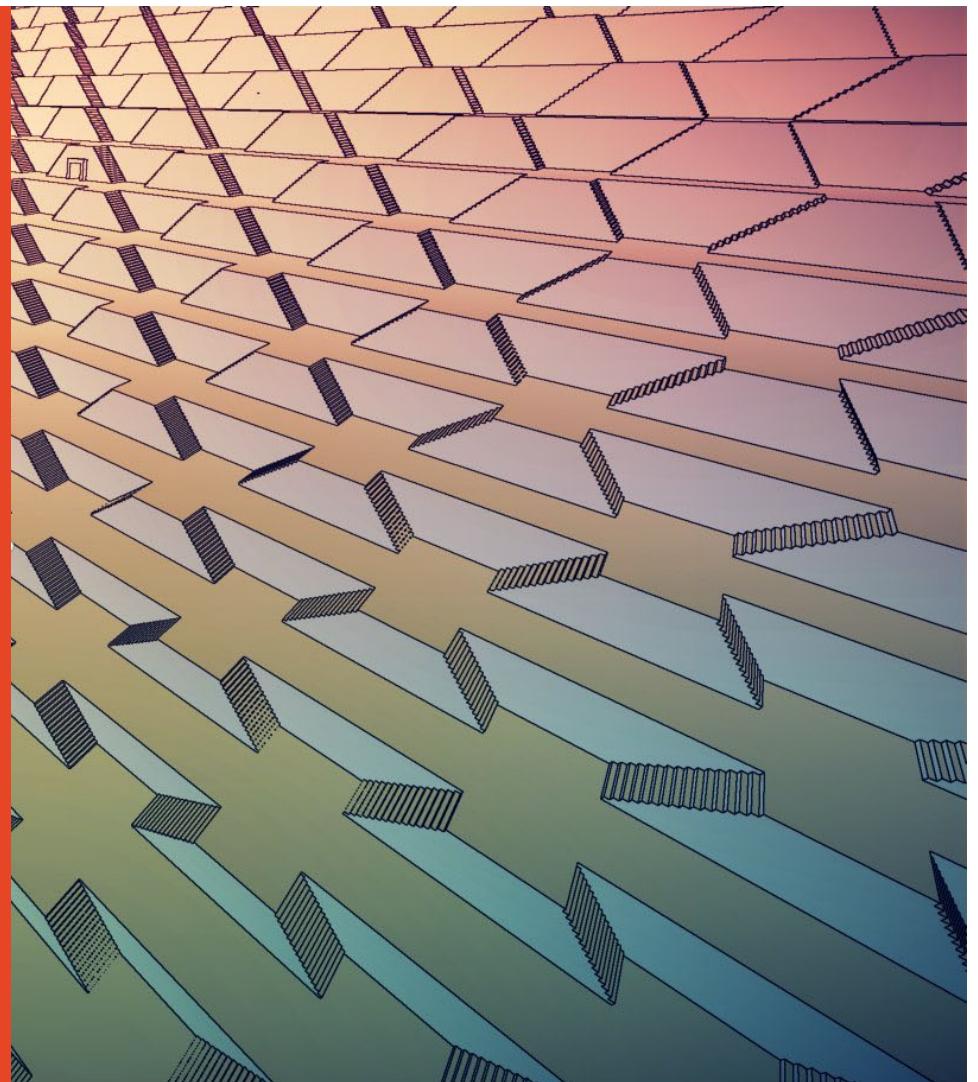


Multivariate Statistical Analysis 1: Dimension Reduction Methods

Presented by
Alex Shaw
Sydney Informatics Hub
Core Research Facilities
The University of Sydney



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Suggested wording:

General acknowledgement:

"The authors acknowledge the technical assistance provided by the Sydney Informatics Hub, a Core Research Facility of the University of Sydney."

Acknowledging specific staff:

"The authors acknowledge the technical assistance of (name of staff) of the Sydney Informatics Hub, a Core Research Facility of the University of Sydney."

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How to use this workshop

Workshops developed by the Statistical Consulting Team within the Sydney Informatics Hub form an integrated modular framework. Researchers are encouraged to choose modules to **create custom programmes tailored to their specific needs**. This is achieved through:

- **Short 90 minute workshops**, acknowledging researchers rarely have time for long multi day workshops.
- Providing **statistical workflows applicable in any software**, that give **practical step by step instructions which researchers return to when analysing and interpreting their data or designing their study** e.g. workflows for designing studies for strong causal inference, model diagnostics, interpretation and presentation of results.
- Each one focusing on a specific statistical method while also integrating and referencing the others to give a **holistic understanding of how data can be transformed into knowledge from a statistical perspective** from hypothesis generation to publication.

For other workshops that fit into this integrated framework refer to our training link page under statistics <https://www.sydney.edu.au/research/facilities/sydney-informatics-hub/workshops-and-training.html#stats>

Research Workflows

– So... what is a workflow?

- The process of doing any statistical analysis follows the same general “shape”.
- We provide a general research workflow, and a specific workflow for each major step in your research (currently **experimental design, power calculation, analysis using linear models/survival/multivariate/survey methods**)
- You will need to tweak them to your needs

– Why do we need a research workflow?

- As researchers we are motivated to find answers quickly
- But we need to be *systematic* in order to
 - Find the right method
 - Use it correctly
 - Interpret and report our results accurately
- The payoff is huge, we can avoid mistakes that would affect the quality of our work and get to the answers sooner



Using this workshop after today

These slides should be used after the workshop as reference material and include these **workflows for you to follow**

- Todays workshop gives you the **statistical workflow**, which is software agnostic in that they can be applied in any software.
- In future, there may also be accompanying **software workflows** that show you how to do it. We won't be going through these in detail. But if you have problems we have a monthly hacky hour where people can help you.

1on1 assistance You can request a consultation for more in-depth discussion of the material as it relates to your specific project. Consults can be requested via our Webpage (link is at the end of this presentation)

During the workshop

 Ask short questions or clarifications during the workshop. There will be breaks during the workshop for longer questions.

 Slides with this blackboard icon are mainly for your reference, and the material will not be discussed during the workshop.



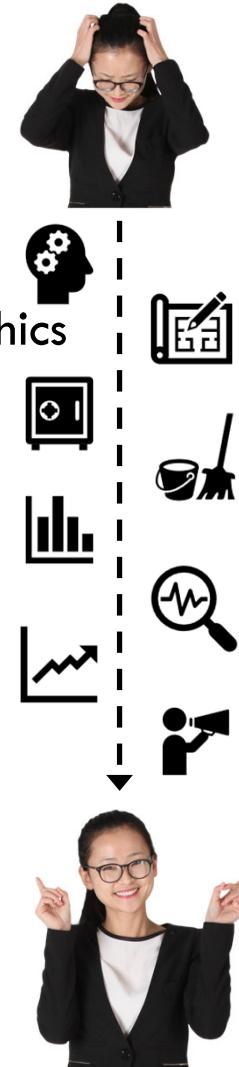
Challenge Question

- A wild boar is coming towards you at 200mph. Do you?:
 - A. Ask it directions
 - B. Wave a red flag
 - C. Wave a white flag
 - D. Begin preparing a trap



General Research Workflow

- 1. Hypothesis Generation** (Research/Desktop Review)
- 2. Experimental and Analytical Design** (sampling, power, ethics approval)
- 3. Collect/Store Data**
- 4. Data cleaning**
- 5. Exploratory Data Analysis (EDA)**
- 6. Data Analysis aka inferential analysis**
- 7. Predictive modelling**
- 8. Publication**

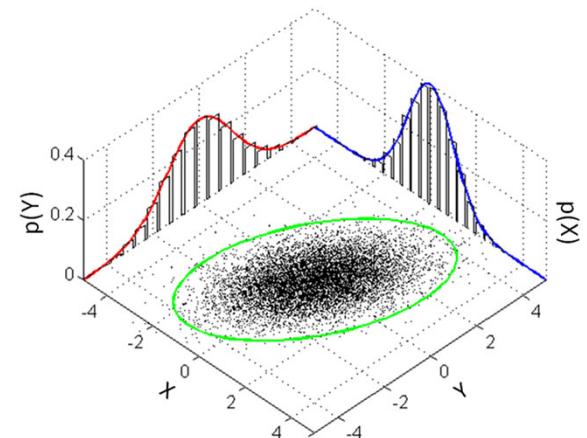


Learning Objectives

- Understanding the motivation for using multivariate methods
- Understanding the goals of multivariate methods
- A workflow for dimension reduction methods
- Introduction to major dimension reduction methods:
 - Principal Components Analysis and Factor Analysis
 - Correspondence Analysis
 - nMDS
- Not covered in this workshop:
 - Multivariate regression
 - Multivariate hypothesis tests

Multivariate Statistics

- Multivariate statistics is a subbranch of stats concerned with the simultaneous analysis of more than one *random* variable.
- A random variable is essentially a variable in your analysis for which we model a probability distribution (usually an outcome variable)
- It is common to have more than one variable in your study, but we often treat some variables as ‘fixed’ (i.e. no probability distribution). *E.g. in univariate linear models, the explanatory variables are fixed.*
- Multivariate statistics applies when you are considering multiple random variables in combination e.g. *in linear models with multiple outcome variables.*
- We are usually interested in the relationships between these random variables, i.e. how the variables vary together. Otherwise, we could just perform [a simpler] univariate analysis on each.



https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Why multivariate statistics?

- **Multivariate statistics** is a very broad topic with a huge array of different techniques. The motivation for using one of these techniques may include:
 - **Investigation of dependence:** relationships among variables, either explanatory or outcome variables
 - **Sorting and grouping:** identify groups among the entities/subjects under study
 - **Data reduction:** summarise multiple variables through a smaller set of ‘synthetic variables’
 - **Hypothesis testing:** group differences for multiple outcome variables
 - **Prediction:** based on a multivariate model

Which of these has brought you to this workshop?

Special cases of multivariate statistics

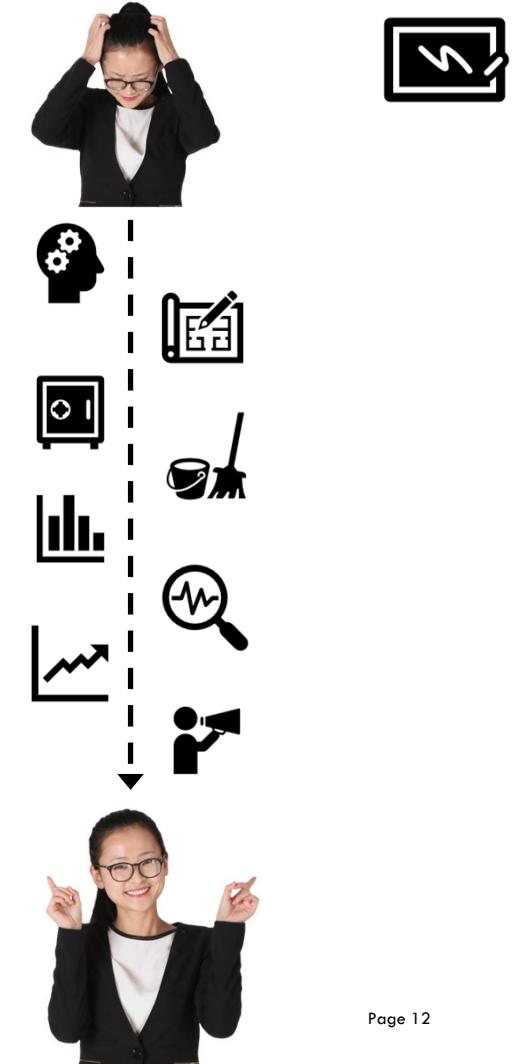


- Multivariate statistics also come in to play in situations where we have repeated measurements on the same individual, usually longitudinal data
- Although these are indeed important applications of multivariate statistics, they are a special case and outside the scope of this workshop
- See our Linear Models series of workshops and/or book a consult with us to discuss analysis of repeated measures data

General Research Workflow

1. Hypothesis Generation (Research/Desktop Review)
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4. Data cleaning
5. Exploratory Data Analysis (EDA)
6. Data Analysis aka inferential analysis
7. Predictive modelling
8. Publication

Discovery projects to generate new hypotheses by characterising individuals (new cell populations, human populations)



General Research Workflow

1. Hypothesis Generation (Research/Desktop Review)
2. Experimental and Analytical Design (sampling, power, ethics approval)
3. Collect/Store Data
4. **Data cleaning**
5. Exploratory Data Analysis (EDA)
6. Data Analysis aka inferential analysis
7. Predictive modelling
8. Publication

Multivariate techniques are an important part of QC (Quality Control) in high-throughput biology

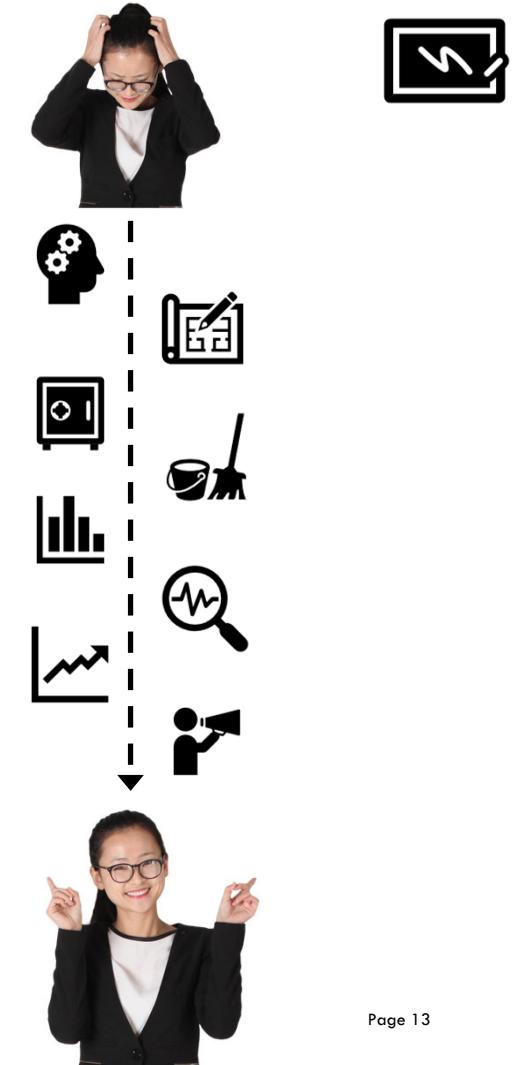
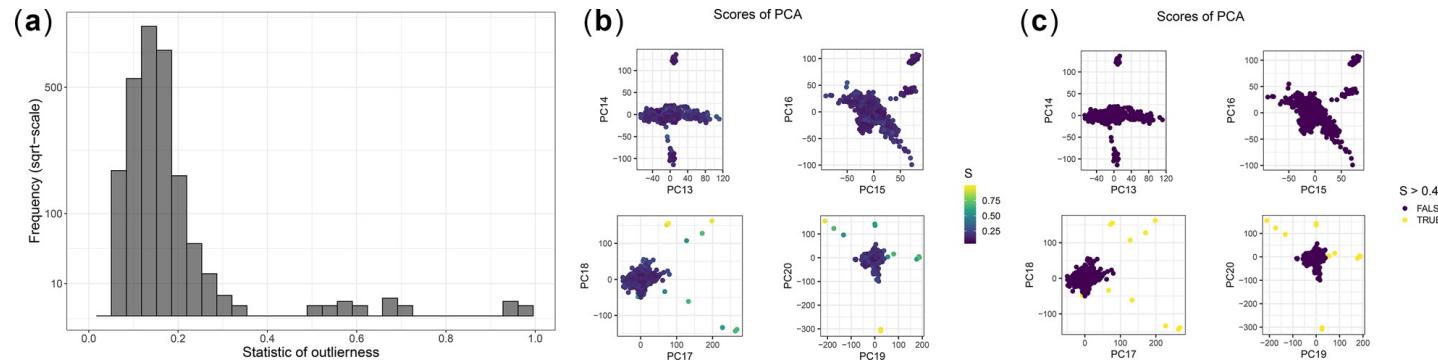




Fig. 2. Outlier detection in the 1000 Genomes (1000G) project, using prob_dist (Section 3.4)



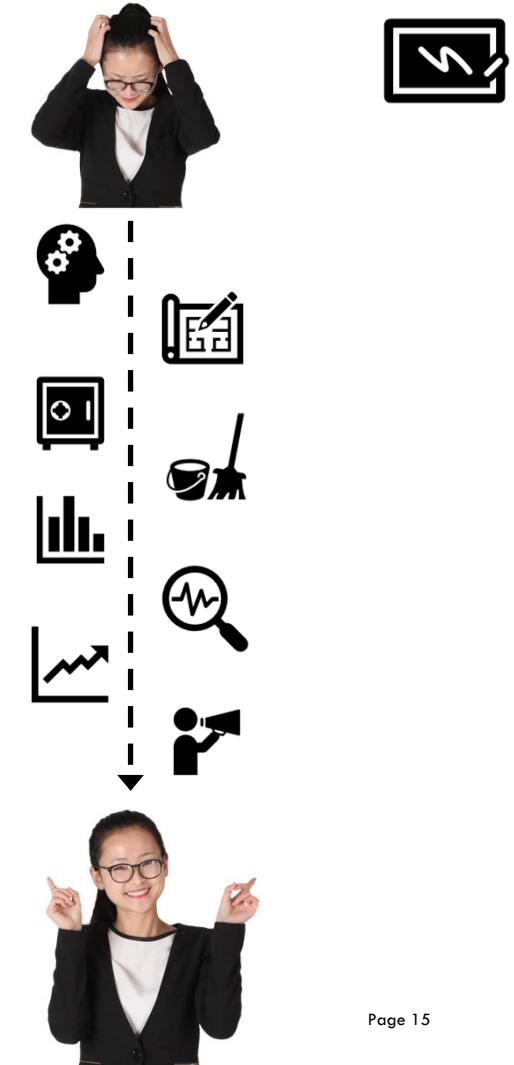
Bioinformatics, Volume 36, Issue 16, 15 August 2020, Pages 4449–4457, <https://doi.org/10.1093/bioinformatics/btaa520>

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General Research Workflow

1. Hypothesis Generation (Research/Desktop Review)
2. Experimental and Analytical Design (sampling, power, ethics approval)
3. Collect/Store Data
4. Data cleaning
5. **Exploratory Data Analysis (EDA)**
6. Data Analysis aka inferential analysis
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8. Publication

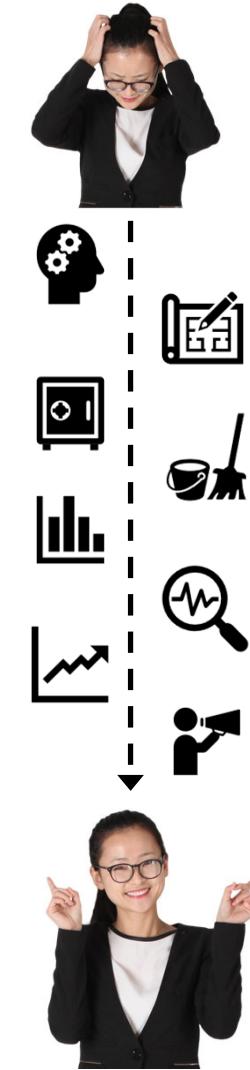
An important component of the research workflow. When there are multiple predictors, characterising the higher-order relationships between them is useful. See **Model Building Workshop**.



General Research Workflow

1. Hypothesis Generation (Research/Desktop Review)
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8. Publication

- Regression with multivariate outcome
- Measurement model with latent variables
- Prediction of class for new subjects



Statistical Principles Background



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Multivariable analysis

- Is simple (or multiple) linear regression an example of multivariate statistics?
- No, because the explanatory (x) variables are considered **fixed**, we only model the variability in our outcome (y) directly
- So although we call x the explanatory **variables**, they are not an outcome variable, and merely act as the ‘levels’ at which we examine variability around the outcome variable’s mean



From Linear Models II

$$Y_i = \beta_0 + \beta_1 X_{1i} + \varepsilon_i$$

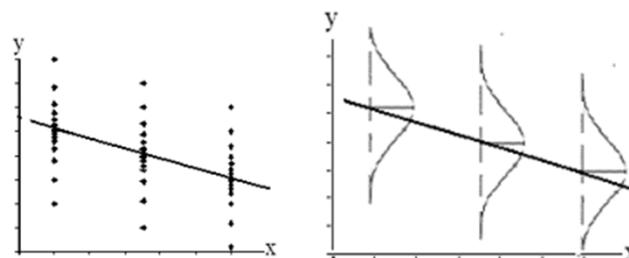
Data

Y_i ~ Response of Observation i

X_{1i} ~ Predictor X_1 of Observation i

Random (Stochastic) Model & Parameters

ε_i ~ Error of Observation i from Deterministic model

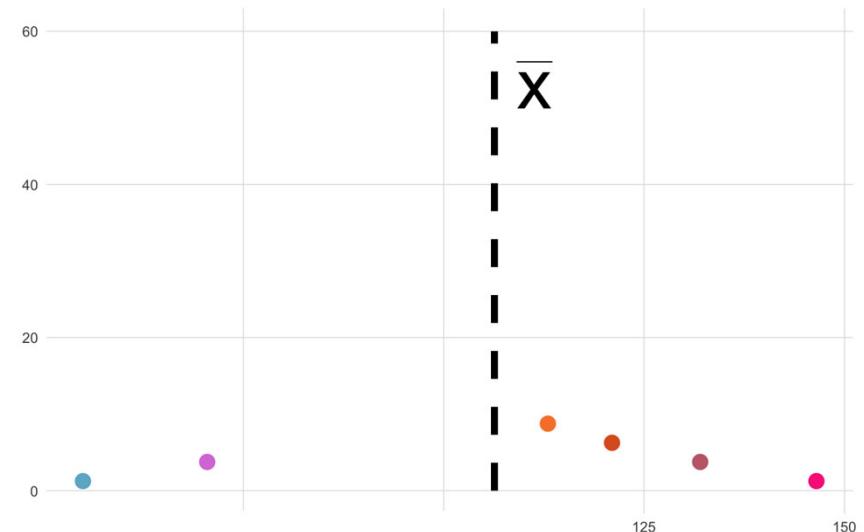


Relationships between variables

- How do we measure the relationship between two variables?
- It depends on the type of variable:
 - For continuous variables we examine their patterns of **covariance/correlation**
 - For categorical variables we examine their patterns of **association**

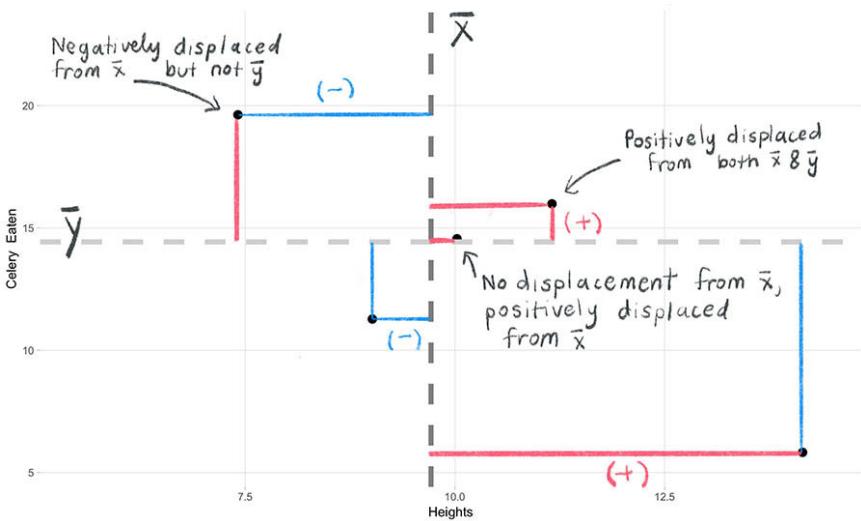
Covariance

- For two continuous variables we need the concept of covariance
- Variance: take the distance of each observation from the mean, square it, and add the squares together. Then divide by the sample size



Covariance

- Covariance extends the concept of variance to the relationship between two variables
- How do two different variables vary together?
- Here, we need to consider the sign and the magnitude of the deviation from the mean of both variables
- Instead of adding squares as per variance, we add (and cancel out) signed cross-products



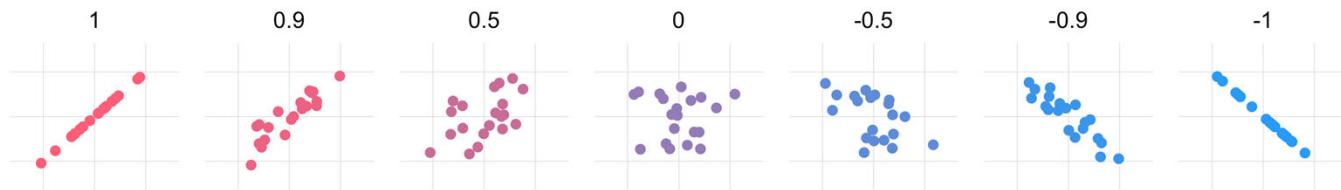
Correlation

- A problem with covariance: it's difficult to interpret and scale dependent

$$\text{cov}(x, y) = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})$$

- The solution is correlation:

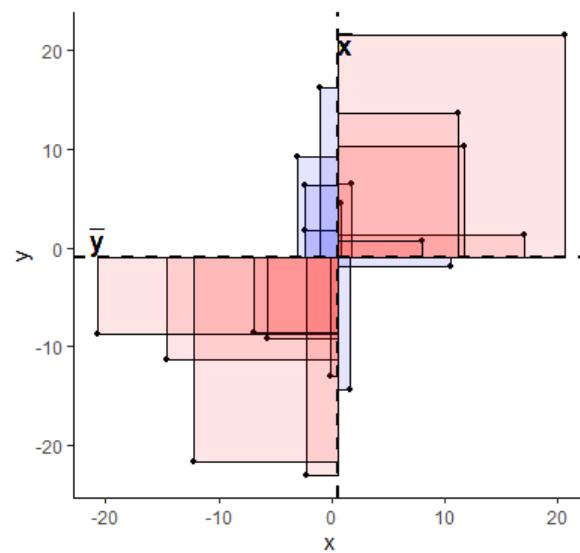
$$r(x, y) = \frac{\text{cov}(x, y)}{s_x s_y}$$



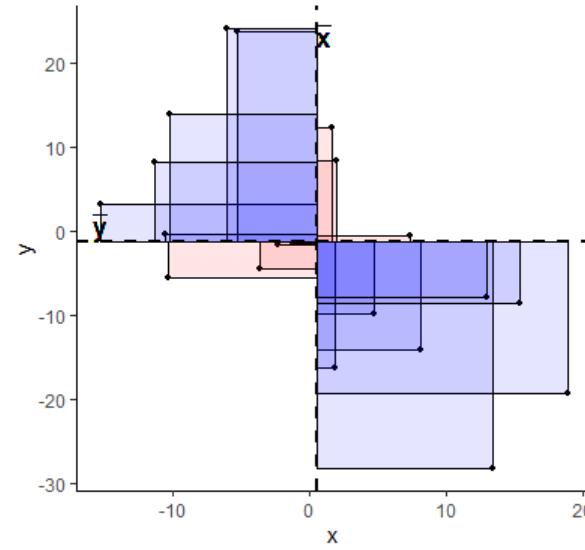


Eyeball test

Is the correlation of these pairs of variables positive, negative or close to 0?



Positive correlation

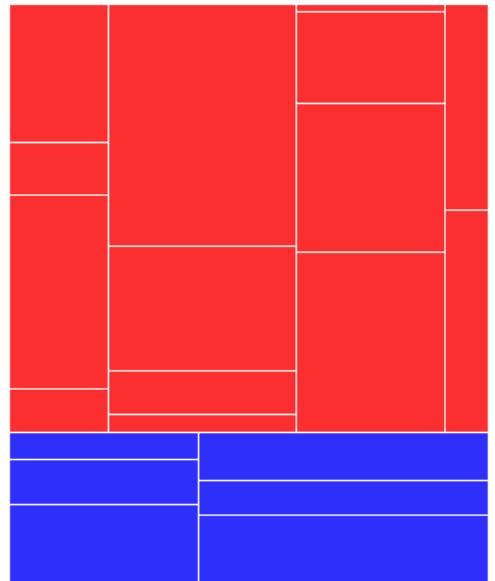


Negative correlation



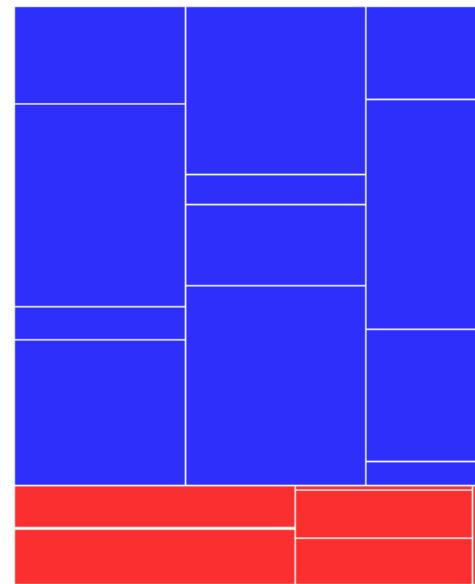
Eyeball test

Is the correlation of these pairs of variables positive, negative or close to 0?



sign
■ -
■ +

Positive correlation



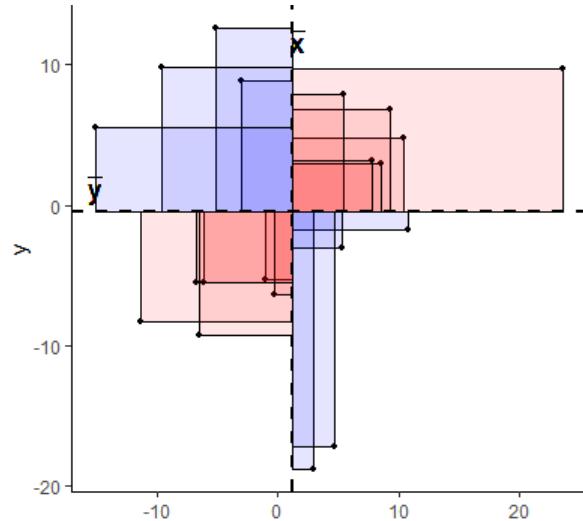
sign
■ +
■ -

Negative correlation

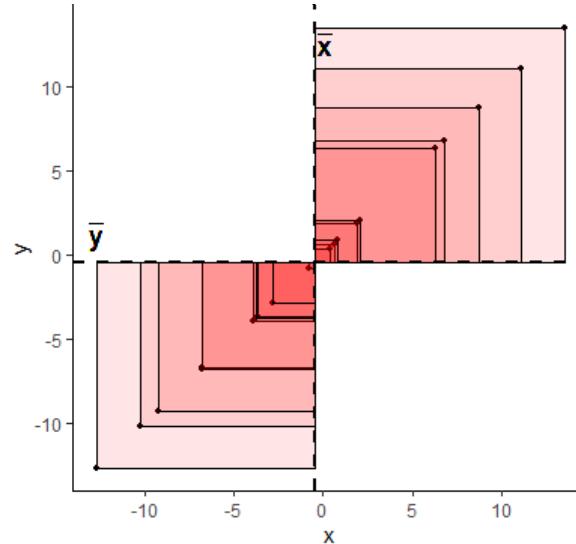


Eyeball test

Is the correlation of these pairs of variables positive, negative or close to 0?



Close to 0 correlation



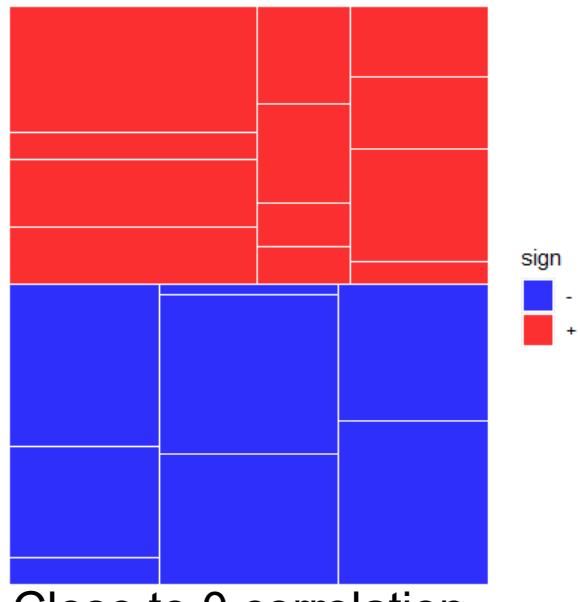
Correlation of 1

Variance = Covariance of a variable with itself

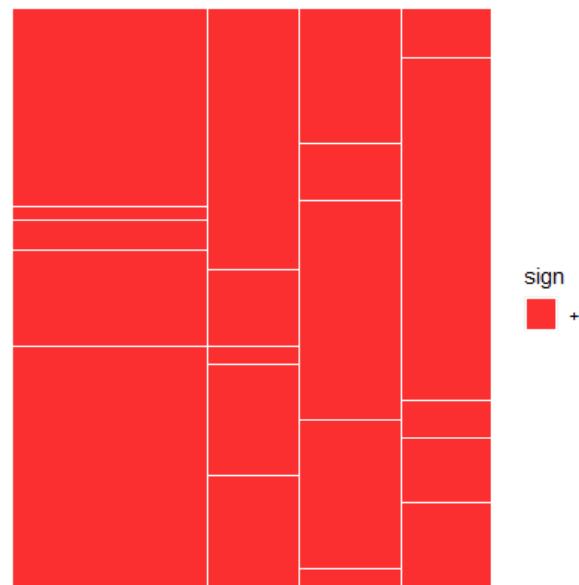


Eyeball test

Is the correlation of these pairs of variables positive, negative or close to 0?



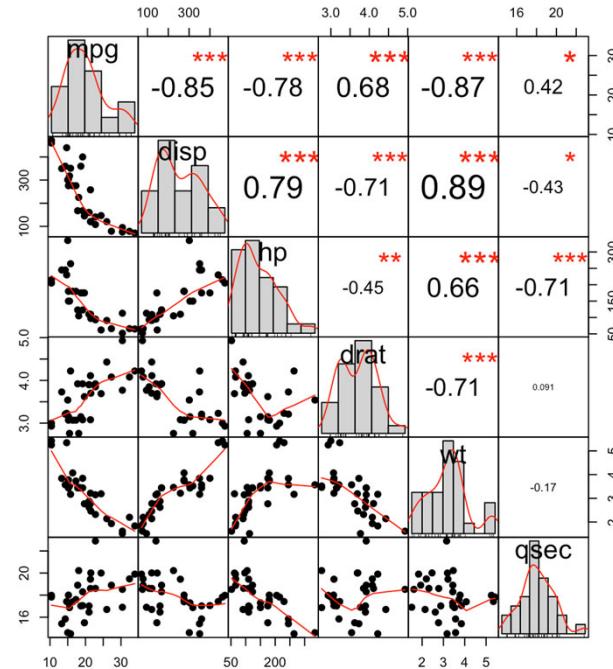
Close to 0 correlation



Correlation of 1
Variance = Covariance of a variable with itself

Correlation matrix

- Covariance and correlation are a summary of the relationship between two variables
- For more than two variables, a correlation is calculated between each pair of variables
- We can create a correlation matrix from these pairwise correlations
- This matrix is useful for exploratory data analysis in itself, and is used extensively in the mechanics of the analysis techniques that follow. It's a summary of the relationships between all variables in your analysis.

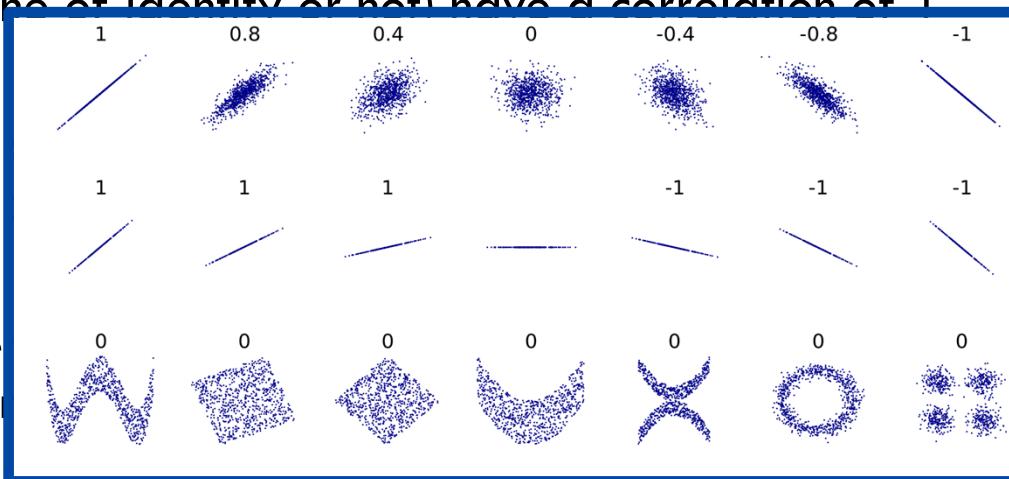


Types of correlation

- You may have noticed that points in a scatter plot that fall along a straight line (whether line of identity or not) have a correlation of 1
- This is actually called Pearson correlation coefficient, and it is only capable of capturing and quantifying a linear relationship between two variables
- There are other options for non-linear relationships, the most used being Spearman's rank correlation
- So please keep in mind, Pearson correlation coefficient, or a method that uses a [Pearson] correlation matrix as input, is only meaningful for linear relationships

Types of correlation

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- So please keep in mind, Pearson correlation coefficient, or a method that uses a [Pearson] correlation matrix as input, is only meaningful for linear relationships



Association

- The categorical variable equivalent of correlation is usually termed association.
- Potential association between two categorical variables is usually examined using a contingency table

	Dislikes Crosswords	Likes Crosswords
Dislikes Statistics	0.1	0.4
Likes Statistics	0.1	0.4



- Let's assume that the proportions shown are the actual proportions in the population.
- Now I choose a new person from the population. If I know that someone likes statistics, does that tell me anything about whether they like crosswords?



Association

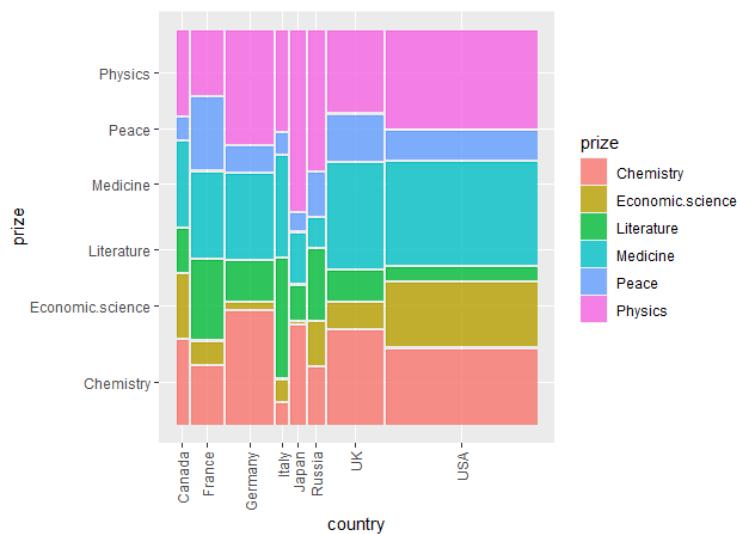
- How about the table on the right? If I know that someone likes statistics, does that tell me anything about whether they like crosswords?

	Dislikes Crosswords	Likes Crosswords		Dislikes Crosswords	Likes Crosswords
Dislikes Statistics	0.1	0.4	Dislikes Statistics	0.1	0.4
Likes Statistics	0.1	0.4	Likes Statistics	0.4	0.1

- We use a chi-squared test (or similar) to examine evidence against the null hypothesis of independence for a given sample. This provides a good summary of association for a 2×2 contingency table.
 - But what about if there are more than two categories in either or both variables?

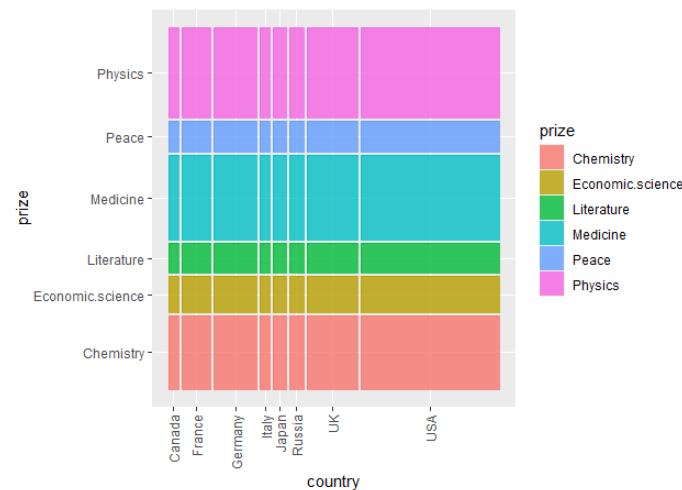
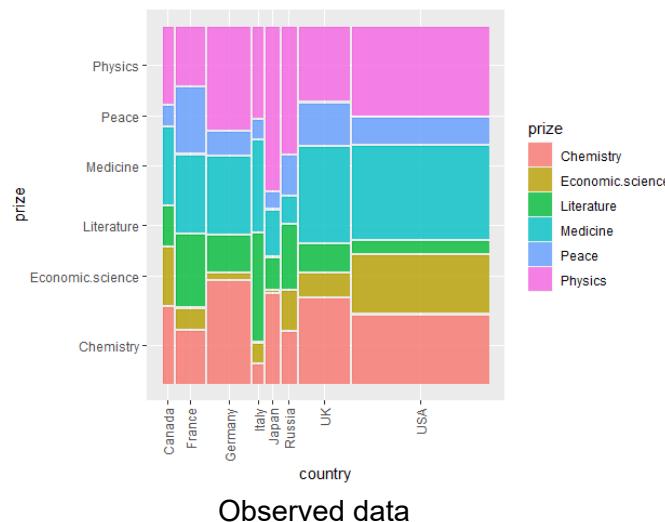
Example: Nobel Prize Data

- Nobel prize winners by country from 1901 to 2015. Just G8 countries, and excluding mathematics.
- We could use a contingency table, or a mosaic plot as shown below.
 - The width of the columns represents the column proportions (country)
 - The area of the blocks represents the proportion of all prizes (prize x country)



Comparing to the independence model

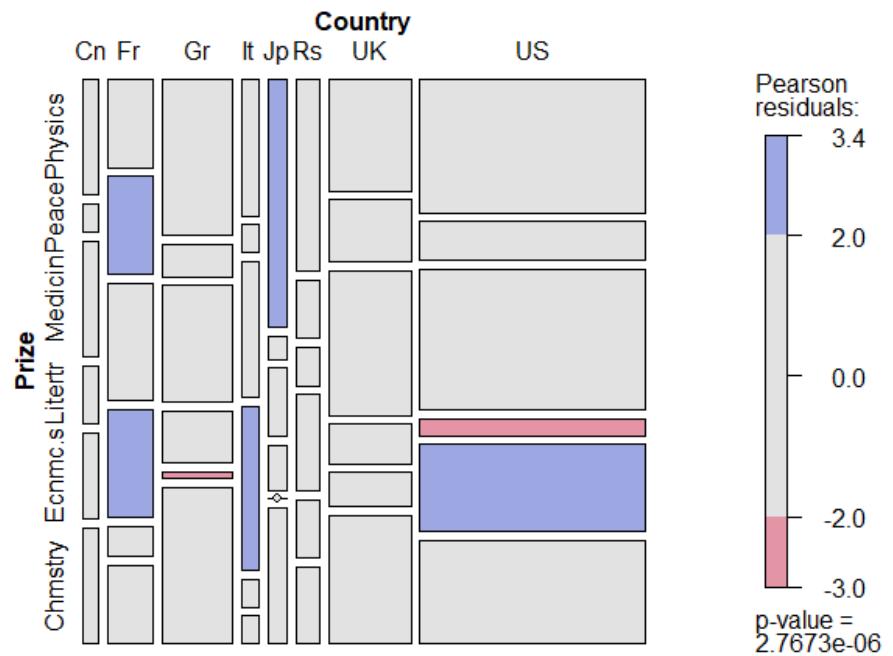
- Is there an association between country and type of Nobel prize won?
- We can compare the observed areas to the independence model.
- Is there an association, and if so what is the nature of this association?



Null hypothesis,
INDEPENDENCE

Comparing to the independence model

- We can perform a Chi-squared test for independence of the two variables (strongly significant)
- We can also look at the Pearson residuals to see which combination of categories have observed values furthest away from expectation under the independence model



Dimensionality Reduction Techniques

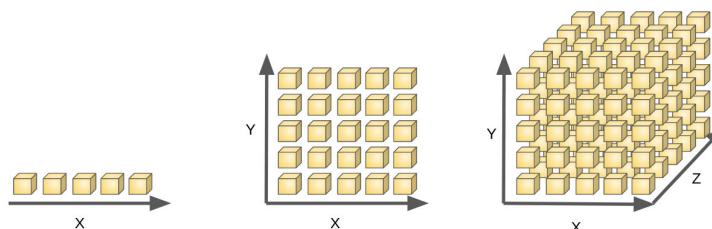


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Why do we need dimension reduction?

- Multicollinearity – situations where predictors are very similar to each other.
 - Consequence: Difficulty accurately estimating effect of each predictor on the outcome. See **Model Building Workshop**
- Situations where $k \approx n$ or $k > n$, we have as many measurements on each subject as we have subjects (or more). **Sometimes referred to as the ‘curse of dimensionality’** (Common in high throughput biological assays gene expression, neuroimaging etc)
 - Consequence: Can’t fit a model, not easy to compare individuals to assess their similarity or group membership

“Even if the number of collected data points is large, they remain sparsely submerged in a voluminous high-dimensional space that is practically impossible to explore exhaustively”



Why do we need dimension reduction?

- Synthetic Variables: We reduce the number of variables in our analysis by replacing original variables with a smaller number of synthetic variables. By ‘synthetic variable’, I mean one that *synthesises* information from multiple ‘original variables’
- **Body Mass Index (BMI)** is a simple example of a synthetic variable:

$$\frac{\text{Weight in kg}}{(\text{Height in m})^2}$$

- You may have heard of latent variables, these are unobserved variables that are a type of synthetic variable representing meaningful concept that can’t be observed directly (e.g. personality, stage of disease progression)
- Dimension reduction techniques combine information across variables* to create useful synthetic variables.

*For simplicity and consistency I will mostly call the original variables just ‘variables’ and the synthetic variables ‘dimensions’.

A workflow for dimension reduction

0. Identify your variable types and perform appropriate Exploratory Data Analysis
1. Run dimension reduction analysis
2. Examine the relationships between variables
3. Examine the relationships between subjects
4. Further summarising/interpretation. Choose how many dimensions to keep/examine.
5. Downstream analysis

Step 0 – Exploratory Data Analysis

- EDA is an important step in our general research workflow
 - See the EDA step in our Research Essentials workshop
 - Useful for choosing the right Dimension Reduction method
- Once you have chosen, dimension reduction methods need their own EDA:
 - Want to make sure that the method is appropriate
 - Want to make sure that we use the right settings for our data and analysis questions
- Even if our intention for the dimension reduction is purely exploratory, it is still an analysis method and we need to make sure we get meaningful and interpretable output

Step 1 – Run Dimension Reduction Analysis

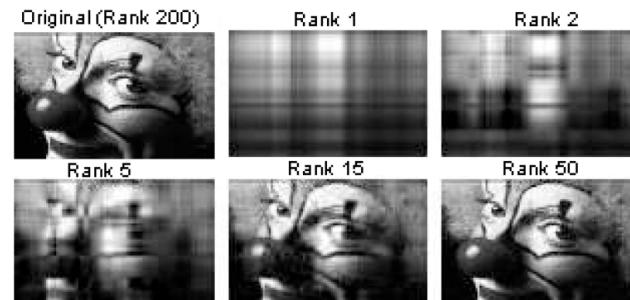
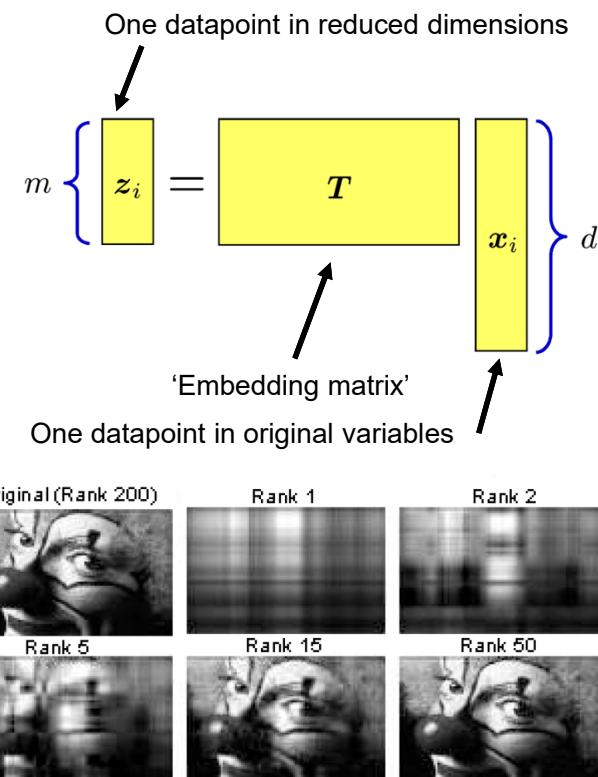
- The purpose of this workshop is to introduce the theory behind dimension reduction
- You may have a single dimension reduction method you want to use, or you may want to run multiple methods and compare outputs
- Dimension reduction analysis can be performed in several statistical software packages
- Often the best resource is to find a tutorial using the software package you intend to use for your own data

Dimensionality Reduction Techniques: PCA-like



Why do we need dimension reduction?

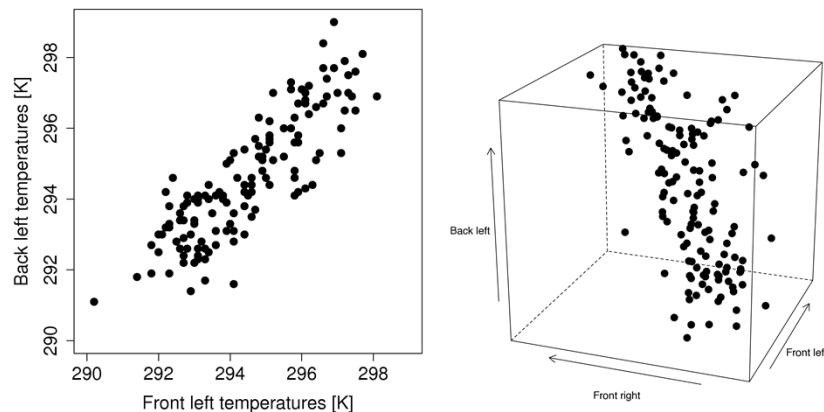
- You can think of dimension reduction as using the relationships between variables to extract information dispersed throughout the original variables and 'concentrate' it in a lower number of dimensions
- Every datapoint in the space of original variables can be transformed to a point on in the reduced dimensional space
- Although you may end up with as many dimensions as you had original variables ($m = d$), there will be dimensions that contain relatively little information, you can discard them (if doing pre-processing) or ignore them (if identifying latent variables)



https://www.researchgate.net/publication/33427320_Latent_Semantic_Indexing_and_Information_Retrieval-A_quest_with_BosSE

Mechanics of Dimension Reduction

- To get a geometric intuition of what PCA-like dimension reduction methods are doing, we need to think of our original measurements as a ‘cloud’ of points in space. Each original variable defines an axis, and each observation is located at a point in space defined by its measurements



Can we describe these points in fewer dimensions while still retaining as much as possible of the shape of this point cloud?



Challenge question: Dimension reduction

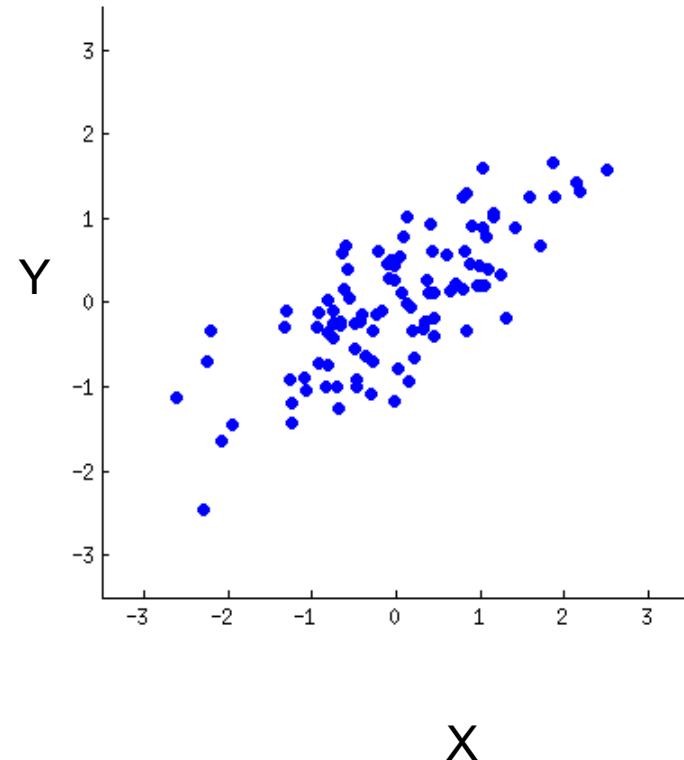
The scatter plot on the right represents measurements on two variables (X and Y) that have been mean centred

Draw a line through the points that will form a new axis (or measurement scale)

All points will ‘fall on to the line’ by following a perpendicular path to this new axis.

Choose the axis so the new scale will preserve the most information, so that points that had relatively high measurements on both original variables have higher numbers in the new scale.

Is this line of best fit, like that in a simple linear regression?



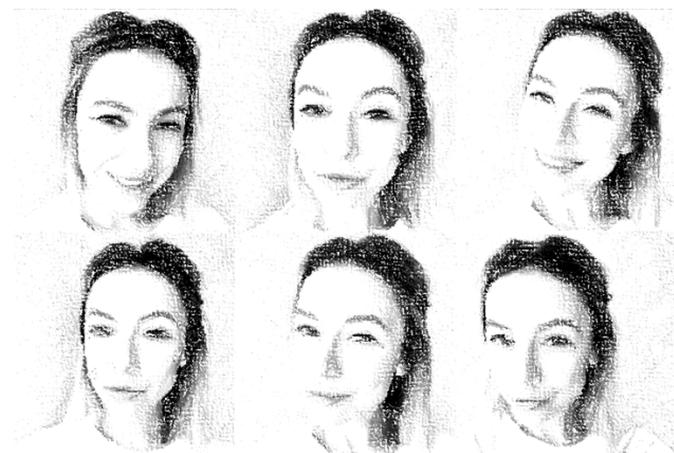
Principal Component Analysis (PCA)



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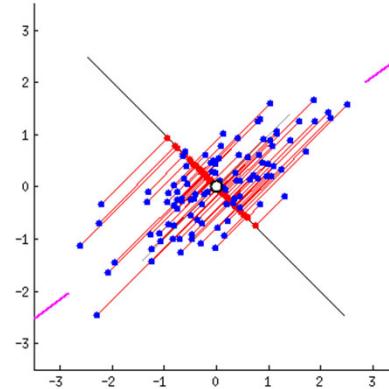
Principal Components Analysis (PCA): Ever taken a selfie?

- There are many sites that advise on how to take the best selfie
- One element that is clearly important is, which angle? You're reducing from a 3D person to a 2D image so you are losing information
- We might choose the angle to highlight certain features of our face
- A PCA is like a selfie for your data. Your data points are in high dimensions. PCA chooses an angle in this space that captures as much information as possible in a lower number of dimensions.



The PCA approach

- PCA chooses a new coordinate system, by choosing a series of ‘principal directions’. Projection of your original data points along these directions form Principal Components (PCs)
- How are the principal directions chosen?
 - Maximises variation in the initial principal component (PC), PC1
 - All subsequent principal components are orthogonal/uncorrelated, while maximising variation sequentially
- **3D example:**
 - <https://setosa.io/ev/principal-component-analysis/>
- **2D example:**



<https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues>



What are the outputs from a PCA?

- Mathematically, each principal component is a linear combination or weighted sum of the original variables. Similar to a regression equation, where your outcome is related to your explanatory variables with a series of coefficients.
 - E.g. $PC1 = Ax + By + Cz \dots$ where A, B and C are scalar coefficients/weights and x, y and z are points in the original coordinate system
 - The **loadings** (coefficients)* allow us to calculate the projection of our data from the original variables to a **PC score** on each individual principal component
 - The PCA outputs are mathematically related to your covariance/correlation matrix
 - The principal directions are **eigenvectors** of the covariance/correlation matrix
 - The corresponding **eigenvalues** quantify the variation captured in the relevant principal component
- Technical note: Different R packages provide either unscaled (eigenvectors), or scaled (loadings) as a summary. Terminology can vary, see <https://stats.stackexchange.com/questions/143905/loadings-vs-eigenvectors-in-pca-when-to-use-one-or-another>

An example dataset: Decathlon

- Some of the concepts are best explained using a concrete example
- Let's use the **decathlon** data set, which contains the performance of athletes in the 10 events of the decathlon
- So we have data from 41 performances across 10 variables
- Unless stated, all subsequent outputs are from this example

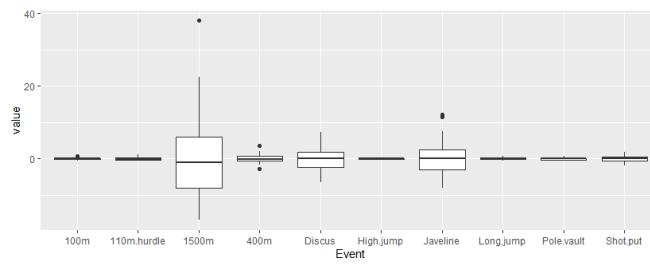
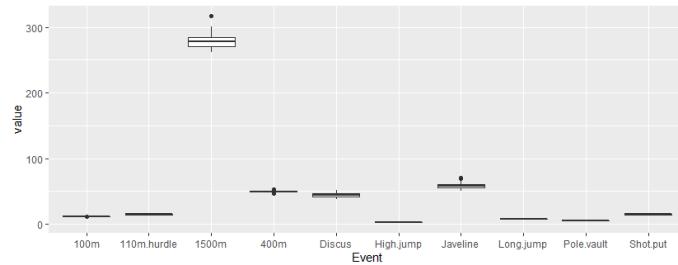


```
library(FactoMineR)
library(factoextra)
data(decathlon)
```

A workflow for dimension reduction

0. **Identify your variable types and perform appropriate Exploratory Data Analysis**
1. Run dimension reduction analysis
2. Examine the relationships between variables
3. Examine the relationships between subjects
4. Further summarising/interpretation. Choose how many dimensions to keep/examine.
5. Downstream analysis

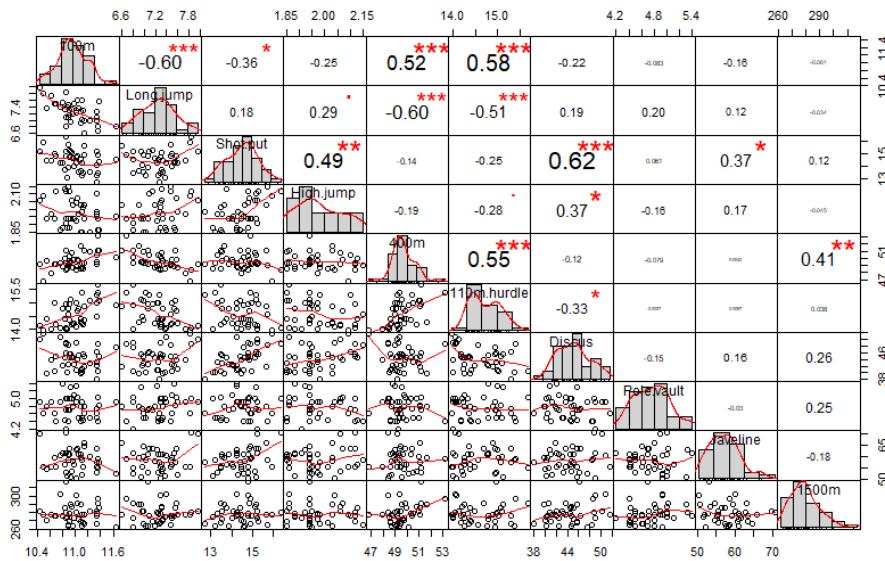
Decathlon Dataset. Step 0: EDA



- We always mean centre the data (subtract the mean value from each variable) before PCA. Remember that we are using correlation, so the mean must be subtracted otherwise biases are introduced.
- It is also clear in this example that the different variables are on a different scale of measurement (different length track events with time in s, field events are distances in m)
- Beyond this, the variances for our variables are quite different to each other. We need to ‘rescale’ this data to get useful results (divide by the sample standard deviation).

```
data_long %>% ggplot(aes(x=Event,y=value)) + geom_boxplot()  
data_long_centred %>% ggplot(aes(x=Event,y=value)) + geom_boxplot()
```

Decathlon Dataset. Step 0: EDA



- Clear correlations between the similar field events, and similar track events
- Negative correlations reveal the track events have a different polarity to the field events.
 - A big number is a good thing in long jump (you jumped far)
 - A big number is a bad thing in 100m (you took a long time)

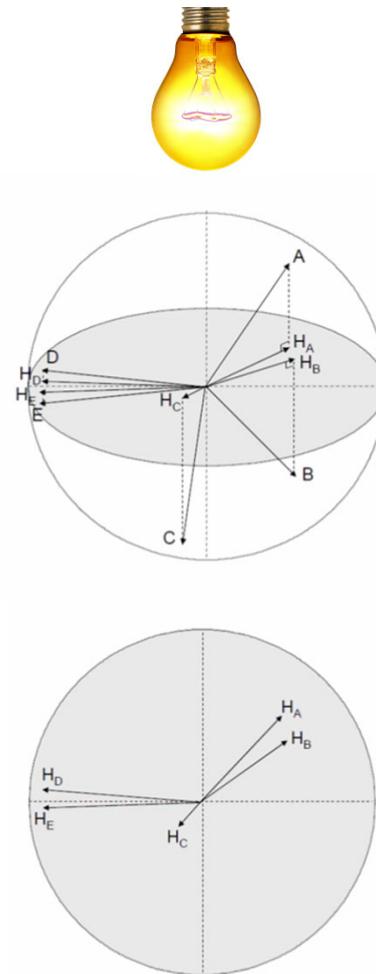
```
chart.Correlation(data_wide %>% select(-Athlete))
```

A workflow for dimension reduction

0. Identify your variable types and perform appropriate Exploratory Data Analysis
1. Run dimension reduction analysis
- 2. Examine the relationships between variables**
- 3. Examine the relationships between subjects**
4. Further summarising/interpretation. Choose how many dimensions to keep/examine.
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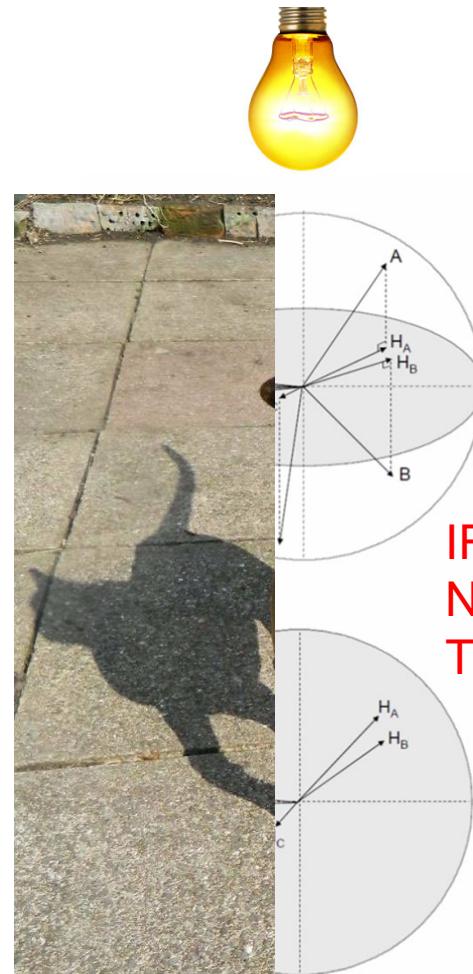
Step 2 and 3 examine plots

- We can't see in more than 3 dimensions, but if you have a 3D space we can visualise what projections of different vectors look like onto a 2D plane.
- The length of some vectors (D, E) is close to the length of their projections, while for others (C), the projection length is much shorter. This depends on the size of the vector and the angle between the vector and the plane
- The closer the actual vector length is to the length of its projection, the more accurately it is being represented by its projection



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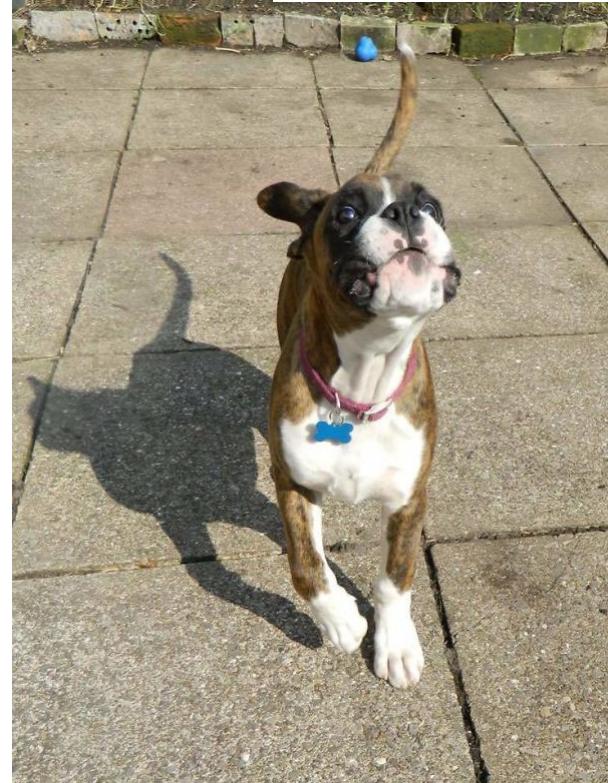


IF AN OBJECT IS
NOT CLOSE TO
THE PLANE

Step 2 and 3 examine plots

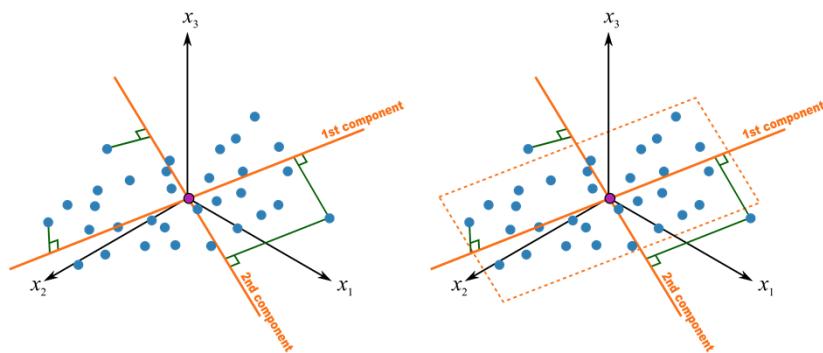
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- The closer the actual vector length is to the length of its projection, the more accurately it is being represented by its projection

**THEN IT IS NOT WELL
REPRESENTED BY ITS
PROJECTION!**

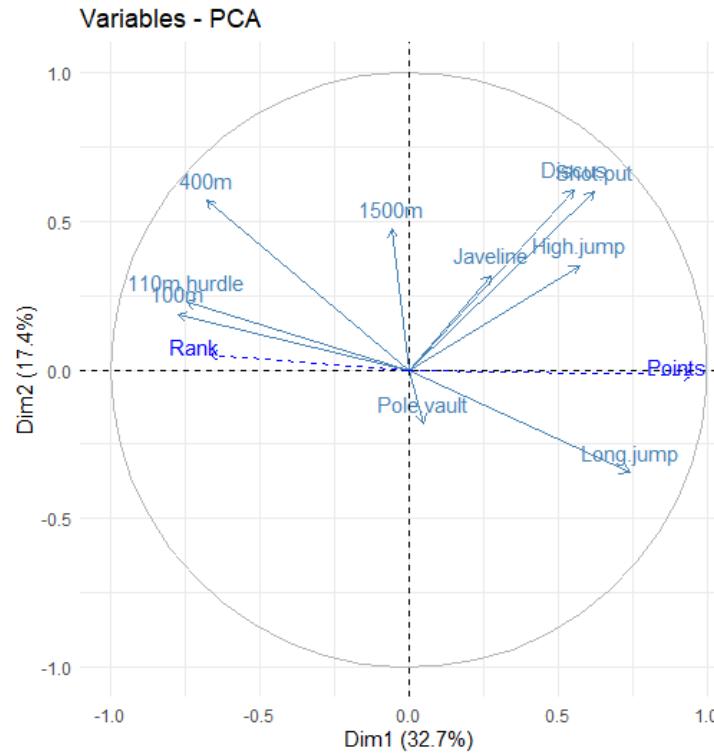


Step 2 and 3 examine plots

- Projection is an important geometrical concept to understand in dimension reduction
- In a (PCA-style) loading plot:
 - The vectors represent original variables
 - The orientation of the plane is the PCA solution (principal directions)
 - Projection of the variables (shown as vectors) shows us the **loadings plot**
 - Subjects can also be projected onto the plane (shown as points) **subjects plot**
 - Or both variables and subjects **biplot**



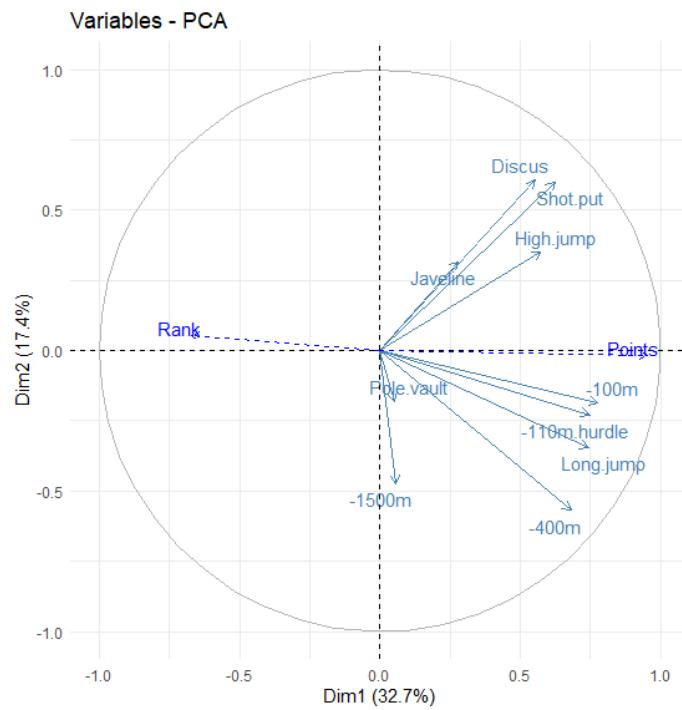
Decathlon Dataset. Step 0: EDA



- Let's run the PCA and look at the loading plot
- Sometimes you may have supplementary variables available that are not used in PCA analysis but correlate with PCs. In this case we can use the 'Points' and 'Rank' which give the number of points achieved and the Rank of that athlete. These can be added to the loading plot by calculating their Pearson's correlation with each PC.
- Not surprisingly, these are negatively correlated with each other wrt to the PCs. A smaller rank means a better performance, for which more points are awarded.
- The 'polarity' separates track events and field events on this plot, which is not helpful. Making all track times negative (multiply by -1) allows us to compare track and field events more readily.*

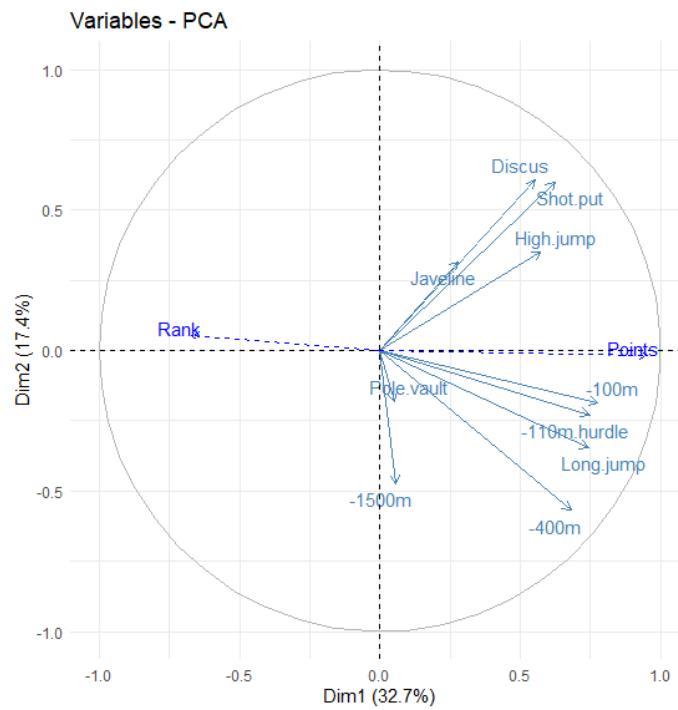
PCA Step 2: Examine the variable plot

- The loadings plot is where we see the dimension reduction in action. All of the original variables have been projected onto the 2D plane of two chosen PCs.
- The correlation of the original variables with each PC is shown by the position of the arrowhead. Drop a perpendicular line from the arrowhead to each axis to see the correlation with that PC (unit circle shows the [-1,1] limits of correlation).
- Those original variables with shorter vectors are less captured by the PCs (e.g. Pole Vault). Recall that the principal directions chosen in PCA preserve as much information as possible, so the variables poorly represented are less important for explaining variability



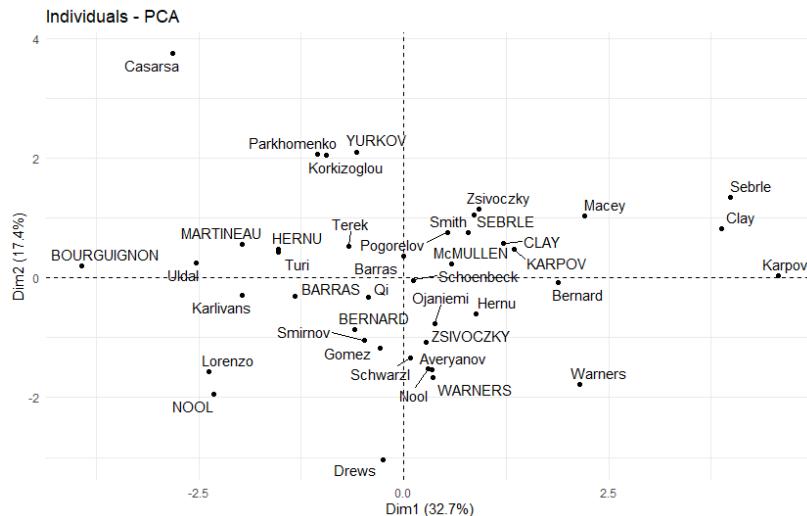
PCA Step 2: Examine the variable plot

- Interpreting the PCs as latent variables:
 - Clearly PC1 represents performance of the athlete. A **weighted sum** of all events – all variables are positively correlated. Those with higher PC1 scores, have higher points and lower rank. Despite explaining the most variability (33%), this is not particularly interesting as a *latent variable*.
 - PC2 appears to represent specialisation of athletes. It is a **contrast** between events that involve sprinting, and those that don't, which have opposite signed correlations with PC2*. Sprint specialists achieve by running really fast. Non-sprint specialists achieve most of their points by being good at other field events. Despite explaining about half as much of the variability as PC1, PC2 has a more interesting interpretation as a *latent variable*. If specialisation is not present, this PC will not appear reliably.



*A technical note: the sign of the PC itself is arbitrary! The sign of the correlation between the variable and the PC is not arbitrary.

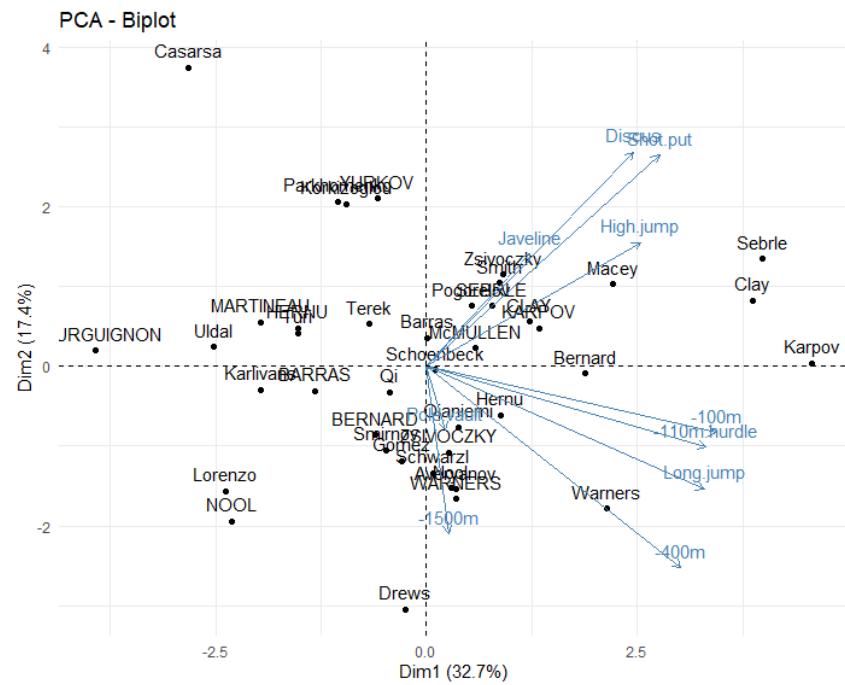
PCA Step 3: Examine the subject plot



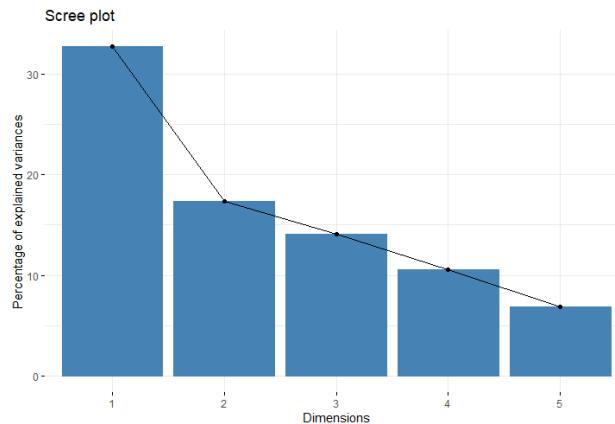
- We can plot the individual observations plotted in PC space, often called the score plot. Their PC scores for 2 dimensions at a time
- This is again a projection into PC space, but not of the variables, but instead the individual measurements
- Observations close to each other have similar values for the depicted PCs (but not necessarily similar overall). Recall latent variable interpretation for each PC.
- In some examples (not this one) there may be distinct clusters, and you can perform various types of clustering on observations in the PC space.

PCA Step 2 & 3: Examine the variable and subject plot

- The subjects and the variables can be examined on the same plot (often you will have overplotting issues)
- Note that the axes are the same as in the subject plot, and reflect the PC scores
- The original variables can be thought of as additional axes showing the approximate* + relative position of each of the subjects on the original variable



How many PCs should we consider?

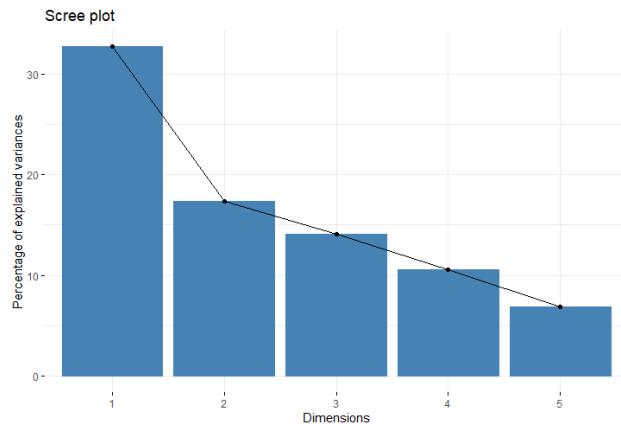


- We have seen that the first 2 PCs capture about 50% of the total variance and we have plausible latent variable interpretation for each
- There are as many PCs as there were variables from the output
- Each PC captures some amount of the total variance (across all original variables = across all dimensions), and this decreases for each subsequent PC
- The size of the eigenvalue corresponds to the variance of each PC. We can divide by the total variance to find the % total variance of each PC.

```
res.pca = PCA(decathlon[,1:10], scale.unit=TRUE, ncp=5)
fviz_screenplot(res.pca, ncp=5)
```



How do you choose how many PCs?



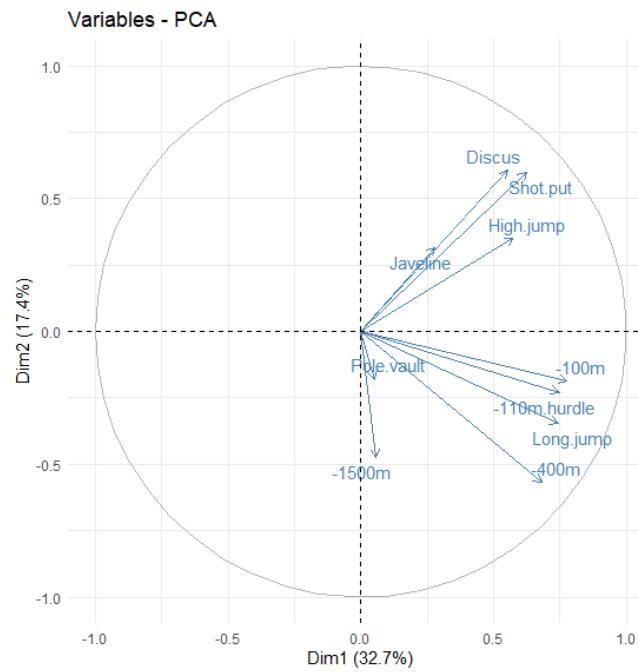
- A ‘scree plot’ is a plot of % of total variance captured in each PCA
- The steeper the drop between bars, the less information is being captured in the k th PCs compared to the first ($k - 1$) PCs. We can consider dropping the k th and higher PCs
- Rules of thumb:
 - Smallest # of PCs that together hold 80-90% of variance
 - Keep components with an eigenvalue greater than the average of eigenvalues/Keep components with an eigenvalue > 1 when working with standardised variables
- If we collected many samples, we would probably find that the first dimensions were more stable in their (relative) directions between samples whereas the last dimensions would keep changing. This would show us that the first dimensions contain more ‘signal’, and the last dimensions contain more ‘noise’.

```
fviz_screepplot(res.pca, ncp=5)
```

Challenge question – correlation between original variable and PC



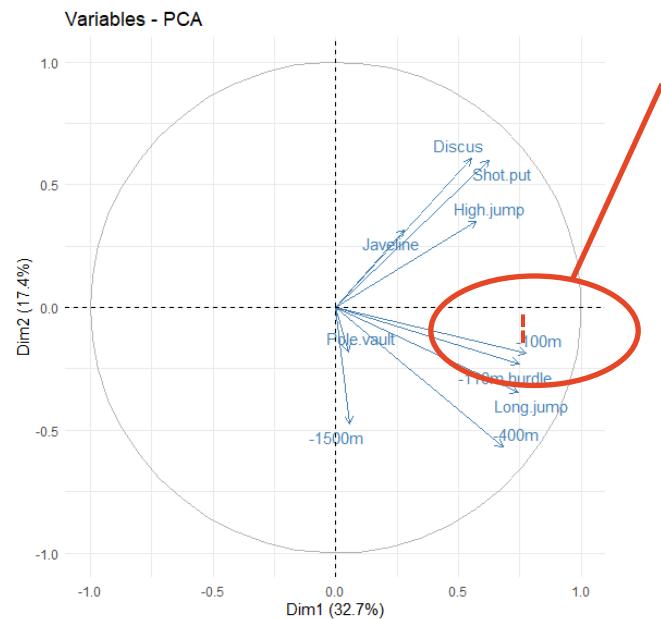
What is the correlation between -100m (i.e. 100m time with a minus sign) and PC1 score?



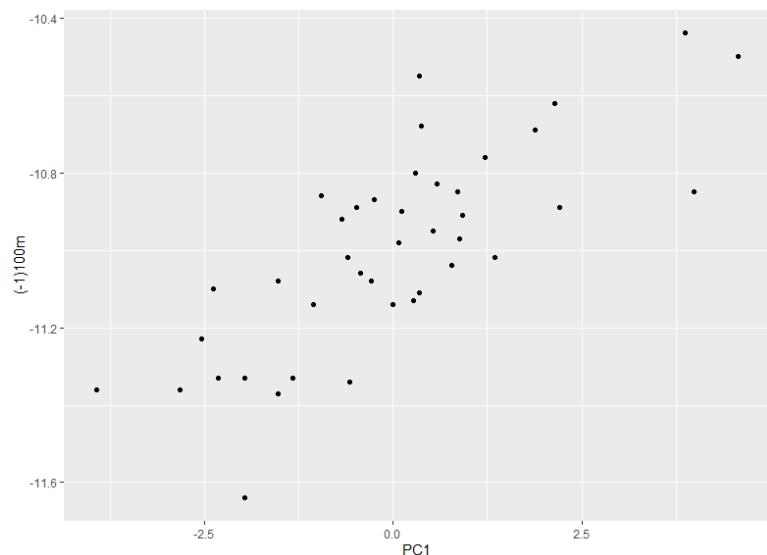
Challenge question – correlation between original variable and PC



- We can see a strong positive correlation ($r=0.77$) between PC1 and -100m



- Scatterplot for these two variables



Challenge question – correlation between PCs

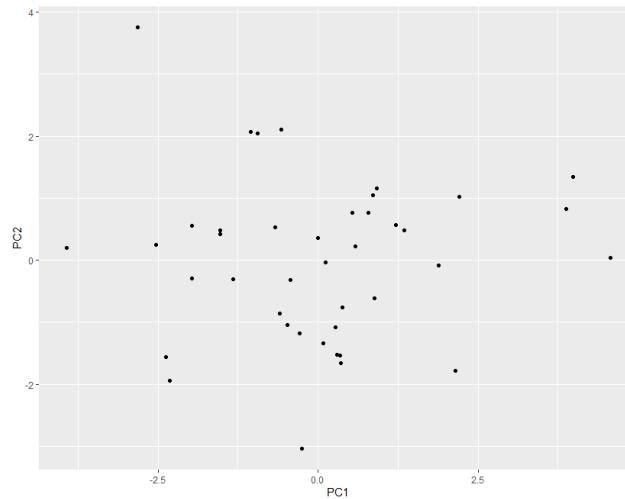


What is the correlation between PC1 and PC2 scores?



Challenge question – correlation between PCs

- Recall that the PCs are uncorrelated.
Here is a scatterplot between PC1 and PC2
- Recall the red and blue boxes, if you drew them for this scatterplot how would their total areas compare?
- What would be the correlation coefficient?

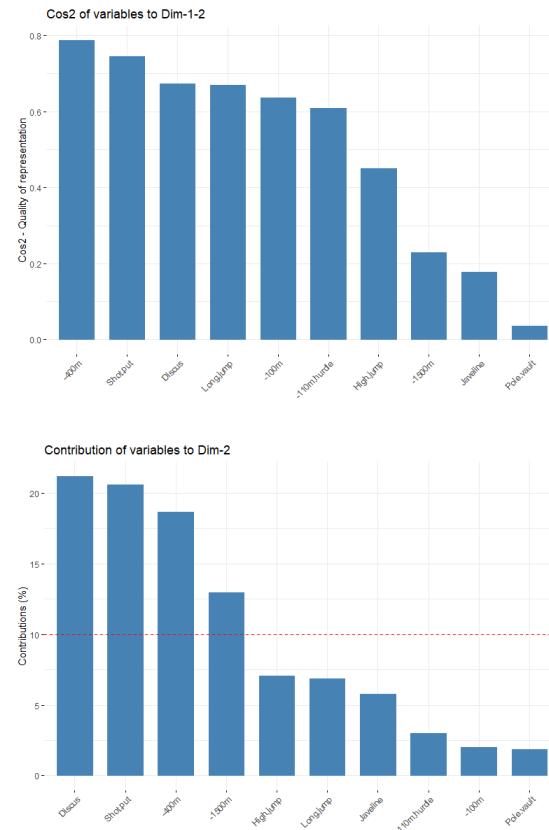


```
cor(tidy(res.prcmp) %>% filter(PC==1) %>% .$value,tidy(res.prcmp)
%>% filter(PC==2) %>% .$value)
[1] 9.627521e-17
```

= 0 (allowing for numerical precision of computers)

PCA Step 4: Further summarisation

- Other interpretation aids:
 - Quality of representation for variables and individuals on a given map
 - Contribution of variables and individuals to each PC



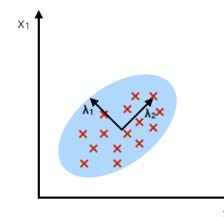
PCA Downstream analysis

- Possible uses of PCA downstream:
 1. Pre-processing for clustering subjects
 2. Looking for outliers or time dependency in subjects
 3. As predictors in multiple regression (PCR-Regression)
 4. As a pre-processing step for further dimension reduction

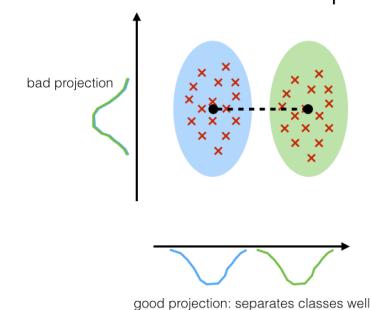
Method Extension: Linear Discriminant Analysis (LDA)

- PCA can be modified towards a different goal by imposing a different constraint.
Recall that in [classic] PCA we want to maximise variability on each principal component
- If your goal is to find principal components that separate two or more different classes of subject, you could use LDA
- It is a modified version of PCs. LDA calculates PCs that maximise the separability between your classes

PCA:
component axes that maximize the variance



LDA:
maximizing the component axes for class-separation



https://sebastianraschka.com/Articles/2014_python_lda.html

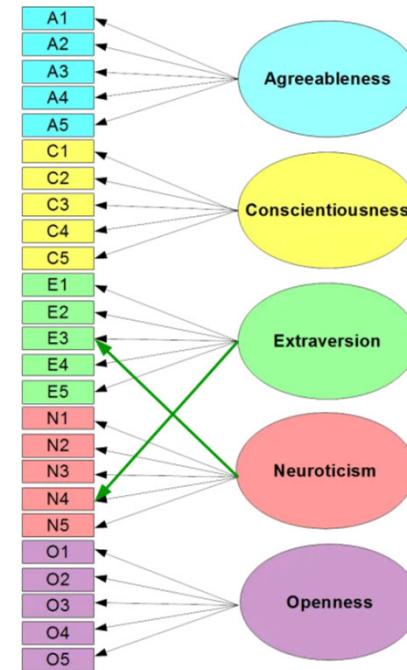
Factor Analysis (FA)



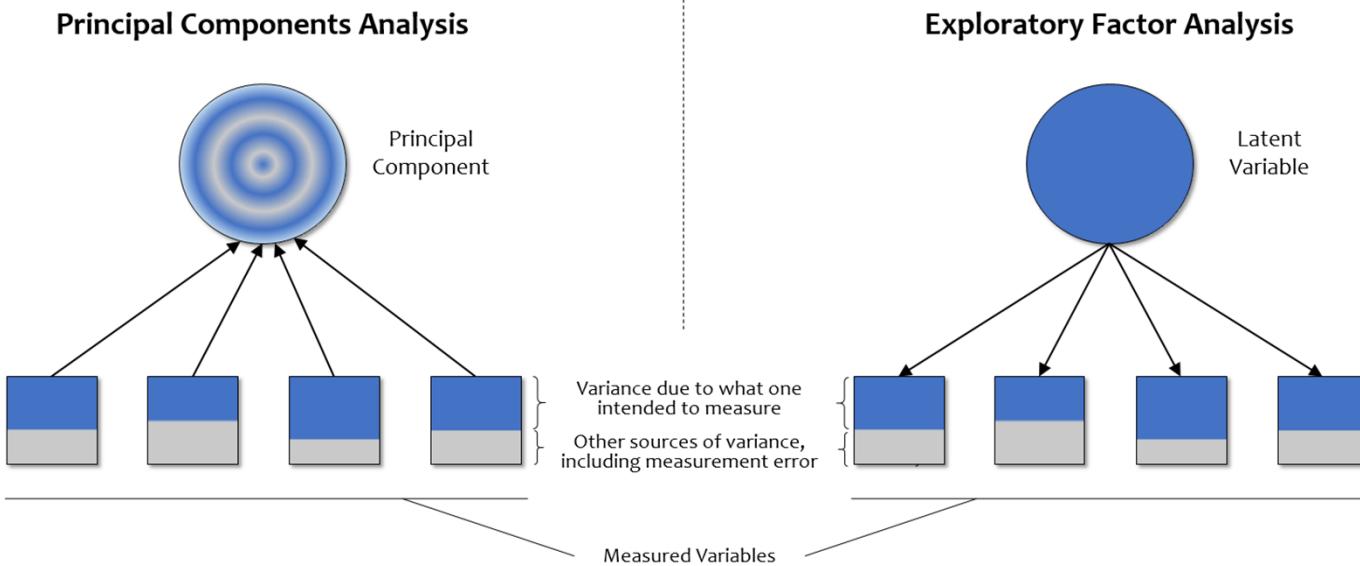
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Factor Analysis

- Another major dimension reduction technique with continuous variables as input
- Similar to PCA in many respects, but differences in the methods reflect different aims and applications
- Most often used to define latent variables with the aim of producing an explicit, and testable model for how these interact with each other and measured variables
- Common in psychometrics. Things like personality traits can't be measured directly but are of interest. Think building a theoretical/functional model using a probabilistic model.



PCA vs. Factor Analysis

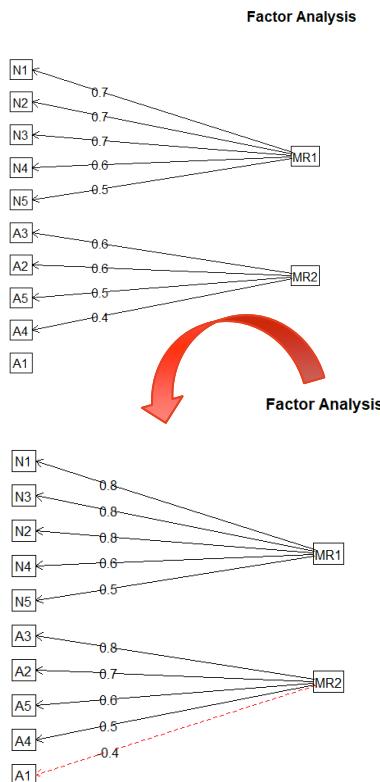


- PCA identified principal components, which capture patterns of variance in measured variables. You can think of any measurement error as being distributed throughout the PCs (but hopefully relegated to PCs that are ignored)
- In factor analysis you will model error in your measured variables, and this is separate from the shared variance from their factor scores.

PCA vs. Factor Analysis

- In SPSS the Factor Analysis menu lists PCA as a method. But most analysts would not consider PCA to be true Factor Analysis. Factor Analysis would only be when using a factor extraction method that partitions variance of a measured variable into unique and common (see previous slide)
- Some people refer to Factor Analysis as Common Factor Analysis, or Exploratory Factor Analysis (EFA) as distinct to CFA (Confirmatory Factor Analysis), or SEM (Structural Equation Modelling) where a defined model is tested for model fit

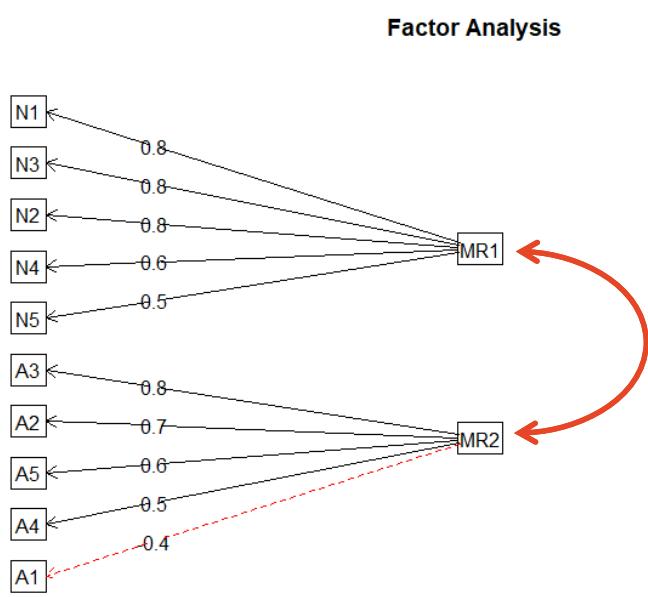
FA. Step 2: Examine the variable space



- The initial ‘unrotated’ solution, in which factors are ordered by the amount of variability they explain (like in PCA) is usually not of much interest in factor analysis
- Rotation of the factor loadings typically aid the interpretability of our factors, which is what we want in FA
- In plotting FA, we often produce loading plots that ignore the loadings from factors below a threshold.
- These loading plots do not look like PCA loading plots. There isn’t a simple projection of original variables onto the factors. Each measured variable has its own unique variance. These plots are part of a ‘path diagram’, as used in FA and SEM.

```
model_unrotated = fa(bfi_trim, 2, rotate="none")
fa.diagram(model_unrotated)
fa.diagram(model) # Oblimin (default)
```

FA. Step 2: Examine the variable space



- There are two classes of rotation:
 - Orthogonal, which assumes no correlation between factors and
 - Oblique, which assumes some level of correlation between factors
- For oblique rotations, an estimate of the correlation between factors is provided by the method output

Factor Analysis Downstream analysis

- The goal of FA is to come up with an explicit and testable model for how measured variables and factors interact. So FA is usually the first step in a longer process.
- Typical downstream steps from Factor Analysis (FA):
 - Confirmatory Factor Analysis
 - Structural Equation Modelling

Correspondence Analysis (CA)



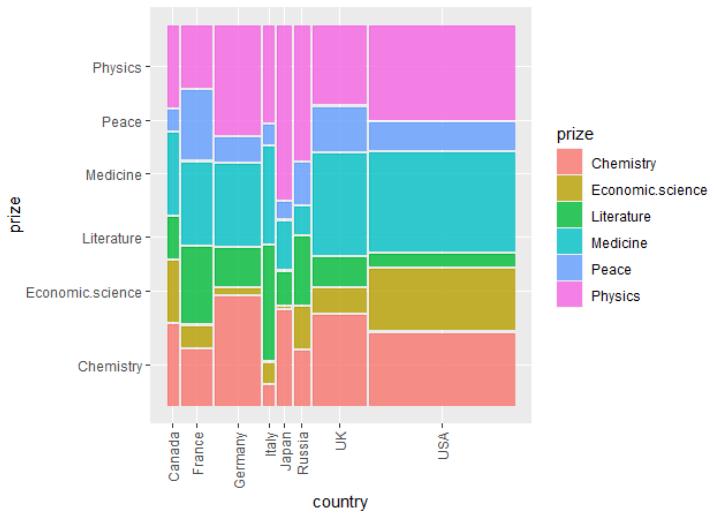
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Correspondence Analysis (CA)

- Very common in surveys with categorical responses. Can also be used for abundance measurements in ecology.
- Often used as categorical/qualitative analogue of PCA
- Input for PCA and factor analysis is continuous observations
- Input for Correspondence Analysis is categorical observations on two variables: contingency table

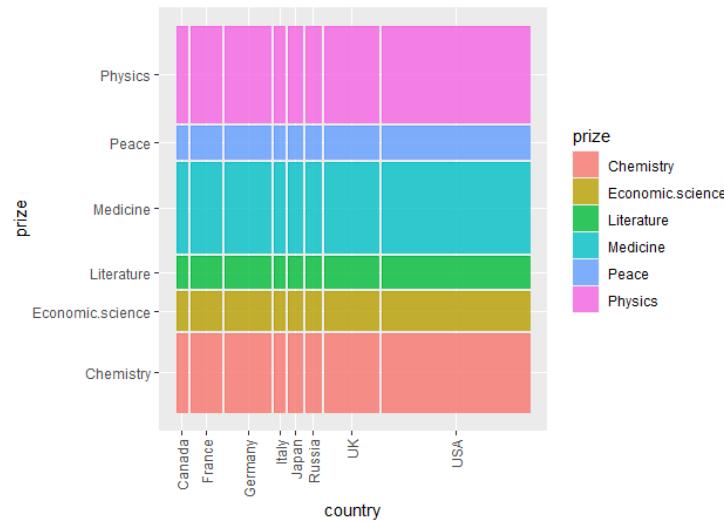
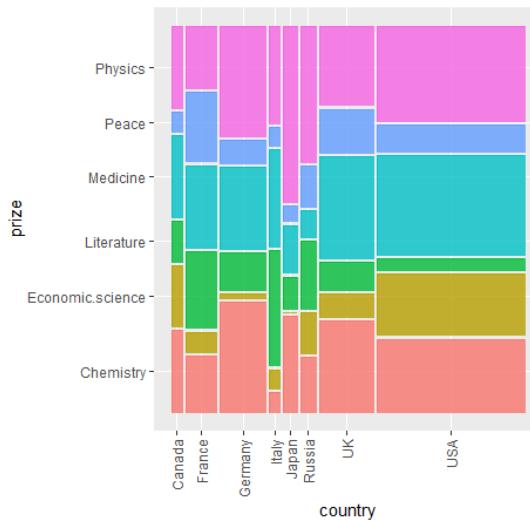
Example: Nobel Prize Data

- Nobel prize data: what is the nature of the association between country and type of Nobel prize won?
- This example and analysis explanations adapted from the excellent CA videos of François Husson



Comparing row profiles to mean row profile

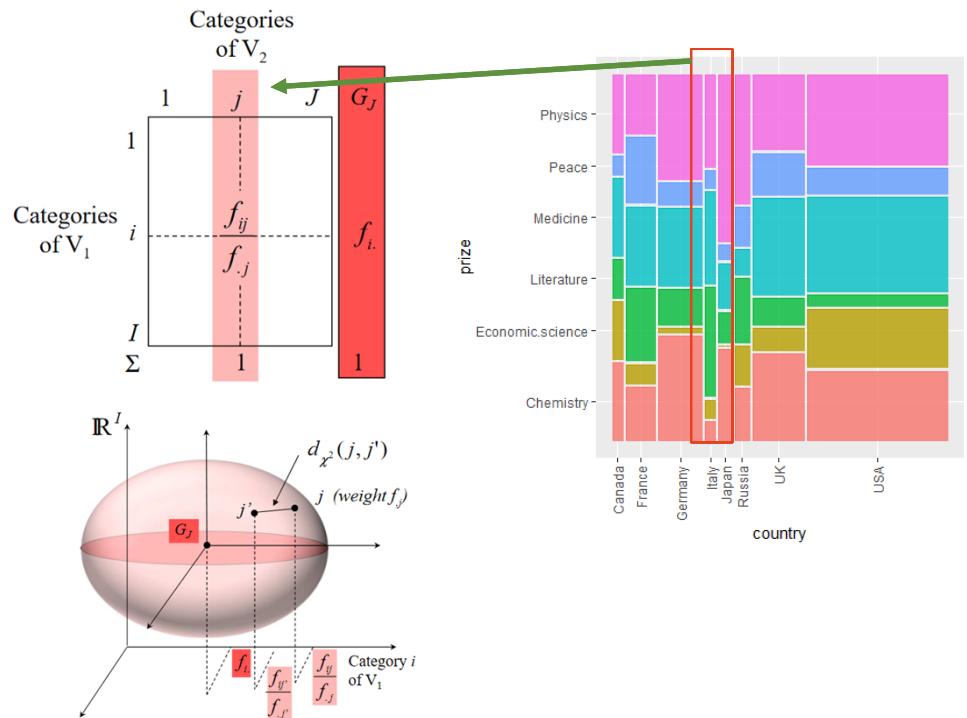
- Can these frequencies be treated as continuous data?
- For each country (column), what is its profile? (Relative frequency of each prize)



```
nobel_sums_long %>% mutate(Country=fct_relevel(Country, "Total", after = Inf)) %>% ggplot(aes(x=Country, fill=name, y=value)) +  
  geom_bar(position="fill", stat="identity") + scale_fill_brewer(palette = "Set2")
```

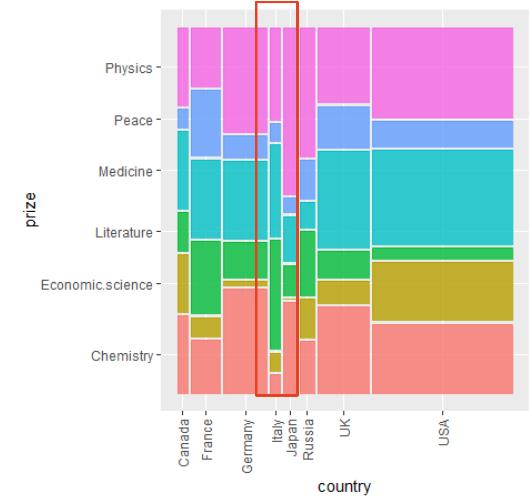
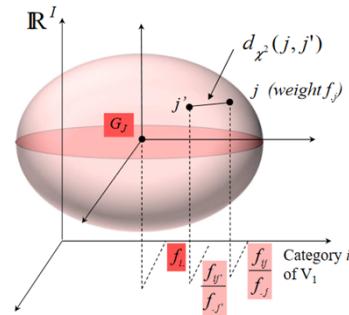
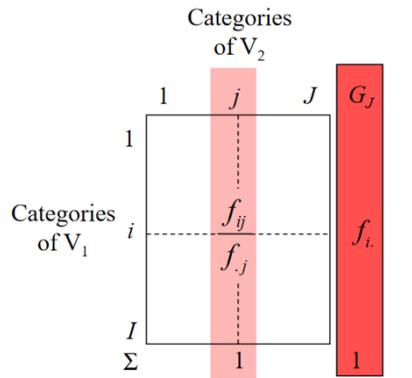
How does correspondence analysis work?

- Each column profile (country) is represented as a point in J-dimensional space, where J is the number of rows (prizes). The location depends on the relative frequency of each row.
- The mean column profile is represented as another point (G_j) that serves as a reference to observed column profiles
- You can calculate a Chi-squared distance between any two column profiles
- The total inertia is made up of the inertia (weighted distance) of each column profile from the mean column profile (i.e. the deviation of that column from independence)



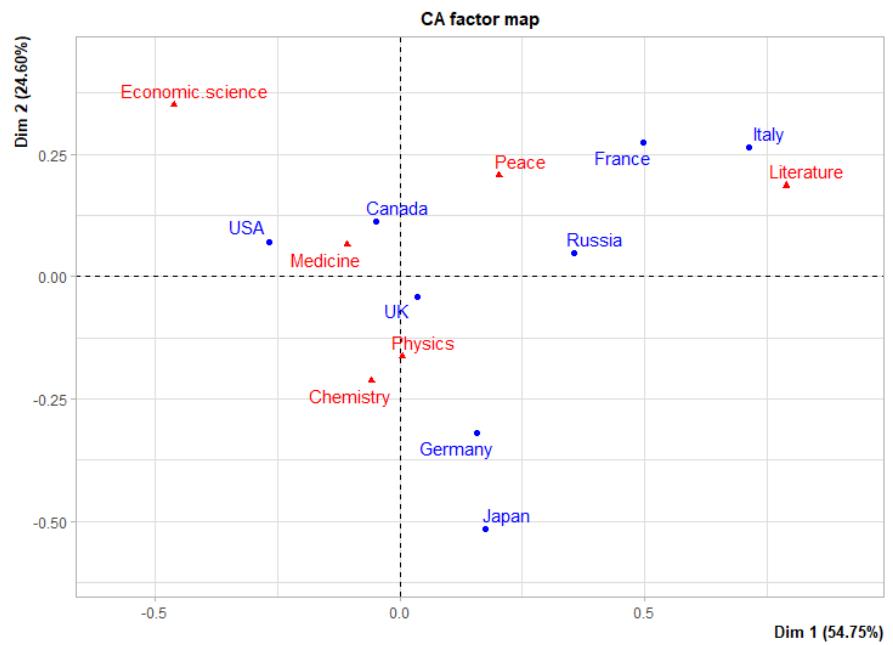
How does correspondence analysis work?

- The set up is analogous to PCA, except that the relative frequencies must add to 1
- Extraction of components proceeds as per PCA, choosing principal directions that maximise the inertia of the first dimension, and subsequent dimensions being orthogonal to previous dimensions
- The same analysis can be performed from the row profile point-of-view. The total inertia is the same. Columns and rows are symmetric in CA. Think association between two variables as not having a direction.

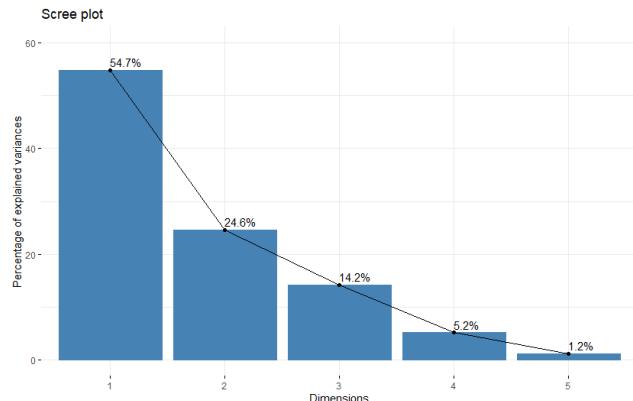


CA Steps 2&3: Correspondence Map

- This is the correspondence map for the Nobel prize data
- Rows (countries) appear in blue
- Columns (prize type) appear in red
- This is an analogue of the biplot for PCA:
 - Rows and columns play symmetric roles in CA
 - We don't usually include vectors and points, as the choice of which is 'variables' and which is 'subjects' is arbitrary.
 - For discussion we will consider countries as subjects and prizes as variables.



CA Steps 2&3: Scree plot



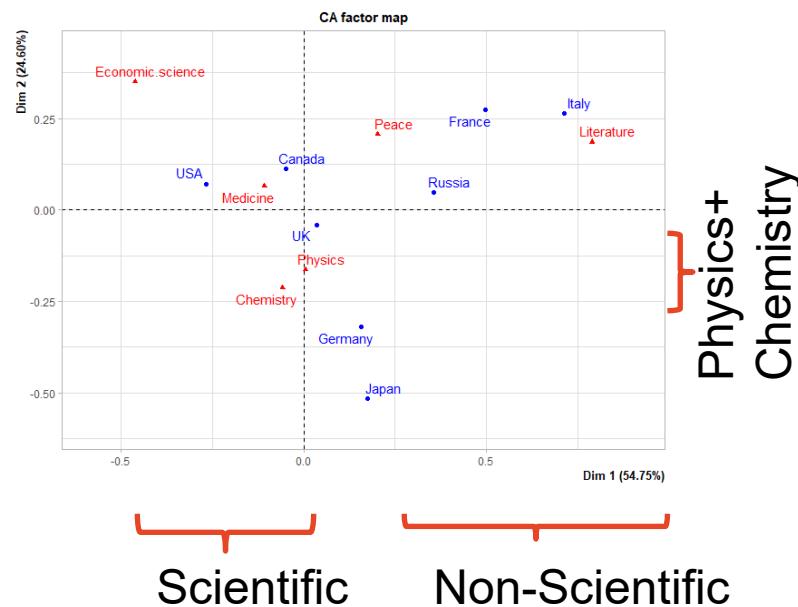
dim 1 dim 2 dim 3 dim 4 dim 5
0.08 0.04 0.02 0.01 0.00

- Scree plot shows the percentage of inertia captured by each dimension
- The first two dimensions capture ~80% of total inertia
- The size of the eigenvalue itself also tells us something, an eigenvalue of 1 means perfect association between 1 column and 1 row (i.e. 1 country had all of its prizes in one category only, and no other countries had a prize in this category)

```
fviz_screepplot(res.ca, addlabels = TRUE, ylim = c(0, 60))  
round(res.ca$eig,2)[,1]
```

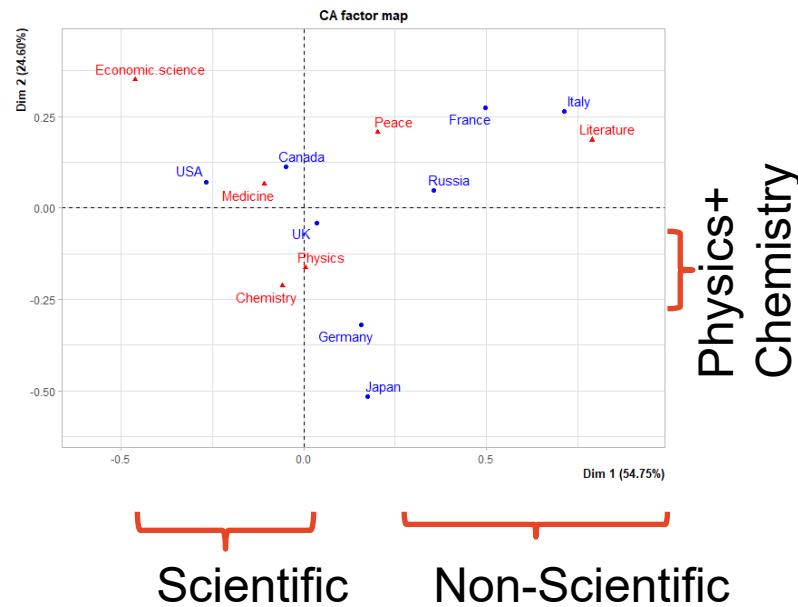
CA Step 2: Examine the ‘variable’ plot

- Dimension 1 appears to contrast the scientific prizes from non-scientific
- Dimension 2 appears to contrast ‘hard sciences’ Physics and Chemistry from the others



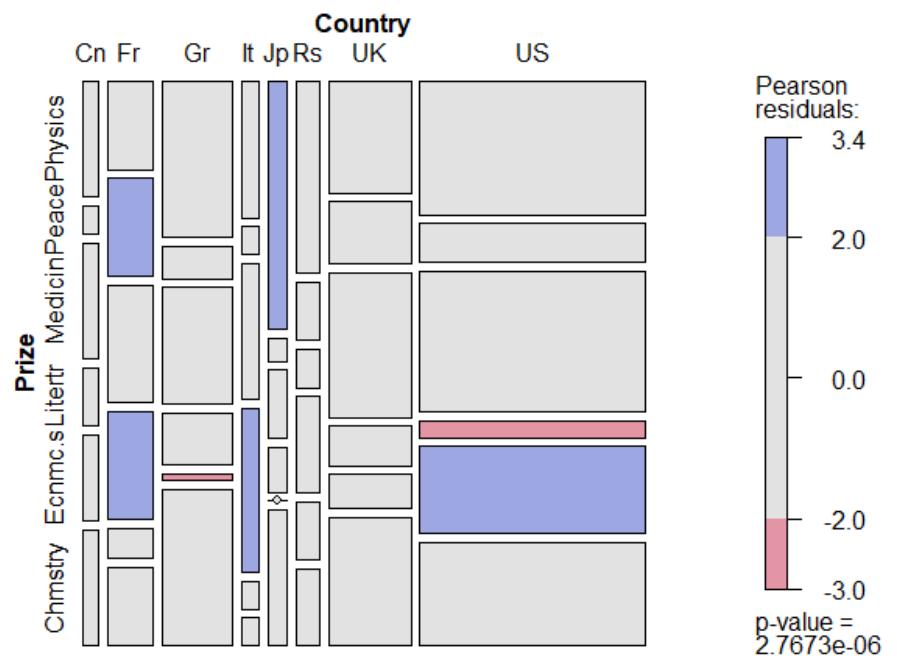
CA Step 3: Examine the ‘subject’ plot

- Same map, but lets concentrate on the rows now (countries, blue points)
- The origin indicates the mean row profile
- Can think of the country being pulled from the origin toward (and potentially beyond) the prizes with which it is most associated with
- The distance between blue and red points on this plot does not have a direct meaning, but rows and columns that are associated tend to be closer together



Comparing to the independence model

- Recall the Pearson residuals from the Chi-squared test between the two variables



Method Extension: Multiple Correspondence Analysis (MCA)

- In multiple correspondence analysis we consider more than two categorical variables
- We no longer start with a contingency table of two categorical variable frequencies, but instead with an 'indicator matrix*' of subjects vs. categories
- Correspondence map can show relation between subjects, variables and categories

How do you take your tea:			
Milk <input type="radio"/>	Lemon <input type="radio"/>	Other <input type="radio"/>	Straight up <input type="radio"/>
Do you have sugar in your tea?			
Yes <input type="radio"/>	No <input type="radio"/>		

The University of Sydney



*Matrix of indicator variables where e.g. (1 = Yes, 0 = No) for the relevant subject x category combination

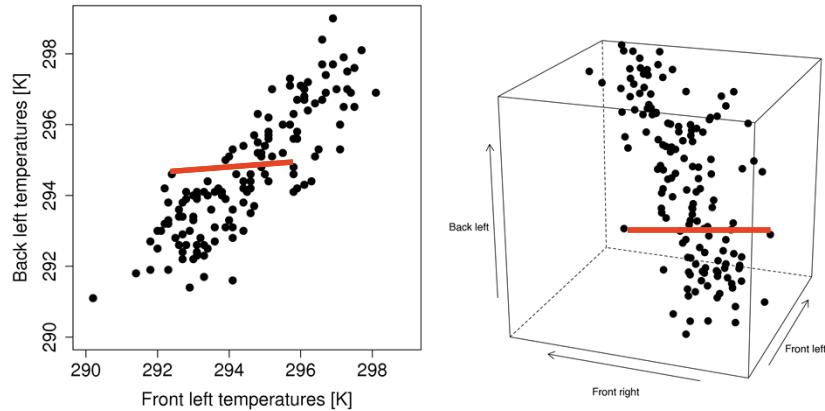
Multidimensional Scaling (MDS)



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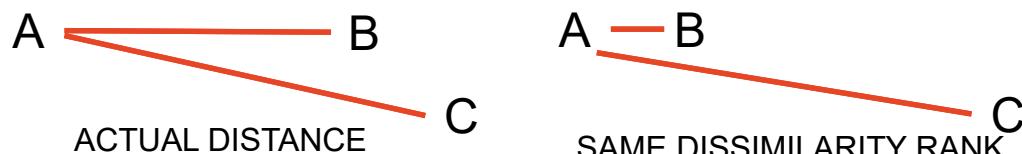
Distance Based Methods

- The starting point of methods so far have been measurements on **variables**, either continuous (PCA, FA) or categorical (CA)
- Multidimensional Scaling (MDS) and similar methods use the distances between **subjects** as their starting point.
- The goal is to produce a low-dimensional map (ordination/embedding) that most accurately visualises the distances between the subjects, i.e. preserves as much as possible the distance information from higher dimensions



MDS Step 1: Run the MDS

- MDS can be run as either metric or non-metric (nMDS). Metric is also called Principle Coordinates Analysis (PCoA)
- Metric is appropriate when you expect there can be a linear relationship between the data distances (original variables) and the ordination distances (ordination map). The method and outputs are very similar to PCA.
- In non-metric MDS (nMDS) the success of the ordination chosen depends on preserving the ranks of dissimilarity between subjects (e.g. site C is more dissimilar to site A than site C is dissimilar to site B).



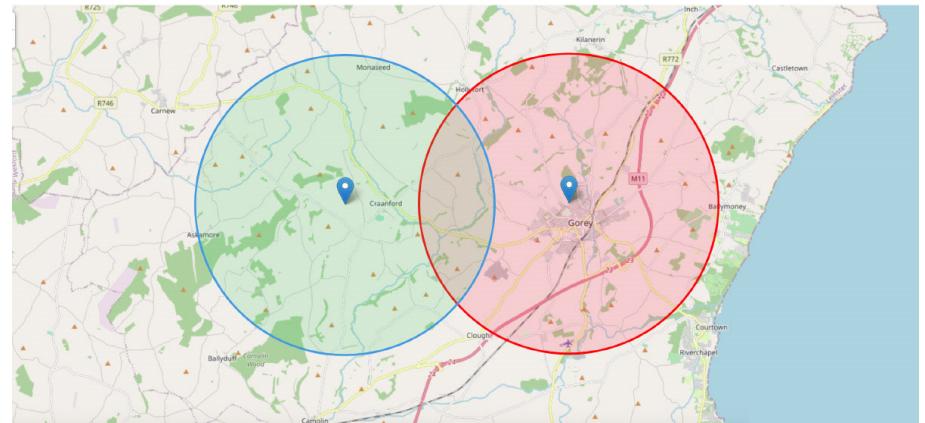
Differences of nMDS from PCA

- The output dimensions are not orthogonal to each other as in PCA
- Ordination map is optimised for a pre-specified number of dimensions
 - The dimensions are not ordered by variance explained as they are in PCA
- Better at accurately capturing local structure (distances between neighbouring subjects), than PCA-like methods, which are better at capturing global structure (distances between all subjects)



What are distances between subjects?

- We're (very) familiar with geographic distances, but what is the distance between subjects?
- The type of data will dictate the appropriate distance measurement. MDS is very flexible in that it can accommodate different kinds of distances.
 - The Euclidian distance is the straight-line distance between two points in your original variable space
 - In ecology, the abundance of species at different sites is measured. Bray-Curtis distance is used, ranges between 0 (identical) and 1 (no similarity)



<https://2kmfromhome.com/>

Example: Mac Nally bird abundance

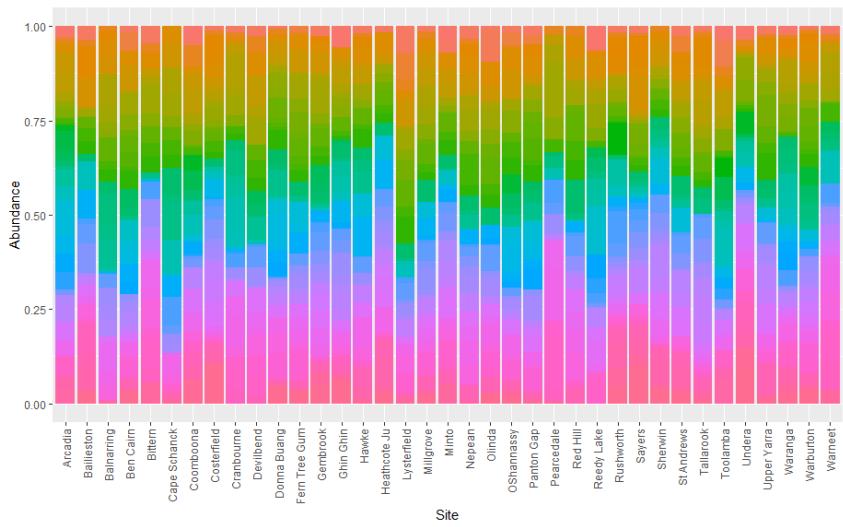
- Let's take an ecology example for MDS: Mac Nally bird abundance data
 - Maximum abundance for 102 bird species
 - 37 sites, 5 different forest types
- Do the bird assemblages differ between forest types?



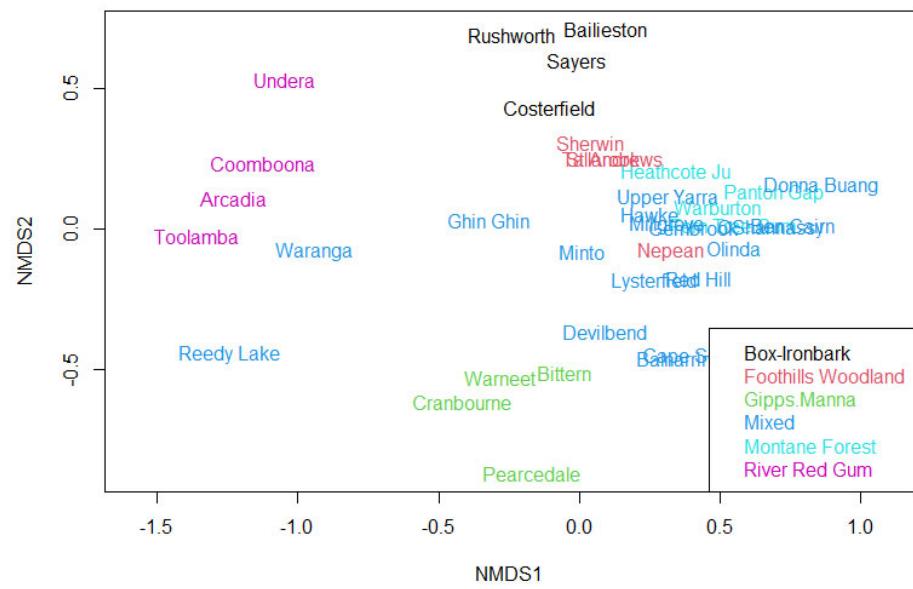
By JJ Harrison (<https://www.jjharrison.com.au/>) - Own work, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=10708260>

EDA

- Very skewed data typical of abundances. A lot of variation in abundance between sites (x-axis) and between birds (colour area)
- Lots of 0s (not shown)
- We need to standardise these abundances to meaningfully compare the composition of the sites
 - Apply Wisconsin double standardisation
 - Could apply other standardisations depending on desired comparisons to make between sites

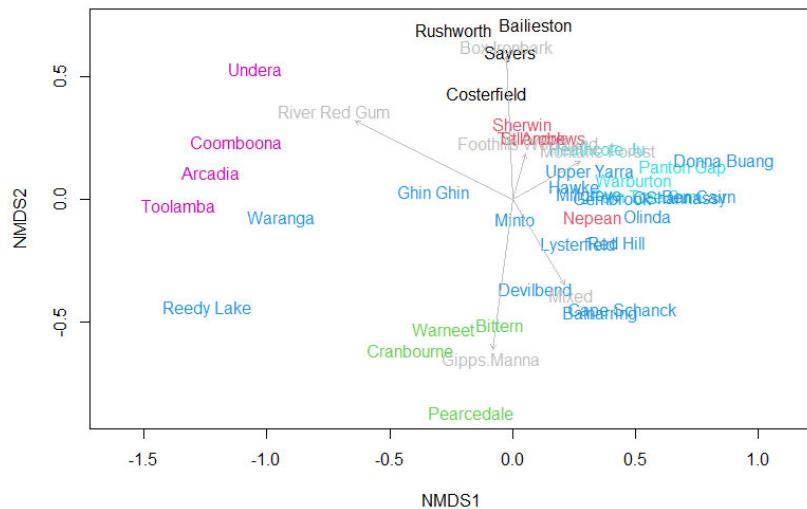


MDS Step 2: Examine the subject (site) plot



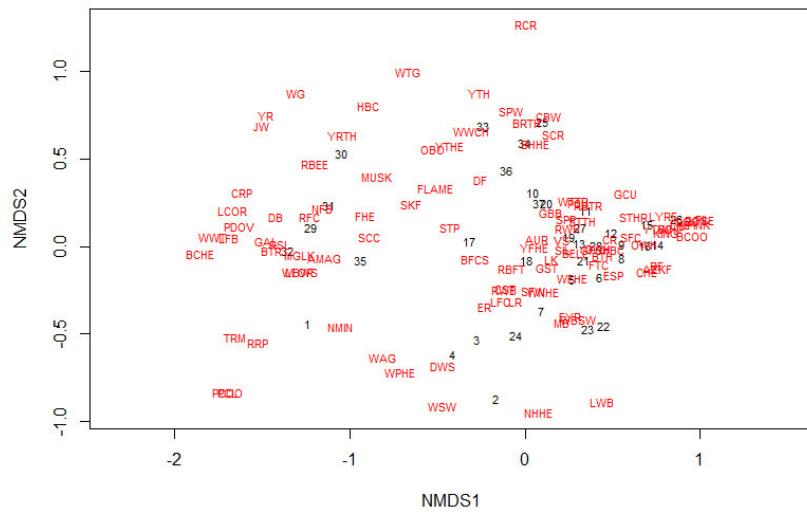
- Forests of the same type (colour label) tend to be closer together. Reflects that bird abundance is related to the forest type.
- Unlike in PCA, the dimensions in MDS are non-orthogonal
 - No longer have a potential interpretation of dimensions as distinct latent variables
 - Dimension scores would not be independent predictors in a regression

MDS Step 2: Examine the subject (site) plot



- Environmental variables can be included in the plot in a similar way to supplementary variables for PCA (i.e. not part of the input, but correlation with each dimension calculated post-hoc)
- Could include things like soil pH, soil composition, altitude, etc.
- In this example we have just used each type of forest as a [binary] variable. The directions generally match the clusters of forest type.

MDS Step 3: Examine the variables plot



- Variable (species) scores are included by taking a weighted average of the site scores
- Species that are closest to the sites in the ordination map are expected to have the highest abundances

Conclusions



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Choosing a method



EDUCATION

Ten quick tips for effective dimensionality reduction

Lan Huong Nguyen¹, Susan Holmes^{2*}

1 Institute for Mathematical and Computational Engineering, Stanford University, Stanford, California, United States of America, **2** Department of Statistics, Stanford University, Stanford, California, United States of America

* susan@stat.stanford.edu

Introduction

Dimensionality reduction (DR) is frequently applied during the analysis of high-dimensional data. Both as a means of denoising and simplification, it can be beneficial for the majority of modern biological datasets, in which it's not uncommon to have hundreds or even millions of simultaneous measurements collected for a single sample. Because of "the curse of dimensionality," many statistical methods lack power when applied to high-dimensional data. Even if the number of collected data points is large, they remain sparsely submerged in a voluminous high-dimensional space that is practically impossible to explore exhaustively (see chapter 12 [1]). By reducing the dimensionality of the data, you can often alleviate this challenging and troublesome phenomenon. Low-dimensional data representations that remove noise but retain the signal of interest can be instrumental in understanding hidden structures and patterns. Original high-dimensional data often contain measurements on uninformative or redundant variables. DR can be viewed as a method for latent feature extraction. It is also frequently used for data compression, exploration, and visualization. Although many DR techniques have been developed and implemented in standard data analytic pipelines, they are easy to misuse, and their results are often misinterpreted in practice. This article presents a set of useful guidelines for practitioners specifying how to correctly perform DR, interpret its output, and communicate results. Note that this is not a review article, and we recommend some important reviews in the references.

Tip 1: Choose an appropriate method

Nguyen LH, Holmes S (2019) Ten quick tips for effective dimensionality reduction. PLOS Computational Biology 15(6): e1006907. <https://doi.org/10.1371/journal.pcbi.1006907>



OPEN ACCESS

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Copyright: © 2019 Nguyen, Holmes. This is an open access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and

- I've given you a broad overview of basic dimension reduction methods
- There are many extensions to these methods and many other methods available
- Many excellent tutorials and other resources are available for implementing a particular method
- Also consider the choice of method after doing some basic EDA

Further Assistance at Sydney University

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Workshops

- Create your own custom programmes tailored to your research needs by attending more of our Statistical Consulting workshops. Look for the statistics workshops on our training page <https://www.sydney.edu.au/research/facilities/sydney-informatics-hub/workshops-and-training.html#stats>. Some we recommend are:
 - Research Essentials
 - Experimental Design
 - Power Analysis
- Other SIH workshops <https://www.sydney.edu.au/research/facilities/sydney-informatics-hub/workshops-and-training.html>
- Training Sign up to our mailing list to be notified of upcoming training:
mailman.sydney.edu.au/mailman/listinfo/computing_training
- Hacky Hour
www.sydney.edu.au/research/facilities/sydney-informatics-hub/workshops-and-training/hacky-hour.html OR Google “Sydney Hacky Hour”
- 1on1 Consults can be requested on our website www.sydney.edu.au/research/facilities/sydney-informatics-hub.html OR Google “Sydney Informatics Hub”

OTHER

- Open Learning Environment (OLE) courses
- Linkedin Learning: <https://linkedin.com/learning/>
 - SPSS <https://www.linkedin.com/learning/machine-learning-ai-foundations-linear-regression/welcome?u=2196204>

We recommend our Experimental Design and Sample Size Workshops

Experimental Design Workshop

- Far too many researchers think they know all they need to in this area. We commonly see designs that could be substantially improved for stronger causal inference and improved results which leads to publication in higher impact journals (amongst other benefits).
- Even if you have already collected your data it is well worth attending since it may improve your write up and analysis e.g. we had a client who didn't realise they had a very strong Before/After Control/Impact (BACI) design.

Sample and Power Workshop

- Shows the steps and decisions researchers need to make when designing an experiments to ensure sufficient sample e.g. Power, minimum required to fit the necessary model, etc.
- Also how much Power the study has i.e. does it have sufficient power to detect the effects you expect to see, or is your study a complete waste of time and resources.

A reminder about Acknowledging SIH



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Acknowledging specific staff:

"The authors acknowledge the technical assistance of (name of staff) of the Sydney Informatics Hub, a Core Research Facility of the University of Sydney."

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We value your feedback

We want to hear about you and whether this workshop has helped you in your research. What **worked** and what **didn't work**.

We actively use the feedback to improve our workshops.

Completing this survey really does help us and we would appreciate your help! It only takes a few minutes to complete (promise!)

Here is the link to the survey!

<https://redcap.sydney.edu.au/surveys/?s=FJ33MYNCRR&training=51>



Glossary of Terms

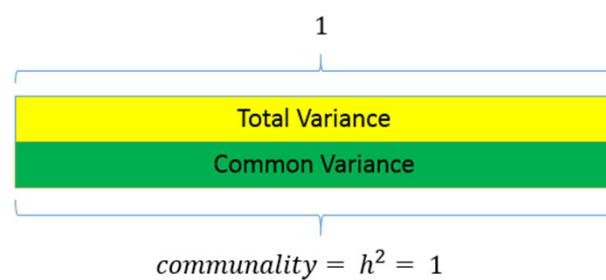
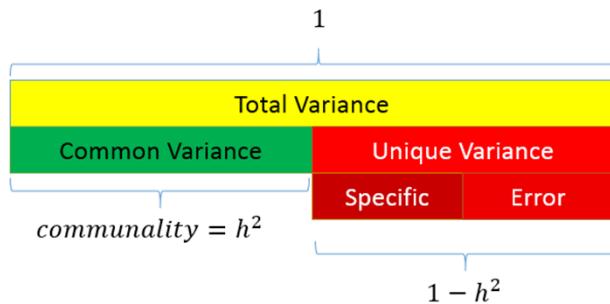
- **Variance** is simply variability of a single variable. Similar to modelling, unexplained variation is a bad thing because it contributes to the error of our estimates, but explained variation is a good thing because we can attribute that variability to a particular factor, and turn ‘noise’ into a meaningful ‘signal’. When we try to “maximise variability” in PCA, you can think about this as trying to maximise explained variability or “information”.
- **Total Variance/Total inertia** usually refers to the variance or inertia summed across all variables/dimensions
- **Dimension/Components/Factors** Dimension reduction techniques employ linear algebra, which often uses terminology from geometry. Mathematically, we can think about each original variable, or synthetic variable as being a dimension (I use ‘dimension’ to refer exclusively to the dimensions identified by the various dimension reduction methods These dimensions have differing names depending on the technique being used.)

Extra slides on Factor analysis



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Partitioning Variance



- For each measured variable in a factor analysis, the **communality** is a measure of the proportion of variance deemed common variance, ranging from 0 to 1

An example dataset: Big Five Personality Traits

- Dataset is a 10-question subset from the big five personality measures dataset, preloaded with the psych package in R
- Measured on a 6-point LIKERT scale (Very Inaccurate (1) -> Very Accurate (6))
- N=2800
- 25 personality self-report items taken from the International Personality Item Pool (ipip.ori.org) were included as part of the Synthetic Aperture Personality Assessment (SAPA) web-based personality assessment project.

A1
Am indifferent to the feelings of others.
(q_146)

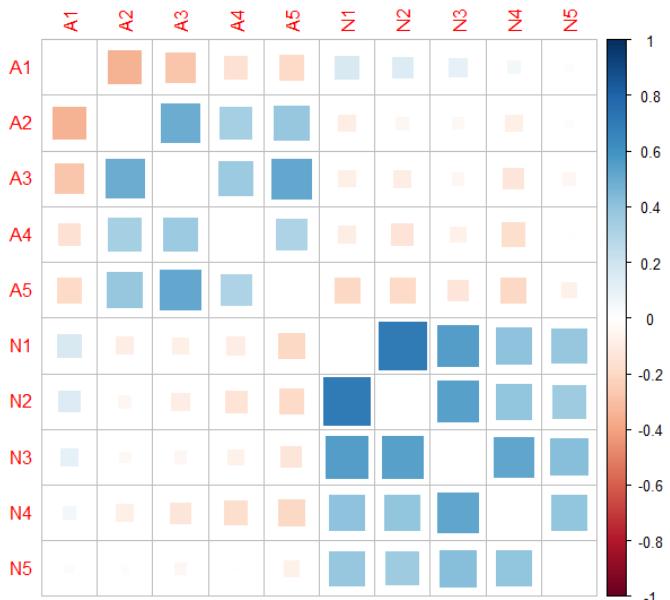
A2
Inquire about others' well-being. (q_1162)

A3
Know how to comfort others. (q_1206)

A4
Love children. (q_1364)

A5
Make people feel at ease. (q_1419)

Factor Analysis Step 0 EDA



- Scatterplots are not terribly useful for 6-point LIKERT scale, so this is a correlation only plot.
- Pretty clear structure: correlation between the 'A' questions and the 'N' questions. Note that Q1 “am indifferent to the feelings of others” is negatively correlated with other Agreeableness questions
- We will perform a two-factor analysis to see whether we reconstruct two factors for Agreeableness and Neuroticism

```
bfi_trim = bfi %>% select(matches('^A[1-5] | ^N'))  
corrplot(cor(bfi_trim,use="complete.obs"),method="square",diag=F)
```

FA. Step 2: Examine the variable space

```
Factor Analysis using method = minres
Call: fa(r = bfi_trim, nfactors = 2)
Standardized loadings (pattern matrix)
based upon correlation matrix
```

	MR1	MR2	h2	u2	com
A1	0.07	-0.36	0.14	0.86	1.1
A2	0.05	0.69	0.47	0.53	1.0
A3	0.03	0.76	0.56	0.44	1.0
A4	-0.05	0.47	0.24	0.76	1.0
A5	-0.12	0.60	0.39	0.61	1.1
N1	0.78	-0.03	0.61	0.39	1.0
N2	0.76	-0.02	0.58	0.42	1.0
N3	0.77	0.05	0.58	0.42	1.0
N4	0.58	-0.08	0.36	0.64	1.0
N5	0.54	0.08	0.29	0.71	1.0

- First thing to examine is the communality **h2** column (h^2)
- Fairly high for most items.
- The **u2** column is the uniqueness ($1-h^2$)
- The **com** column is the item complexity, a summary of how much each item reflects a single construct (1=loading on to one factor, 2 = loading on to two factors)

```
model = fa(bfi_trim, 2)
```

```
model
```

FA. Step 2: Examine the variable space

	MR1	MR2	h2	u2	com
A1	0.07	-0.36	0.14	0.86	1.1
A2	0.05	0.69	0.47	0.53	1.0
A3	0.03	0.76	0.56	0.44	1.0
A4	-0.05	0.47	0.24	0.76	1.0
A5	-0.12	0.60	0.39	0.61	1.1
N1	0.78	-0.03	0.61	0.39	1.0
N2	0.76	-0.02	0.58	0.42	1.0
N3	0.77	0.05	0.58	0.42	1.0
N4	0.58	-0.08	0.36	0.64	1.0
N5	0.54	0.08	0.29	0.71	1.0

	MR1	MR2
SS loadings	2.44	1.78
Proportion Var	0.24	0.18
Cumulative Var	0.24	0.42
Proportion Explained	0.58	0.42
Cumulative Proportion	0.58	1.00

```
model = fa(bfi_trim, 2)
```

```
model
```

- The first two columns are the factor loadings. The two factors are MR1 and MR2, after the factor extraction method (minimum residual)
- Note that one of the two factors loads much more highly than the other onto each item.
- Factor 1 and Factor 2 explain 24% and 18% respectively of total variance.