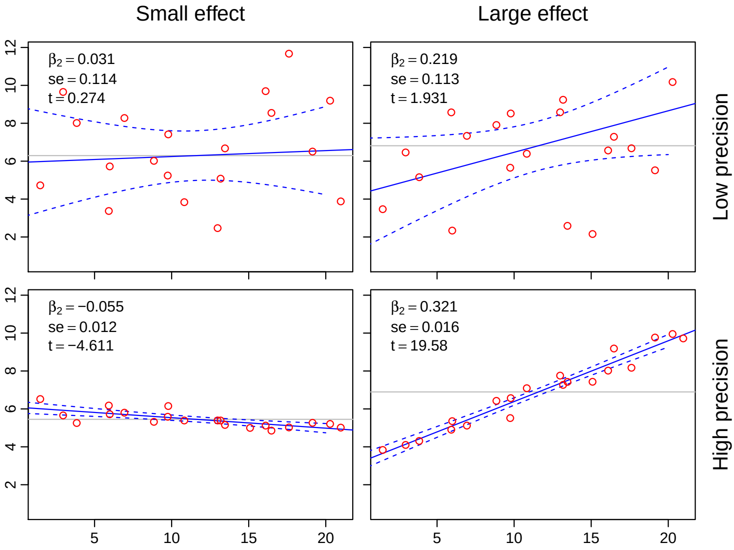
Large is good: bigger changes

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

Small is good: known more precisely

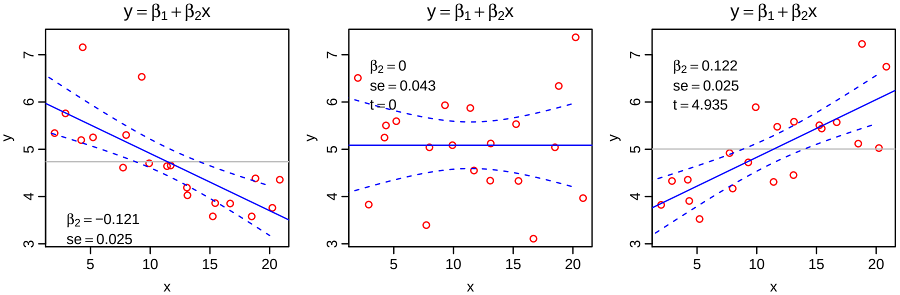
- The value of a coefficient in a model is an *effect size*
- How much does changing that predictor variable change the response variable?
- The *standard error* estimates how precisely we know the value

# Variation in effect size and precision



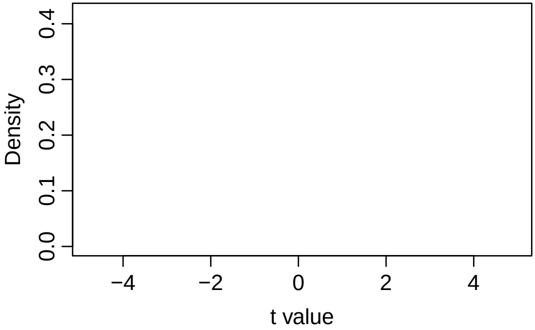
# What it really means: $t$ values by chance

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



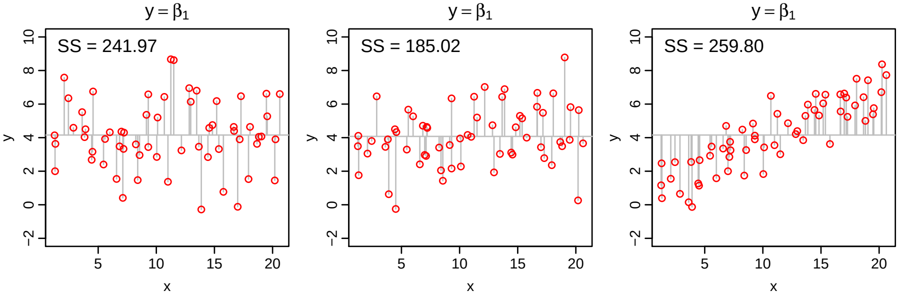

- Simulate 10,000 datasets where nothing is going on ($H_0$ is true)
- Calculate $t$ for each random dataset under $H_1$
- $H_1$ typically has a $t$ near zero but can be strongly positive or negative *by chance*

# 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.

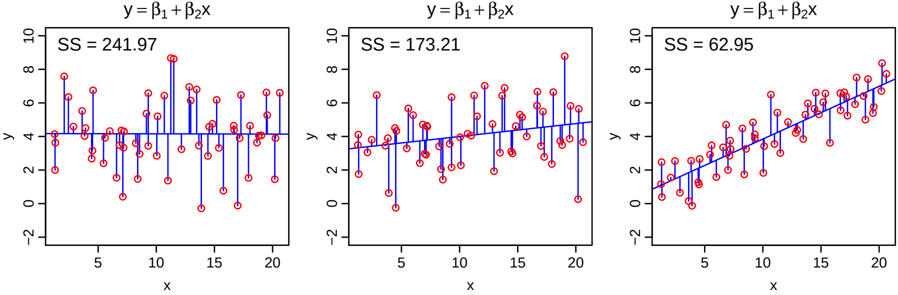
# SOME MORE EXAMPLES OF LINEAR MODEL FITTING




- The null hypothesis ($H_0$): Nothing is going on (model is just $\beta_1$!)
- 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

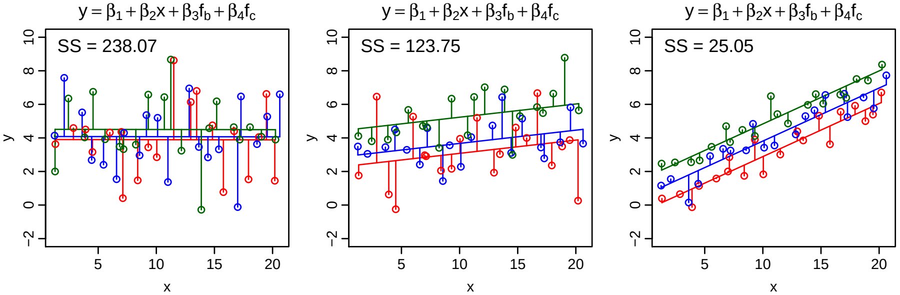
*First try: Add one continuous term*




- 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

*Second try: Add one continuous term*




- 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