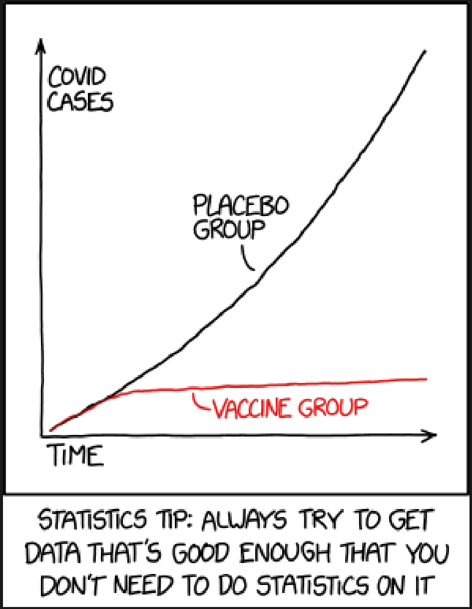
Towards Modern Statistical Testing

Daniel Lawson University of Bristol

Lecture 02.2 (v2.0.2)

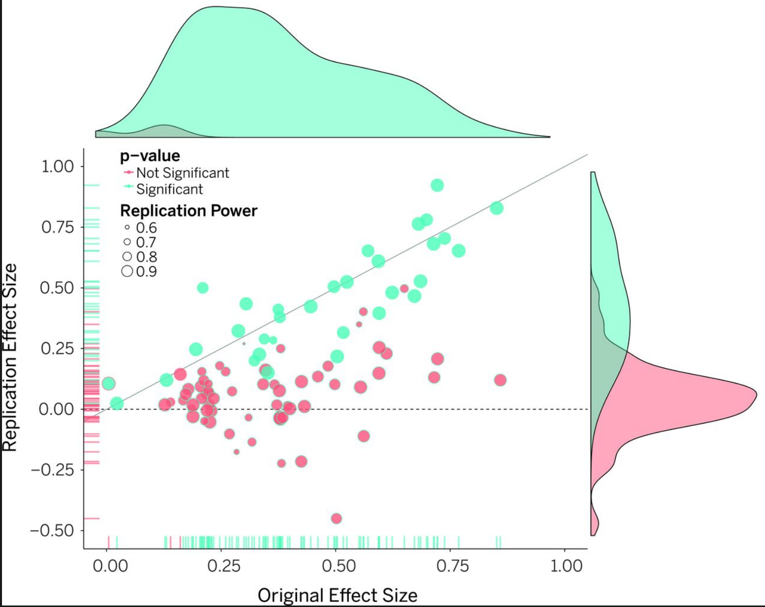


https://xkcd.com/2400/

Signposting

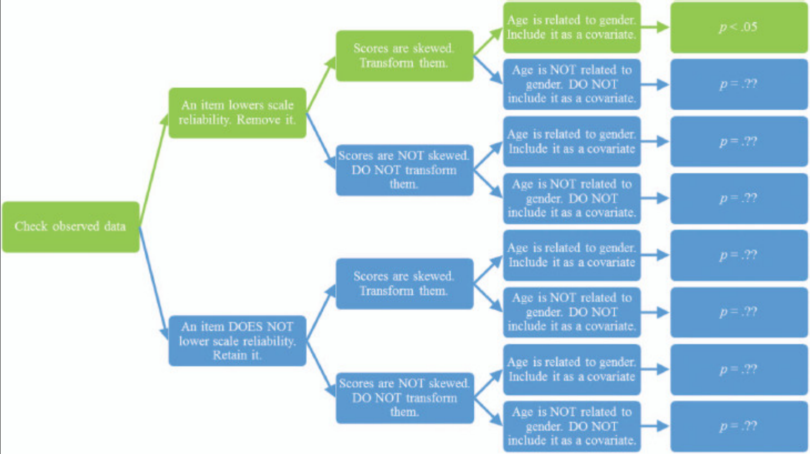
- This lecture covers three main topics:
  - Classical testing (and when its still ok to use it)
  - Modern testing (and how to use it well)
  - General Cross Validation (and why you should always do it)

The replication crisis



Estimating the reproducibility of psychological science. Science 2015

The garden of forking paths



Rubin: Four Solutions to the Forking Paths Problem, Rev. Gen. Psych. 2017

Questions

- Why might statistical testing have a bad reputation?
- What is the point of testing in large-scale data science?
- What is Monte-Carlo testing?
- What does(n't) Cross Validation save you from?

Null hypothesis test

- Given some data $\{y\}$:
  - Null Hypothesis **H0**: A statement is true about $\{y\}$.
  - Alternative Hypothesis **H1**: The statement is not true.
- We then compute a **test statistic** $T(\{y\})$ whose distribution is **computable under H0**.
  - By convention, large T is evidence against the null.
- Then compute p-value $p(T \geq T(\{y\}))$, the probability of observing a test statistic at least as large as that observed given H0 is true.
  - Example: H0: $\mathbb{E}(y) = \mu$ with $\mu = 0$. H1: $\mu \neq 0$.
  - This is **not model selection**. We favour H0 and must find evidence against it to accept H1.

Null hypothesis significance testing

- Hypothesis testing is asking: are my data consistent **with this hypothesis** when **using this measure**?
  - If you choose a silly hypothesis, testing will dutifully say "no"
  - If you use a weak measure, testing will dutifully say "yes"
  - Nothing is learned by this!
- The correct use of statistical testing is where:
  1. the **null hypothesis might plausibly be true**, or
  2. it might not be true, but you care how much **power the data has to reject the null**

When to use hypothesis testing

- Some valid use cases include:
  - To **rank hypotheses** by how much evidence there is against them
  - To obtain a **standardised scale** (0-1) for combining evidence
  - When **data are scarce**
- Also when testing plausible nulls, such as:
  - **validating simulations** with a known simulator;
  - **independence** or other non-parametric tests.
  - **broad null hypotheses**, such as testing a range of parameters.

Types of error

- The **p-value** defines *the probability that H0 is true, but is rejected*.
- The **power of the test** is *the probability that H0 is false but is accepted anyway*.
  - Low power situations are to be avoided: see e.g. Andrew Gelman's blog[1].
- Power is a surprisingly important problem because there are many *researcher degrees of freedom*.
  - so if power is low, we tend to find significant results anyway, through the (often unintentional) use of the data to choose the test.

[1] https://andrewgelman.com/2018/02/18/low-power-replication-crisis-learned-since-2004-1984-1964/

Types of error

Error notation

.	H0 true	H0 false
H0 accepted	Correct	Type II error
H0 rejected	Type I error	Correct

Types of error

Error notation

.	H0 true	H0 false
H0 accepted	Correct	Type II error
H0 rejected	Type I error	Correct

- Under the convention that $H0 = 0 =$ "negative" case and $H1 = 1 =$ "positive case":

Alternative notation

.	H0 holds	H1 holds
H0 accepted	True Negative	False Negative
H0 rejected	False Positive	True Positive

t-tests

- Can be one-tailed (**H0**: $\mu \leq \mu_0$) or two-tailed (**H0**: $\mu = \mu_0$)
- Assumes:
  - independence (note: paired tests are possible) and identically distributed
  - the **data are Normal**
  - the standard deviation is either known (t is then Normal) or estimated from the data (t is then t distributed).
- Used in regression, paired tests, etc.
- *NB Incomplete notes as this is a prerequisite!*

Chi squared test

- The χ^2 test is for categorical data comparing two variables.
- **H0**: No relationship between the variables; **H1** Some relationship between them.
- The **test statistic** for N datapoints from k classes, with x_i observations of type i, with expected value $m_i = Np_i$ where p_i is the expected probabilities, is (under the null):

$$X^2 = \sum_{i=1}^{k} \frac{(x_i - m_i)^2}{m_i} \sim \chi^2(k-1)$$

- This is most often used for **contingency tables** though appears elsewhere.
- See also **Fishers exact test** for small samples.
- *NB Incomplete notes as this is a prerequisite!*

Other important tests

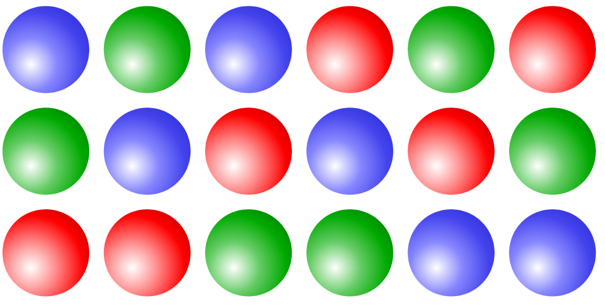
- Nonparametric tests:
  - **Mann-Whitney U or Wilcoxon rank sum** test: are two samples are drawn from the same distribution? by comparing their ranks.
  - **Wilcoxon signed-rank** test - as rank sum test, for paired data.
  - **Kolmogorov-Smirnov** test - are two samples from the same distribution? by comparing the empirical cumulative distribution function.
- There are many online cookbooks which state exactly which circumstances each test should be used in. You should be able to use them.
- *NB Incomplete notes as this is a prerequisite!*

Resampling

- The main types of resampling tests include:
  - **jacknifing**, which is analysing subsets of data to estimate (variance of) parameter estimates
  - **bootstrapping**, which is resampling with replacement, to estimate (variance of) parameter estimates
  - **permutation**, which is resampling without replacement, to test a null hypothesis
  - **cross-validation**, which is analysing subsets of data to estimate out-of-sample prediction, for model performance
- Each of these methods can be applied to a wide variety of problems, and often requires thought to use appropriately.

Permutations

All permutations of three colors (each column is a permutation):



- Figure from Wikipedia[2]. There are in general $n!$ permutations.

[2] https://upload.wikimedia.org/wikipedia/commons/4/4c/Permutations_RGB.svg

Generating permutations

```
> set.seed(1)
> n = 5
> x = seq(0,20,length=n)
> x
[1]  0  5 10 15 20
> x[sample.int(n)]
[1]  5 20 15 10  0
> x[sample.int(n)]
[1] 20 15  5 10  0
```

Use of permutations in testing

- Consider the following general class of problem:
  - H0: y is independent of x.
  - H1: y is dependent on x.
- x may be continuous, categorical, etc and y may depend on a number of other things.
- A **permutation test** will:
  - resample x, y pairs **under H0**,
  - Construct a test statistic T,
  - test if T is extreme in the real data, compared to the permutations?

Why permutations

- Asymptotically correct and distribution free. We only (**!**) have to assume **exchangeability**.
- Exchangeability of what?
  - what would be **equal if the null hypothesis is true**, and
  - would be **different if the alternative hypothesis is true**?
- The test is correct if we **maintain any true correlation structure**.
- For example, if the indices were originally correlated, permutation testing will fail.
  - as from e.g. a time-series.

Some main types of test (1)

x1	x2	x3	y1	y2
4	12	-3	2	-24

- Permutation of **indices**:

x2	y1	x3	y2	x1
4	12	-3	2	-24

Some main types of test (1)

x1	x2	x3	y1	y2
4	12	-3	2	-24

- Permutation of **indices**:

x2	y1	x3	y2	x1
4	12	-3	2	-24

- Permutation of **signs**, retaining magnitudes:

x1	x2	x3	y1	y2
4	-12	3	-2	24

Some main types of test (2)

x1	x2	x3	y1	y2
4	12	-3	2	-24

- Permutation of **group** labels:

x1	y1	y2	x2	x3
4	12	-3	2	-24

Some main types of test (2)

x1	x2	x3	y1	y2
4	12	-3	2	-24

- Permutation of **group** labels:

x1	y1	y2	x2	x3
4	12	-3	2	-24

- Permutation **within group** labels:

x1	x2	x3	y1	y2
12	-3	4	-24	2

Monte-Carlo testing

- There are in general $n!$ permutations. This is typically too many for $n > 20$.
- We instead choose N **random permutations** from all the possible ones.
- Monte-Carlo testing is an important subject in its own right.
- Its often possible to place guarantees on the p-value from very few samples.

Monte-Carlo test

- To conduct a Monte-Carlo test, we construct N random datasets and add our real dataset.
- We then ask, is the **real dataset an outlier** with respect to the random datasets?
- Specifically, the p-value for a test T applied to X (where large values are considered strange) is:

$$\frac{\mathrm{Rank}(T(X); T(\{x_i\}))}{N+1}$$

- where Rank simply counts the number of cases as large or larger.

Permutation testing summary

- **Distributional assumptions** are often invalid (regular tests)
- **Exchangeability assumptions** are often plausible (permutation tests)
- It is still possible to get misleading inference if the assumptions of a test don't hold

Model Selection

- Imagine that we have run two different inference procedures (models) on our data.
- We want to decide which of these gives the **best** description of the data.
  - (we might pretend we want to know which one is **right**. . .)
- Model selection formalises how to make this assessment.

General considerations

- To make Cross-Validation work, we need to be able to define our inference goal cleanly. Some scenarios:
  - **Same source, single datapoint**: Within a single datastream, how well can we predict the **next** point?
  - **Same source, segment of data**: Within a single datastream, how well could we predict everything that happens within an hour?
  - **New but understood source**: We have multiple datastreams, each of which might be different but all are generated by a similar process. How well can we predict a new such datasource?
  - **Unexpected source**: We have many classes of datastream. How well can we predict what would happen on a new class of datastream?

Problems with LOOCV

- We might worry that leaving out one datapoint at a time isn't enough:
  - **Cost**. It is straightforward to apply LOOCV to an arbitrary loss function, including a Likelihood. However, it can be costly.
  - **Quality**. LOOCV estimates of out-of-sample loss has high variance because each test datapoint using $n-2$ of the **same training datapoints**...
    - Empirically, we often choose a different model on different data generated under the same distribution!
  - **Correlation**. Any correlation breaks LOOCV.

K-fold CV

- Naive **k-fold CV** addresses the first issue by creating a **bias-variance tradeoff**: we introduce a bias (towards simpler models) but also significantly reduce the variance of the MSE estimation.
- More complicated sampling in k-fold settings can also address correlation.
- **Split** the data into k "folds" $f(i)$, that is, **random non-overlapping samples** of the data of size n/k. Then:
- **For each fold** i:
  - Call $X^{-(f(i))}$ the "training" dataset and $X^{(f(i))}$ the "test" dataset
  - Learn parameters $\hat{\theta}_i$ with data $X^{-(f(i))}$
  - Evaluate $l_i = \text{Loss}(X^{(f(i))}|\hat{\theta}_i)$
- And report $\frac{1}{n}\sum_{i=1}^{k} l_i$

How many folds?

- k-fold CV loses a fraction of the data, whereas LOOCV only loses a constant.
- This means that (under the assumption that the **true model is not in the model space**) k-fold CV will choose a **simpler model** with less predictive power than was possible.
- However, smaller k can make the inference more consistent across different data.
- For **small data**, LOOCV is recommended. For **larger data**, $k = 10$ is often chosen:
  - **cost**. k defines the minimum number of times you need to run the models. If you can afford to run a model once, you can probably afford 10 times.
  - **practicality**. If you had only 10% more data you might expect to get the same performance as LOOCV. We frequently lose this amount of data to quality control, etc.

Handling correlation

- **Correlation** structures can be handled in k-fold CV by **careful sampling**:
  - a-priori there is a correlation in time or space expected. we can therefore **remove windows**.
  - the data have some associated covariate, which can be removed en-masse.
  - empirical correlation structures can be used to select a point i and all points correlated with it above some **correlation threshold**.
- Some of these can be used in other contexts. Examples include:
  - **block bootstrap**
  - Using a different definition of a “datapoint” in a leave-one-out context, for example: datapoints are countries instead of countries at timepoints

Reflection

- You should understand how to:
  - Define and use a null hypothesis significance test,
  - Contrast classical and resampling tests, and judge appropriate uses,
  - Use statistical testing appropriately in projects.

Further reading

- Classical Testing
  - Chapter 4 of Statistical Data Analysis by Glen Cowan
  - Statistical tests, P values, confidence intervals, and power: a guide to misinterpretations by Greenland et al
  - Andrew Gelman's blog has many examples of statistical testing failures in social science and medicine
- Modern Testing
  - Cosma Shalizi's Modern Regression Lectures (Lectures 26,28)
  - Cross Validation and Bootstrap Aggregating on Wikipedia
  - Chapters 18.7 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
- Cross Validation
  - Chapters 2.3 and 7.10 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
  - Cosma Shalizi's Modern Regression Lectures (Lectures 20, 26)

Appendix: How many permutations?

- The **smallest possible p-value** with N permutations is $1/(N+1)$. So 999 permutations gives a minimum of 0.001.
- The **variance** around a chosen threshold, say $p = 0.05$, is determined by the sampling distribution of the Binomial:

$$\mathrm{sd}(p) = \mathrm{sd}\left(\mathrm{Bin}(N, p)\right) = \sqrt{\frac{p(1-p)}{n}}$$

  - p is of course the true unknown probability, not the observed one.
  - But variance is an increasing function of p (for $p < 0.5$)
- A heuristic rule is: to be 95% confident that $p \leq t$ we need the empirical p-value to be less that $t - 1.96\mathrm{sd}(p = t)$
- For $N = 999$ and $t = 0.05$, $\mathrm{sd}(p = t) = 0.0135$ and therefore $p < 0.036$
- A similar calculation shows $N = 999$ wouldn't be enough to be sure we were less than 0.005.
- This is conservative... only if the distribution is Normal....(**!**) **Plot the distribution of T**!