Non-linear, Multivariate & Bayesian Statistics

Lecture 9

LSM 3257

AY22/23; Sem 2 | Ian Z.W. Chan



Summary (Learning Objectives)

Non-linear Modelling

- GAM

Multivariate Statistics

- Theory: Response variables, purposes, dissimilarity matrices
- Understanding structure
 - Clustering: AHC, PAM, K-means
 - Unconstrained ordination: PCA, PCoA, NMDS, CA
- Interpreting/Making predictions
 - Constrained ordination: RDA, CAP, CCA
 - "Modelling": MANOVA, PERMANOVA, MANCOVA & Multivariate GLM

Bayesian Statistics

- Bayes' Rule and a stan_glm() example



Non-linear Modelling



GAM

Generalised Additive Model

What is a GAM?

Used to create (very) complex non-linear models

- Uses splines to fit a curve to the data: splines are curves with constantly changing radius that are made to pass through a series of fixed points.

The curvature that is introduced should improve the predictive performance (Maximum Likelihood) of the model

splines: f(x) is complicated Source: Bolker (2007)

But the model will be penalised for the curvature (because this increases its complexity).

Fitting a GAM

Load package and dataset:

```
require(mgcv)
data(columb)
str(columb)
```

Let's use <home.value> to explain <crime>

Visualise data:

plot(crime~home.value, data=columb)

Is this linear or non-linear?

Fit a linear model:

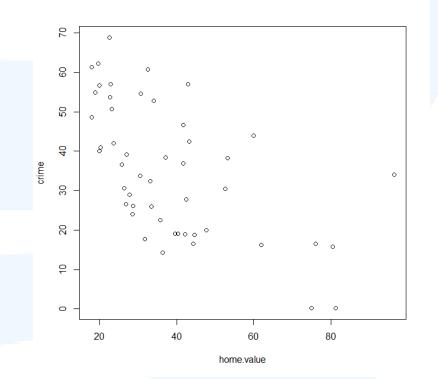
mod3.lm=gam(crime~home.value,data=columb)

Function to fit a GAM

This is equivalent to a linear model

Dataset on <crime> rates as a function of <area> of the district, average <home.value>, average <income> and <open.space> in the area.

```
> str(columb)
'data.frame': 49 obs. of 8 variables:
$ area : num 0.3094 0.2593 0.1925 0.0838 0.4889 ...
$ home.value: num 80.5 44.6 26.4 33.2 23.2 ...
$ income : num 19.53 21.23 15.96 4.48 11.25 ...
$ crime : num 15.7 18.8 30.6 32.4 50.7 ...
$ open.space: num 2.851 5.297 4.535 0.394 0.406 ...
$ district : Factor w/ 49 levels "0","1","2","3",..: 1 2
$ x : num 8.83 8.33 9.01 8.46 9.01 ...
$ y : num 14.4 14 13.8 13.7 13.3 ...
```



Fitting a GAM

Fit the GAM non-linear model:

```
mod3.g=gam(crime~s(home.value),data=columb)
```

This s(...) tells R to use splines on the variable. R decides how many splines to use on its own (you can specify this number "s(home.value, k=20)" and some other things, check ?gam). This can only take continuous variables. You can add categorical variables as "linear variables", i.e. without the s(...).

Note: you would still have to specify the correct error distribution using "family=": poisson, binomial, quasipoisson, quasibinomial, or nb (negative binomial).

Compare the two:

```
AIC (mod3.lm, mod3.g) > AIC (mod3.lm, mod3.g)

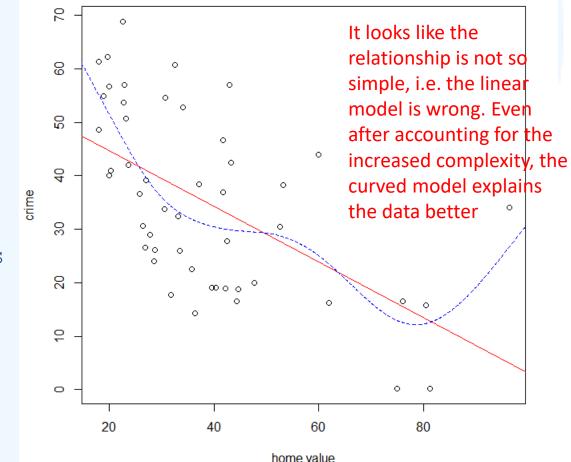
df AIC

mod3.lm 3.000000 400.5179

mod3.g 6.137319 394.3689
```

Visualise the 2 models:

```
plot(crime~home.value,data=columb) #points
abline(mod3.lm,col="red") #linear model
xv=seq(0,100,0.1)
yv_3.g=predict(mod3.g,list(home.value=xv))
lines(xv,yv_3.g,col="blue",lty=2) #GAM
```



Interpreting results

Check the model:

```
par (mfrow=c(2,2))
gam.check(mod3.g)
```

Tells you whether the model converged. If not, try to simplify your model.

> gam.check(mod3.g)

Method: GCV Optimizer: magic

Smoothing parameter selection converged after 4 iterations.

The RMS GCV score gradient at convergence was 0.001427689 .

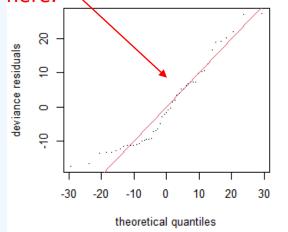
The Hessian was positive definite.

Model rank = 10 / 10

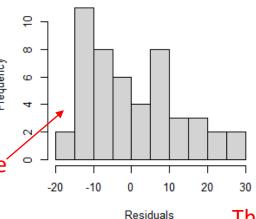
Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

```
k' edf k-index p-value
s(home.value) 9.00 4.14 1.05 0.52
```

p-value < 0.05 would be bad (indicates that residuals are not randomly distributed) – try increasing the "k" specified for the variable to more than the value here. Here it is OK. This looks at whether the residuals are normally distributed. They should follow the red line. A little marginal here.

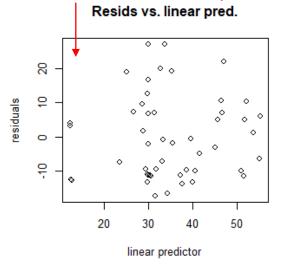


Histogram of residuals

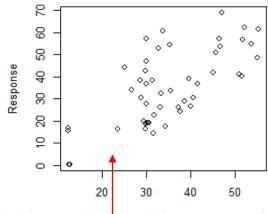


This also looks at the normality of the residuals. It should look like a normal distribution.

This should be randomly distributed. Looks OK in general (cannot expect too much from a GAM)



Response vs. Fitted Values



This looks at how well your model fits the data. It should be as close as possible to the y = x diagonal line.

Interpreting results

View results:

summary(mod3.g)

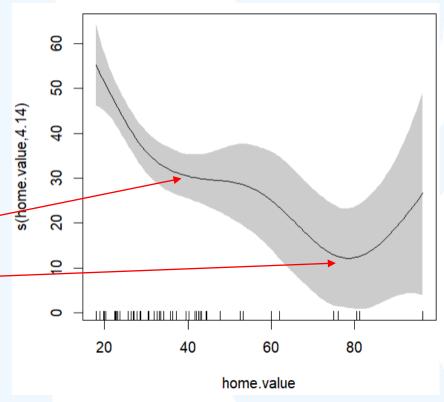
Linear terms are reported here (there are none in this model)

The non-linear term for <home.value> is significant and uses 4.137 effective degrees of freedom

Graphically:

```
plot (mod3.g, shift=coef (mod3.g) [1], shade=T)
```

All else being equal, there are about 30 crimes for properties worth about \$40k, and about 12 crimes for those worth about \$80k



Fitting more complicated GAMs

Note: You can also fit random effects using gamm(). There are 2 ways to do it. See: ?gamm and http://r.qcbs.ca/workshop08/booken/quick-intro-to-generalized-additive-mixed-models-gamms.html.

Fit a GAM with multiple terms and an interaction:

mod3.g2=gam(crime~s(home.value)+s(area)+te(income,open.space),data=columb)

Simplify:

```
Approximate significance of smooth terms:
                            s(home.value)
summary(mod3.g2)
                            te(income,open.space) 4.586
```

mod3.g3=update(mod3.g2, ~.-s(area))

```
summary (mod3.g3)
```

AIC (mod3.g, mod3.g2, mod3.g3) mod3.g2 12.687751

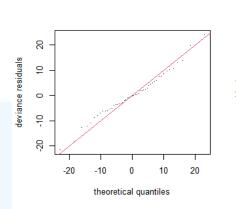
#I decide to follow the AIC: mod3.g2 is the best (my personal interpretation)

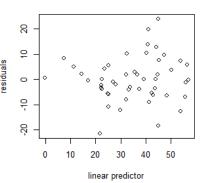
Check:

gam.check(mod3.g2)

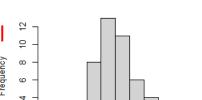
The residuals of this new model look much more normally distributed than in mod3.g

This te() tells R to allow <income> and <open.space> to interact.

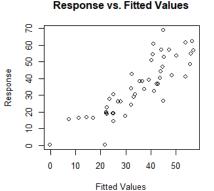




Resids vs. linear pred.



Histogram of residuals



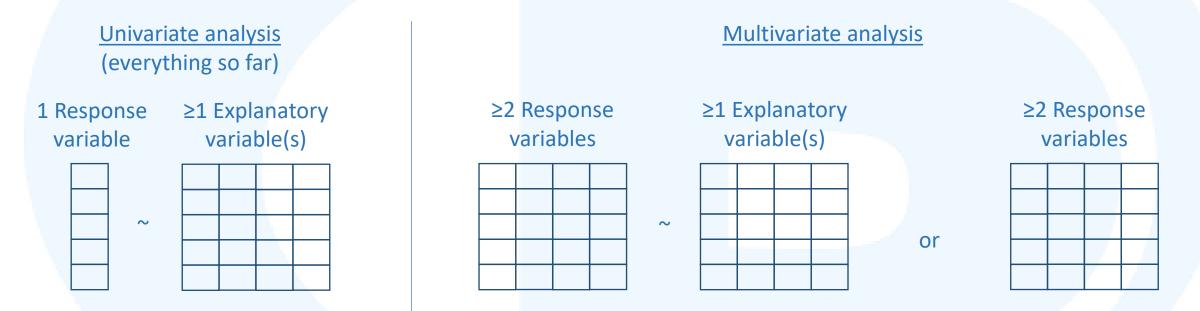
There is A LOT more... a great starter resource: https://noamross.github.io/gams-in-r-course/



Multivariate Statistics

What are Multivariate Analyses

Used to analyse 2 or more response variables at the same time.



Many (many many) different analyses: I will only introduce the most common

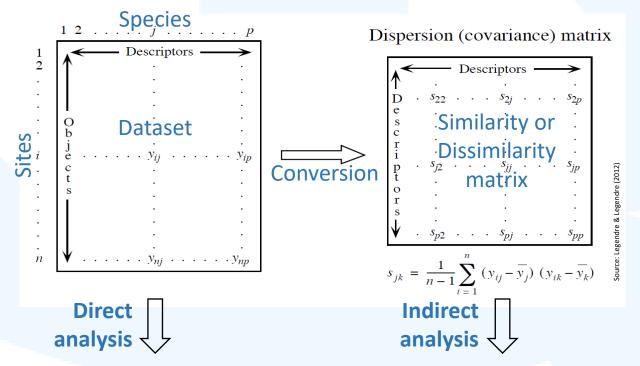
- Read up details on how they work, their strengths and weaknesses, etc.
- Google for alternative analyses

Purposes, Datasets and (Dis)similarity matrices

In general, multivariate analyses have 2 purposes:

- 1) Understanding structure: visually looking for groupings within your matrix of response variables (i.e. no explanatory variables and no p-values).
- 2) Interpreting/Predicting: using a matrix of explanatory variables to explain a matrix of response variables.

General concept:



Interpretation/Prediction (using a dataset of explanatory variables)
Structure (without using explanatory variables)

(Dis)similarity/Distance matrices

A matrix of dissimilarities/distances between the values in your original dataset.

Euclidean

Note: Distance ≠ Dissimilarity, read more here.

Many different <u>distance measures</u> in statistics.

- Commonly-used in ecology:

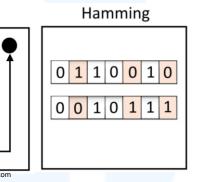
Euclidean: direct distance between two points for continuous data.

Manhattan: x-distance + y-distance between two points. Preferred in datasets with many variables (i.e. high dimensionality).

Hamming: counts the number of variables that are different. For categorical variables.

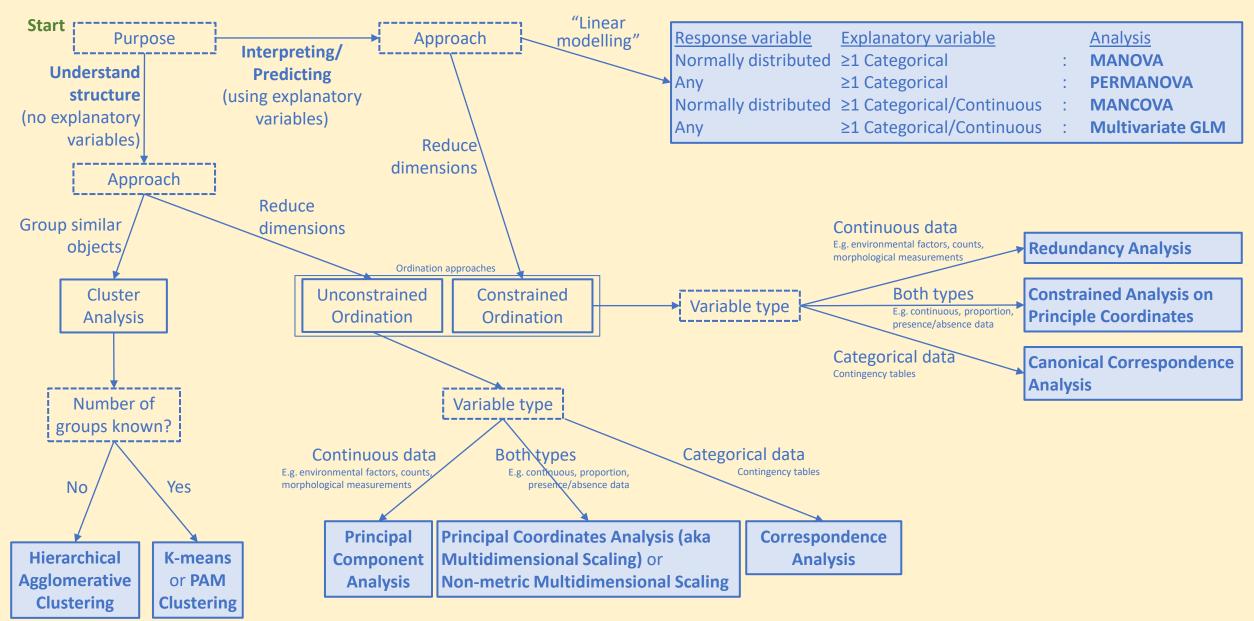
Bray-Curtis: Based on counts of similar species at different sites. Preferred for species matrices.

Fuller guide to choosing the right distance measure.



Manhattan

Multivariate analyses – Analysis decision tree





Cluster Analysis

HAC, PAM, K-means

What is clustering?

Clustering tries to split your data into groups based on how similar they are.

Two most common types...

- 1) Connectivity-based (Hierarchical): when number of groups is not known.
- Agglomerative: starts with individual datapoints (singletons) then groups the closest together.
- Divisive: starts with all datapoint in one cluster and then splits them into groups.
- 2) **Centroids-based** (Partitioning): Repeatedly reassigns points to a pre-specified number of groups and minimises the distances of the points to their centroids.

Before you cluster:

- Remove all NAs.
- Consider scaling your variables using scale() (changes all your variables to have a mean of 0 and s.d. of 1): places the same importance on all variables.

Hierarchical Agglomerative Clustering

If you don't know how many clusters (groups) you want.

Load dataset, remove NAs and scale data:

```
require (car)

d1=Freedman #dataset on characteristics of cities in the US

d1=na.omit(d1)

Akron 675 7.3 746 2602

Albany 713 2.6 322 1388
Allentown 534 0.8 491 1182

Anaheim 1261 1.4 1612 3341

Atlanta 1330 22.8 770 2805

Bakersfield 331 7.0 41 3306
```

Calculate dissimilarity matrix with Euclidean distances (AHC needs this as input):

```
d1_dist=dist(d1.1) #Note: can specify other distances with "method="
```

Perform clustering:

```
ahcmod1=hclust(d1 dist)
```

Hierarchical Agglomerative Clustering

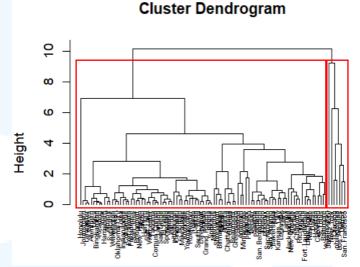
View dendrogram to decide on number of clusters you want:

```
plot(ahcmod1,cex=0.5,hang=-1)
#I decide that I want 2 clusters
```

Cut into 2 clusters to save results:

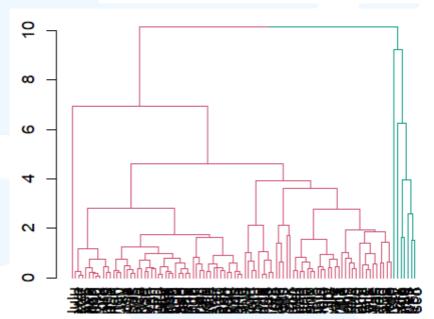
ahcmod2=cutree(ahcmod1, k=2)
d1\$cluster=as.integer(ahcmod2)

These are your results: which cluster each row is assigned to



Plot results:

require(dendextend)
ahcdend1=as.dendrogram(ahcmod1)
ahcdend2=color_branches(ahcdend1, k=2)
plot(ahcdend2)



Centroid-based: K-means and PAM Clustering

If you know how many clusters (groups) you want:

- K-means uses centroids (imaginary points).
- PAM uses medoids (actual points, more robust to outliers).

Read in dataset:

d2=Freedman

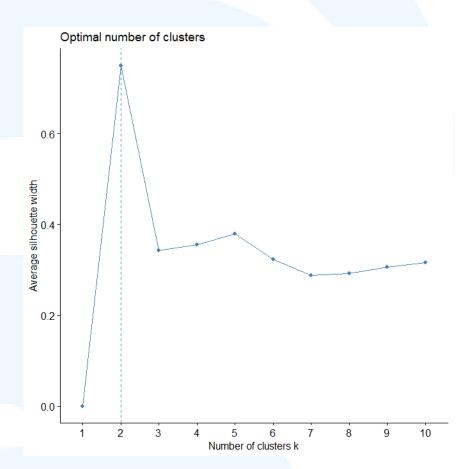
d2=na.omit(d2)

Determining optimal number of clusters:

require (factoextra)

fviz_nbclust(d2,FUNcluster=kmeans,method="silhouette") #2

Change to "pam" for PAM clustering

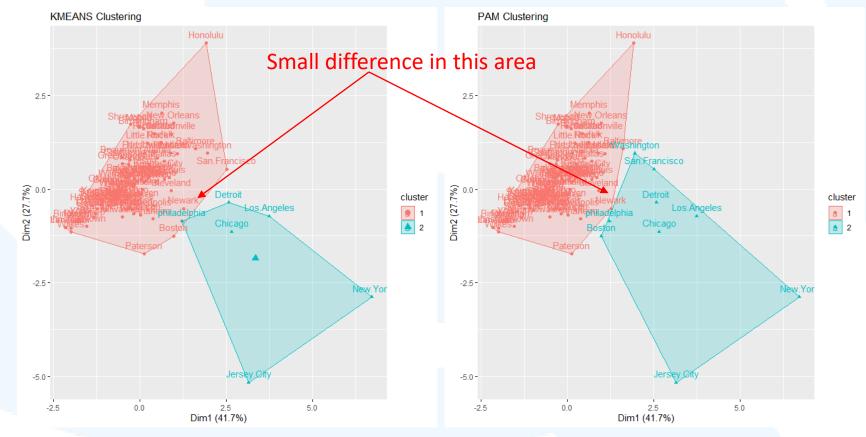


Centroid-based: K-means and PAM Clustering

Do the clustering:

Change to "pam" for PAM clustering

kmmod=eclust(d2,FUNcluster="kmeans", k=2)
pammod=eclust(d2,FUNcluster="pam", k=2)



Saving results:

d2\$cluster=as.integer(kmmod\$cluster)

Interpreting results

Clustering just tells you visually which datapoints are more similar to one another (similar to Unconstrained Ordination). There are no p-values.

It is then up to you to interpret these results based on biological intuition.

Example (from PAM results):

The cities in Cluster 2 are all large, metropolitan cities, suggesting that this has an effect on the variables in the dataset.





Unconstrained Ordination

PCA, PCoA, NMDS, CA

What is Unconstrained Ordination?

When you have many variables, it's difficult to see relationships in the dataset:

- E.g. if you have 10 variables, to compare all of them, you would need to plot 55 graphs at least; even more to investigate interactions and combinations of variables.

Unconstrained Ordination helps to make it easier to visualise what variables are important:

- 1) We first plot all the datapoints in multivariate space (e.g. 10-D space for 10 variables).
- 2) We then rotate this scatterplot so that we are looking at it from the direction where the points are most spread out, i.e. so that the x- and y- axes are the axes with the most variance. The axes we see are hence combinations of the original variables.
- 3) We then flatten (aka project) this scatterplot onto 2 dimensions for easy viewing and interpreting.

There are no p-values.

What is Unconstrained Ordination?

Different types of ordination for different types of data.

| Method | Distance preserved | Variables |
|--|--|--|
| Principal component analysis (PCA) | Euclidean distance | Quantitative data, linear relation- ships (beware of double-zeros) |
| Correspondence analysis (CA) | χ^2 distance | Non-negative, dimensionally homogeneous quantitative or binary data; species frequencies or presence/absence data |
| Principal coordinate analysis (PCoA), metric (multidimensional) scaling, classical scaling | Any distance measure | Quantitative, semiquantitative, qualitative, or mixed |
| Nonmetric multidimensional scaling (nMDS) | Any distance measure Source: Legendre & Legendre (2012) | Quantitative, semiquantitative, qualitative, or mixed |

Note: It is NOT compulsory that the data are normally distributed, but PCA tends to work better when they are (read this).

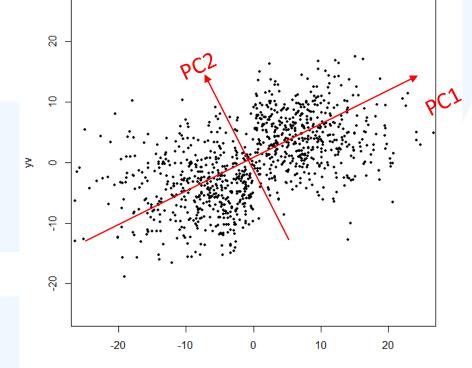
Direct, unconstrained ordination for continuous data. Assumes a linear relationship. Uses Euclidean distance.

Visualises the data so that the x-axis of the PCA plot (aka PC1) is the axis with the most variation, and the y-axis (aka PC2) is the axis with the most variation while

being orthogonal (i.e. at right angles) to PC1.

Each PC is a linear combination of the original variables.

- The first few PCs explain most of the variation.
- Looking at what variables are in PC1 and PC2 allows us to identify important variables.



Note: eigenvector = PC; eigenvalue = the variance along that PC.

Loading a dataset of 9 variables:

```
d3=mtcars[,c(1:8,11)]
```

Running the PCA and viewing the results:

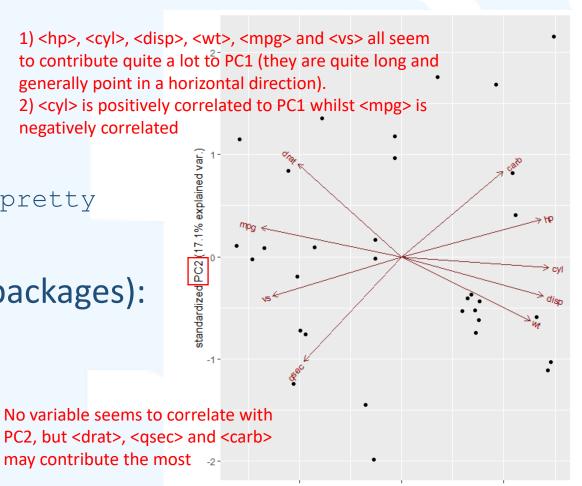
Visualising (a little annoying to install the packages):

```
install.packages("devtools")
library(devtools)
install_github("vqv/ggbiplot")
require(ggbiplot)
ggbiplot(pcal) #nicer
```

> summary(pcal) Importance of components: PC1 PC2 PC3 PC4 PC5 Standard deviation 2.4732 1.2390 0.75052 0.50607 0.47234 Proportion of Variance 0.6796 0.1706 0.06259 0.02846 0.02479 Cumulative Proportion 0.6796 0.8502 0.91277 0.94123 0.96601

Notice how the first 2 PCs already explain >85% of the variation in the dataset

standardized PC1 (68.0% explained var.)



For more plotting options, see: https://www.datacamp.com/community/tutorials/pca-analysis-r27

Calculating loadings (how much each variable contributes to the PCs) to see which variables are important:

<mpg>contributes

```
loadings
                                                              to 13.6% of PC1
func1=function(rotation, sdev) {rotation*sdev}
func2=function(varcos, compcos) {varcos*100/compcos}
varcos=(t(apply(pcal$rotation,1,func1,pcal$sdev)))^2
compcos=apply(varcos, 2, sum)
                                                       Just change these
                                                                                  7.077041 20.0395319
                                                       to your PCA
loadings=t(apply(varcos, 1, func2, compcos))
                                                                          Summary:
                                                       model object and
loadings
                                                                          1) a lot of variables are
                                                        run the whole
                                                                          important in PC1
                                                       chunk of code
                                                                          2) <drat>, <qsec> and <carb>
```

Interpretation: the various cars differ mostly due to a combination of fuel efficiency <mpg>, number of cylinders <cyl>, size <disp> and power <hp>.

are important in PC2.

If you have pre-defined groups based on some variable, you can see how well these groups spread out from one another.

Assigning grouping by country manually:

```
d3groups=c(rep("Japan", 3),
rep("US", 4), rep("Europe",
7), rep("US", 3), "Europe", rep("Japan",
3), rep("US", 4), rep("Europe", 3),
"US", rep("Europe", 3))
```

Replaces the points with the names of the cars

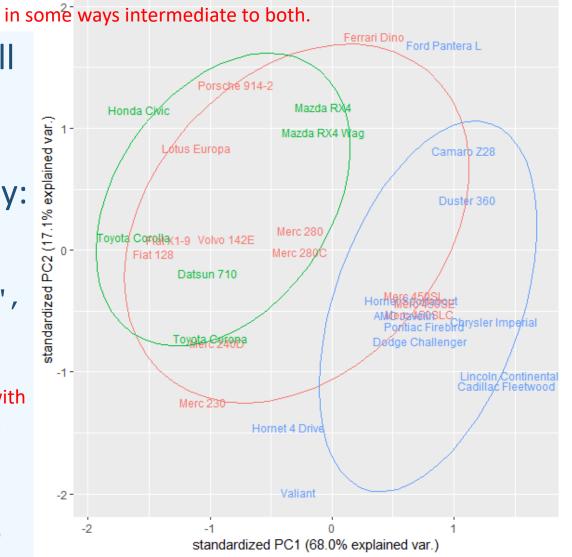
Plotting different countries by colour:

```
ggbiplot (pca1, labels=rownames (d3),
groups=d3groups,ellipse=T,var.axes=F)
```

groups

Assign coloured Draws ellipsés based on 68% confidence, change to 95% by adding "ellipse.prob=0.95"

Gets rid of the arrows (we are now interested in groupings)



European and Japanese cars tend to be

more similar to each other but different

to US cars, although European cars are

groups Europe

Principle Coordinates Analysis (PCoA)

Also known as Multidimensional Scaling (MDS). Indirect, unconstrained ordination for many types of data. Assumes a linear relationship.

Dataset:

```
d3=mtcars[,c(1:8,11)]
```

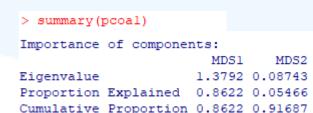
Note: distances available are "bray" (the default), "manhattan", "euclidean", "canberra", "kulczynski", "jaccard", "gower", "altGower", "morisita", "horn", "mountford", "raup", "binomial" or "chao". If you choose "Euclidean", it's the same as a PCA. Use "bray" for abundance data. Use "jaccard" for presence/absence data.

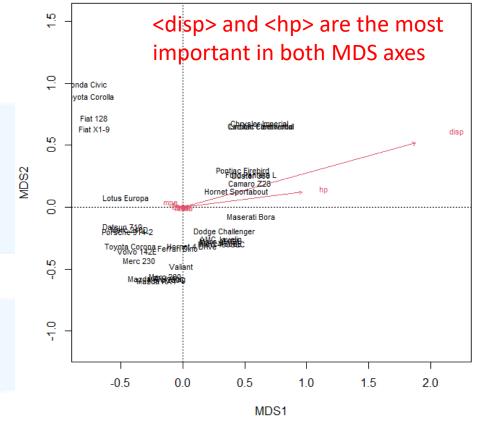
Fit the PCoA:

```
require(vegan)
pcoal=capscale(d3~1, distance="bray")
```

View results:

```
summary(pcoal)
biplot(pcoal)
```





Non-metric Multidimensional Scaling (NMDS)

Indirect, unconstrained ordination for many types of data. **Better for ordinal data** (e.g. Likert scales). Uses ranks rather than actual data. Fits by trial and error (so you may get different results with successive runs).

Stress is an indication of

Load dataset:

see: "No convergent solutions", try require (vegan) increasing the "trymax" argument.

data(varespec) #from vegan

Fit NMDS:

Chooses number of dimensions

Iteration produced a solution. If you

nmds1=metaMDS(comm=varespec, k=2,
distance="bray", trymax=100)

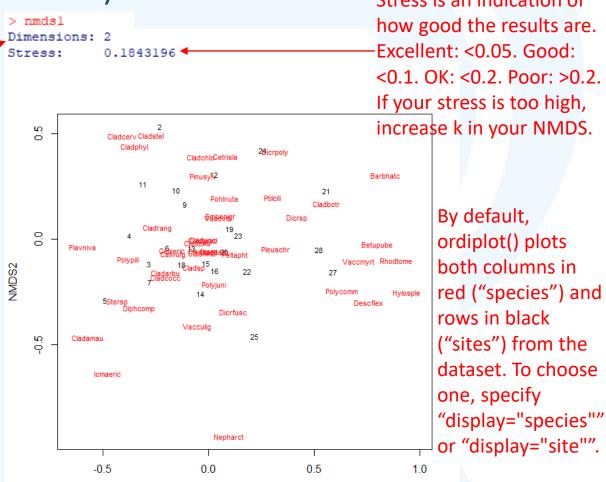
View results:

Also many different distance measures available

nmds1

ordiplot(nmds1, type="t")

For more plotting ideas, see: help(ordiplot), https://jonlefcheck.net/2012/10/24/nmds-tutorial-in-r/ and https://jkzorz.github.io/2019/06/06/NMDS.html.



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NMDS1

Correspondence Analysis (CA)

Unconstrained ordination for categorical data (chi-square distance). Assumes a unimodal relationship. Data should be in the form of a contingency table.

Load dataset:

require(FactoMineR) #for performing the analysis
require(factoextra)

data(housetasks) #dataset from factoextra

Has to be a

contingency

table

Perform analysis:

cal=CA(housetasks,graph=F)

View results:

summary(ca1)

plot(ca1)

For more: http://www.sthda.com/english/articles/31-principal-component-methods-in-r-practical-guide/113-ca-correspondence-analysis-in-r-essentials/.

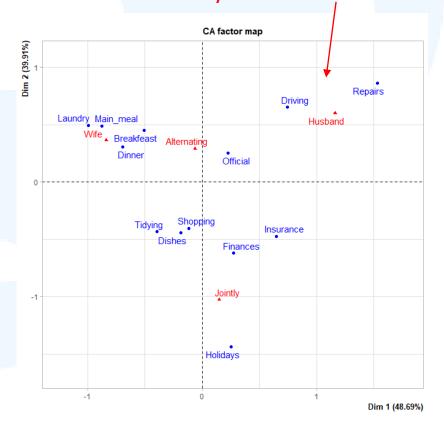
> housetasks Wife Alternating Husband Jointly

| | 1111 | Arocinating | Habbana | COLHELY |
|------------|------|-------------|---------|---------|
| Laundry | 156 | 14 | 2 | 4 |
| Main_meal | 124 | 20 | 5 | 4 |
| Dinner | 77 | 11 | 7 | 13 |
| Breakfeast | 82 | 36 | 15 | 7 |
| Tidying | 53 | 11 | 1 | 57 |
| Dishes | 32 | 24 | 4 | 53 |
| Shopping | 33 | 23 | 9 | 55 |
| Official | 12 | 46 | 23 | 15 |
| Driving | 10 | 51 | 75 | 3 |
| Finances | 13 | 13 | 21 | 66 |
| Insurance | 8 | 1 | 53 | 77 |
| Repairs | 0 | 3 | 160 | 2 |
| Holidays | 0 | 1 | 6 | 153 |
| | | | | |

> summary(cal

| | Dim.1 | Dim.2 | Dim.3 |
|----------------------|--------|--------|---------|
| Variance | 0.543 | 0.445 | 0.127 |
| % of var. | 48.692 | 39.913 | 11.395 |
| Cumulative % of var. | 48.692 | 88.605 | 100.000 |

Driving and repairs tend to be more similar to each other, and they tend to be done by the husband alone.



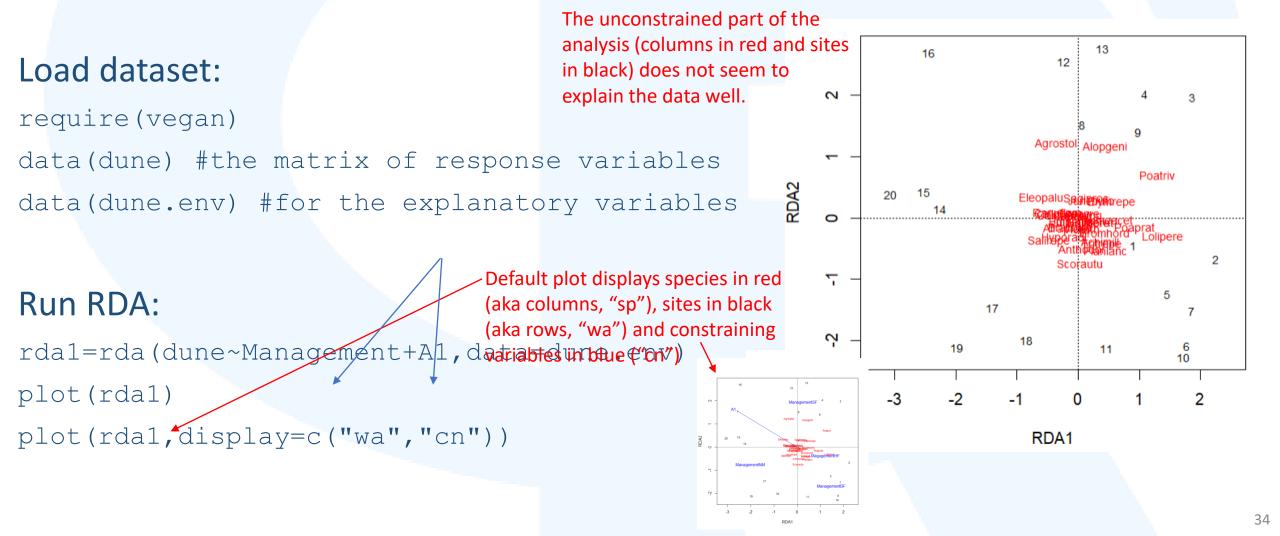


Constrained Ordination

RDA, CAP, CCA

Redundancy Analysis (RDA)

The **constrained equivalent of PCA**. The ordination is constrained by a dataset of explanatory variables (they determine the axes). Data interpretation is visual.



Redundancy Analysis (RDA)

Display results:

```
plot(rda1, display=c("wa", "cn"))
summary(rda1)
```

```
Accumulated constrained eigenvalues
Importance of components:
RDA1 RDA2
```

```
RDA1 RDA2 RDA3 RDA4
Eigenvalue 15.1445 11.8619 4.0532 2.53821
Proportion Explained 0.4508 0.3531 0.1206 0.07555
Cumulative Proportion 0.4508 0.8038 0.9245 1.00000
```

```
Site scores (weighte
```

```
RDA1
           RDA2
0.89393 -0.4471
2.23895 -0.6637
1.86599 1.9795
1.08262 2.0321
1.45165 -1.2385
1.76693 -2.0860
1.85326 -1.5143
0.06223 1.5213
0.97741 1.4042
1.72119 -2.2735
0.46469 -2.1281
-0.24074
         2.5504
0.40046
```

0.1493

0.4329

-2.26001

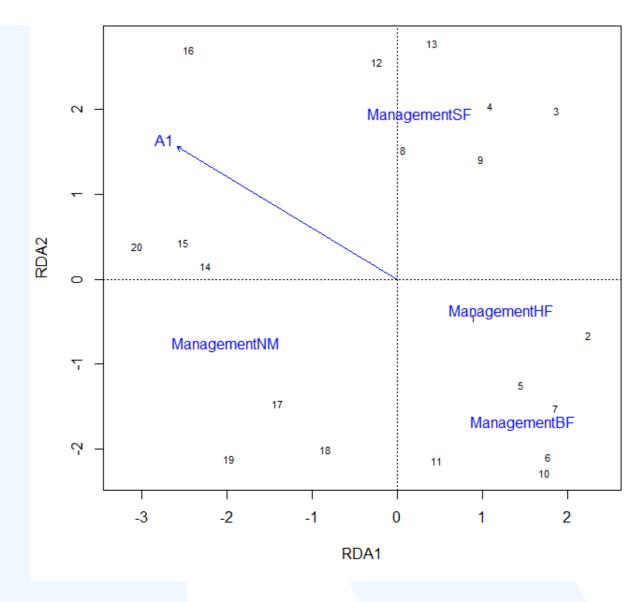
-2.52432

-2.45355 2.6938 -1.40908 -1.4644

18 -0.84683 -1.9976 19 -1.98250 -2.1061 20 -3.06227 0.3849 How much variation is captured by each RDA axis: these two in the plot are already displaying 80% of the variation in the whole dataset

How important each site is in each RDA axis

The constraining variables (blue) do a good job of explaining the differences at the various sites (black)



Constrained Analysis on Principle Coordinates (CAP)

The **constrained equivalent of PCoA**. The ordination is constrained by a dataset of explanatory variables (they determine the axes). Data interpretation is visual.

Code is similar to previous.

- Same dataset as RDA

Run CAP:

the tilde is a "1" (reflecting the fact there are no explanatory variables

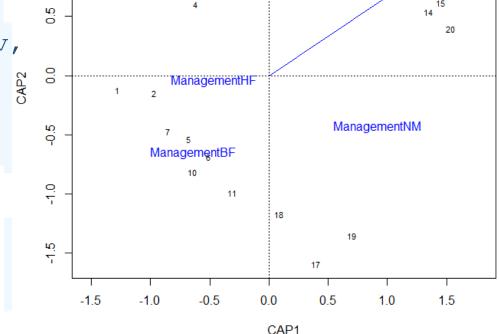
Display results: in unconstrained ordination)

plot(cap1)

plot(cap1, display=c("wa", "cn"))
summary(cap1)

Results are similar to previous, but the plot looks different because Bray-Curtis distance was used (instead of Euclidean).

The unconstrained part of the analysis (red and black points in the small graph) similarly does not explain the data well. But the constraining variables (blue) do a good job of explaining the differences at the various sites (black)



Canonical Correspondence Analysis (CCA)

The **constrained equivalent of CA**. The ordination is constrained by a dataset of explanatory variables (they determine the axes). Data interpretation is visual.

> housetasks

Same dataset as CA:

```
data(housetasks) #response contingency table

Laundry 156 14 2 4

Main_meal 124 20 5 4

Dinner 77 11 7 13

Breakfeast 82 36 15 7

Tidying 53 11 1 57

Dishes 32 24 4 53

physical=c(4,3,3,3,4,4,5,3,7,3,3,9,3),

math=c(F,F,F,F,F,T,T,F,T,T,F,F)

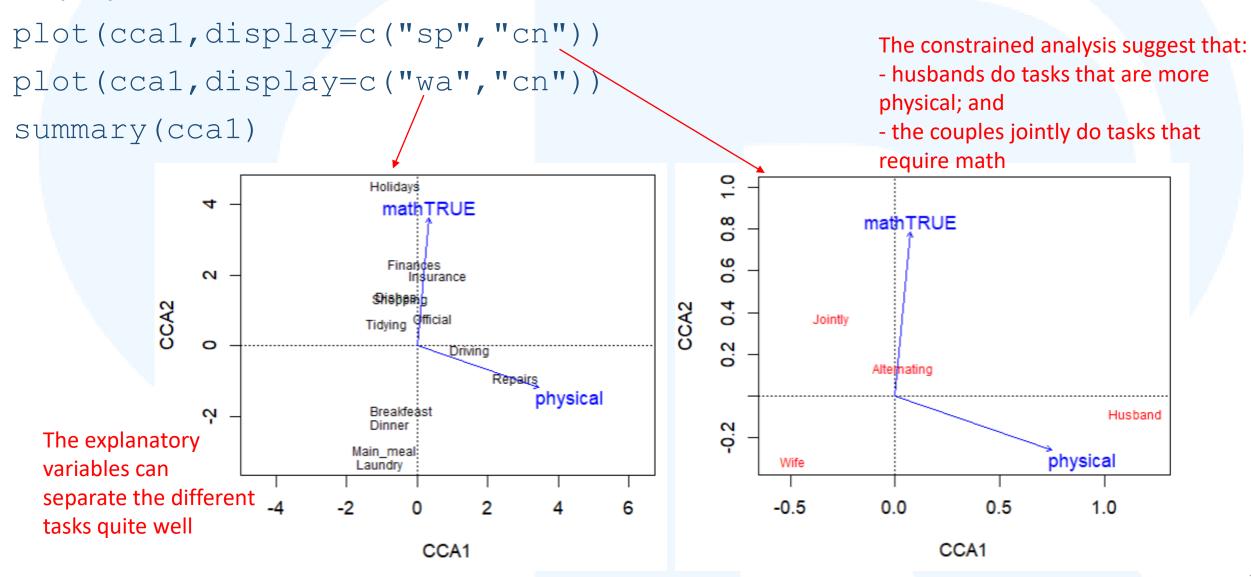
#additional explanatory variables for each task
```

Run CCA:

ccal=cca(housetasks~physical+math, data=task.properties)

Canonical Correspondence Analysis (CCA)

Display results:





"Linear Modelling"

MANOVA, PERMANOVA, MANCOVA, Multivariate GLM

"Linear modelling"-like approaches

Explaining more than 1 response variable (different types need different analyses) using 1 or more explanatory variables whilst accounting for the fact that the response variables may also interact.

Used to test a hypothesis, and therefore will produce p-values.

Analyses available are usually extensions of univariate analyses, with similar requirements and assumptions:

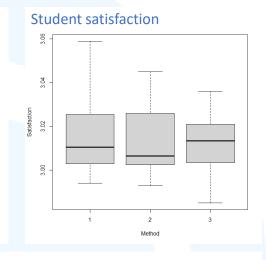
| Univariate basis | Multivariate equivalent(s) | | | | | |
|------------------|----------------------------|-----------|--|--|--|--|
| ANOVA — | → MANOVA | PERMANOVA | | | | |
| ANCOVA — | → MANCOVA | | | | | |
| GLM — | → Multivariate GLM | | | | | |

Multivariate ANOVA (MANOVA)

Explaining > 1 normal continuous response variable using ≥1 categorical variables.

Assumptions: similar to ANOVA. not seem to vary much amongst

Each dependent variable does teaching methods. Individually, we would expect a non-significant result



Load dataset – teaching <Method> to explain student <Test> scores and <Satistfaction>:

d4=read.csv("testScores.csv")

When plotted together, it can be seen that:

i) <Test> scores and <Satisfaction> are correlated; and

Test scores

ii) the <Test> scores for Method <3≥ are higher than

Methods 1 & 2 for a given <Satisfaction>

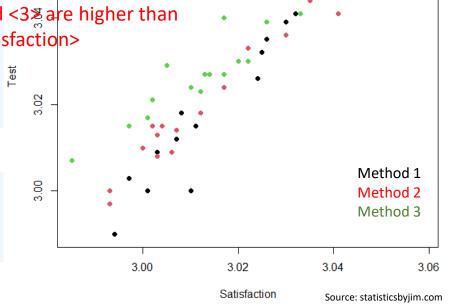
Perform MANOVA:

manoval=manova(cbind(Test, Satisfaction)~ Method, data=d4)

summary (manoval)

Residuals 46 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Note: cannot simplify using update().



Permutational MANOVA (PERMANOVA)

Any response variable type, one or more <u>categorical</u> explanatory variables. Tests many permutations of the data (i.e. rearranges them over and over again) and sees how many result in an increase or decrease in the measured "correlation".

Assumptions:

- Assumes objects in the datasets are exchangeable (i.e. are independent and have similar amounts of dispersion), e.g. if the values are very different, you may have to scale them first
- Does not assume any distribution; is insensitive to multicollinearity; allows for multiple variables; is insensitive to data with many zeros

Note: ANOSIM does something similar (although slightly different) but can only take 1 categorical variable, so I do not cover it. You can learn about it here: https://jkzorz.github.io/2019/06/11/ANOSIM-test.html.

Permutational MANOVA (PERMANOVA)

Load dataset:

```
require (vegan)
data(dune) #the response variables, counts of different plant species
data(dune.env) #contains explanatory variables <Management> and <Moisture>
                                                        Make sure to choose the correct
                                                        type of distance for your response
                                                        variables (Google is your friend)
```

Perform analysis:

perm1=adonis (dune~Management*Moisture, data=dune.env, method="euclidean")

perm1

Continue to simplify manually according to what we have learnt (update() works!)

```
> perm1
Call:
adonis(formula = dune ~ Management * Moisture, data = dune.env,
                                                                    method = "euclidean")
Permutation: free
Number of permutations: 999
Terms added sequentially (first to last)
                   Df SumsOfSqs MeanSqs F.Model
Management
                         555.38 185.128 3.3438 0.34747
Moisture
                         326.69 108.897 1.9669 0.20439
                         273.36 54.672 0.9875 0.17103 0.493
Management:Moisture 5
Residuals
                         442.92 55.365
Total
                                                1.00000
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' '1
```

Multivariate ANCOVA (MANCOVA)

Different ways of calculating significance. Pillai's trace is usually considered the most reliable

Univariate Tests

Explaining > 1 normal continuous variable using one or more <u>categorical and/or</u> <u>continuous</u> variables.

Run a MANCOVA using the mtcars dataset:

No need to simplify, just use results

Note: PERMANCOVA is not available in R (have to use PRIMER), you can use multivariate GLM instead.

<am> has a significant effect on both <qsec> and <hp> together MANCOVA Multivariate Tests F value df1 df2 р 0.0008036 Pillai's Trace 0.43453995 9.6058940 25 Wilks' Lambda 9.6058940 0.5654601 0.0008036 Hotelling's Trace 0.76847152 9.6058940 0.0008036 0.76847152 9.6058940 0.0008036 Roy's Largest Root Pillai's Trace 0.72974539 33.7526794 < .0000001 Wilks' Lambda 0.2702546 33.7526794 25 < .0000001 Hotelling's Trace 2.70021435 33.7526794 < .0000001 2.70021435 < .0000001 Roy's Largest Root 33.7526794 0.1803688 Pillai's Trace 0.01422425 0.8360392 0.9857757 0.1803688 Wilks' Lambda 0.8360392 Hotelling's Trace 0.01442950 0.1803688 25 0.8360392 Roy's Largest Root 0.01442950 0.1803688 0.8360392 Pillai's Trace 0.03144342 0.4058026 0.6707527 Wilks' Lambda 0.9685566 0.4058026 0.6707527 Hotelling's Trace 0.03246421 0.4058026 0.6707527 Roy's Largest Root 0.03246421 0.4058026 0.6707527 0.37520672 Pillai's Trace 7.5066172 25 0.0027971 0.6247933 7.5066172 0.0027971 Wilks' Lambda Hotelling's Trace 0.60052937 7.5066172 25 0.0027971 7.5066172 Roy's Largest Root 0.60052937 0.0027971

| | Dependent Variable | Sum of Squares | df | Mean Square | F | p |
|-----------|--------------------|-----------------|----|-----------------|--------------|------------|
| am | qsec | 5.230139474 | 1 | 5.230139474 | 4.924711499 | 0.0354097 |
| | hp | 8619.498481781 | 1 | 8619.498481781 | 5.451895339 | 0.0275391 |
| vs | qsec | 62.495550579 | 1 | 62.495550579 | 58.845955849 | < .0000001 |
| | hp | 69789.621491764 | 1 | 69789.621491764 | 44.142442034 | 0.0000005 |
| am:vs | qsec | 0.152447177 | 1 | 0.152447177 | 0.143544617 | 0.7078587 |
| | hp | 577.091258620 | 1 | 577.091258620 | 0.365014409 | 0.5509704 |
| drat | gsec | 0.002548780 | 1 | 0.002548780 | 0.002399938 | 0.9613023 |
| | hp | 963.937223484 | 1 | 963.937223484 | 0.609697289 | 0.4419536 |
| mpg | qsec | 3.494957886 | 1 | 3.494957886 | 3.290860478 | 0.0812239 |
| | hp | 24670.478788701 | 1 | 24670.478788701 | 15.604256859 | 0.0005322 |
| Residuals | gsec | 27.612506104 | 26 | 1.062019466 | | y |
| | hm | 41106 247755650 | 26 | 1501 000520062 | | |

Looking at each response variable individually: <mpg> has a significant effect on <hp> but not on <qsec> (marginally)

Multivariate GLM

To more than one response variable of various types (must be the same type within the analysis) using one or more categorical and/or continuous explanatory variables. No random effects.

Load dataset:

```
require (mvabund) #also needed for the manyglm() function data(spider) #a List with 2 datasets in it: "abund" and "x"
```

Response variables: counts of 12 different spiders

Y=as.matrix(spider\$abund) #must be matrix

Explanatory variables: 6 environmental variables

X=as.data.frame(spider\$x) #must be dataframe to use the variables in it

Multivariate GLM

Matrix of response variables

Explanatory variables from the X dataframe, can take interactions and nesting

Perform the multivariate GLM:

```
mod1=manyglm(Y~soil.dry*reflection+fallen.leaves/moss,data=X,

family="poisson"

Choose the summary(mod1) #for simplification (according to what we've learnt)

On the same of the same of
```

Check for heteroscedasticity:

plot (mod1)

```
Test statistics:
calculate.
                                 wald value Pr(>wald)
               (Intercept)
                                        14.99
                                                  0.001 ***
p-value
              soil.drv
                                        13.62
                                                  0.003 **
              reflection
                                        15.83
                                                  0.002 **
              fallen.leaves
                                        24.99
                                                  0.001 ***
              soil.dry:reflection
                                        17.25
                                                  0.001 ***
                                        15.86
                                                  0.005 **
              fallen.leaves:moss
              Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Choose the error distribution based on the same rules in GLM. Default is negative binomial. Note: no "quasi" distributions yet.

Interpretation of results is usually done visually, by plotting the different groupings with different colours (e.g. using a PCA and grouping based on the levels in the significant explanatory variables). It gets complicated!

- For more info (very well written), see: help(manyglm).

Note: To fit Gaussian errors, use manylm()

Note: although it is possible to use AIC() to compare different models (e.g. for simplification), I personally find the results to be unreliable so I currently don't suggest you use it.



Bayesian Statistics

A (very) gentle introduction from my viewpoint



Frequentist viewpoint

In experiments, we assume that the data follow a given distribution, then we gauge how well our data represent the truth by...

P(Hypothesis|Evidence) = P(Evidence|Distribution)

Probability that the hypothesis is true given the evidence that we have

Probability of observing our data given that the population and/or errors follow the assumed distribution. This is related to our p-value.

The crux of the matter:

- We assume that there is a "truth" out there (e.g. Lecturers are more handsome than Pilots).
- We go out and collect the data (measure the good-looking score of Lecturers and Pilots).
- Then we say: **given the data** we have **and the distribution** we assume the population follows, it is **very likely true** (p-value < 0.001) that Lecturers are more handsome than Pilots

Bayesian viewpoint: Bayes' rule

Basis of Bayesian statistics:

P(Hypothesis|Evidence) =

Probability that the hypothesis is true given the evidence that we have. This is known as the **POSTERIOR**.

 $P(\text{Evidence}|\text{Hypothesis}) \cdot P(\text{Hypothesis})$

P(Evidence)

What we previously believed about whether the hypothesis is true. This is known as the **PRIOR**.

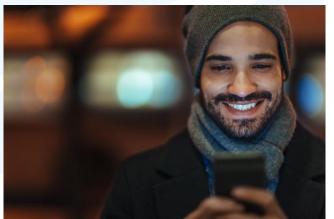
We update our PRIOR belief based on evidence to get our new POSTERIOR belief.

Example: You're going on a blind date.

You love Star Wars! You wonder whether your date does too.







Bayesian viewpoint: Bayes' rule

You think it's maybe a 50% chance that a random person likes Star Wars.



Your **POSTERIOR belief**: what you think now that you've seen your new data
$$P(\text{Hypothesis}|\text{Evidence}) = \frac{0.99 \cdot 0.5}{0.6}$$
P(Hypothesis)
The PRIOR belief.

You don't want to be too obvious, so you say:

"I just watched The Rise of Skywalker? Have you seen it?"

Your date replies: "YES, I have! It was great!"



You get excited!! You think that the probability that someone would have seen the movie given that they're a fan is 99%! (Some may be in comas.)

But wait! What's the overall likelihood that someone went to watch the movie in the first place? It was a bit of a flop, so let's say 60%.



So you now believe the chance your date is a fan is ... 82.5%!! Love at first sight!

Bayesian viewpoint

In typical experiments, *P*(Evidence) is a constant, so we can reduce Bayes' equation to:

 $P(\text{Hypothesis}|\text{Evidence}) = P(\text{Evidence}|\text{Hypothesis}) \cdot P(\text{Hypothesis})$

Probability that the hypothesis is true given the evidence that we have. This is known as the **POSTERIOR**.

The probability of getting our data given that the hypothesis is true. We calculate this from our experiment.

What we previously believed about whether the hypothesis is true. This is known as the **PRIOR**.

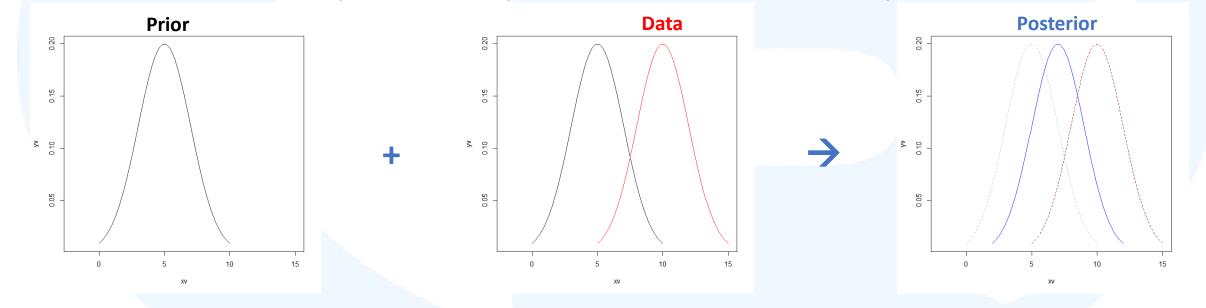
The crux of the matter:

- We are updating a previous belief using the new evidence we just collected.
- We are **not specifically interested in how well our data represents a "truth"**, hence there's usually no p-value.
- We just interpret the new estimates/effect sizes.

Bayesian statistical methods

There are Bayesian versions for many of the advanced and multivariate analyses

Whenever we run a Bayesian analysis, we need to define a prior.

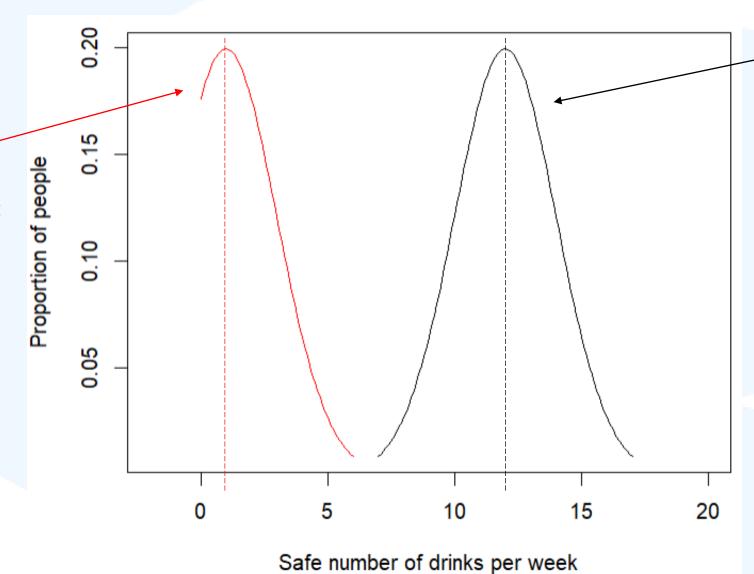


Using the data, the analysis will then give us the final posterior through repeated trial and error (e.g. Markov Chain Monte Carlo aka MCMC).

- Recall: Some R functions (e.g. stan_glmer) can supply the prior for us based on our error family, but for others (e.g. MCMCglmm), we need to learn how to do it ourselves.

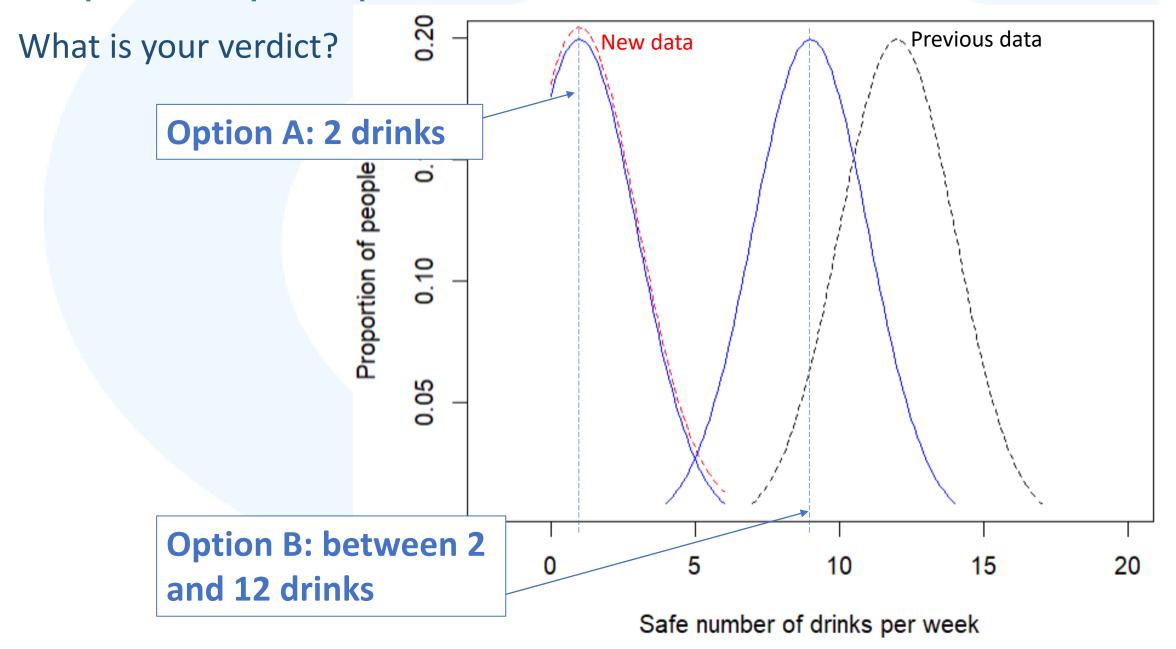
Example: how many drinks per week is safe?

New data: the latest experiment shows (with statistically significant data) that the safe number is 2 on average

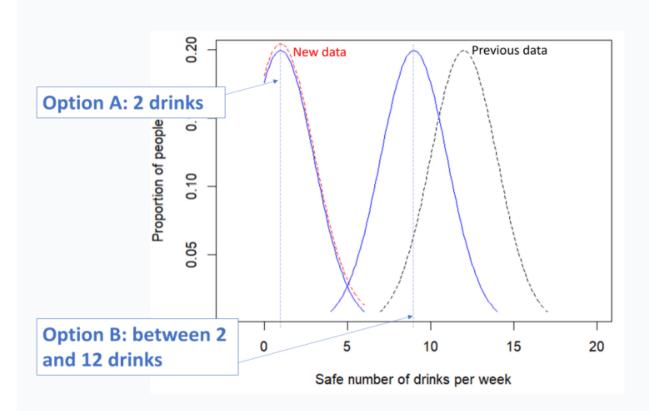


Previous data: based on existing experiments, the consensus is that the safe number is 12 on average

Example: how many drinks per week is safe?



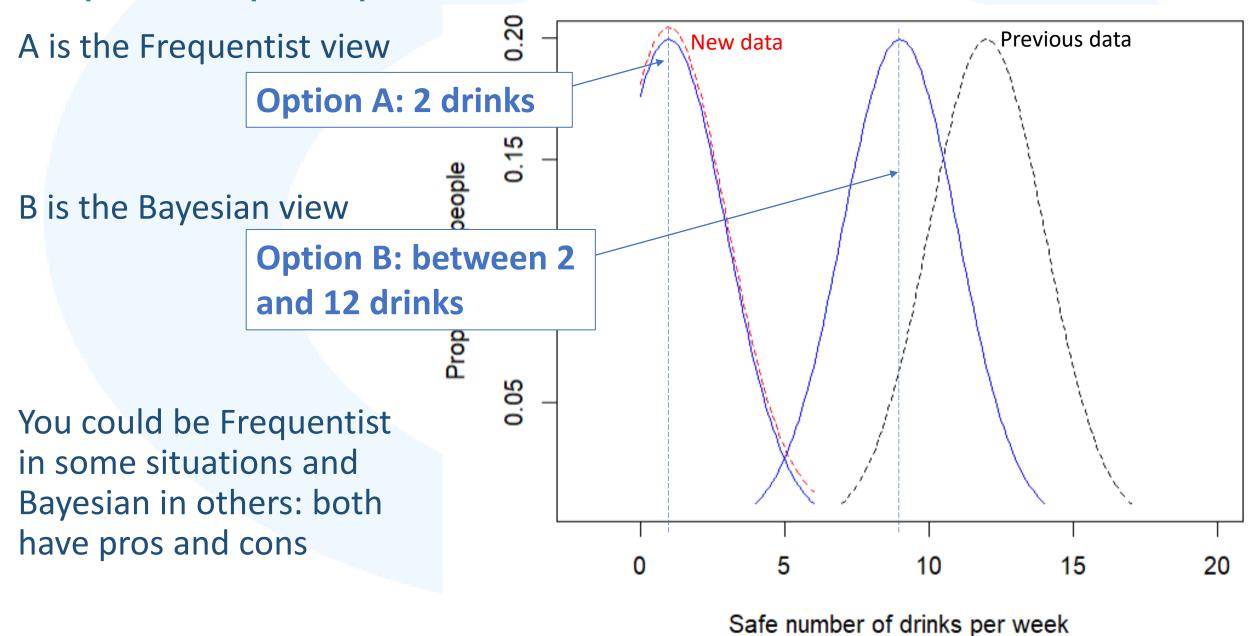
What's your verdict?



Option A

Option B

Example: how many drinks per week is safe?



Fitting a Bayesian GLM

Example using stan glm()

If published studies suggest that your y-variable's:

- Intercept follows a normal distribution of mean = 0 and S.D. = 1
- Slope follows a normal distribution of mean = 3 and S.D. = 0.5

Then you fit the model like this:

modl=stan_glm(Y~X,data=d1,family=Gamma,prior_intercept=normal(0,1),
prior=normal(3,0.5))

The prior for the slope

More information on priors in "rstanarm"

- ?normal #after loading rstanarm
- Read more <u>here</u>.

The prior for the intercept

```
Usage:
    normal(location = 0, scale = NULL, autoscale = FALSE)
    student_t(df = 1, location = 0, scale = NULL, autoscale = FALSE)
    cauchy(location = 0, scale = NULL, autoscale = FALSE)

    hs(df = 1, global_df = 1, global_scale = 0.01, slab_df = 4, slab_scale = 2.5)

    hs_plus(
        df1 = 1,
        df2 = 1,
        global_df = 1,
        global_scale = 0.01,
        slab_df = 4,
        slab_scale = 2.5
)
```

Summary (Learning Objectives)

Non-linear Modelling

- GAM

Multivariate Statistics

- Theory: Response variables, purposes, dissimilarity matrices
- Understanding structure
 - Clustering: AHC, PAM, K-means
 - Unconstrained ordination: PCA, PCoA, NMDS, CA
- Interpreting/Making predictions
 - Constrained ordination: RDA, CAP, CCA
 - "Modelling": MANOVA, PERMANOVA, MANCOVA & Multivariate GLM

Bayesian Statistics

- Bayes' Rule and a stan_glm() example

Overview

LSM3257

AY22/23; Sem 2 | Ian Z.W. Chan



BL5233 at a glance

- A) If you have only one response variable: univariate statistics
 - If you have simple controlled experiments:

Basic Tests

- If you have complex studies with potential confounding effects:

Advanced Analyses

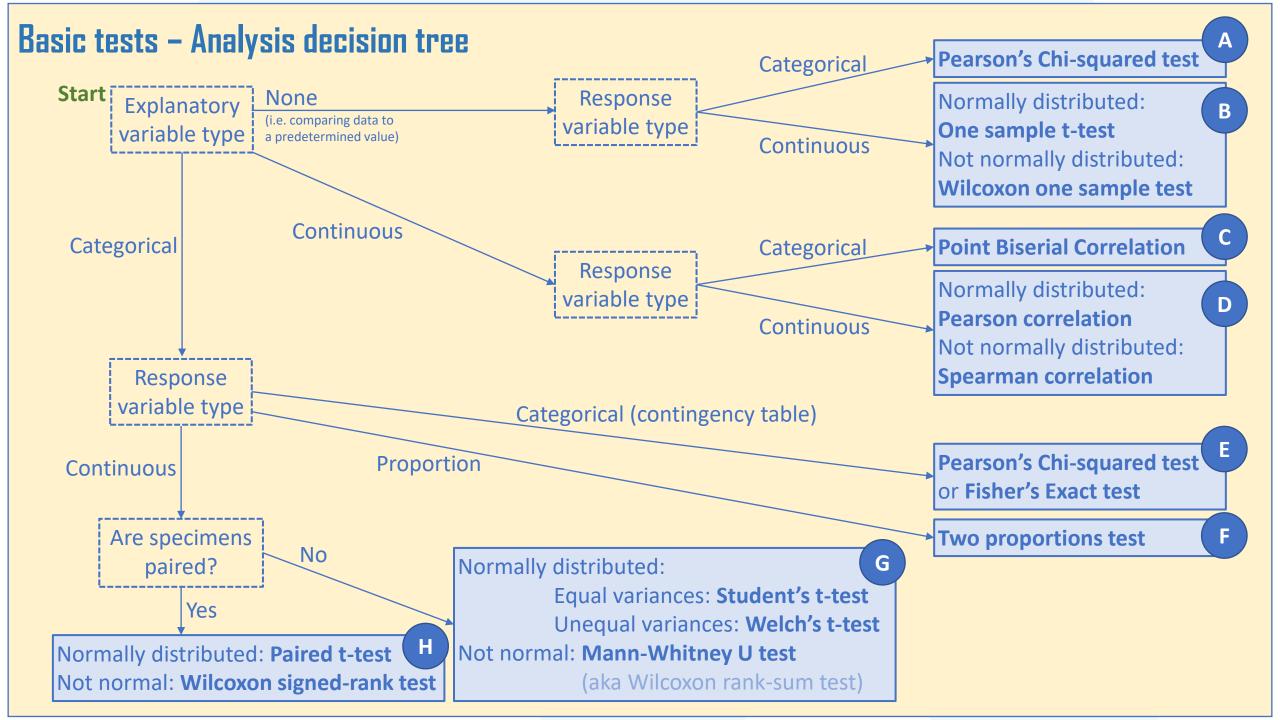
(including non-linear modelling)

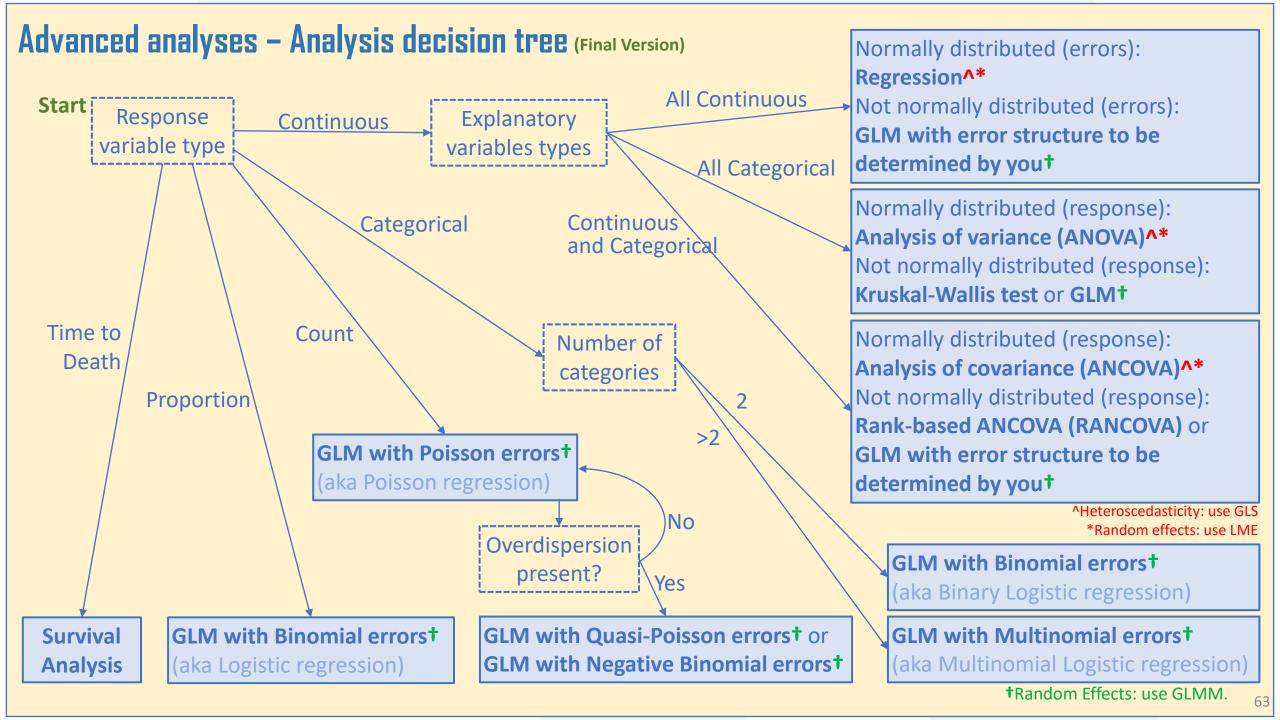
(has Bayesian alternatives)

B) If you have more than one response variable: multivariate statistics

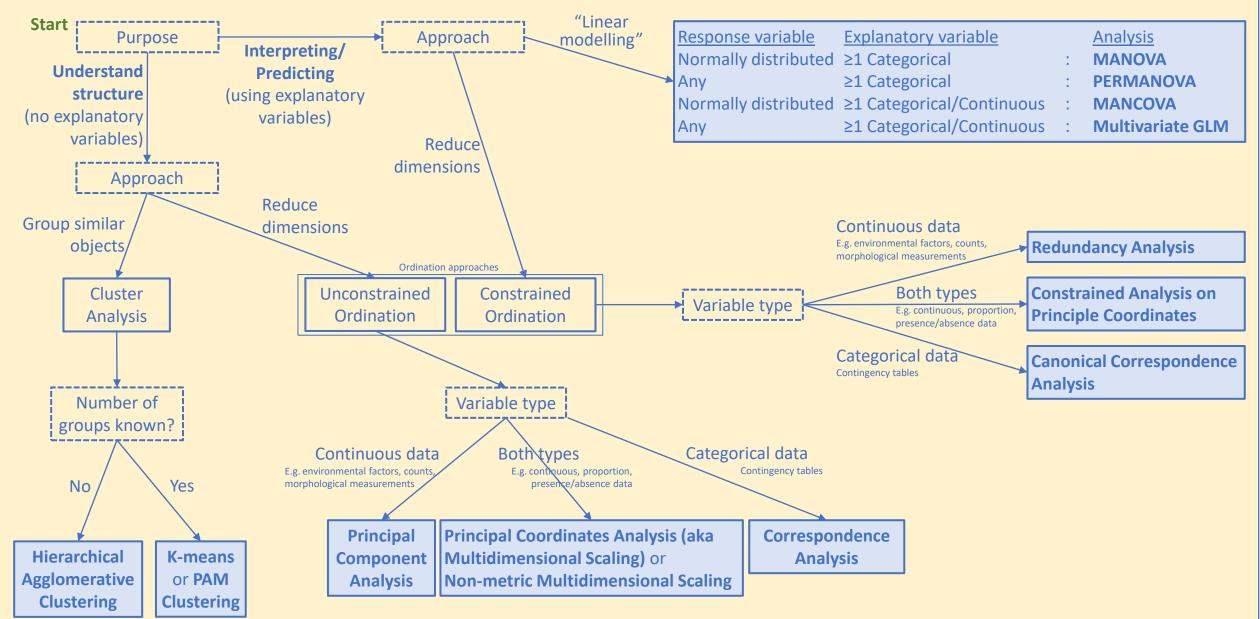
Multivariate Analyses

(has Bayesian alternatives)





Multivariate analyses – Analysis decision tree



Further information: Now the learning moves to your home/office!

For specific questions

1) Built-in R help:

```
help(glmmPQL)

?glmmPQL #same thing as help()

??glmmPQL #if you haven't installed the package yet
```

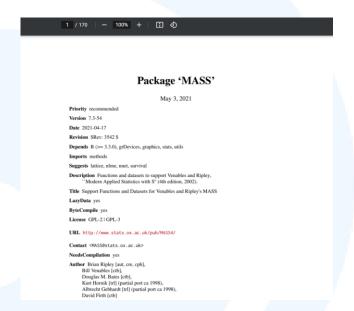
2) Vignettes of packages:

The vignette contains the documentation written by the authors. It's the best bet for getting information and finding out what the function can do, e.g. glmmPQL() is from the "MASS" package, so google: "MASS vignette R".

3) Forum posts, e.g. https://stats.stackexchange.com/

For general knowledge

Special interest groups: on <u>Facebook</u>, in the <u>R community</u>.



SEARCH and READ...

then

be BRAVE and TRY!!!



AC2

Released tonight; Material from Weeks 7 to 9

Due 31 Mar, 2359h

OPEN UNIVERSE; BUT PLEASE DO NOT DISCUSS



Projects

Project Presentation (Group)

10-min presentation, followed by Q&A (about 5 mins)

- Weeks 12 and 13: you're only required to attend the week that you're presenting

| Project Projec | esentation | Timings (a) | pproximate) | | | | | | | | |
|--|------------|-------------|-------------|-----------|-----------|---------|----------|----------|----------|----------|----------|
| Week 12 | | | | | | Week 13 | | | | | |
| 1000 | Group 2 | Jian Xi | May Ching | Huile | Yin Chuan | 1000 | Group 7 | Judith | Regina | Wen Xin | Yan Zhi |
| 1020 | Group 16 | Jerome | Jin Chi | Zhi Cheng | | 1020 | Group 4 | Shannon | Iliya | Isaac | Kate-Lyn |
| 1040 Group 1 | Group 14 | Benedick | Shin Yin | Kaizeng | Victoria | 1040 | Group 5 | Justin | Wee Meng | Jia Le | Jing Wei |
| | Break | | | | | | Break | | | | |
| 1110 | Group 18 | Wen Han | Yee Qi | Amanda | Benjamin | 1110 | Group 19 | Ruth | Kendrick | Gen Koh | Wei Kai |
| 1130 | Group 17 | Clara | Lixuan | Kelly | Alicia | 1130 | Group 13 | Ler Shan | Maryam | Diya | |
| | Group 12 | Samuel | Ophelia | Sarita | Vera | 1150 | Group 1 | Kimberly | Sin Yu | Wan Ling | Jing Min |
| | Break | | | | | | Break | | | | |
| 1220 | Group 8 | Ho Ning | Shuna | Dana | | 1220 | Group 11 | Jun Ning | Raine | Michelle | |
| 1240 | Group 6 | Cian Jin | Ryan | Gen Fong | Min Xian | 1240 | Group 9 | Vicki | Divina | Si Ying | Rachel |
| 1300 | Group 3 | Sherry | Anna | Sarah-Ann | Jia Wei | 1300 | Group 15 | Choon | Sophia | Boon Hao | |
| 1320 | Group 20 | Phoebe | Salman | Han Lin | Clive | 1320 | Group 10 | Kai Le | Hao Yu | Danish | Whelan |

- Week 11: consultations, email me to arrange

Project Report (Individual)

Deadline: 28 Apr 2023, 2359h

Scientific Communication tips

Remember you're telling a story (in BOTH presentations and reports)

Stories need to **be interesting** so each section in a Research paper/report is designed to help you tell the story...

- Tell us about the existing situation and knowledge: Background
- You run into a problem: Research Question
- What did you do to solve it?: Materials & Methods
 - How the authors (of the original dataset) collected the data (brief): context for understanding
 - How you analysed the data: what variables and analysis did you use?
- The climax of the story—how you saved the day!: Results
- The happy-ever-after: Discussion/Conclusions

Presentation tips

Design your slides to tell the story: each slide communicates one or two points and advances the story

Use as few words as possible in each slide

- Main points are written, your explanations are verbal
- My lecture slides are NOT a good example because they're designed as hybrid presentation and notes for your future use

Choose the right visuals to illustrate your points

Practise, practise!

- Decide how you want to say things in advance
- Keep within the time limit: usually 1 slide = about 1 minute

Teammate grading is available upon request (as a last resort)

IMPORTANT: Asking other groups (friendly and constructive) questions is part of the grading rubric!!

Report tips

Again: tell the story!

- The Title is one sentence summarising the main result from your whole story
- The Abstract is a TL;DR form of your report (don't copy and paste from your proposal): it should have 2 sentences of Introduction/Research Question, 2 sentences of M&Ms, 2 sentences of Results and 1 sentence of Discussion/Conclusion
- The rest of the sections follow the purposes described above

Refer to published journal articles and try to follow them:

- The sections and what information is in each section
- The referencing
- The professional tone of language

From Presentation to Report

- Your M&Ms and Results can be similar to your group members (but NOT word-for-word identical)
- Your Abstract, Introduction and Discussion should be quite different (even if the main points are similar)
- Bottomline: So long as you sit down and write your report yourself, it will be fine

Proof-read to eliminate typos and grammatical errors