BENV0091 Lecture 3: Introduction to Supervised Learning

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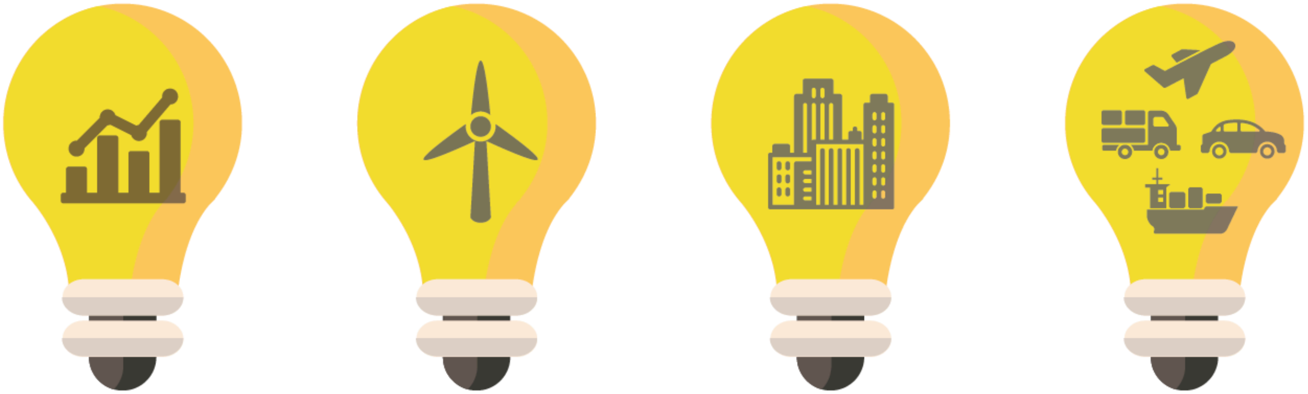


Lecture Overview

1. Tidy Data
2. Using Facets
3. Supervised Learning

Tidy Data

- R and especially the tidyverse packages like **tidy data**
- In tidy data:
  - Every column is a variable
  - Every row is an observation
  - Every cell is a single value
- Tidy data is easier to plot!
- Most commonly, untidy data is in **wide format**, and should be converted to **long format**

This data below gives the height of 2 people over 3 years. It is in wide format: a variable (year) is spread across columns – not tidy and hard to plot!

```
# A tibble: 2 × 4
  name  `2016` `2017` `2018`
  <chr>  <dbl>  <dbl>  <dbl>
1 andy     160    165    167
2 bella    170    180    182
```

The data has been tidied using pivot_longer() below

```
# A tibble: 6 × 3
  name   year height
  <chr> <int>  <dbl>
1 andy   2016    160
2 andy   2017    165
3 andy   2018    167
4 bella  2016    170
5 bella  2017    180
6 bella  2018    182
```

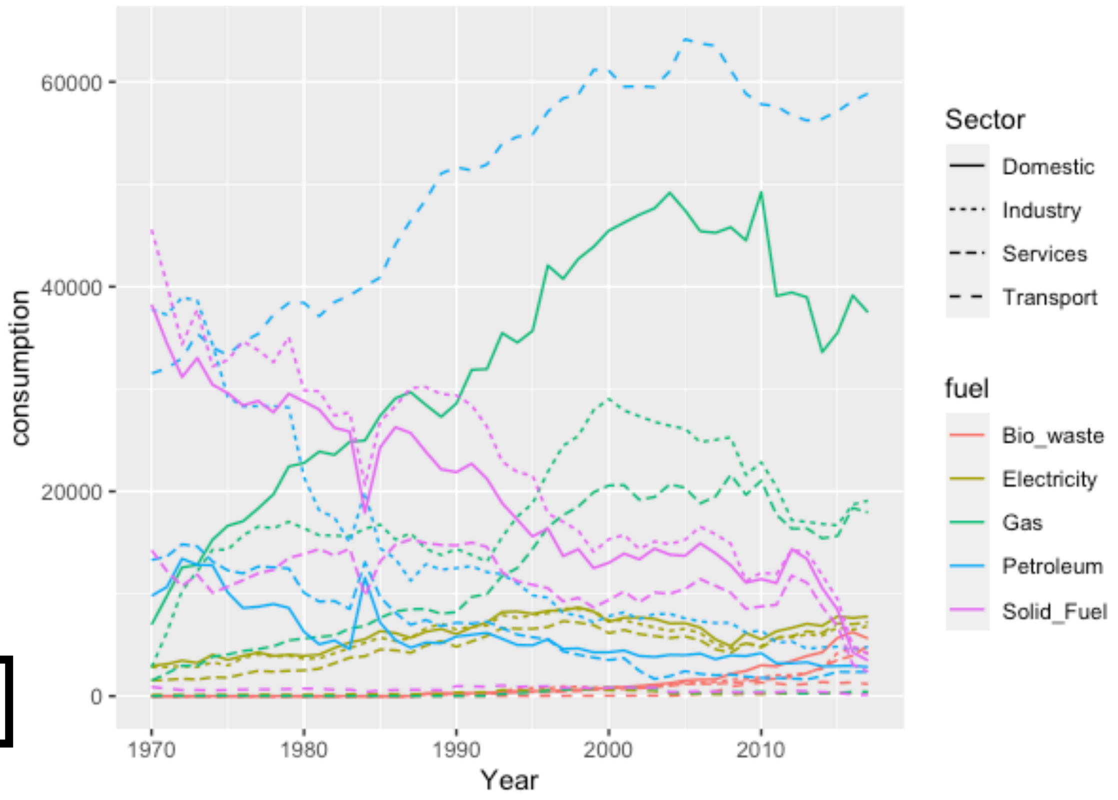
Pivoting

- Read the energy consumption data, assigning to an object named `energy`
- How should we transform the data to create the plot on the right?
- Task: use pivot_longer() to make the energy data tidy
- Task: create the plot on the right with ggplot2 and geom_line()

Use the `linetype` aesthetic

Original data

	Year	Solid_Fuel	Petroleum	Gas	Bio_waste	Electricity	Sector
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<chr>
1	1970	45573.	37758.	2808.	0	2820.	Industry
2	1970	899.	31515.	1.23	0	107.	Transport
3	1970	38262.	9798.	6979.	0	2976.	Domestic
4	1970	14260.	13296.	1511.	0	1532.	Services
5	1971	40284.	37250.	6219.	0	2846.	Industry
6	1971	745.	31998.	8.57	0	107.	Transport



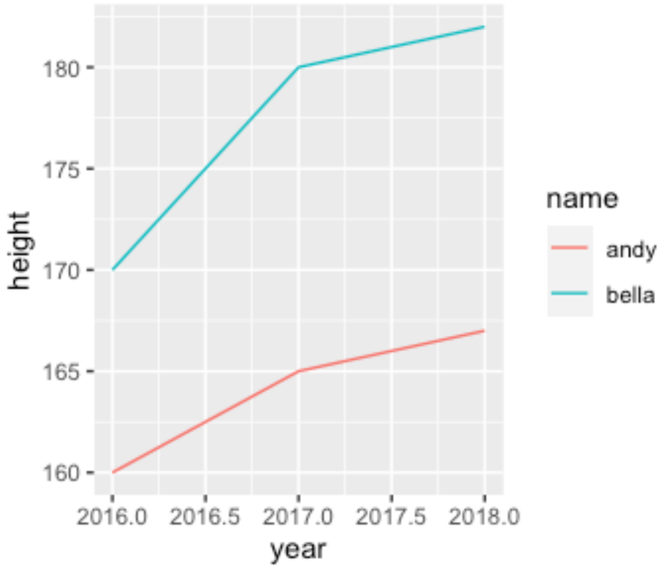
Pivot Wider

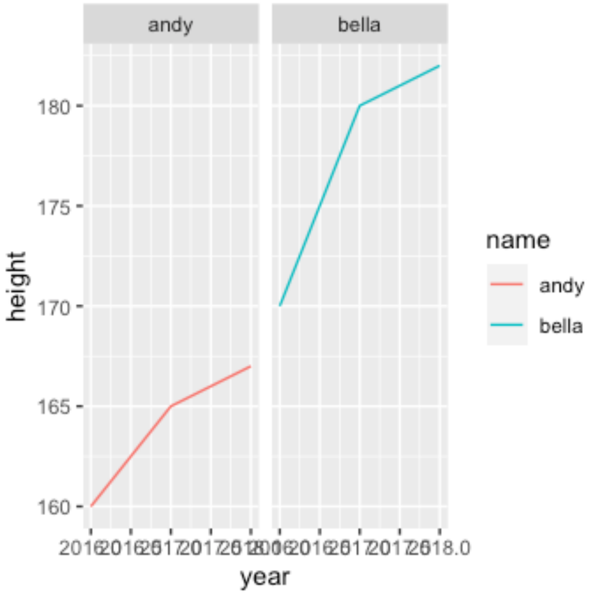
- pivot_wider() does the opposite of pivot_longer()
- You won't need it so often but it's good to know
- Task: use pivot_wider() to return the pivoted energy data frame back to its original
- Task: use pivot_wider() to create a new data frame with the following columns: Sector, fuel, 1970, 1971,…2017 (see below)

	Sector	fuel	`1970`	`1971`	`1972`	`1973`	`1974`	`1975`	`1976`	`1977`	`1978`	`1979`	`1980`
	<chr>	<chr>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	Indust…	Soli…	45573.	40284.	34345.	37748.	32206.	32822.	34644.	33783.	32615.	35081.	29877.
2	Indust…	Petr…	37758.	37250.	38944.	38626.	34362.	29229.	28290.	28333.	28332.	28197.	21386.
3	Indust…	Gas	2808.	6219.	10297.	12204.	14297.	14315.	15685.	16569.	16402.	17029.	16387.
4	Indust…	Bio_…	0	0	0	0	0	0	0	0	0	0	0
5	Indust…	Elec…	2820.	2846.	2925.	2840.	3311.	2994.	3731.	4084.	3847.	3944.	3648.

Facets

- The line plot we made of energy consumption by fuel and sector was pretty busy
- There are sometimes advantages to plotting variables on different **panels**
- We can use facet_grid() and facet_wrap() to do this
- facet_grid() is used to plot the interaction **two variables** across rows and columns
- facet_wrap() splits the plot across **one variable**





Facets: Wrap

- Task: use facet_wrap() to create a bar plot for each sector (see right)
- Task: use the `scales` argument to allow each panel to be freely scaled by consumption (each panel has its own y-axis limits)
- Task: create a bar plot of consumption vs. year, coloured by Sector, faceted by fuel

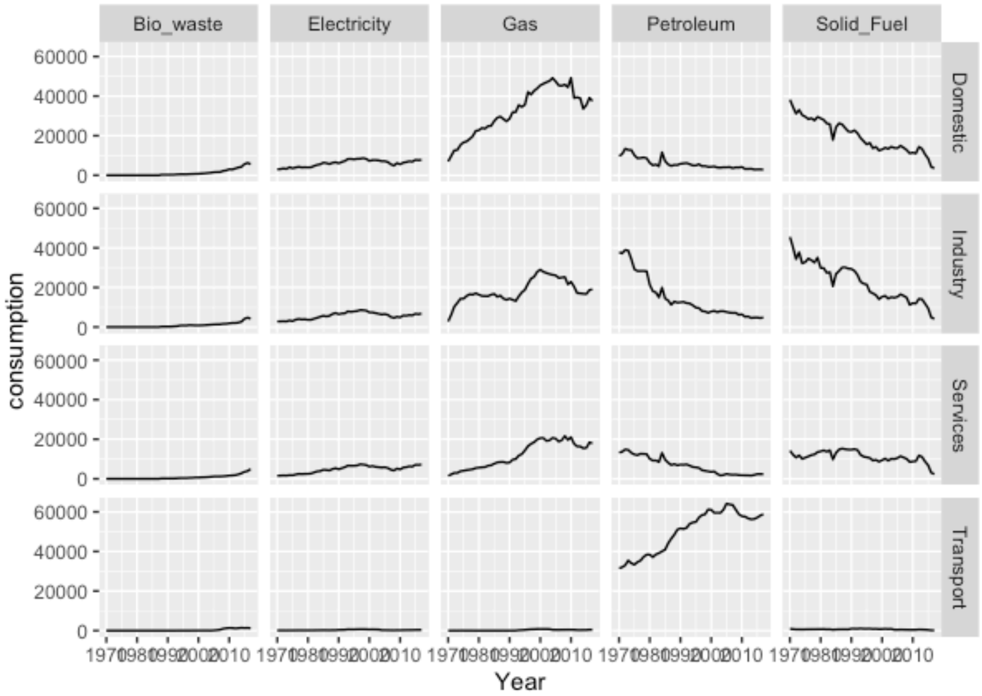
What happened here?

Use ggplot(data) + … + facet_wrap(~var) to create a panel for each value of var

You will need geom_col() and the fill aesthetic to colour bars

Facets: Grid

- Suppose we want to disaggregate the plot further, seeing each fuel and sector combination separately
- Task: use facet_grid() to create a line plot for each fuel and sector (see right)
- Task: look carefully at what happens when you set the scales argument to "free"
- Task: replace facet_grid() with facet_wrap() and set the y scale to be free



Use facet_wrap(var1 ~ var2) to spread var1 across rows and var2 across columns

Supervised Learning

The Task of Supervised Learning

- Supervised learning is the task of fitting a **model** (function) that maps inputs to outputs based on **labelled examples**
- The most common purposes of a supervised learning model are:
  - To predict things we don’t have data for:
    - What will the temperature be tomorrow? (**Regression**)
    - What does this image show? (**Classification**)
  - To better understand or quantify (possibly causal) relationships between variables:
    - What are the drivers of fuel poverty?
- At a high level, both purposes use the same methods, but some models are less **interpretable** or have better **predictive power** than others

Modelling MPG

- We will fit two models on the `mpg` dataset from ggplot2
- We will predict the highway MPG (`**hwy**`) with the following variables: **displ**, **cyl**, **drv**, **class**
- We will try a **linear regression model** and a **decision tree**
- Task: create a new data frame `df` which has only the following columns:
  - hwy
  - displ
  - cyl
  - drv

Splitting Data

- The models will be trained on a subset of the data (**training set**), and tested on the remainder (**testing set**) to determine how well they generalise to new data and avoid **overfitting**
- Task: split the data into `train` (75%) and `test` (25%) sets:
  - There are several methods: this one uses `sample_frac()` and `anti_join()`:

*Use set.seed(x) to set the **random seed**: this makes your results reproducible*

Use sample_frac(df, x/100) to sample x% of rows randomly from df

```
set.seed(123)

train <- sample_frac(df, 0.75) # Take 75% of the rows from df
test <- anti_join(df, train) # All rows in df that are NOT in train
```

Dummy Variables

- When dealing with categorical variables (factors), we need to convert them to something which we can deal with numerically
- drv has 3 classes: f (front wheel drive); r (rear WD); 4 (4 WD)
- We could naively assign these to 3 values (e.g. 1, 2, 3) but this assumes an ordinal characteristic which is not there!
- Dummy variables spread N classes across N-1 binary variables, with a 1 indicating the class
- R makes dummy variables **automatically** when fitting a model

Wrong way!

drv
f
r
4

→

drv
1
2
3

👎

Right way!

drv
f
r
4

→

drvf	drvr
1	0
0	1
0	0

👏

Note that `4` doesn't have a column: it is the case where all other values are 0

Formulae

- To fit a model, we need to specify a **formula**
- From the modelr package, you can use model_matrix() to see the model equation in matrix form
- This will also show you how dummy variables are going to be created

Explicit formula

```
hwy ~ displ + cyl + drv + class
```

Predict hwy with everything else

```
hwy ~ .
```

modelr::model_matrix(df, formula) returns the model equation explicitly in matrix form

	`(Intercept)`	displ	cyl	drvf	drvr	classcompact	classmidsize	classminivan	classpickup
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	1	1.8	4	1	0	1	0	0	0
2	1	1.8	4	1	0	1	0	0	0
3	1	2	4	1	0	1	0	0	0
4	1	2	4	1	0	1	0	0	0
5	1	2.8	6	1	0	1	0	0	0
6	1	2.8	6	1	0	1	0	0	0

Linear Model

- Linear regression models have the form:

Intercept

Coefficient

Noise/residual

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + b_N x_N + \epsilon$$

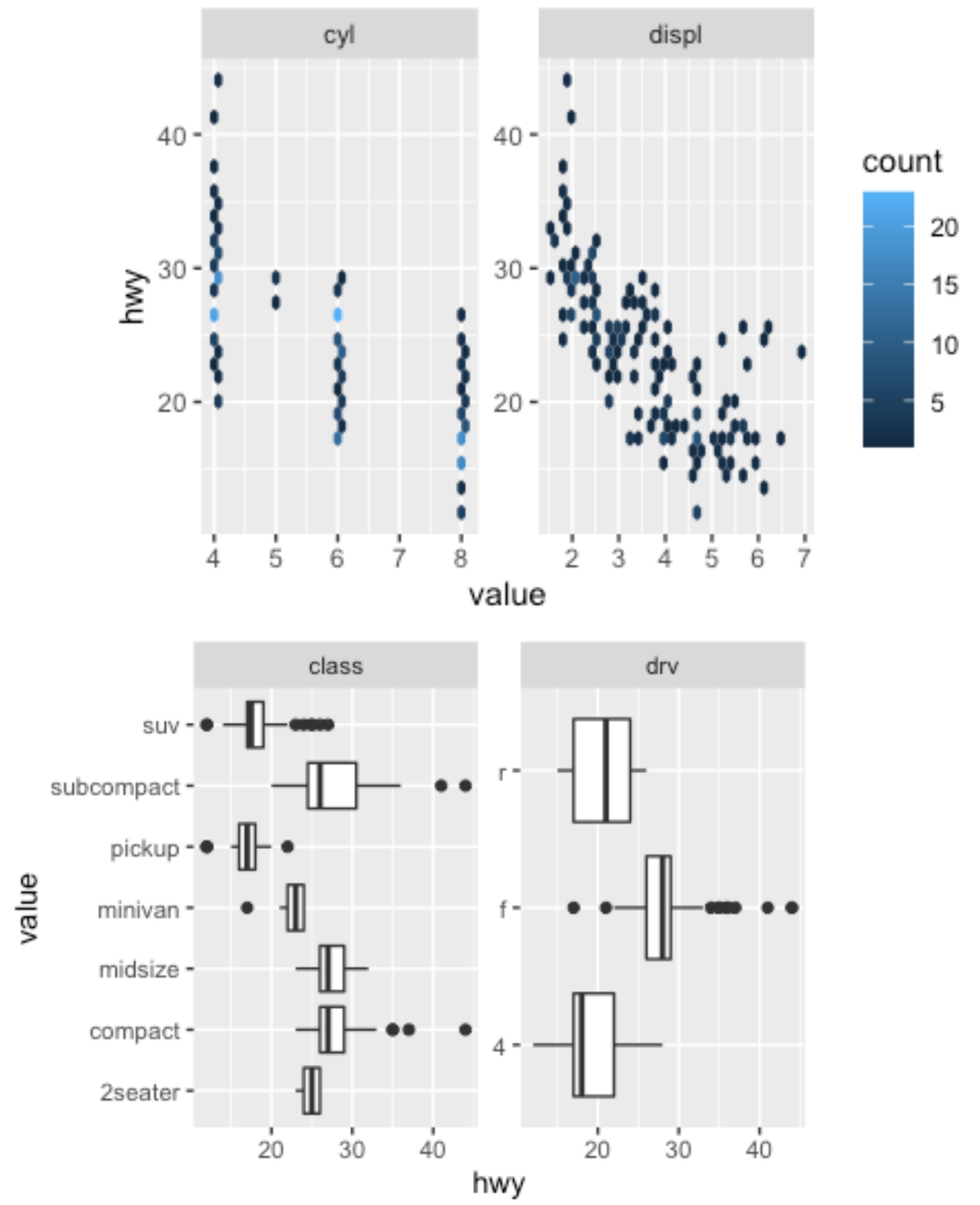
Dependent variable

Independent variable

Exploratory Analysis

- Before we fit the models, it's useful to have some intuition about what we <u>expect</u> to find
- Task: reproduce the right hand plot using facet_wrap()
- Given the plots on the right, what coefficients do you expect from the model?

Exploratory plots



Fitting the Linear Model

- We will now fit the linear model using the `lm()` function (which uses **ordinary least squares**)
- Task: fit the model **to the training data**
- We can use `summary(model)` to get some useful information about the model:
  - Summary statistics about the residuals
  - Coefficients and p-values
  - R^2 value
- From the broom package, `tidy()` can be used to summarise information about a model object in a tidy data frame
- How do the coefficients and p-values confirm/challenge your expectations?
- What can you say about the estimated MPG of 4 wheel-drive cars?

```
linear_model <- lm(hwy ~ ., data = train)
```

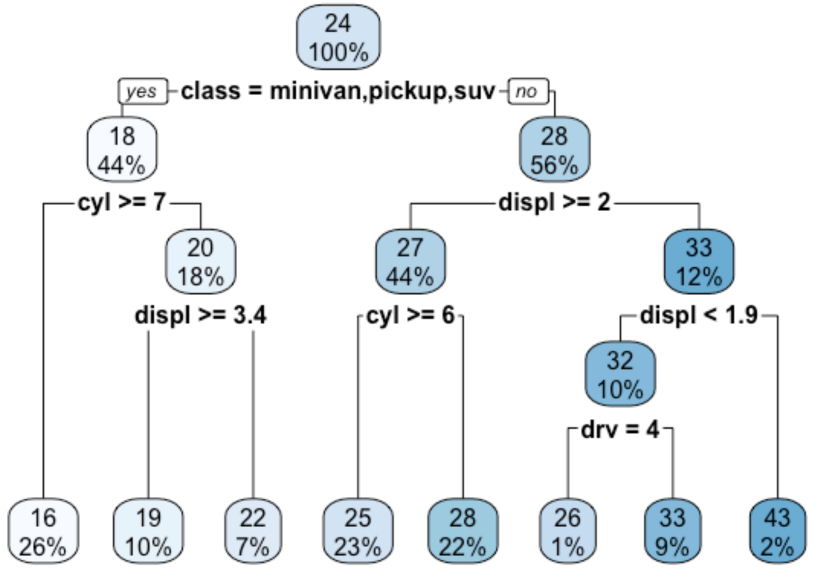
broom::tidy(model) summarises a linear model in a tidy data frame

```
# A tibble: 11 × 5
   term          estimate std.error statistic  p.value
   <chr>            <dbl>     <dbl>     <dbl>    <dbl>
 1 (Intercept)     37.0       2.08     17.8   3.21e-40
 2 displ           -0.417     0.564    -0.739 4.61e- 1
 3 cyl             -1.36      0.367    -3.71  2.79e- 4
 4 drvf             3.89      0.748     5.20  5.71e- 7
 5 drvr             1.39      0.886     1.57  1.19e- 1
 6 classcompact    -4.19      1.75     -2.40  1.77e- 2
 7 classmidsize    -4.93      1.73     -2.85  4.89e- 3
 8 classminivan    -9.29      1.84     -5.05  1.15e- 6
 9 classpickup     -8.71      1.67     -5.23  5.14e- 7
10 classsubcompact -3.52      1.70     -2.07  4.00e- 2
11 classsuv        -8.04      1.55     -5.19  6.07e- 7
```

Fitting the Decision Tree

Use rpart(formula, df) to fit a decision tree for formula, using data df

- The mechanics of fitting a model can generally be applied to several model types
- Fitting a decision tree with \`rpart()\` uses the same syntax as \`lm()\`, although the other arguments are more important too:
- Task: fit a decision tree to the model with \`rpart()\` and:
  - minsplit = 10
  - minbucket = 2
  - cp = 0.01



Plot a decision tree with rpart.plot(dt)

Making Predictions

- In R, model objects can be operated on with similar functions:
  - predict() to make predictions
  - summary() to see summary statistics
- A fitted model object can be applied to make predictions using `predict(model, data)`
- Task: use predict() to retrieve the predictions for the linear model and decision tree on the training data
- Task: use mutate() to add two columns to the `train` data frame with the linear model and decision tree predictions (like below)

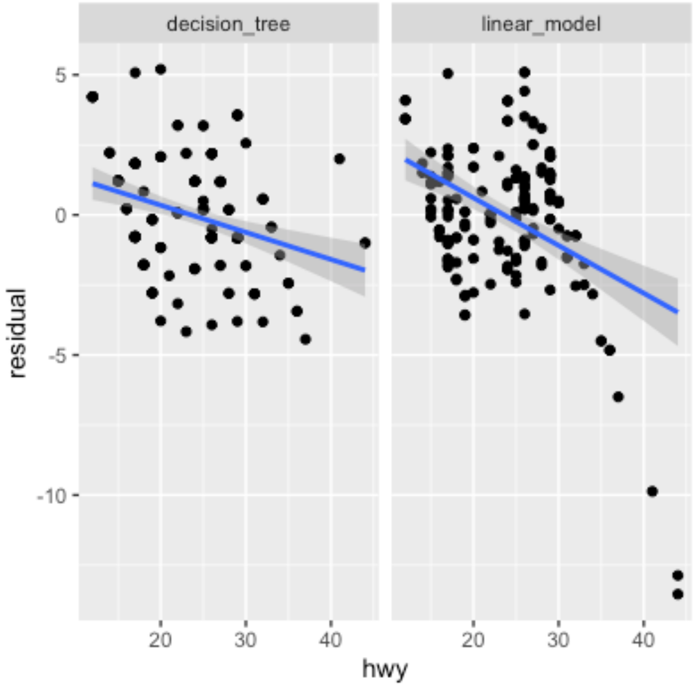
Actual ***Precictions***

hwy	displ	cyl	drv	class	linear_model	decision_tree
<int>	<dbl>	<int>	<fct>	<fct>	<dbl>	<dbl>
25	5.3	8	f	midsize	22.8	25.2
20	4	6	4	pickup	18.4	18.8
17	4.7	8	4	suv	16.1	16.2
25	3.1	6	4	compact	23.3	25.2

Plotting Residuals

hwy	displ	cyl	drv	class	model	predicted
<int>	<dbl>	<int>	<fct>	<fct>	<chr>	<dbl>
25	5.3	8	f	midsize	linear_model	22.8
25	5.3	8	f	midsize	decision_tree	25.2
20	4	6	4	pickup	linear_model	18.4
20	4	6	4	pickup	decision_tree	18.8
17	4.7	8	4	suv	linear_model	16.1
17	4.7	8	4	suv	decision_tree	16.2

- It is important to understand the **residuals** (difference between predicted and actual values) of your model
- Task: use pivot_longer() to make \`train\` a tidy data frame like the one on the right
- Task: add a \`residual\` column to \`train\` predicted – hwy
- Task: produce a scatterplot of residuals vs. hwy



Residuals are heteroskedastic

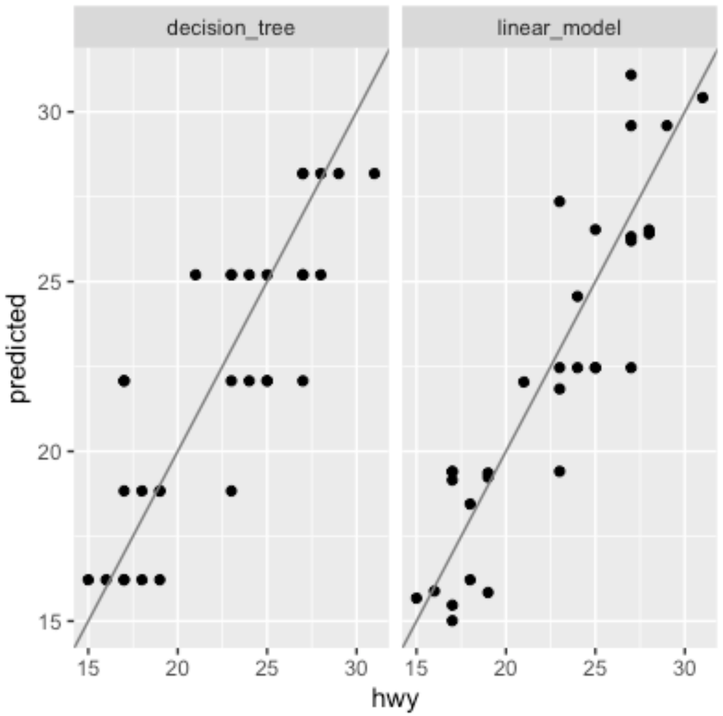
Use geom_smooth(method='lm') to add the linear fit

Use facet_wrap(~model) to add a panel for each model

Making Predictions on Test Data

- Now we will make predictions on the unseen test data and see which one has the best accuracy
- Task: add two columns to the `test` data frame giving predictions from linear model and decision tree using `predict()` (like we did for `train`)
- Task: pivot the data frame, creating a `model` column and `predicted` column
- Task: plot predicted versus actual values (as in the right hand plot)

Predicted vs. actual



The line y=x on the predicted vs. actual graph indicates perfect predictions

Accuracy Metrics (Regression)

- To compare the two models, we need a quantitative accuracy metric
- Common metrics for regression include:
  - Mean absolute error (MAE)
  - Mean squared error (MSE)
  - Root mean squared error (RMSE)
  - R2 (usually valid for linear models only)
- Task: write functions for MAE, RMSE and MAE
- Task: use group_by(), summarise(), and your accuracy functions to create a table of accuracy metrics for each model

Accuracy metrics for regression

Metric	Equation
Mean absolute error (MAE)	$\frac{1}{N}\sum_{i=1}^{N}\lvert y_i - \hat{y}_i\rvert$
Mean squared error (MSE)	$\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$
Root mean squared error (RMSE)	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$
R^2	$1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}$

y_i := predicted value for observation i
$\hat{y}_i$:= actual value for observation i
$\bar{y}$:= mean of actual values

Conclusions

- Which model was most accurate?
- Which model would you choose to use in practice?
- How confident would you be in each model to generalise to new data?
- What were the limitations of our approach?
- How could our method be improved? **Topics for next week!**

Mentimeter