ETC5510: Introduction to Data Analysis Week 10, part A

Regression and Decision Trees

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Monash Institute of Pharmaceutical Sciences

Pharmaceutical ociety of Australia



networks

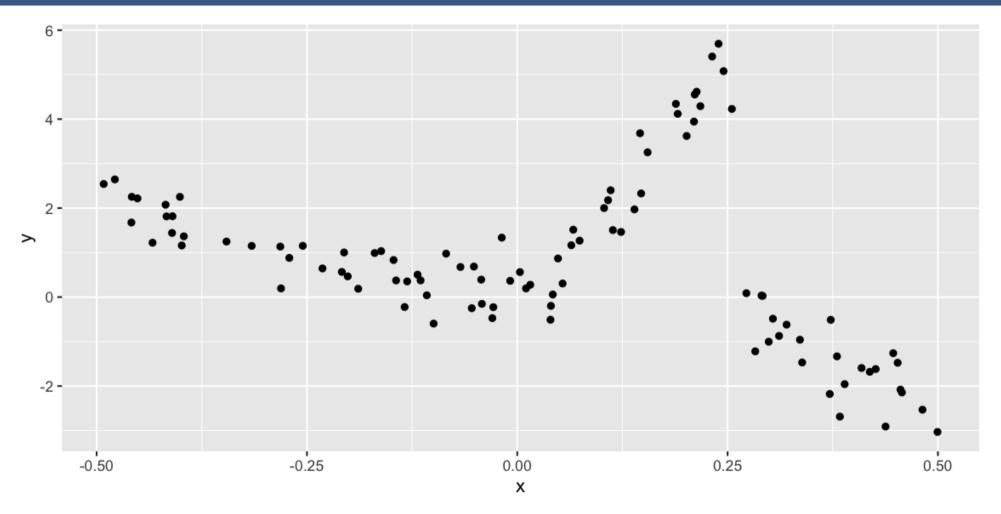
Upcoming

- Peer evaluation of assignment #2 on Wednesday
- Project milestone #3 due this Friday, if you need guidance attend consultation

Overview

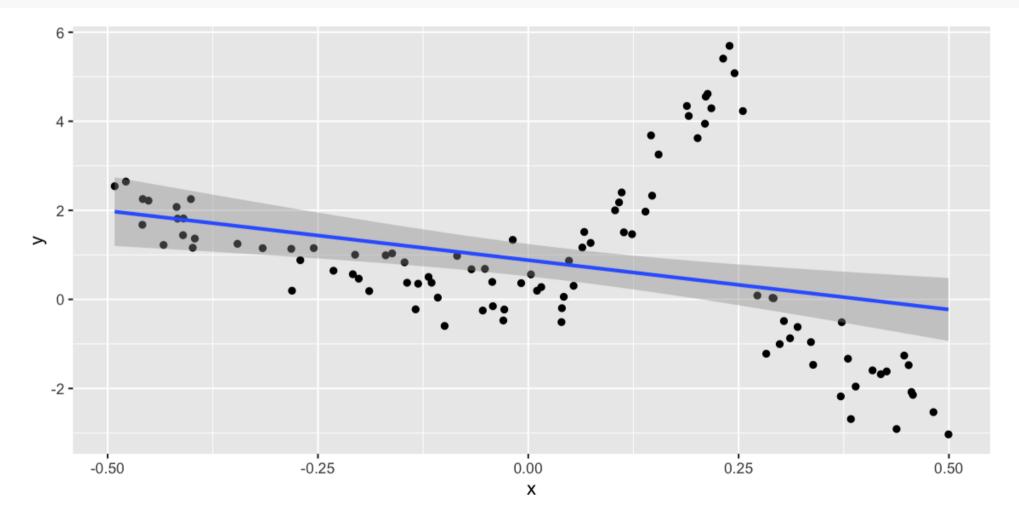
- What is a regression tree?
- How is it computed?
- Deciding when its a good fit
 - rmse
- Comparison with linear models
- Using multiple variables
- Next class:
 - How a classification tree differs from a regression tree?





Let's predict Y using a linear model

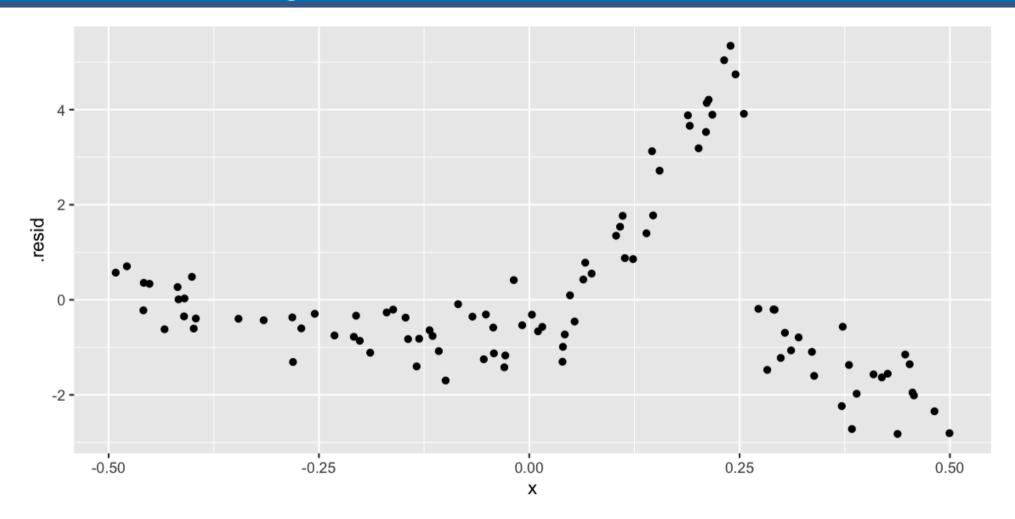
$df_lm <- lm(y \sim x, df)$



Assessing model fit

- Look at residuals
- Look at mean square error

Looking at the residuals: this is bad!



It basically looks like the data!

Looking at the Mean square error (MSE)

$$MSE(y) = \frac{\sum_{i=1}^{i=N} (y_i - \hat{y}_i)^2}{N}$$

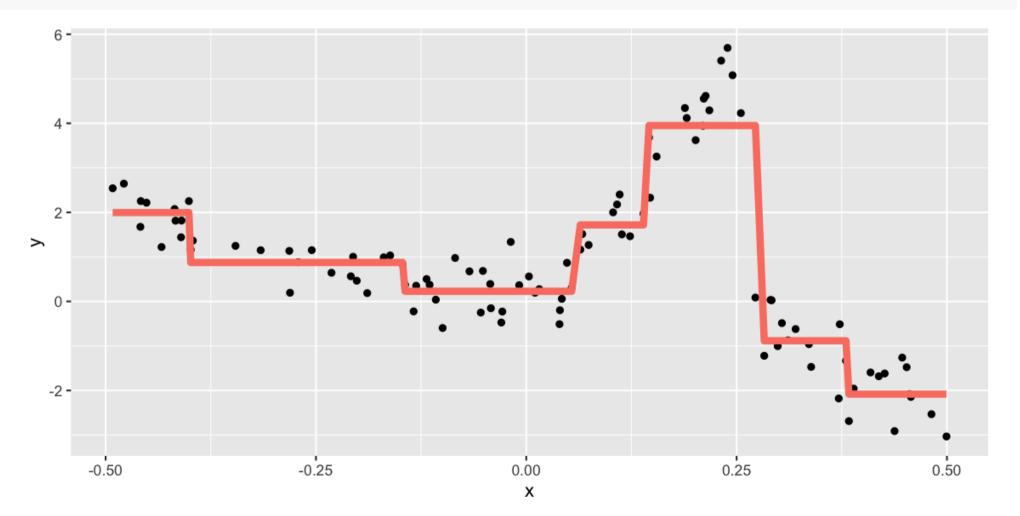
In R code:

calculate example of linear model MSE

Let's use a different model: "rpart"

library(rpart)

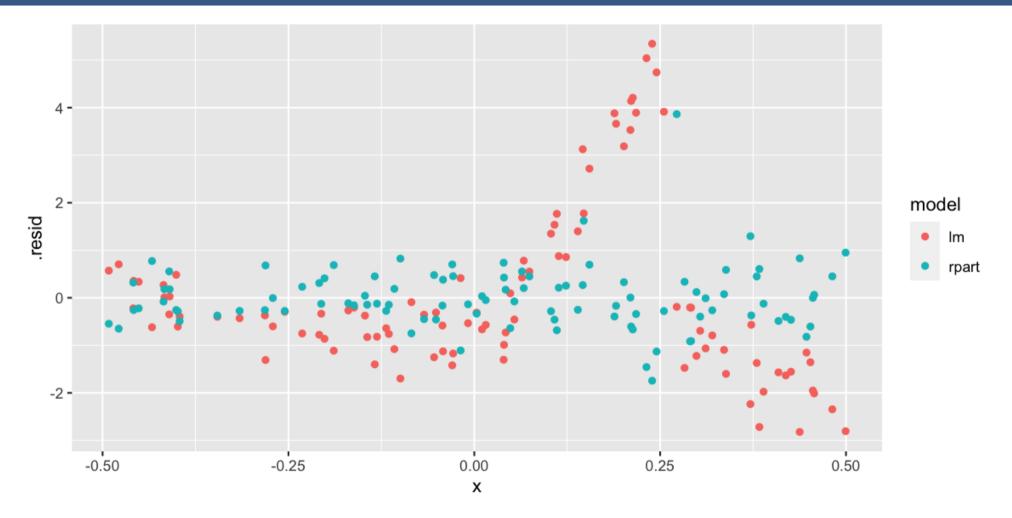
df_lm <- lm(y~x, data=df) - similar to lm! But rpart. df_rp <- rpart(y~x, data=df)</pre>



Look at residuals

Look at MSE

Comparing Im vs rpart



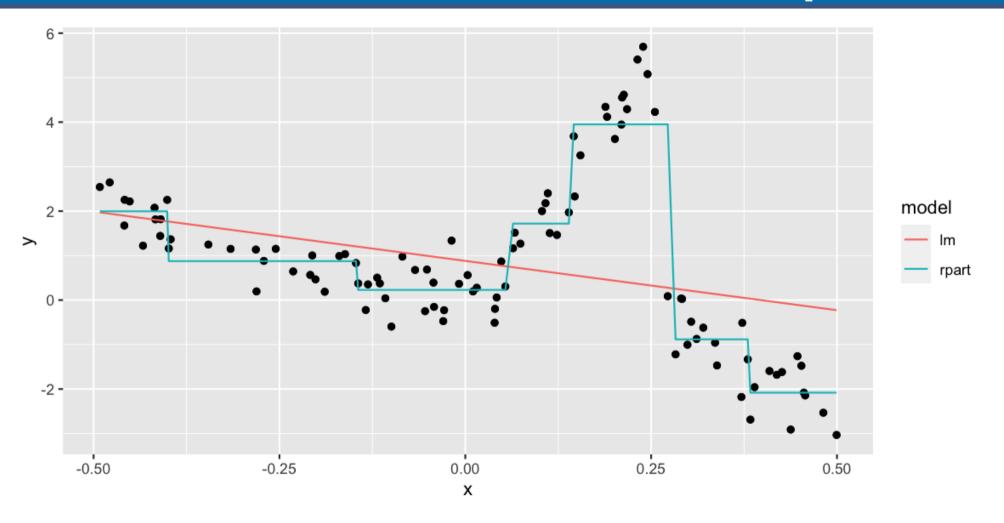
What the output of a linear model looks like

##
Call:
Call:
lm(formula = y ~ x, data = df)
##
Coefficients:
(Intercept) x
0.8806 -2.2165

What the output of a rpart looks like

n= 100
##
node), split, n, deviance, yval
* denotes terminal node
##
1) root 100 359.245100 0.8081071
2) x>=0.2775916 24 16.840100 -1.4822830
4) x>=0.3817438 12 3.832238 -2.0814410 *
5) x< 0.3817438 12 4.392090 -0.8831252 *
3) x< 0.2775916 76 176.745400 1.5313880
6) x< 0.1426085 61 41.562800 0.9365995
12) x>=-0.3999242 50 24.519860 0.7035330
24) x< 0.05905847 41 11.729940 0.4807175
48) x>=-0.1455513 25 5.653876 0.2281914 *
49) x< -0.1455513 16 1.990829 0.8752895 *
25) x>=0.05905847 9 1.481498 1.7185820 *
13) x< -0.3999242 11 1.981477 1.9959930 *
7) x>=0.1426085 15 25.842970 3.9501960 *

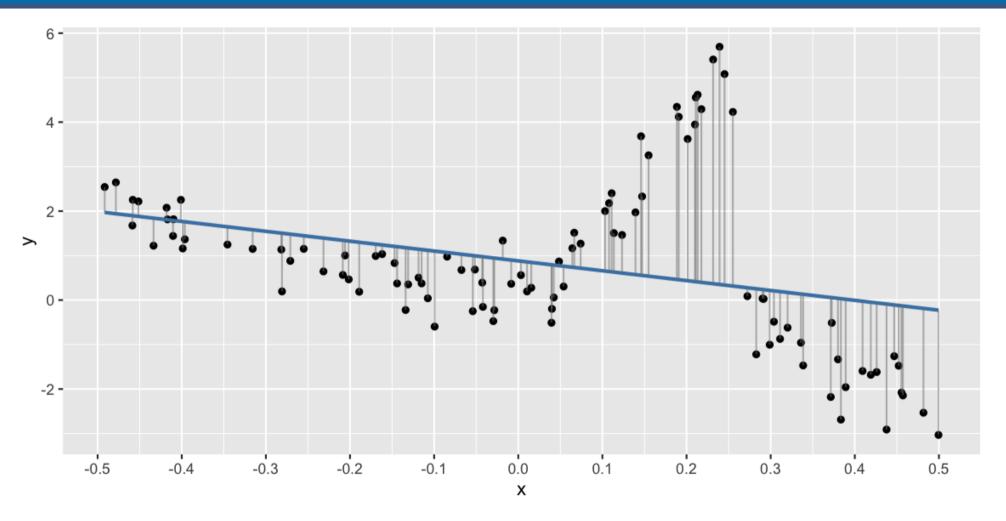
Predictions from linear model vs rpart



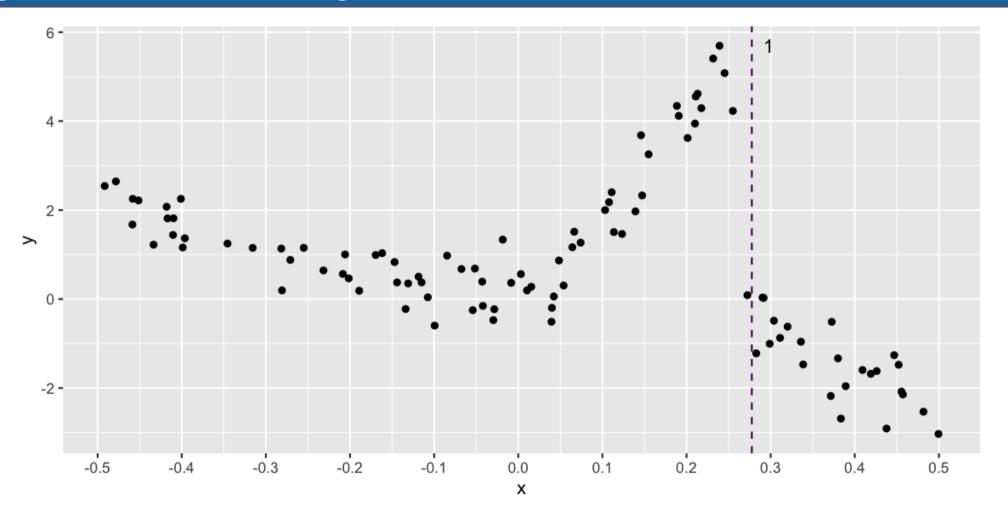
So what is going on?

- A linear model asks "What line fits through these points, to minimise the error"?
- A decision tree model asks "How can I best break the data into segments, to minimize some error?"

A linear model: draws the line of best fit



A regression tree: segments the data to reduce some error



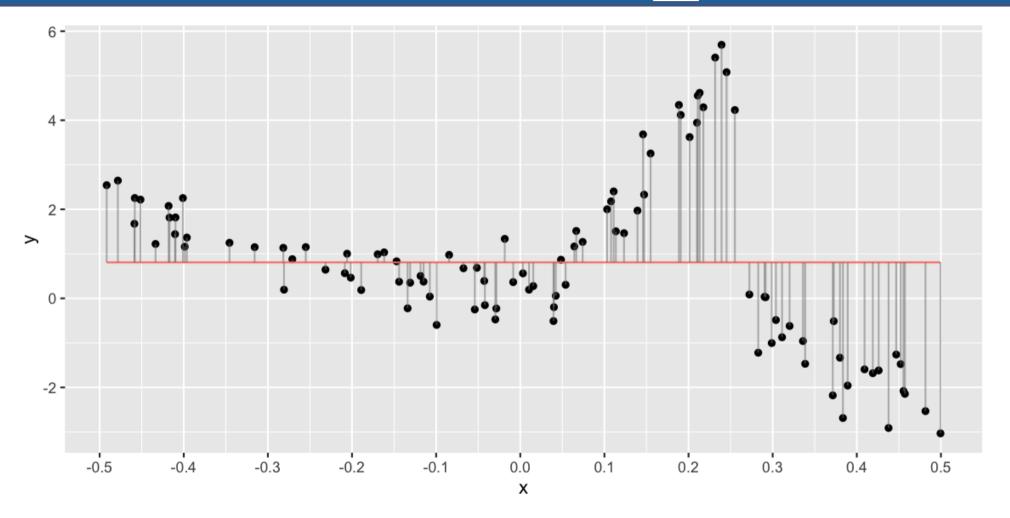
Regression trees

- Regression trees recursively partition the data, and use the average response value of each partition as the model estimate
- It is a computationally intense technique that examines all possible partitions, and choosing the BEST partition by optimizing some criteria
- For regression, with a quantitative response variable, the criteria is called ANOVA:

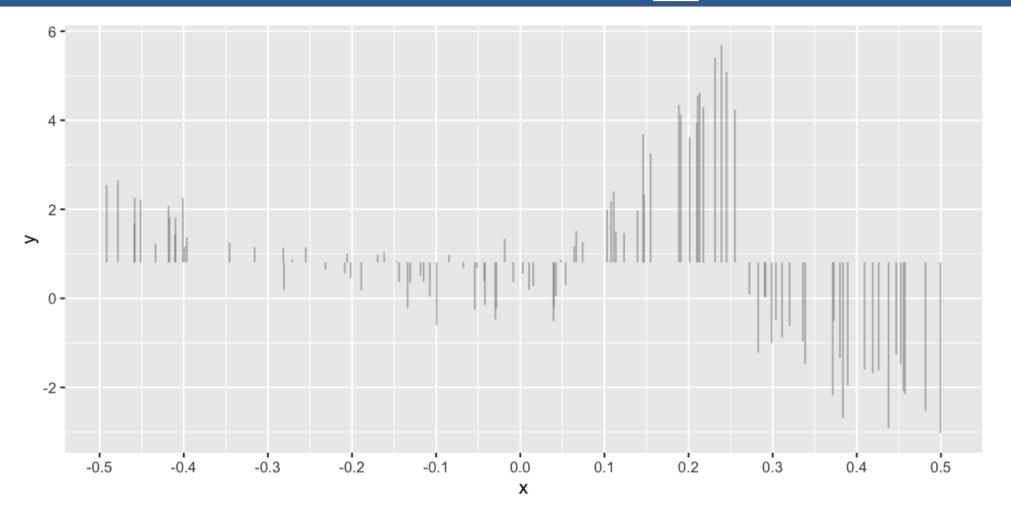
$$SS_T - (SS_L + SS_R)$$

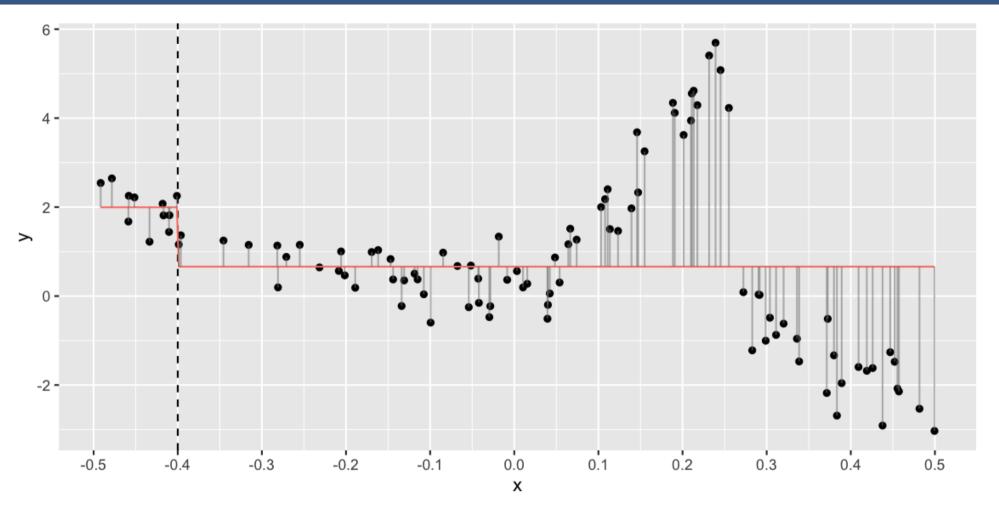
where $SS_T = \sum (y_i - \bar{y})^2$, and SS_L , SS_R are the equivalent values for the two subsets created by partitioning.

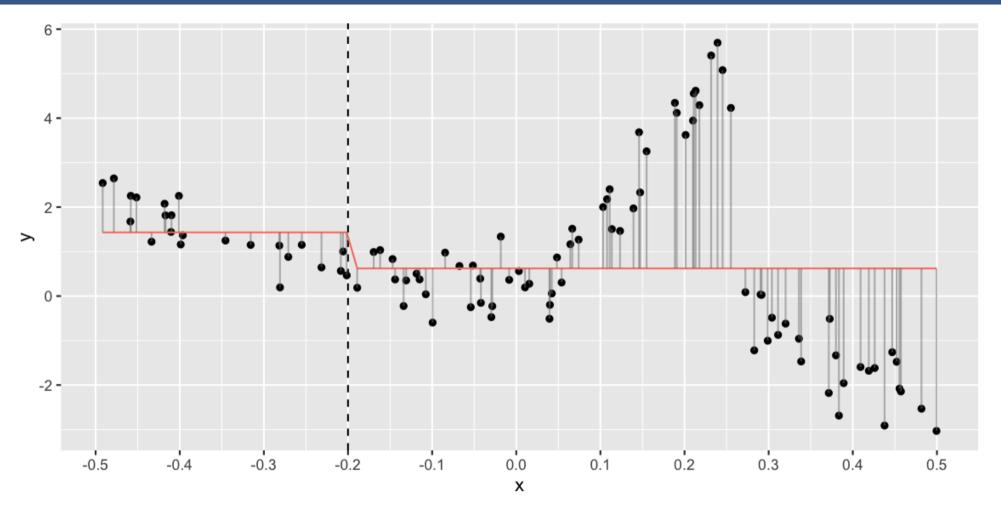
Break down: What is $SS_T = \sum (y_i - \bar{y})^2$?

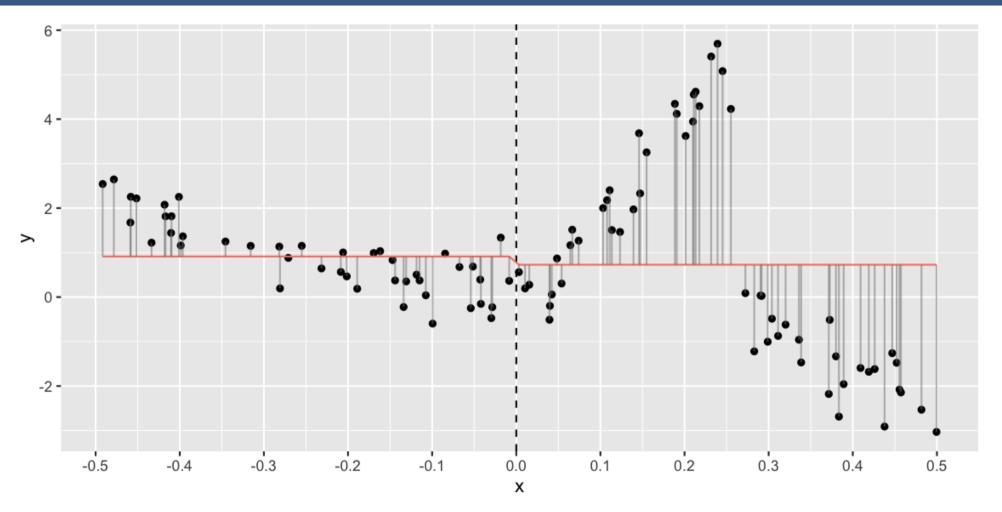


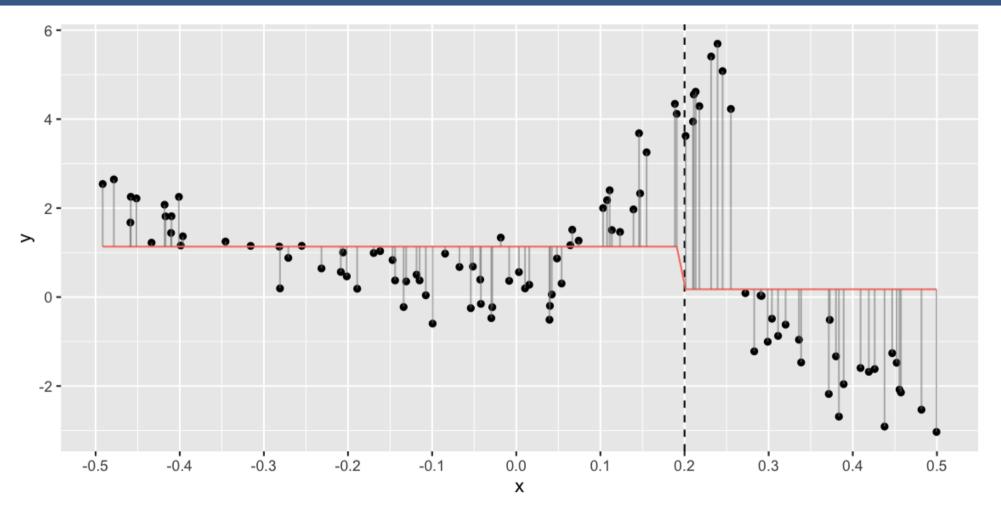
Break down: What is $SS_T = \sum (y_i - \bar{y})^2$?

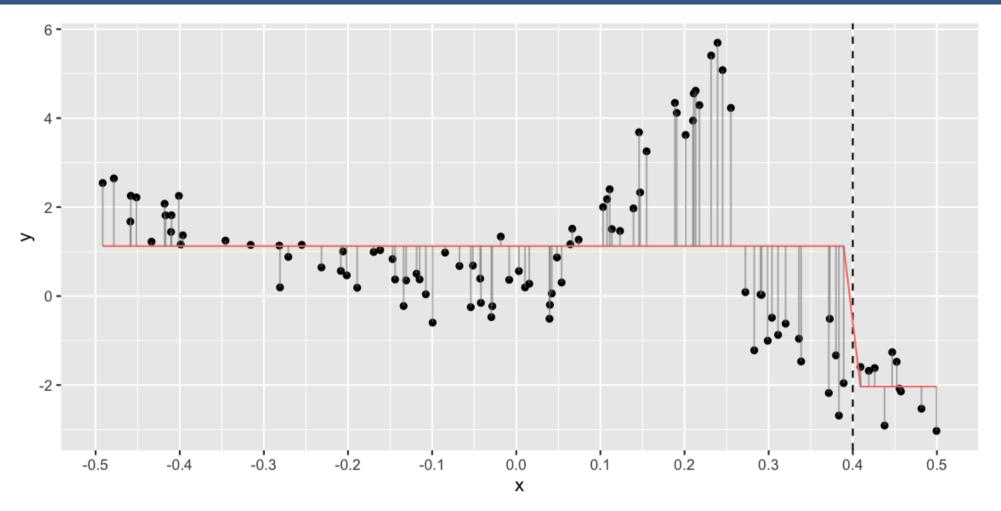








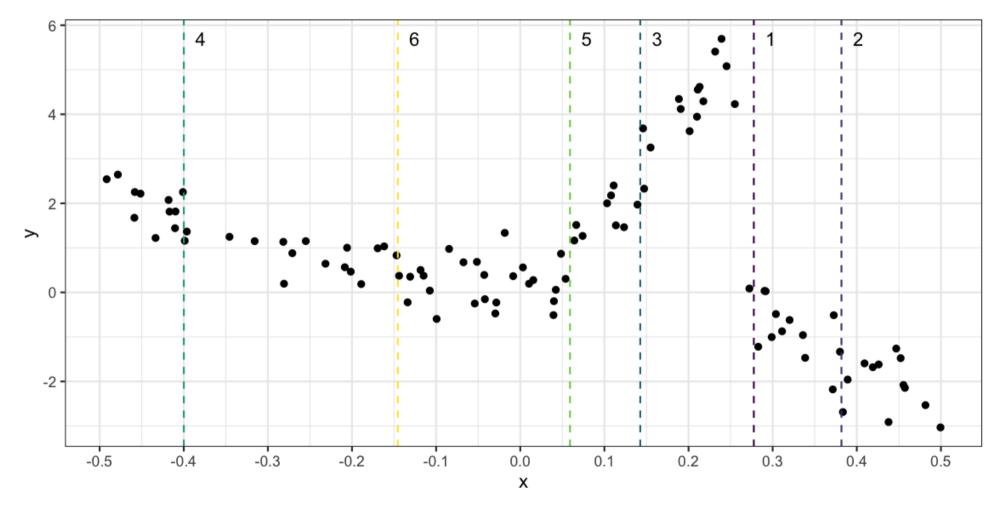




Across all values of x?

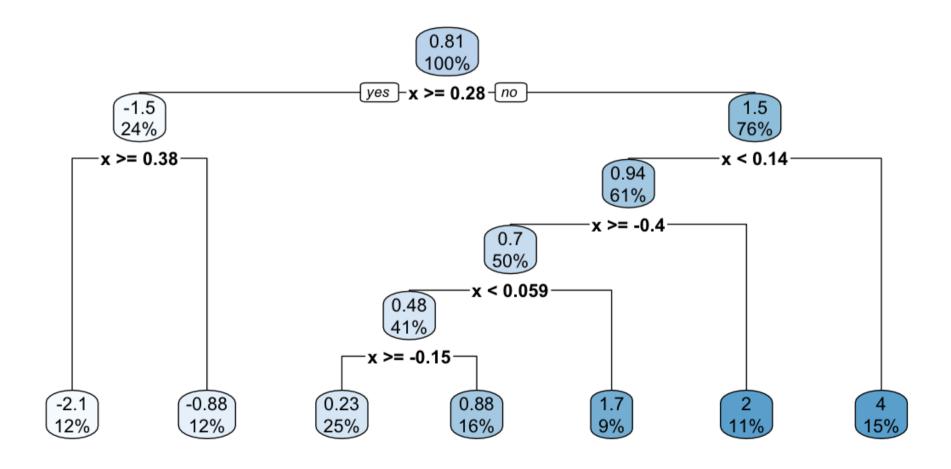
And if we repeated this again

This is how the data is split:



We can represent these splits in a tree format:

library(rpart.plot)
rpart.plot(df_rp)



Your turn: compute a regression tree

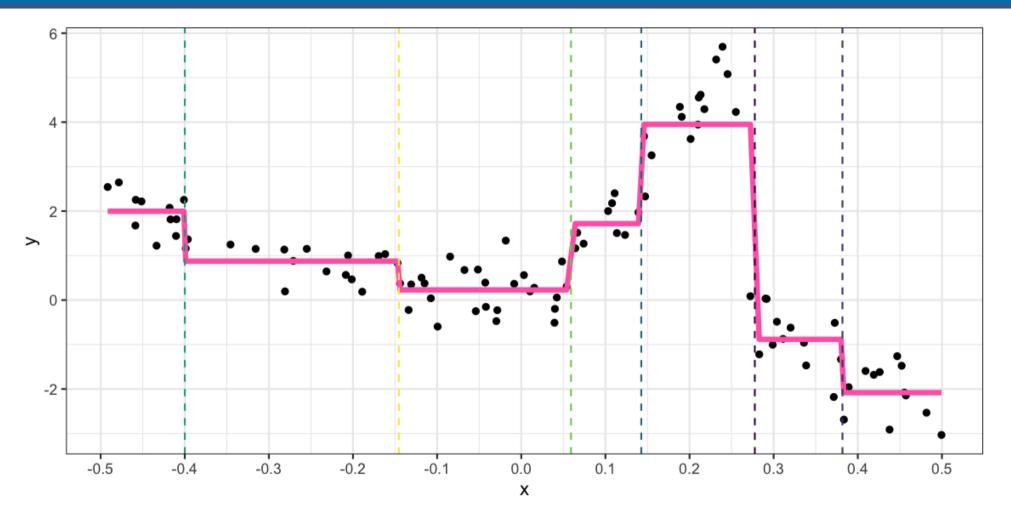
Using the small data set, manually compute a regression tree model for the data. Sketch the model.

```
d <- tibble(x=c(1, 2, 3, 4, 5), y=c(10, 12, 5, 4, 3))
d
ggplot(d, aes(x=x, y=y)) +
geom_???()</pre>
```

Understanding rpart

df_rp	d
## n= 100	#
##	#
## node), split, n, deviance, yval	#
## * denotes terminal node	#
##	#
## 1) root 100 359.245100 0.8081071	#
## 2) x>=0.2775916 24 16.840100 -1.4822830	#
## 4) x>=0.3817438 12 3.832238 -2.0814410 *	#
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This is how the model looks:



Stopping rules

- Its an algorithm. Why did it stop at 7 terminal nodes?
- Stopping rules are needed, else the algorithm will keep fitting until every observation is in its own group.
- Control parameters set stopping points:
 - minsplit: minimum number of points in a node that algorithm is allowed to split
 - minbucket: minimum number of points in a terminal node
- We can also look at the change in value of $SS_T (SS_L + SS_R)$ at each split, and if the change is too *small*, stop.

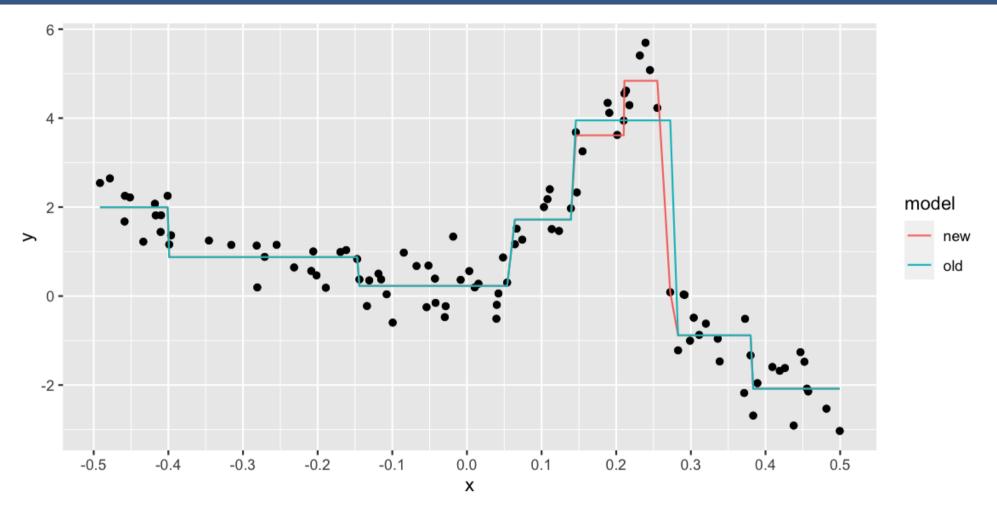
You can change the options to fit a different model

An re-fit, the model will change. Here we reduce the minbucket parameter.

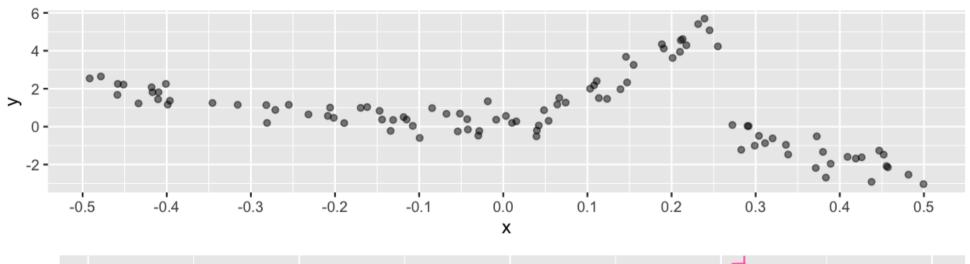
df_rp_m10 <- rpart(y~x, data=df,</pre>

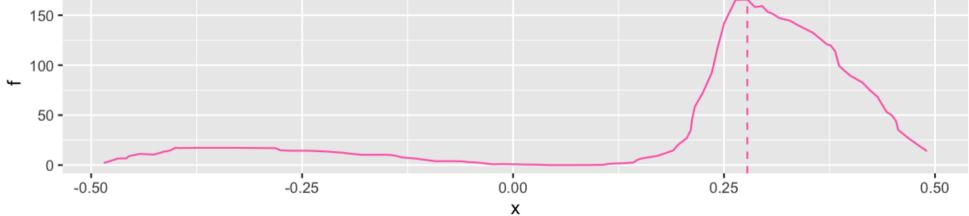
control = rpart.control(minsplit = 2))

This yields a (slightly) more complex model.

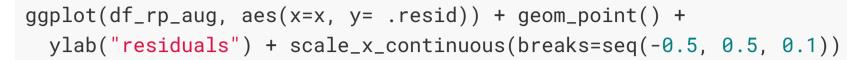


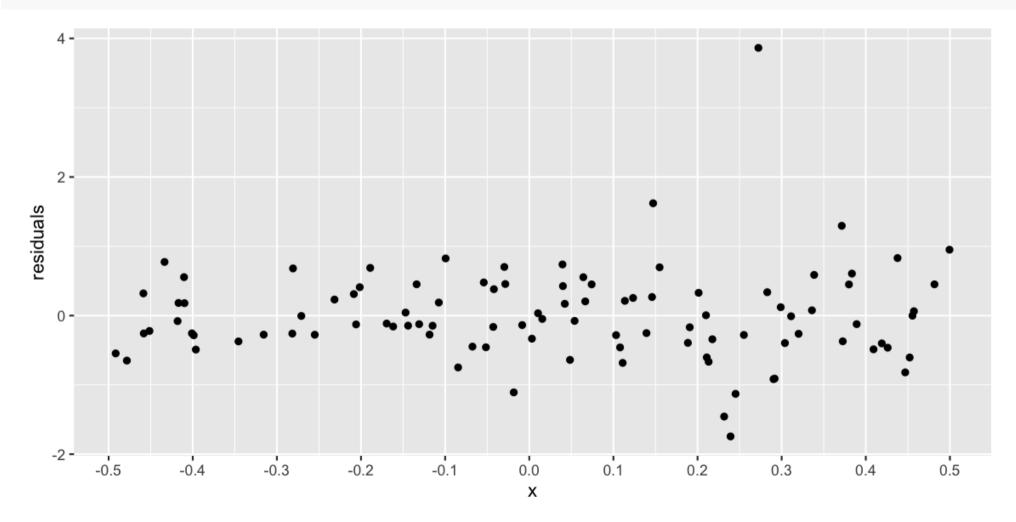
What's computed?





Residuals





Goodness of fit - Root Mean Square Error

```
gof <- printcp(df_rp, digits=3)</pre>
##
## Regression tree:
## rpart(formula = y \sim x, data = df)
##
## Variables actually used in tree construction:
## [1] x
##
## Root node error: 359/100 = 3.59
##
## n= 100
##
##
  CP nsplit rel error xerror xstd
## 1 0.4611 0 1.000 1.008 0.1426
## 2 0.3044 1 0.539 0.580 0.0891
           2 0.235 0.301 0.0643
## 3 0.0419
               3 0.193 0.248 0.0621
## 4 0.0315
## 5 0.0240
           4 0.161 0.246 0.0623
           5 0.137 0.218 0.0617
## 6 0.0114
## 7 0.0100
               6 0.126 0.216 0.0616
```

goodness of fit?

The relative error is $1 - R^2$. For this example, after 6 splits it is 0.1371214. So $R^2 = 0.8628786$.

1-sum(df_rp_aug\$e^2)/sum((df\$y-mean(df\$y))^2)

Strengths

- There are no parametric assumptions underlying partitioning methods
- Can handle data of unusual shapes and sizes?
- Can identify unusual groups of data
- Provides a tree based graphic that is fun to interpret
- Has an efficient heuristic of handling missing values.
- The method could be influenced by outliers, but it would be isolating the effect to one partition.

Weaknesses

- Doesn't really handle data that is linear very well
- Can require tuning parameters to get good model fit
- Also means that there is not a nice formula for the model as a result, or inference about populations available

Next week: Classification trees

When the response is categorical, the model is called a classification tree. The criteria for making the splits changes also. There are a number of split criteria commonly used. If we consider a binary response (y=0, 1), and p is the proportion of observations in class 1.

- Gini: 2p(1-p)
- Entropy: $-p(\log_e p) (1-p)\log_e(1-p)$

Which rewards splits where the observations are all one class.

Your Turn: Lab exercise

- Return of the paintings data
- Just predict price with year

```
pp <- read_csv(here::here("slides/data/paris-paintings.csv"))
pp_lm <- lm(logprice ~ Height_in + Width_in, data = pp)</pre>
```

```
pp_rp <- rpart(logprice ~ Height_in + Width_in + year, data = pp)</pre>
```

```
pp_lm_aug <- augment(pp_lm)
pp_rp_aug <- augment(pp_rp)
library(rpart.plot)
rpart.plot(pp_rp)</pre>
```

