#### Outliers

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Lecture 04.2 (v2.0.2)

Why did you exclude all these responses?



freshspectrum.com

We define outlier as someone who doesn't like our program



### Signposting

- ► How do we identify Bad Data? That is, data that is misleading either due to missingness out atypicality.
  - ► This is one of the key ways that Data Science Goes Wrong.
  - ► Most researchers and practitioners do less than they should to understand their data.
- ► Today is about outliers. The workshop handles missing data.

# Bad Data: Missing and Misleading data

- ► The most time-consuming part of any real-world data analysis is data cleaning.
- ► This takes two main forms:
  - ► Imputing missing data where possible
  - ► Removing bad data where necessary
- ► It is vital that this is handled properly in order to gain appropriate insight from data.

# Quality Control: Diagnosing bad data

- Most of QC is about figuring out whether your data are really what you thought they were.
  - ▶ Did you measure what you set out to measure?
  - Are there systematic effects that were unexpected?
- ▶ In many disciplines there are well-defined ways to spot issues.

#### Statistical tools for bad data

- ► There are two main tools available:
- 1. Exploratory Data Analysis (Block 1)
  - ▶ Does it look generally look the way it should?
  - ► Methods involve both plots and data summaries
- 2. Outlier Detection
  - ▶ What specific parts of the data look unusual?
  - Methods focus on anomaly detection

### Key questions to ask

- 1. Do my data contain important missingness?
  - ▶ What aspects of the truth am I not seeing?
  - ► How would I know?
  - What impact could missingness have on my analysis?
- 2. Do my data containing important outliers?
  - ► What do we mean by an outlier?
  - What impact will they have on my subsequent analysis?
  - What should I do about them?

### **Anomaly Detection**

- ► Anomaly detection uses the core methods we have seen throughout.
- ► For example, Density estimation (Block 4), cluster analysis (Block 3), regression (Block 2), etc.
- ▶ These models:
  - provide a baseline measure of what is Normal?
  - Against which Unusual is measured.

## Measuring "Unusual" with p-values

- ► It is straightforward to use any model that can output a p-value as a measure of anomaly.
- ► Since a p-value is a Uniform random variable under the null, there is a wide literature available to assess whether the dataset as a whole is anomalous.
- ▶ The problem: If there is no plausible null hypothesis,
  - ▶ The data will "look weird" by any statistical measure.

## Measuring "Unusual" with descriptive statistics

#### Thresholding:

- ▶ We saw in the "boxplot" that outliers were defined as all observations at least 3/2 IQR above  $Q_3$  or below  $Q_1$ .
- ► This comes from reasoning about Normal distributions...
- Thresholding can be applied to p-values when they are not interpreted literally.
- ► Removed values should be investigated to understand why they are unusual.
- ► Thresholds might be obtained by:
  - reference to other datasets,
  - theory,
  - bootstrapping,
  - ▶ ... etc!

### Measuring "Unusual" with models

- Many modelling paradigms explicitly handle outliers. Some examples:
- ► Regression:
  - leverage of each point (not always the same as outliers)
  - Robust regression methods fit better in the presence of outliers
- **▶ Density-based** clustering (DBSCAN)
  - Points in low density regions may be outliers
  - An empirical p-value can be constructed from the set of points in lower-density regions.
- ▶ Isolation Forests
  - ► Random Forest-based technique (covered later).
  - Based on identifying "points that are easy to distinguish with a decision tree".
- Many other methods offer Pr(data|model).

## Duplicates and sample density

- ► Sample density obviously affects inference.
  - ► The sampling density should reflect the density of the data to be predicted.
- Missing data often makes many records, that should otherwise be different, appear the same.
  - ► This dramatically affects density estimation.
- ▶ One solution is to work only with unique records.
  - ► This solves some types of bias but not others, e.g. overrepresentation of particular regions of continuous variables.
  - ▶ No longer a density, but a plausible region.

#### Batch and similar effects

- Examining associations between features and properties of the data that should not matter are a vital tool in Quality Control.
- Some quantities are known apriori not to affect some feature.
  - For example, if data are observed in batches, the batch number shouldn't matter.
  - ► In regression analyses, minor batch effects can be regressed out (included in the model).
  - Major batch effects require the data to be discarded or treated specially.
- ► As always, Correlation  $\neq$  Causation.
  - So observing that e.g. different hospital wards contain systematically different patients isn't a smoking gun for a QC problem.

### Robust algorithms

- Most algorithms have robust alternatives, e.g.
  - Robust regression, (quantile regression),
  - Robust clustering,
  - ► Robust Kernel Density Estimation,
  - ... etc. Find one for your problem.
- Generally, robustness comes at a cost:
  - ► Increased computational complexity due to e.g. lack of integrability: e.g. Normal kernel replaced by Laplace,
  - ► Harder optimisation problem, e.g. more local minima, non-convex solution,
  - Or just not the model you wanted?
- Robustness is not a general property but defined with respect to some class of models.
  - ► There are many different "Robust algorithms for X" with different properties.
- ► "Too many" outliers will change the model anyway. How many is too many?

### Removing outliers

- ► "An outlier is an observation which deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism." Charu Aggarwal, IBM Research
- ▶ When outliers are detected, what should you do with them?
  - ► Switch to a robust algorithm and take the hit?
  - ► Remove outliers for the purpose of model building?
  - Add an "outlier model", e.g. a larger normal distribution in Gaussian Mixture Modelling?

#### Reflection

- ► How do we know that the class of outliers detected is the "right" ones?
- ▶ Do we expect more outliers in a test dataset?
- ► How might we test that an algorithm is the "right kind" of robust?

## Signposting

- Further Reading:
  - ► "A Survey of Outlier Detection Methodologies" by Victoria Hodge & Jim Austin, Artificial Intelligence Review 22:85–126 (2004).
  - ▶ Outlier Analysis by Charu C. Aggarwal. NB: Not freely available.
  - ► Chapter 10 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani) discusses the robustness to outliers for various methods.