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?

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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...

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. . . and build a mathematical model:

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

What predicts the weights (w) of lecturers?

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

- Height (h) in metres
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. . . and build a mathematical model:

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

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 (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.

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

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THE VARIABLES

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

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- Categorical variables or *factors* have a number of *levels*:

The Variables

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Continuous variables: w, h, e, d

Categorical variables: g_m, c_s, c_a

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- 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

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

- Each explanatory variable is a *term* in the model

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Gender: g_m — Console: c_s, c_a

Height: h — Exercise: e — Distance: d

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The Terms and Coefficients

Gender Console

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Height Exercise Distance

- 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?

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

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  - Continuous variables: the *y intercept*
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- 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:

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- β_1 is the baseline value of *weight* for *women* with *no games console*
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    - for doing 150 minutes of exercise a week?

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  - for being male?

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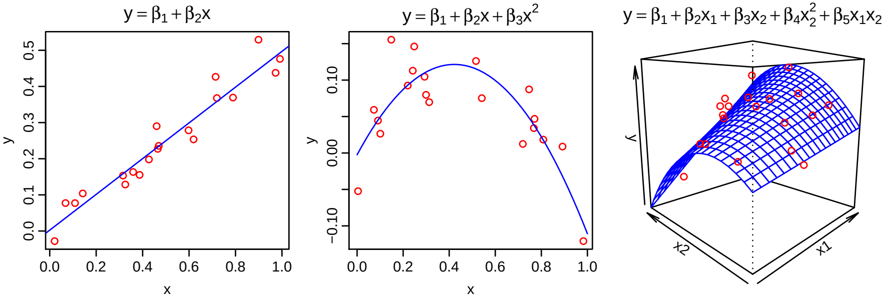
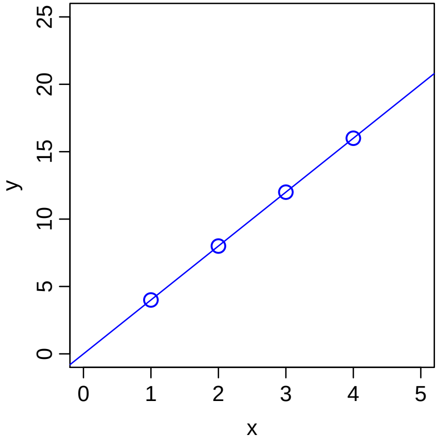
  - for doing 150 minutes of exercise a week?
  - for being male?
  - for living 2416 metres from a Greggs?
  - for owning an Xbox?

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

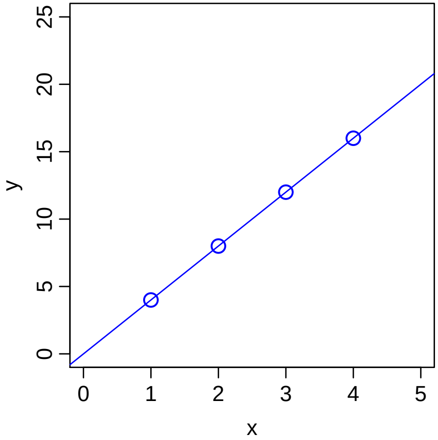


$$y = \beta_1 x$$

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

$$\beta_1 = 4$$

Linear model with one continuous variable



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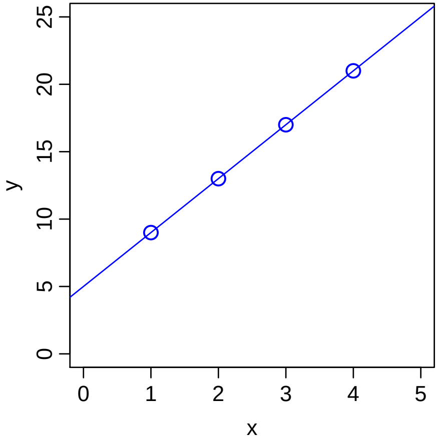
Regression with *known baseline value (intercept)*

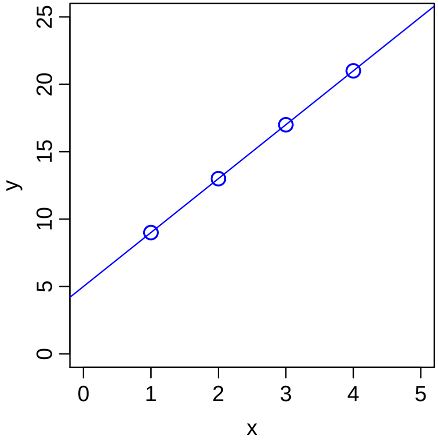
LINEAR MODEL WITH ONE CONTINUOUS VARIABLE



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

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

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



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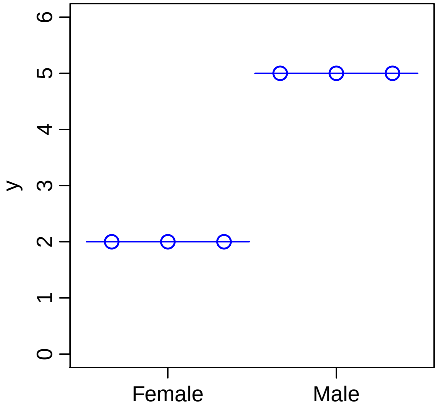
Regression with *unknown baseline value (intercept)*

Linear model with one factor (categorical variable)



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

$$2 = 2 + 3 \times 0$$
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$$2 = 2 + 3 \times 0$$
$$5 = 2 + 3 \times 1$$
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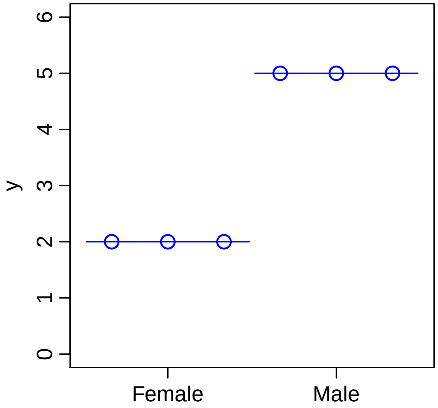
$$\beta_1 = 2; \beta_2 = 3$$

Linear model with one factor (categorical variable)



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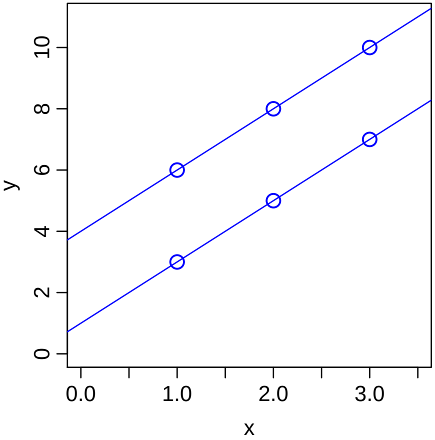
Analysis of Variance (**ANOVA**)

Linear model with one continuous variable and one factor

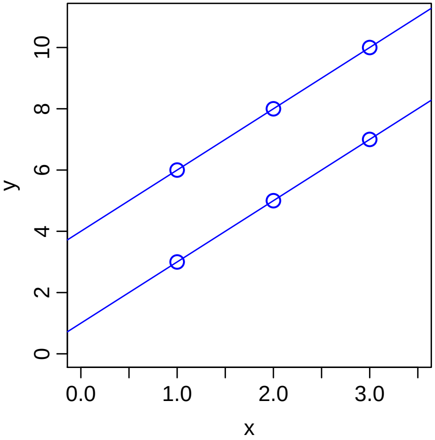


$$y = \beta_1 + \beta_2 x + \beta_3 g_m$$

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

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

Linear model with one continuous variable and one factor



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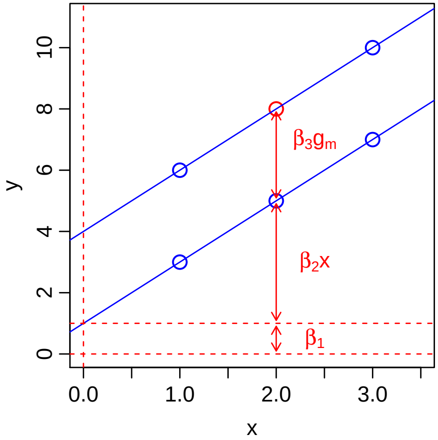
Multiple Expanatory variables, Analysis of Covariance (**ANCOVA**)

Closer look at the ANCOVA example



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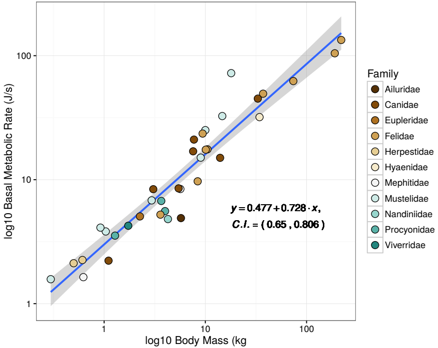
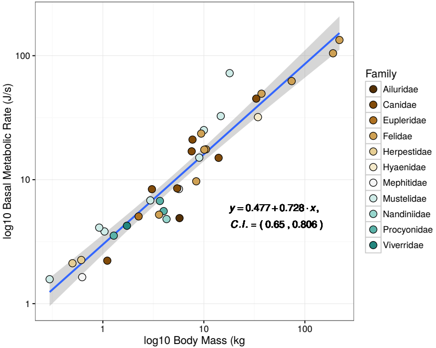
“FITTING” A LINEAR MODEL TO DATA



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)

“Fitting” a linear model to data



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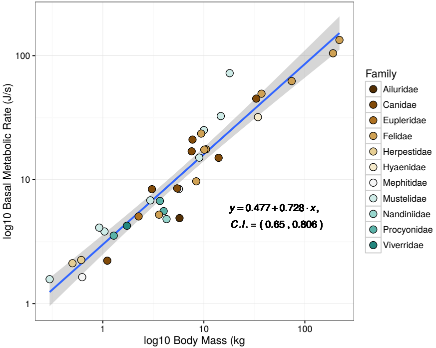

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  - Measurement error
  - Stochastic variation

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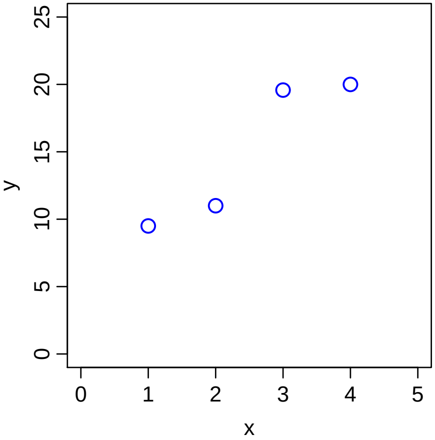

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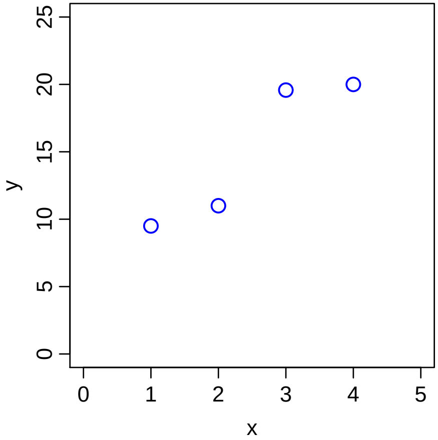

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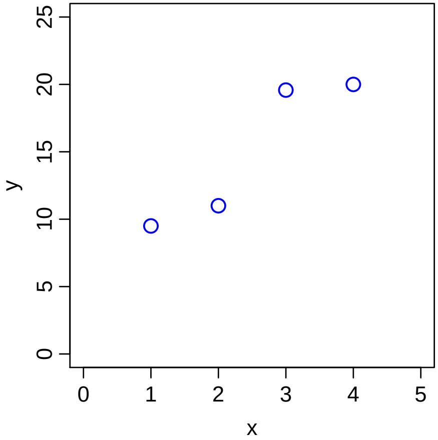
Fitting a Linear Model to Data

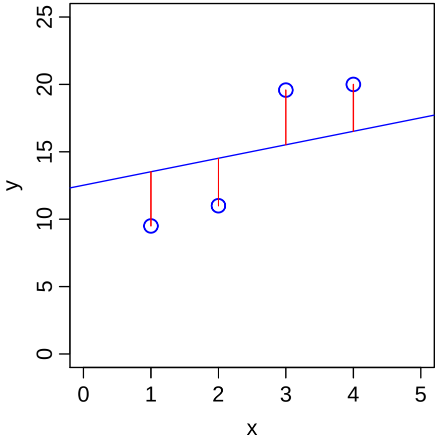


What line best passes through (describes) these data?

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

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

Fitting a Linear Model to Data: Guess

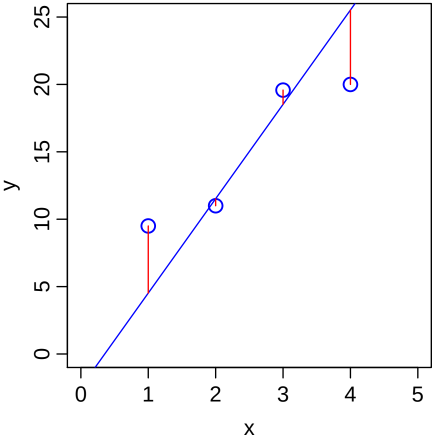


$$y = \beta_1 + \beta_2 x + \varepsilon$$

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

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

Fitting a Linear Model to Data: Guess again!

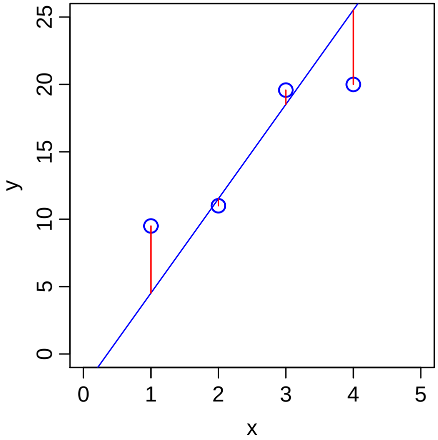


$$y = \beta_1 + \beta_2 x + \varepsilon$$

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

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

Fitting a Linear Model to Data: Guess again!



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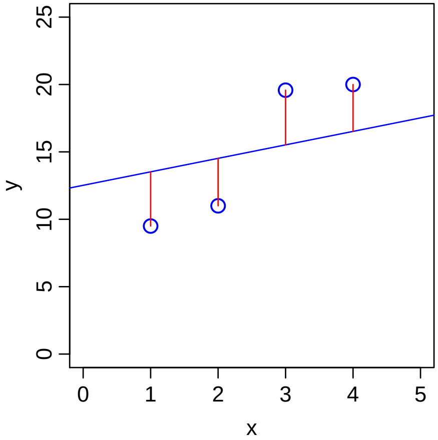
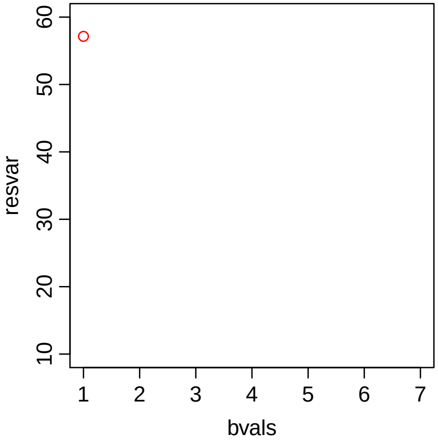
$$\beta_1 = -2.48; \beta_2 = 7$$

There must be a better way to do this!

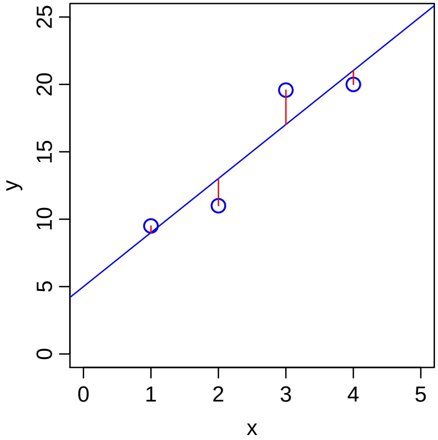
Fitting a Linear Model: Least squares solution

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

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

Observed values

Coefficients

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

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$$\underbrace{\begin{bmatrix} 9.50 \\ 11.00 \\ 19.58 \\ \color{red}{20.00} \end{bmatrix}}_{\text{Observed values}} = \underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ \color{red}{1} & \color{red}{4} \end{bmatrix}}_{\text{Model matrix}} \underbrace{\begin{bmatrix} \color{red}{5} \\ \color{red}{4} \end{bmatrix}}_{\text{Coefficients}} + \underbrace{\begin{bmatrix} 0.50 \\ -2.00 \\ 2.58 \\ \color{red}{-1.00} \end{bmatrix}}_{\text{Residuals}}$$

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

Given these . . .

. . . 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

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

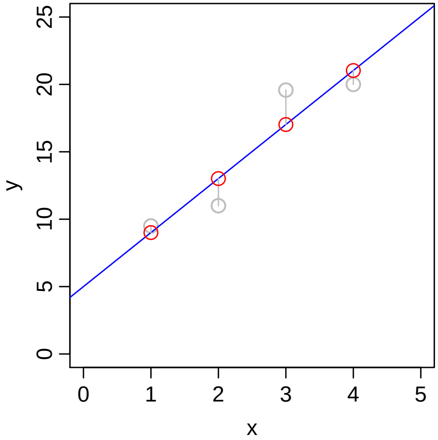
Predicted or fitted values

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

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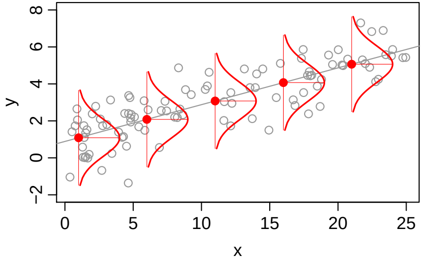
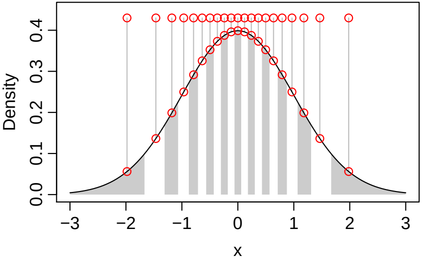
- The last one needs can be tested *after* fitting a linear model

‘THE MODEL HAS CONSTANT NORMAL VARIANCE’

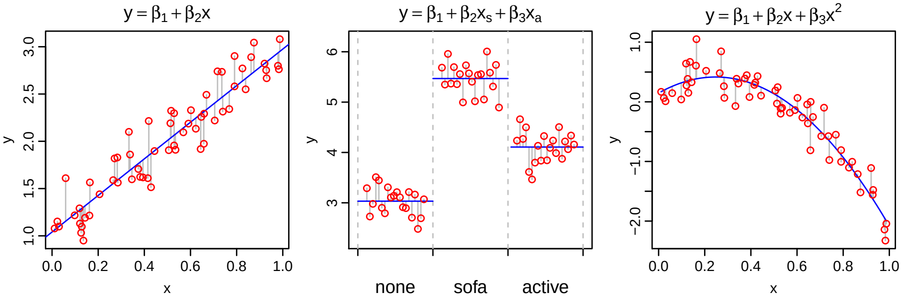


- The data have a similar spread around any predicted point in the model



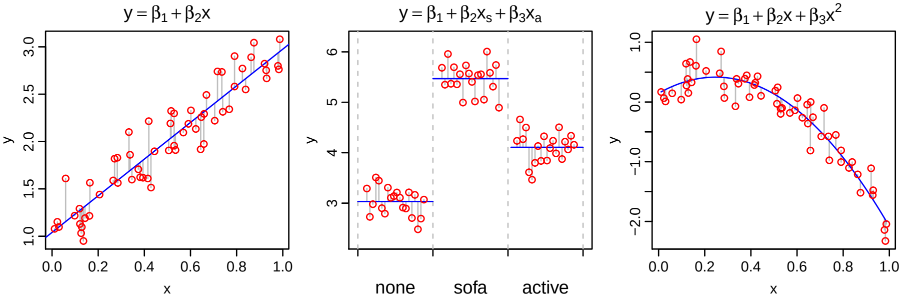
- Overall, the residuals are *normally distributed*: mostly small but a few larger values
- Points *should* be spaced so as to to best capture the normal (gaussian) curve

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?

CHECKING IF THE LINEAR MODEL IS APPROPRIATE



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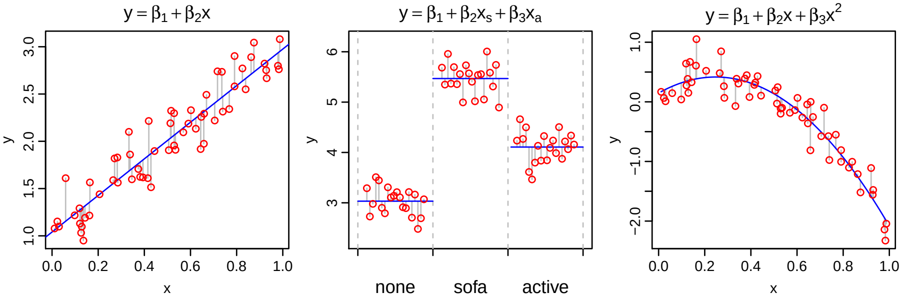

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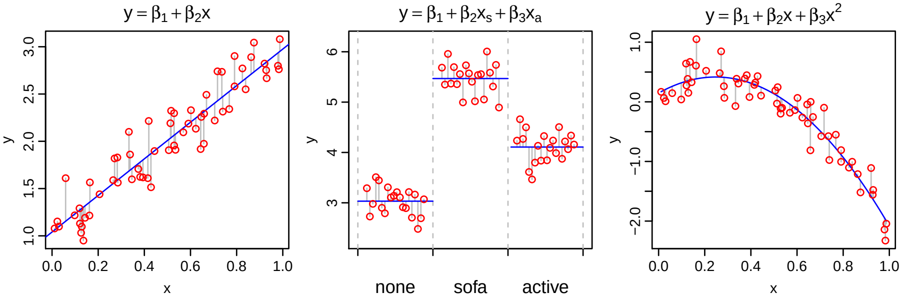

- All these three linear model fits appropriate for the data? Are assumptions of the linear model fit satisfied?
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  - But are the residuals normally distributed?

DIAGNOSTICS FOR A FITTED LINEAR MODEL

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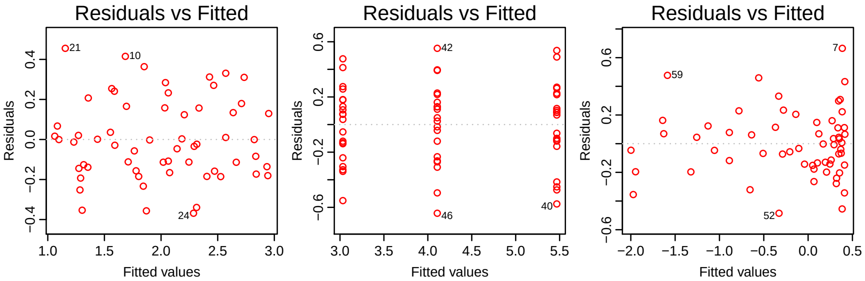

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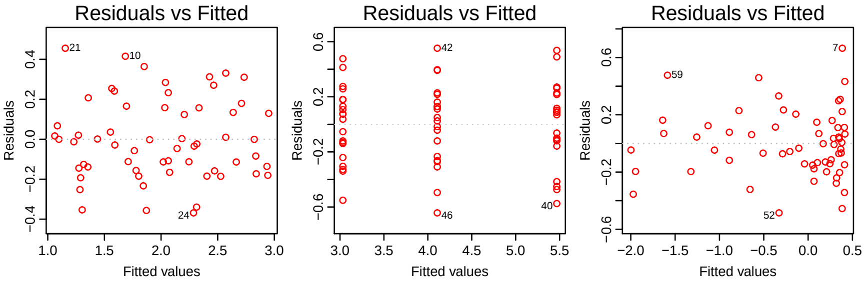

- That is, the residuals have about the same spread irrespective of the fitted values

Diagnostics for a fitted linear model

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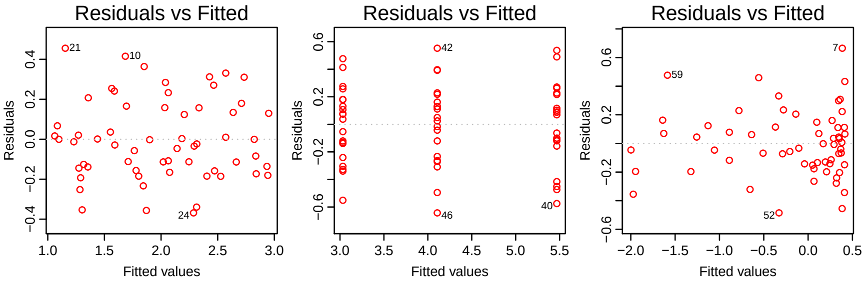

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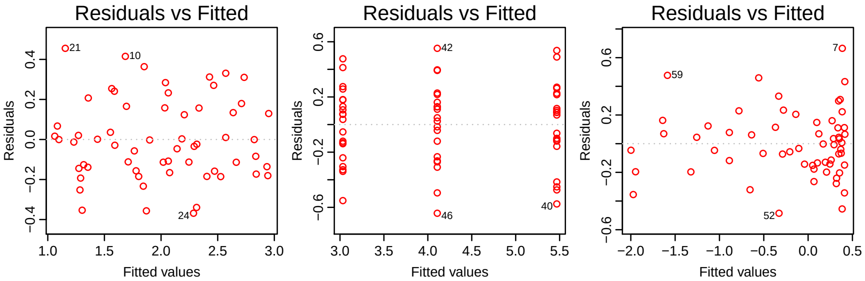

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- The three numbered points in each plot are the three most 'badly behaved' data points.
  - Each number is the datum's row number in the R data frame

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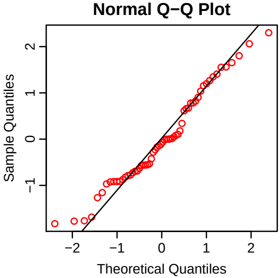

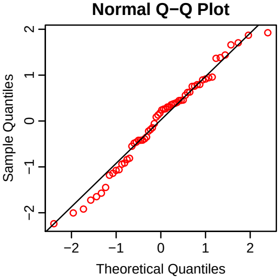

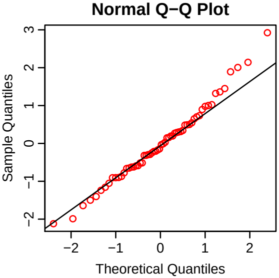

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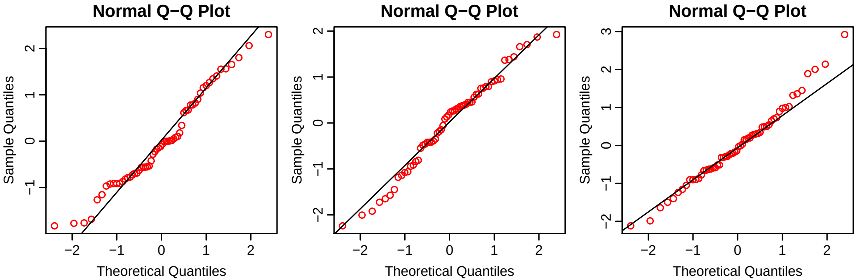
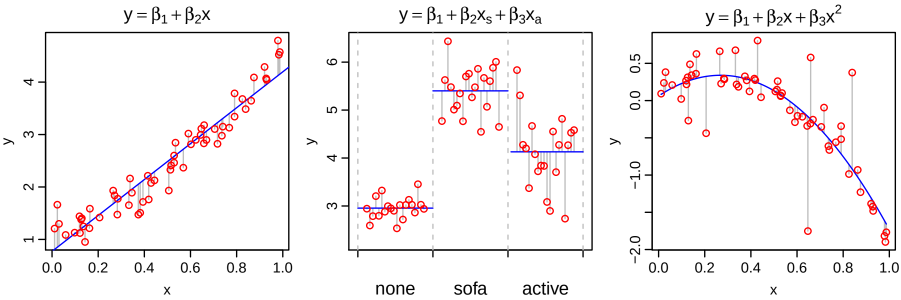


- Residuals from the first (simple regression) and third (polynomial) model's fits show some deviations from normality at the ends (high and low ends of their distributions), but it's acceptable

Three bad linear model fits



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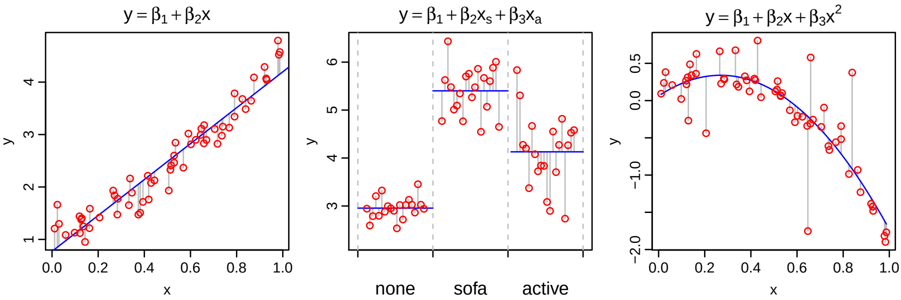
THREE BAD LINEAR MODEL FITS



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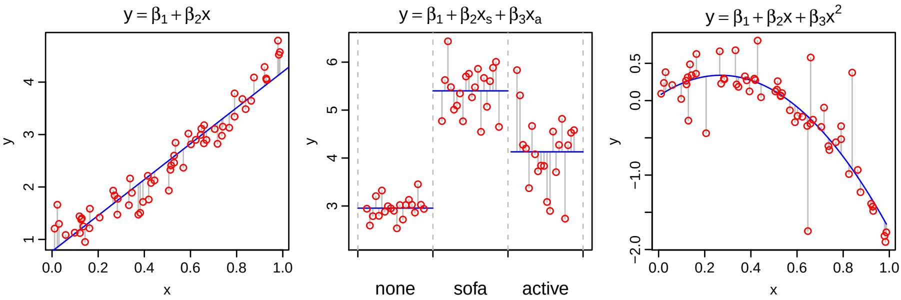

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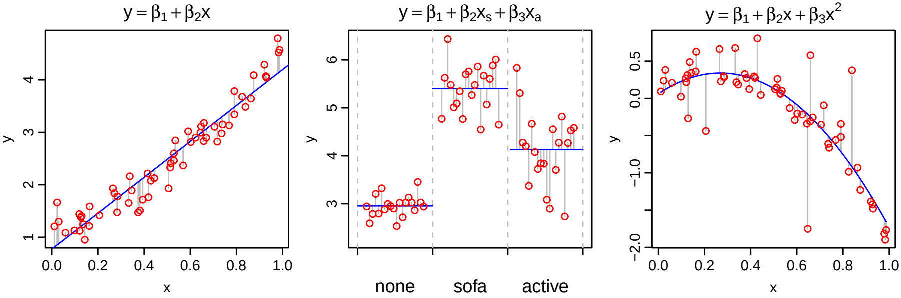

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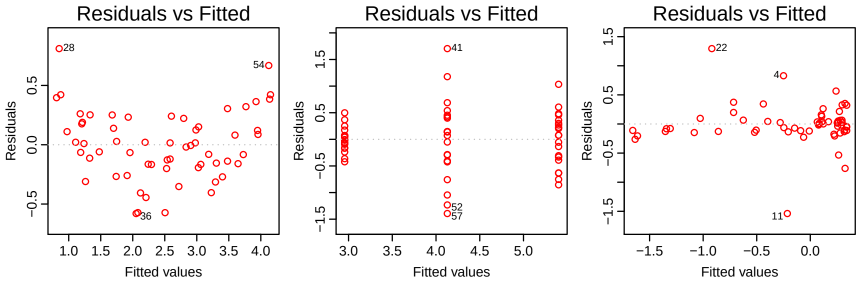
Diagnostics for a (badly) fitted linear model



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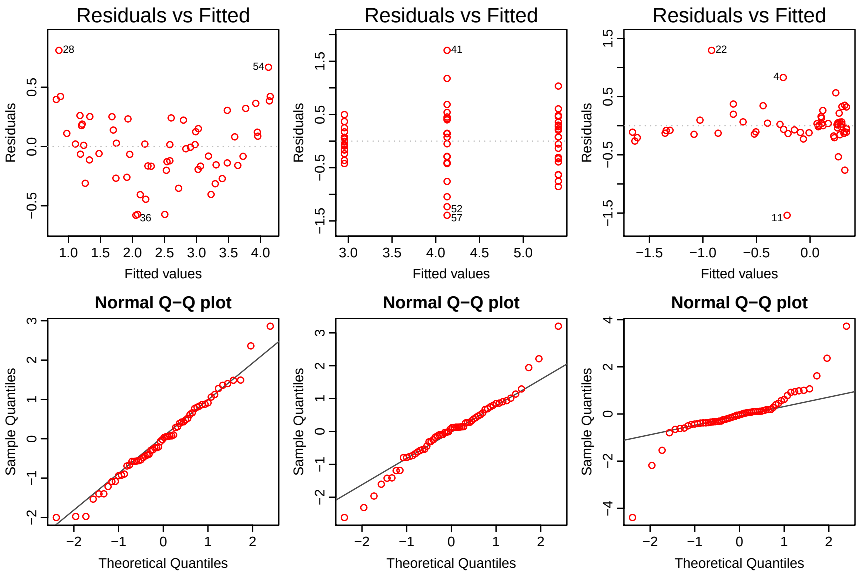

Plot the data!
Plot the residuals!

How explanatory is the fitted linear model?

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HOW EXPLANATORY IS THE FITTED LINEAR MODEL?

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    - 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 = $\sum_{i=1}^{n}(y_i - \bar{y})^2$
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Is the fitted linear model significant?: F test

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- **Residual sum of squares** (RSS): Sum of the squared differences between the observed y and the predicted $\hat{y}$ (residuals), or, RSS = $\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$
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IS THE FITTED LINEAR MODEL SIGNIFICANT?: F TEST

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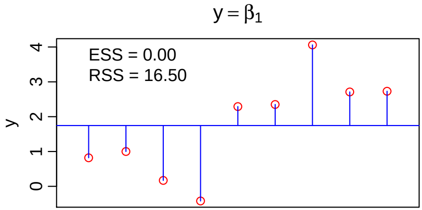
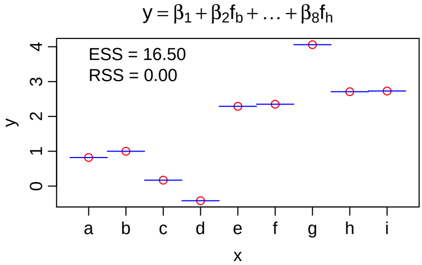
- Of course, TSS = ESS + RSS

Null vs. over-specified models: two endpoints

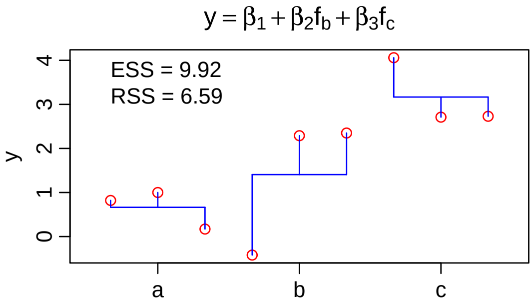


- The null model (H_0)
- Nothing is going on
- Biggest possible residuals
- Residual sum of squares (RSS) is as big as it can be



- 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

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

F STATISTIC OF THE FITTED LINEAR MODEL

Large ESS is good

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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?

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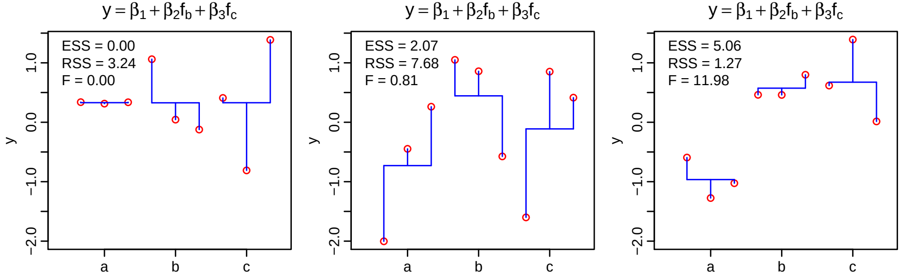

WHAT IT REALLY MEANS: F VALUE BY CHANCE?

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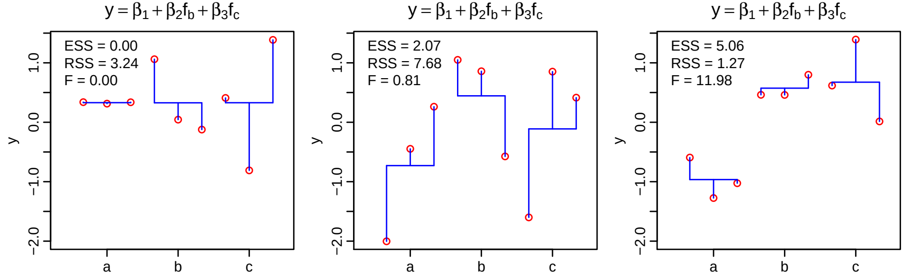

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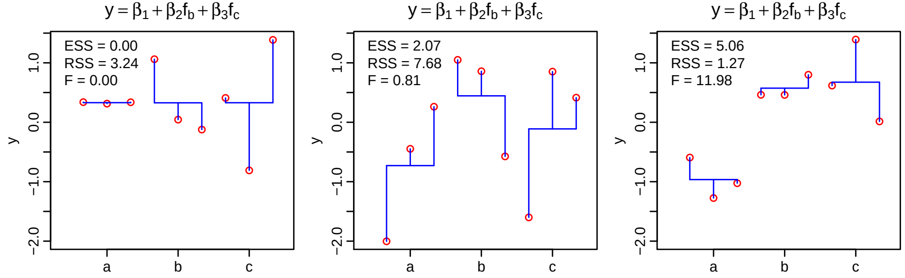

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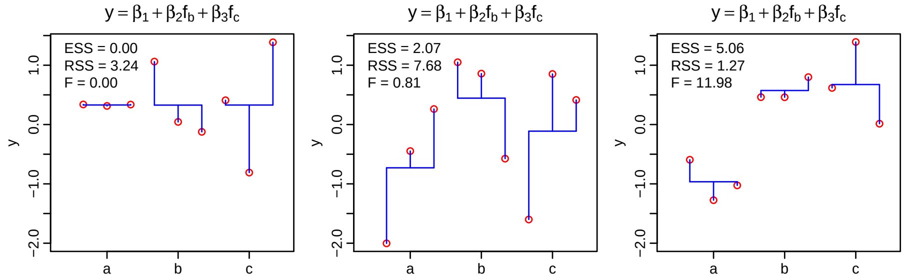

- Simulate 10,000 datasets where nothing is going on (H_0 is true)
- Calculate F for each random dataset under H_1
- H_1 typically has a low F – but sometimes it is high *by chance*

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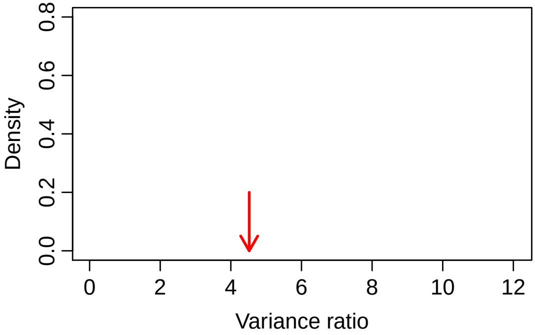

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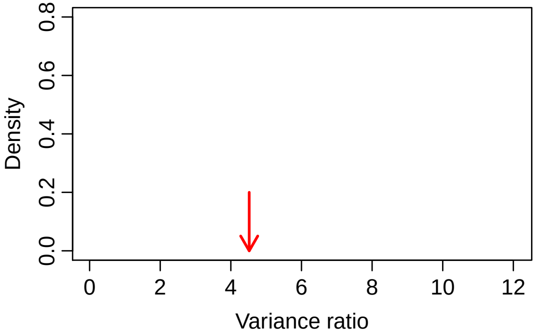

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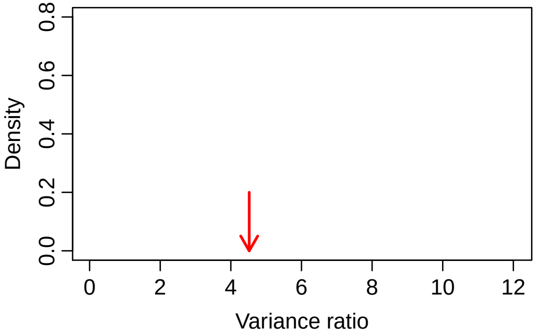

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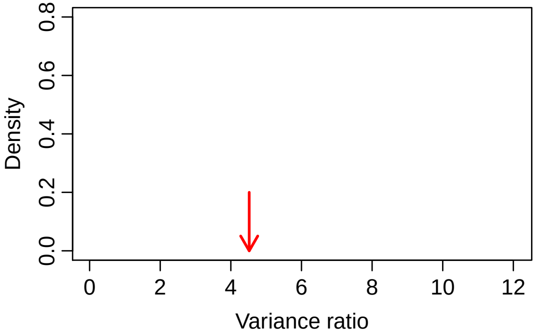

- In our possibly interesting model, $F = 4.52$
- 95% of the random data sets have $F \leq 5.5$
- A model this good would be found by chance 1 in 16 times (p= 0.063)
- Close, but not quite interesting (significant) enough!

Are the coefficients different from zero?

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

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Large is good: bigger changes

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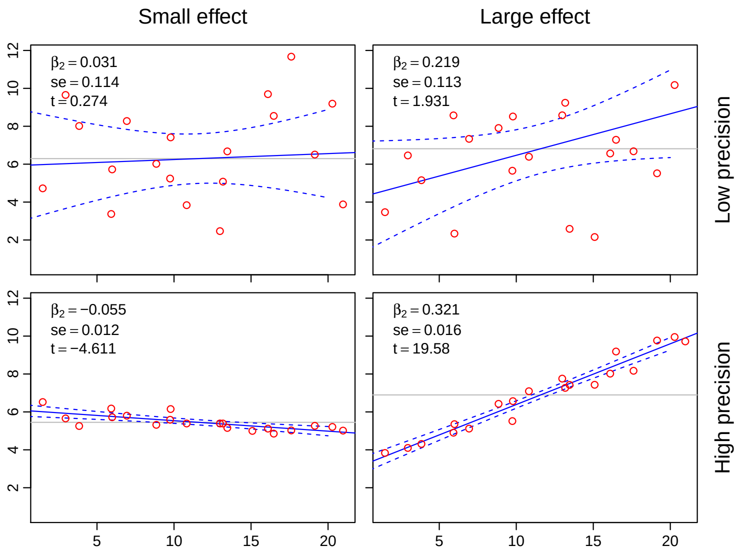
- The value of a coefficient in a model is an *effect size*
- How much does changing that predictor variable change the response variable?
- The *standard error* estimates how precisely we know the value

Variation in effect size and precision



What it really means: t values by chance

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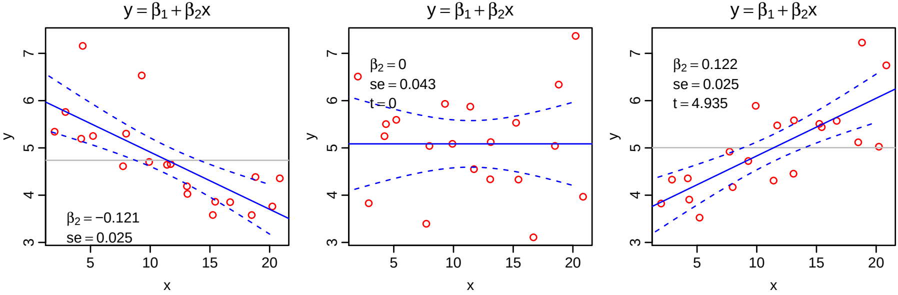

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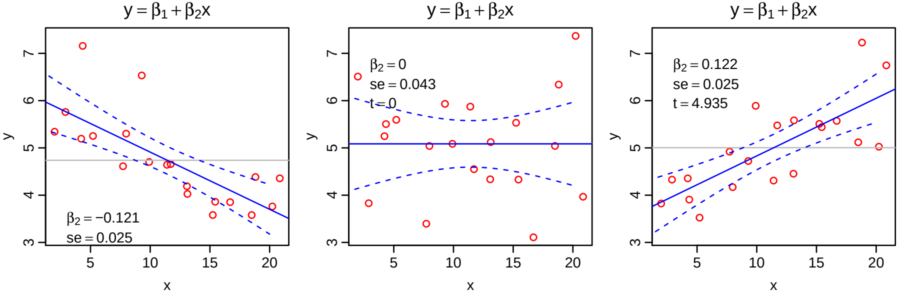

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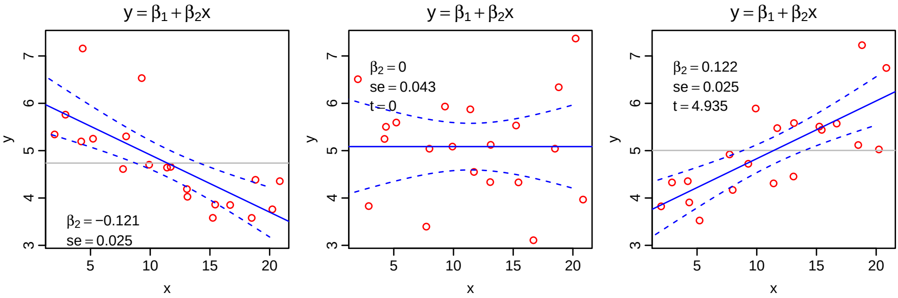

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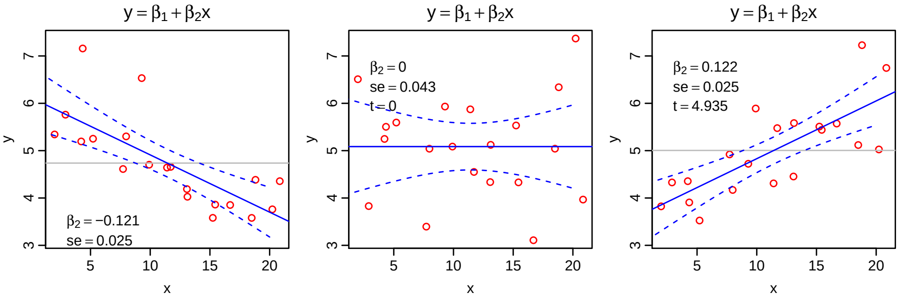
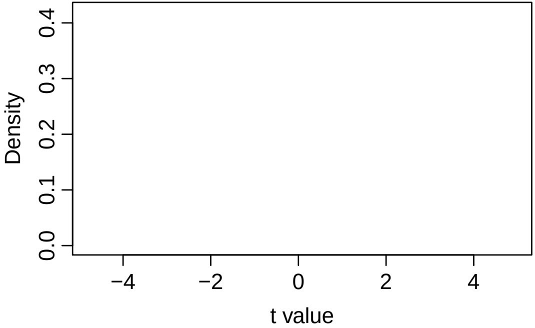
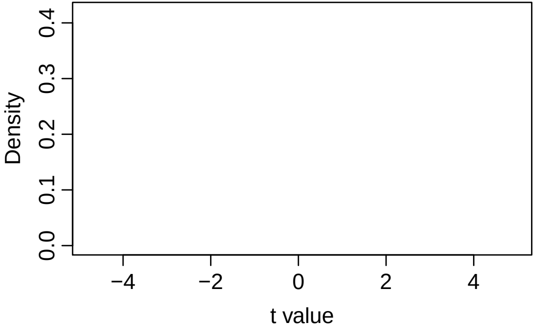


- Simulate 10,000 datasets where nothing is going on (H_0 is true)
- Calculate t for each random dataset under H_1
- H_1 typically has a t near zero but can be strongly positive or negative *by chance*

DISTRIBUTION OF t





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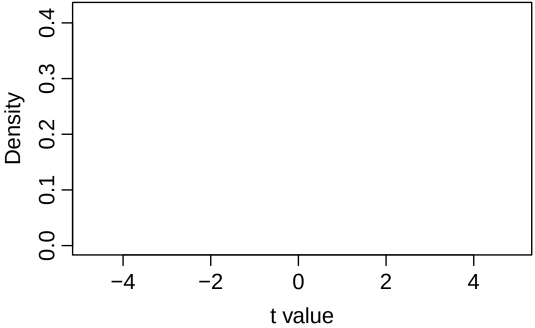
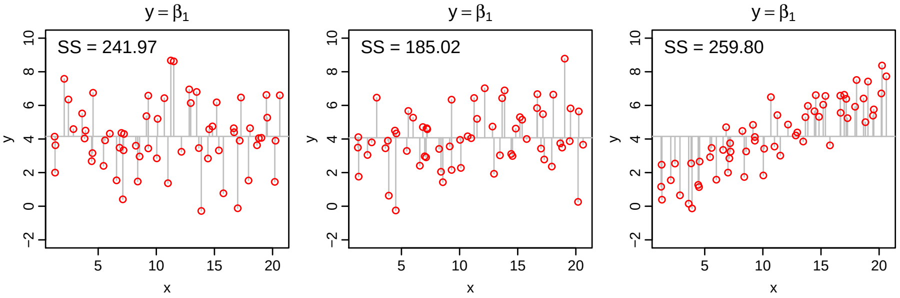


- 95% of the random data sets have $t \leq \pm 2.09$
- Only the two higher precision models are expected to occur less than 1 time in 20 by chance.

Some more examples of linear model fitting



- The null hypothesis (H_0): Nothing is going on (model is just β_1!)

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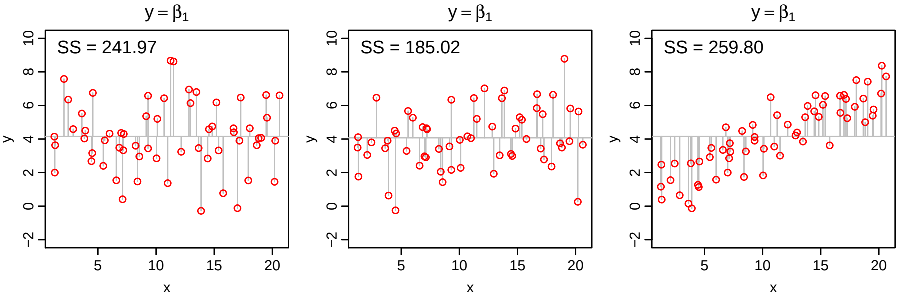

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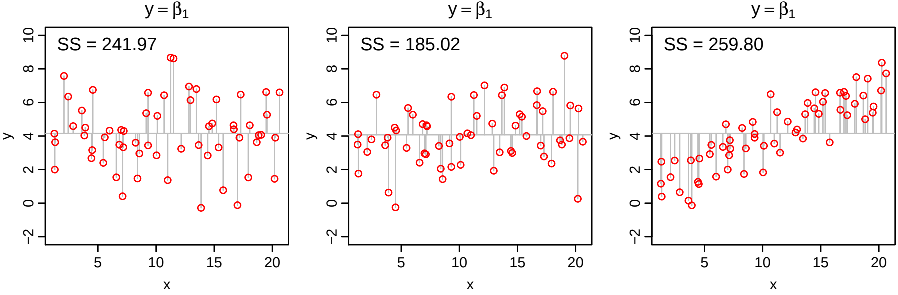

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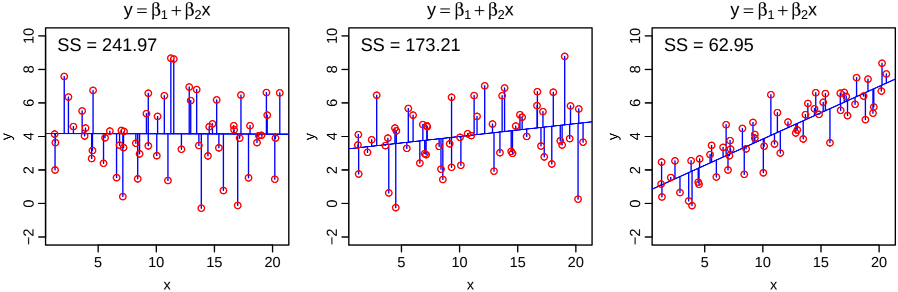
- The residuals (and therefore, RSS) will get *smaller* as we include more terms to the model
- *How much smaller is enough?*

SOME MORE EXAMPLES OF LINEAR MODEL FITTING

First try: Add one continuous term



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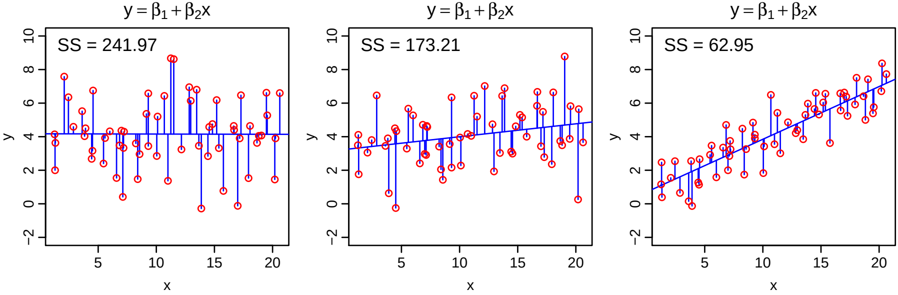

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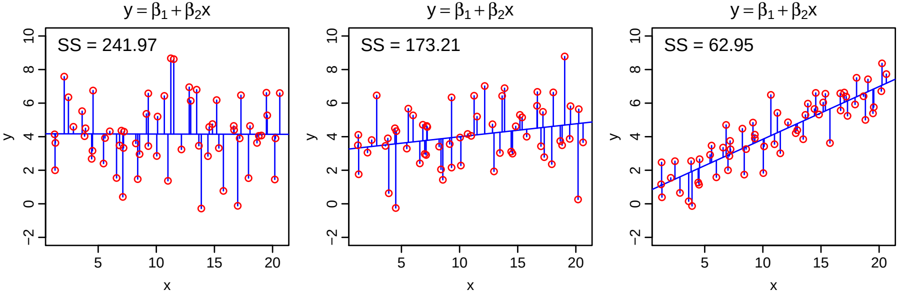
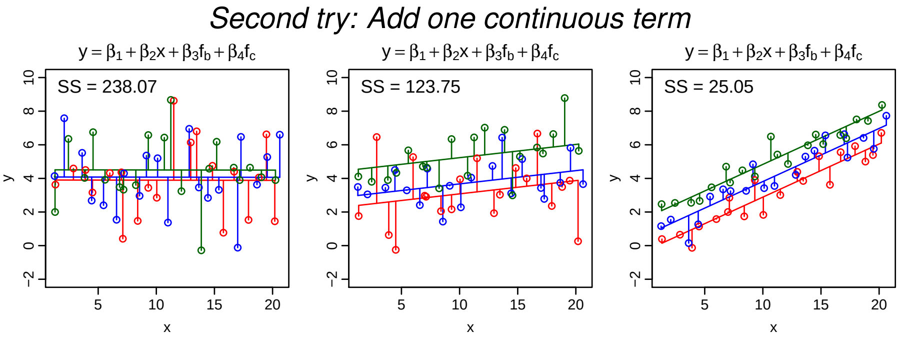


- Fitted an *alternative* model (H_1) using a predictor variable x
- i.e., Added one term (x) to the model to give (H_1)
- Do we reject H_0 and accept this new model?

Some more examples of linear model fitting



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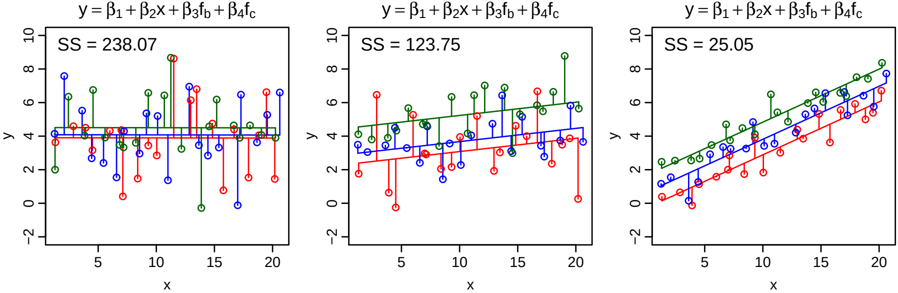

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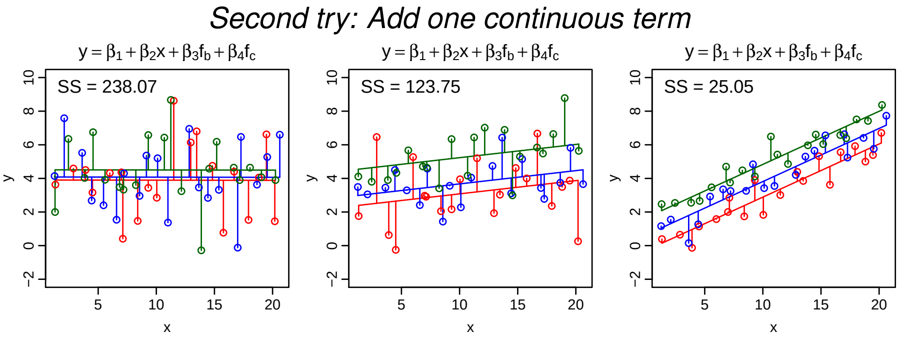

- Fitted another model (H_2) with continuous predictor x and factor f
- The RSS gets still smaller
- Is this *even* better than H_1?

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?

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- 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