BENV0091 Lecture 3: Introduction to Supervised Learning

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Lecture Overview

- 1. Tidy Data
- 2. Using Facets
- 3. Supervised Learning
 - 1. What is supervised learning?
 - 2. Setting up a supervised learning problem

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 - not tidy!

```
# A tibble: 2 \times 4
         `2016`
                `2017`
                         `2018`
          <db1>
                 <db1>
  <chr>
                          <db1>
  andy
            160
                    165
                            167
2 bella
            170
                    180
                            182
```

The data has been tidied using pivot_longer() below

```
# A tibble: 6 \times 3
           year height
  name
  <chr> <int>
                  <db1>
1 and \sqrt{\phantom{a}}
           2016
                     160
2 andy
           2017
                     165
3 andy
           2018
                     167
4 bella
          2016
                     170
5 bella
           2017
                     180
6 bella
          2018
                     182
```

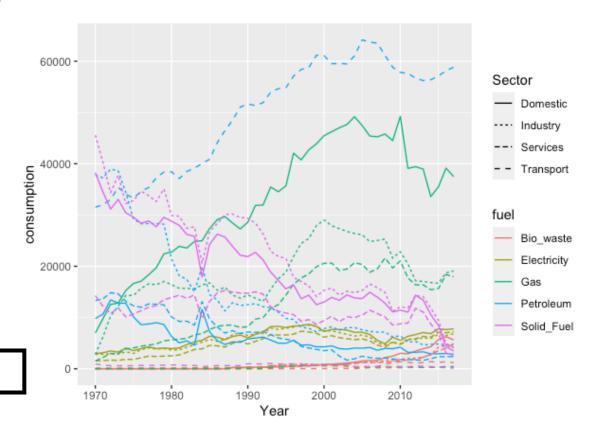
Pivoting

- 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
	<db1></db1>	<db1></db1>	<db1></db1>	<db1></db1>	<db1></db1>	<db1></db1>	<chr></chr>
1	<u>1</u> 970	<u>45</u> 573.	<u>37</u> 758.	<u>2</u> 808.	0	<u>2</u> 820.	Industry
2	<u>1</u> 970	899.	<u>31</u> 515.	1.23	0	107.	Transport
3	<u>1</u> 970	<u>38</u> 262.	<u>9</u> 798.	<u>6</u> 979.	0	<u>2</u> 976.	Domestic
4	<u>1</u> 970	<u>14</u> 260.	<u>13</u> 296.	<u>1</u> 511.	0	<u>1</u> 532.	Services
5	<u>1</u> 971	<u>40</u> 284.	<u>37</u> 250.	<u>6</u> 219.	0	<u>2</u> 846.	Industry
6	<u>1</u> 971	745.	<u>31</u> 998.	8.57	0	107.	Transport



Pivot Wider

- pivot_wider() does the opposite of pivot_longer()
- 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` `1978` `1979` `1980`

      **chr>** chr>** chr** chr>** chr** chr>** ch
```

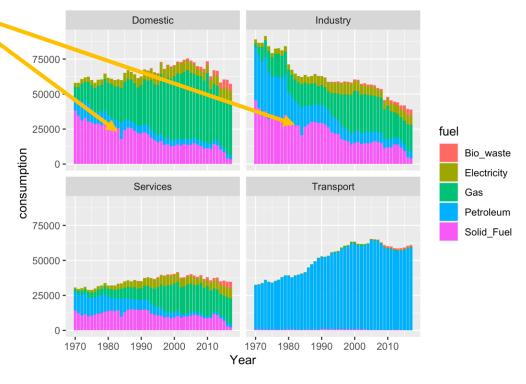
Facets

- The line plot we made of energy consumption by fuel and sector was pretty busy
- There are sometimes advantages to plotting variables across different axes
- 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

What happened here?

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

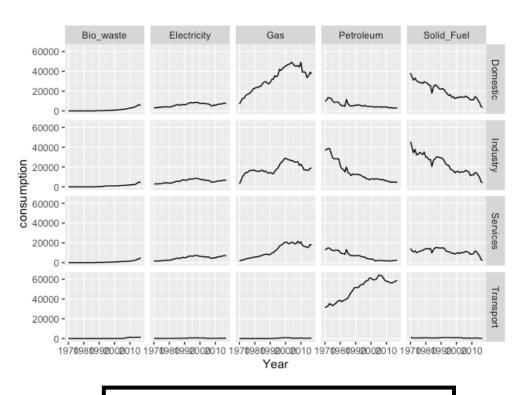


Use ggplot(data) + ... + facet_wrap(~var)

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

Mechanics of Model Fitting

- Let's fit two models on the `mpg` dataset
- 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
- The models will be trained on a subset of the data, and tested on the remainder to determine how well they generalise to new data

Preparing the Data

- Task: create a new data frame `df` which has only the following columns:
 - hwy
 - displ
 - cyl
 - drv
 - class
- There are several ways to split train and test data sets, 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

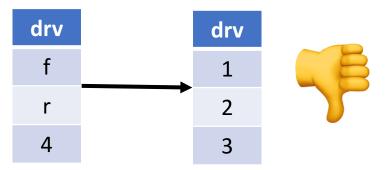
```
set.seed(123)

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</pre>
```

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!



Right way!

drv	drvf	drvr	Ar v
f	1	0	M
r	0	1	
4	0	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 \sim displ + cyl + drv + class

Predict hwy with everything else

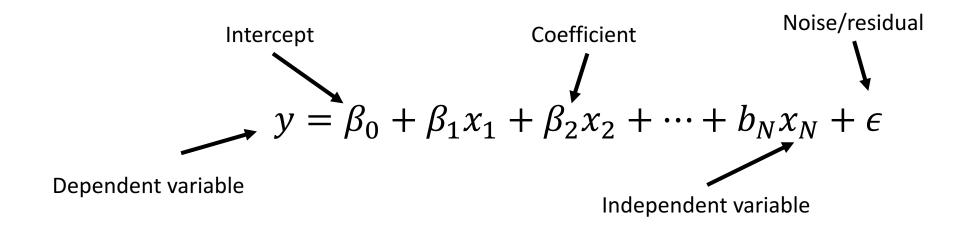
hwy \sim .

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

	`(Intercept)`	displ	cyl	drvf	drvr	classcompact	classmidsize	classminivan	classpickup
	<db1></db1>	<db1></db1>	<db1></db1>	<dbl></dbl>	<db1></db1>	<db1></db1>	<db1></db1>	<db1></db1>	<db1></db1>
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

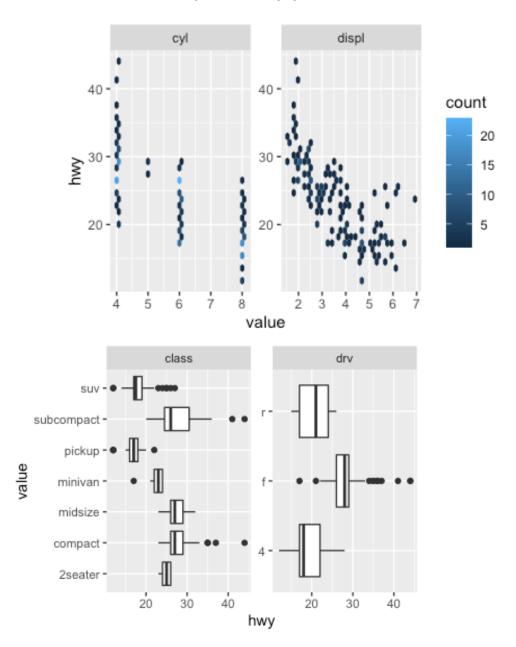
• Linear regression models have the form:



Exploratory Analysis

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

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
 - R² 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?

linear_model <- lm(hwy ~ ., data = train)</pre>

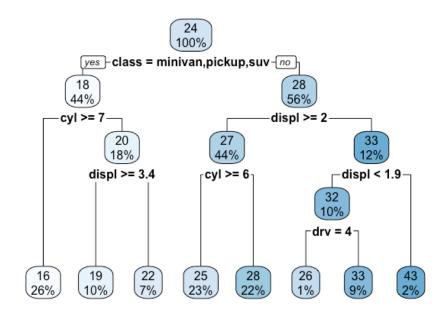
broom::tidy(model) summarises a linear model in a tidy data frame

```
# A tibble: 11 \times 5
                   estimate std.error statistic p.value
   term
   <chr>
                      <db1>
                                <db1>
                                                    <db1>
 1 (Intercept)
                     37.0
                                2.08
                                         17.8 3.21e-40
                     -0.417
                                0.564
                                         -0.739 4.61e- 1
2 displ
 3 cvl
                     -1.36
                                0.367
                                         -3.71 2.79e- 4
4 drvf
                      3.89
                                0.748
                                          5.20 5.71e- 7
                      1.39
                                0.886
                                          1.57 1.19e- 1
5 drvr
                     -4.19
                                         -2.40 1.77e- 2
6 classcompact
                                1.75
 7 classmidsize
                     -4.93
                                1.73
                                         -2.85 4.89e- 3
                     -9.29
 8 classminivan
                                1.84
                                         -5.05 1.15e- 6
9 classpickup
                     -8.71
                                         -5.23 5.14e- 7
                                1.67
10 classsubcompact
                     -3.52
                                         -2.07 4.00e- 2
                                1.55
                                         -5.19 6.07e- 7
11 classsuv
                     -8.04
```

Fitting the Decision Tree

- 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:
 - minsplit
 - minbucket
 - cp
- Task: fit a decision tree to the model with `rpart()`

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



Plot a decision tree with rpart.plot(dt)

Making Predictions on Test Data

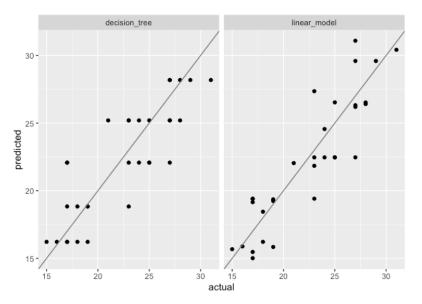
- In R, model objects can be operated on with similar functions:
 - predict() to make predictions
 - summary() to see summary statistics
- A fitted model object can be applied to make predictions using `predict(model, data)`
- Task: create a data frame `preds_df` with the following columns
 - `actual`: actual hwy MPG for test set
 - `linear_model`: predicted hwy MPG using linear model
 - 'decision_tree': predicted hwy MPG using decision tree
- Task: use pivot_longer to make `preds_df` a tidy data frame with the following columns:
 - `actual`: actual hwy MPG for test set
 - `model`: model used to make the prediction (linear model or decision tree)
 - `predicted`: predicted value

model	predicted
<chr></chr>	<db1></db1>
linear_model	30.4
decision_tree	28.2
linear_model	26.5
decision_tree	28.2
linear_model	19.4
decision_tree	25.2
linear_model	24.6
decision_tree	25.2
linear_model	15.8
decision_tree	16.2
	<pre><chr> linear_model decision_tree linear_model decision_tree linear_model decision_tree linear_model decision_tree linear_model decision_tree</chr></pre>

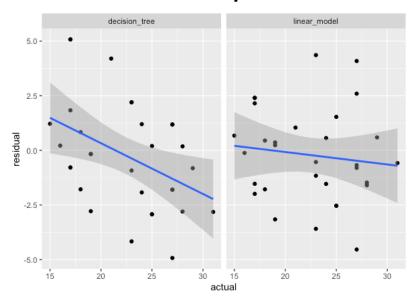
Plotting Residuals

- It is important to understand the **residuals** (error between predicted and actual values) of your model
- Some useful ways to visualise residuals
 - Predicted vs. actual plot
 - Residuals as a function of actual
- Task: add a `residuals` column to `preds_df`
- Task: produce the two plots on the right

Predicted vs. actual



Residual plot



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} y_i - \hat{y}_i $
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

Conclusion

- Which model performed best?
- What were the limitations of our approach?
- How could our method be improved?

Mentimeter