Multivariate models

More than one way of seeing things

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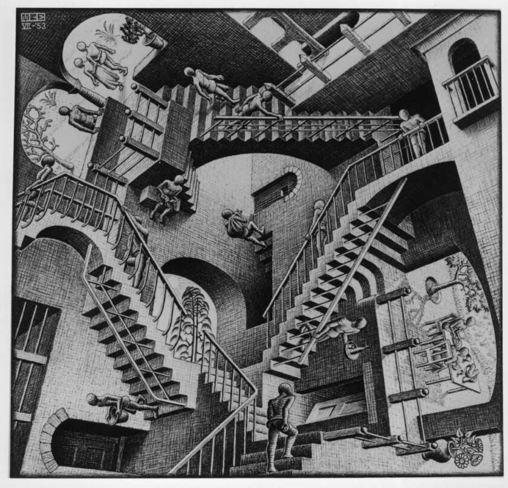
Outline

- What are multivariate data?
- Linear transformations
  - Principle components
  - Some common approaches
- Nonlinear transformations
  - Non-metric dimensional scaling



Some common problems

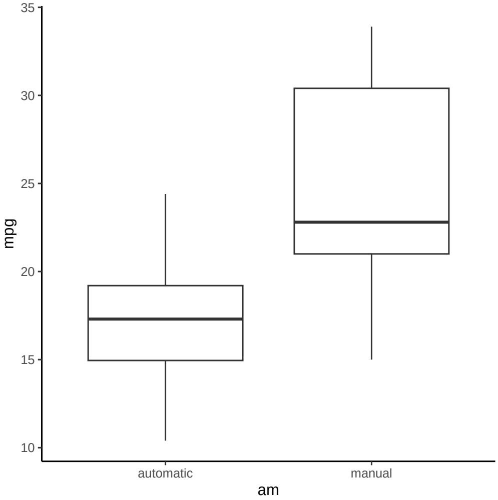
- “I’ve got a zillion predictors that could matter in my model, but they’re all collinear”
- “I measured a zillion things for each site/critter, but I don’t want to fit a zillion models”
- “I measured a zillion things. Do certain things group up into clusters?”
- “My supervisor told me to do a PCA or NMDS for my data, but I have no idea what they’re talking about”

If any of these sound like your situation, then you might need to do **multivariate modeling**!

Part 1: What are multivariate data?

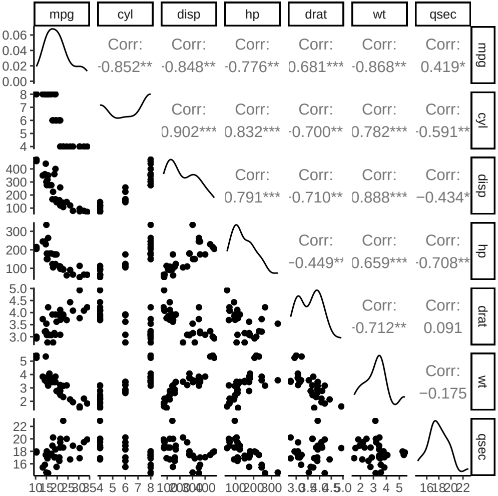
Univariate data

- Up until now, we've dealt mainly with **univariate** data: one thing is changing, and is being affected by other things
- These can be normal, binomial, Poisson, etc. . .
- Single variance term (σ) that controls dispersion



Multivariate data

- With **multivariate** data, we have multiple things changing at once
- *Many things* are changing, with multiple things potentially causing other things
- These are *mostly* normal (non-normal can be tricky)



Multivariate normal

- Normal distributions[1]don't just have a single σ, but actually a *matrix* of values
- If the columns of our data are *independent*, then it looks like this:

$$Y \sim Normal(M, \Sigma)$$

$$M = [\mu_1, \mu_2, \mu_3]$$

$$\Sigma = \begin{bmatrix} \sigma^2 & 0 & 0 \\ 0 & \sigma^2 & 0 \\ 0 & 0 & \sigma^2 \end{bmatrix}$$

- Zeros mean "μ_1, μ_2, & μ_3 aren't related to each other"
- Diagonal elements = *variance*, off-diagonal = *covariance*

[1] Multivariate Normal

Covariance and Correlation

Things may not be independent from each other. For example:

- $\sigma = 2$ (variance $= \sigma^2 = 4$)
- μ_1 and μ_2 are strongly correlated (r=0.7), but μ_3 is not related to anything (r=0). Shown here as a *correlation matrix* (R):

$$R = \begin{bmatrix} 1 & 0.7 & 0 \\ 0.7 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- When multiplied by the variance, this becomes the *covariance matrix* (Σ)

$$\Sigma = \begin{bmatrix} \sigma_a & \sigma_a b & \sigma_a c \\ \sigma_a b & \sigma_b & \sigma_b c \\ \sigma_a c & \sigma_b c & \sigma_c \end{bmatrix} = \begin{bmatrix} 4 & 2.8 & 0 \\ 2.8 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

Covariance vs Correlation

These are similar concepts, but covariance matrix has *units*, while correlation is *dimensionless*

$$\text{Covariance} = \sum_{i=1}^{n} \frac{(x-\bar{x})(y-\bar{y})}{(n-1)}$$

$$\text{Correlation} = \frac{cov(x,y)}{\sigma_x \sigma_y}$$

$$\text{Covariance matrix} = \begin{bmatrix} 4 & 2.8 & 0 \\ 2.8 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

$$\text{Correlation matrix} = \begin{bmatrix} 1 & 0.7 & 0 \\ 0.7 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

How does this help with my data?

- Say you've measured a bunch of things, and they're mostly from normal distributions. . .
- You've gathered data from a *multivariate normal distribution*!
- Now your task is to model this distribution!

$$Y \sim \mathit{Normal}(M, \Sigma)$$

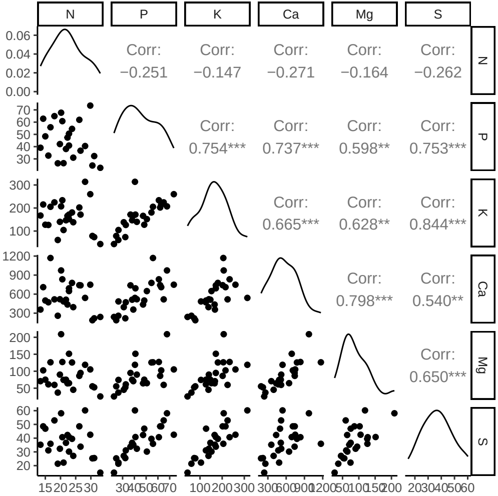
$$M = [\mu_1, \mu_2, \mu_3]$$

$$\mu_1 = b_{01} + b_{11} x_1$$
$$\mu_2 = b_{02} + b_{12} x_1$$
$$\mu_3 = b_{03} + b_{13} x_1$$

Problem: this doesn't really help

- We're *still* stuck with fitting a zillion linear models!
- We also have to estimate the covariance as well as the variance. This might be OK for a few columns, but gets much harder when you've got lots of columns
- We need a better way for dealing with these multivariate normal data...

Another approach



- Say we have a multi-column dataset that looks like this:
- What do you notice about this dataset?
- Looks like most of these columns are pretty strongly related. If we're only interested in the total "information" (variation) from this dataset. . .
- Perhaps we don't need all these columns? Which ones should we throw out or combine?

Part 2: Principal components (linear decompositions)

Matrix Decomposition and Principal Component

- Covariance matrices are a special type of matrix called a *triangular matrix*
- Can be decomposed using a math trick called the *singular value decomposition* that breaks a matrix into its component eigenvectors and eigenvalues
- Transforms data into new coordinate space, where *most variation falls into a few columns* called **principal components**

Covariance matrix

```
##         N      P       K      Ca     Mg      S
## N    30.6  -20.8   -52.6  -364.8  -37.1  -16.9
## P   -20.8  223.4   730.8  2683.9  366.5  131.3
## K   -52.6  730.8  4204.5 10500.6 1669.4  638.4
## Ca -364.8 2683.9 10500.6 59332.2 7974.5 1533.4
## Mg  -37.1  366.5  1669.4  7974.5 1681.9  311.2
## S   -16.9  131.3   638.4  1533.4  311.2  136.1
```

Decomposition: $X = UDV'$

Eigenvectors (V):

```
##      PC1   PC2   PC3   PC4   PC5   PC6
## N   0.01 -0.01  0.02 -0.16  0.83 -0.54
## P  -0.04 -0.10 -0.06  0.88  0.35  0.28
## K  -0.18 -0.95 -0.15 -0.16  0.02  0.08
## Ca -0.97  0.20 -0.11 -0.02 -0.01 -0.03
## Mg -0.13 -0.11  0.98 -0.01  0.05  0.11
## S  -0.03 -0.16  0.09  0.41 -0.43 -0.78
```

Eigenvalues (D):

```
## [1] 62550.01  2371.69   571.21    82.81    31.36    15.21
```

Simple example: 2 dimensions

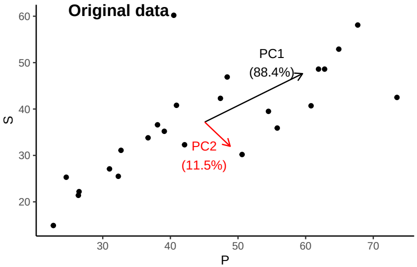
- Principal components are hard to imagine, so let's try it on only 2 dimensions:
- Rotation Matrix (V):
  - Columns $=$ *Principal components*
  - Rows $=$ *Factor Loadings*

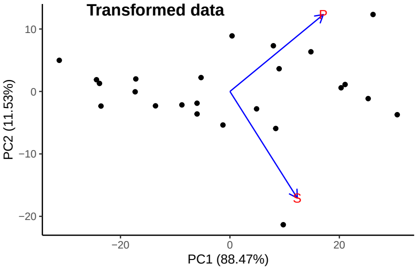
```
##    PC1   PC2
## P 0.81  0.59
## S 0.59 -0.81
```

- SD of principal components ($\sqrt{D}$):
  - Tells you *how strong* the effect of each PC column is

```
round(prcomp(vc_2)$sdev,2)
```

```
## [1] 17.84  6.44
```





Bigger example: full dataset (14 columns)

Use `prcomp` to decompose matrix of `varechem` data:

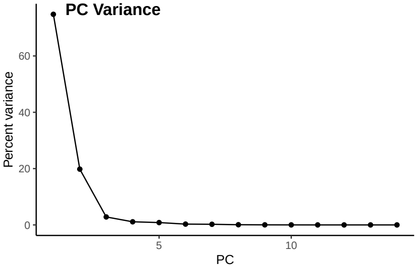
```r
pcVare <- prcomp(varechem)
```

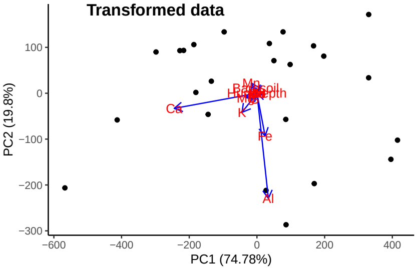
Rotation matrix (PCs and factor loadings)

```
##            PC1   PC2   PC3   PC4   PC5   PC6   PC7   PC8   PC9  PC10  PC11
## N         0.01  0.00 -0.01  0.06  0.01  0.03  0.09  0.16 -0.95 -0.21  0.15
## P        -0.04 -0.03 -0.09  0.03 -0.07  0.17 -0.16 -0.89 -0.22  0.30  0.01
## K        -0.17 -0.16 -0.86  0.03  0.13 -0.42 -0.05  0.05 -0.02  0.06 -0.02
## Ca       -0.96 -0.13  0.22  0.01 -0.11 -0.04  0.03  0.02  0.00 -0.02  0.00
## Mg       -0.13 -0.04 -0.05  0.02  0.84  0.47 -0.14  0.10  0.00  0.13  0.01
## S        -0.02 -0.05 -0.12 -0.06  0.09  0.11 -0.06 -0.30  0.18 -0.88  0.24
## Al        0.13 -0.90  0.02 -0.32 -0.13  0.20  0.04  0.07 -0.01  0.05  0.00
## Fe        0.09 -0.37  0.19  0.86  0.13 -0.21  0.09 -0.09  0.05 -0.05 -0.02
## Mn       -0.07  0.09 -0.38  0.37 -0.43  0.68  0.07  0.19  0.08  0.02  0.00
## Zn       -0.01  0.00 -0.01 -0.02  0.02  0.06 -0.05 -0.04 -0.10 -0.25 -0.95
## Mo        0.00  0.00  0.00  0.00  0.00  0.01  0.00 -0.01  0.00 -0.01 -0.02
## Baresoil -0.01  0.05 -0.08 -0.10  0.15  0.04  0.96 -0.18  0.04  0.03 -0.05
## Humdepth  0.00  0.00  0.00  0.00  0.01  0.01  0.01  0.01  0.01  0.01  0.14
## pH        0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00 -0.01  0.01 -0.01
```

SDs of principal components:

```
##  [1] 253.1 130.2  49.2  30.9  26.8  15.8  14.0   7.8   4.8   3.1   1.2   0.4
## [13]   0.1   0.1
```

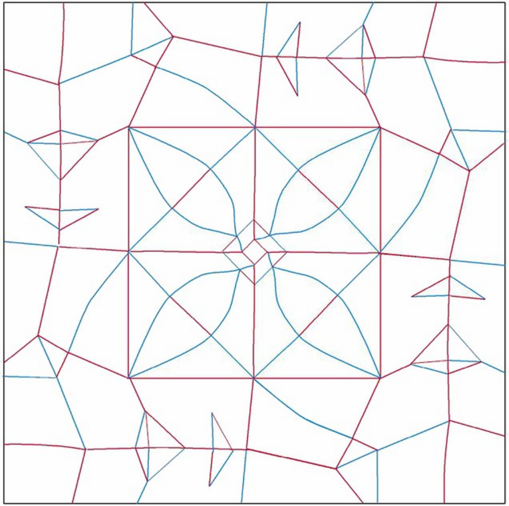




Artistic analogues to this problem

Picasso's *Demoiselle d'Avignon* (1907)

Kawasaki rose crease pattern



First challenge

Let's try this on some biological data

> *"After a severe storm on February 1, 1898, a number of moribund sparrows were taken to Hermon Bumpus' biological laboratory at Brown University, Rhode Island. Subsequently, about half of the birds died, and Bumpus saw this as an opportunity to see whether he could find any support for Charles Darwin's theory of natural selection. . . "*

```
##   Survived Bird Total_length Alar_length BeakHead_Length Humerus_length
## 1      Yes    1          156         245            31.6           18.5
## 2      Yes    2          154         240            30.4           17.9
## 3      Yes    3          153         240            31.0           18.4
## 4      Yes    4          153         236            30.9           17.7
## 5      Yes    5          155         243            31.5           18.6
## 6      Yes    6          163         247            32.0           19.0
##   Keel_length
## 1        20.5
## 2        19.6
## 3        20.6
## 4        20.2
## 5        20.3
```

- Take a look at the bird dataset found here), and perform a PCA decomposition
- Hint: you'll need to transform it into a *matrix* (using `as.matrix` on the relevant columns) before using `prcomp`
- How many PCs are needed to represent *most* of the variation?

First challenge results

Covariance matrix

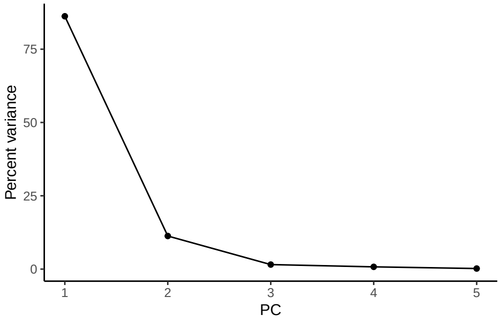
```
##                 Total_length Alar_length BeakHead_Length Humerus_
## Total_length            13.4        13.6             1.9
## Alar_length             13.6        25.7             2.7
## BeakHead_Length          1.9         2.7             0.6
## Humerus_length           1.3         2.2             0.3
## Keel_length              2.2         2.7             0.4
##                 Keel_length
## Total_length            2.2
## Alar_length             2.7
## BeakHead_Length         0.4
## Humerus_length          0.3
## Keel_length             1.0
```

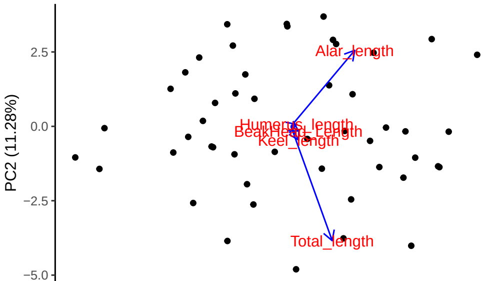
Principal components

```
##                  PC1   PC2   PC3   PC4   PC5
## Total_length    0.54 -0.83 -0.16 -0.04 -0.02
## Alar_length     0.83  0.55 -0.06 -0.07  0.04
## BeakHead_Length 0.10 -0.03  0.24  0.90  0.36
## Humerus_length  0.07  0.01  0.20  0.31 -0.93
## Keel_length     0.10 -0.10  0.94 -0.31  0.11
```

Variance per column

```
## [1] 34.81  4.41  0.64  0.36  0.09
```

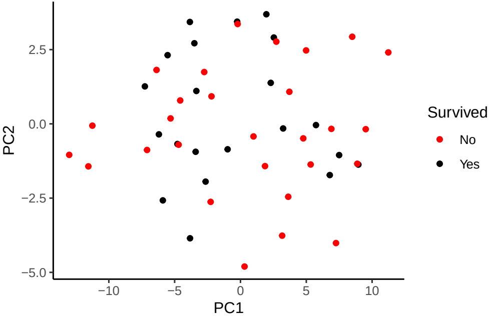


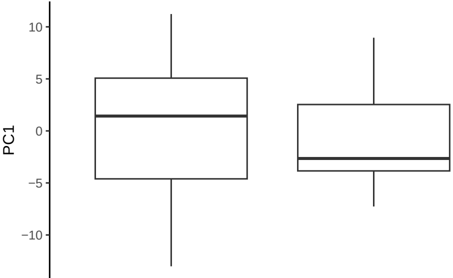


What's next?

- Now that we've reduced our data to only a few *uncorrelated* columns, we can do a couple things:
- Use linear regression (or some other test) on each column, along with some other set of predictor columns
- Use some other test to see if your data are "different" (far away) from each other

First step: plot your data





- Usually we want to see if some other thing is changing our data “somehow” (usually using a linear model)
- The first step is to plot your data. I’ve been using `autoplot` from `ggfortify`, but we can also plot things manually
- These data don’t look particularly different in their centers, but. . .
- They are different in variances! What does this mean biologically?

Formal tests for differences

- envfit from the vegan package is a common way to test for differences between groups (or continuous variables)
- Uses a permutation test to compare "jumbled" data original data. In this case, shows no difference in group averages

```
envfit(birdPCA ~ Survived,data=birds)
```

```
##
## ***FACTORS:
##
## Centroids:
##                 PC1     PC2
## SurvivedNo   0.4453 -0.2392
## SurvivedYes -0.5938  0.3190
##
## Goodness of fit:
##              r2 Pr(>r)
## Survived 0.0087  0.606
## Permutation: free
## Number of permutations: 999
```

- rda and cca from vegan are also popular (older) methods. They basically fit linear regression to each row in the data matrix, then decompose the fitted values
- "Constrained" part is related to variables you provided, "Unconstrained" is leftover variance. You can run anova on this to get variable importance

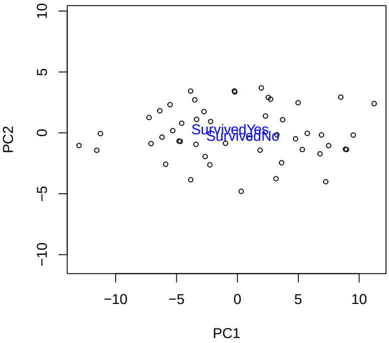
```
rda(birdMat ~ Survived,data=birds)
```

```
## Call: rda(formula = birdMat ~ Survived, data = birds)
##
##                 Inertia Proportion Rank
## Total         40.969439   1.000000
## Constrained    0.357460   0.008725    1
## Unconstrained 40.611979   0.991275    5
## Inertia is variance
##
## Eigenvalues for constrained axes:
##   RDA1
## 0.3575
##
```

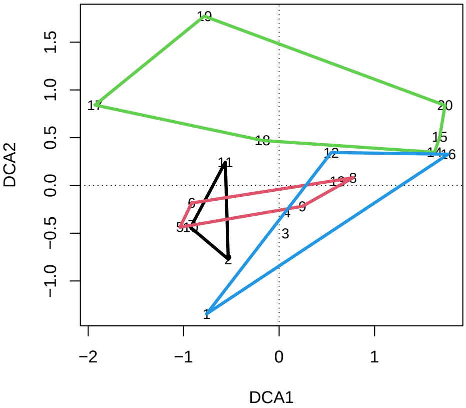
Plotting your results

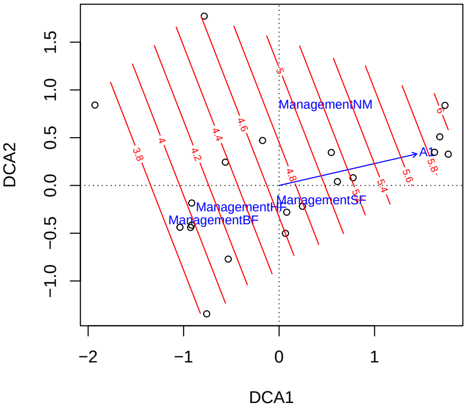
- For plotting your results, you generally want to show the *transformed data* plus the direction of the effects you're interested in
- `ggplot2` has some plotting functionality, but the plots from `vegan` are more purpose-made for these kinds of data
- See the `vegan` vignette (`vignette("intro-vegan")`) for more details

```
ordiplot(birdPCA,type='points',display='sites')
plot(envfit(birdPCA ~ Survived,data=birds))
```



Other kinds of ordination plots





```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## y ~ s(x1, x2, k = 10, bs = "tp", fx = FALSE)
```

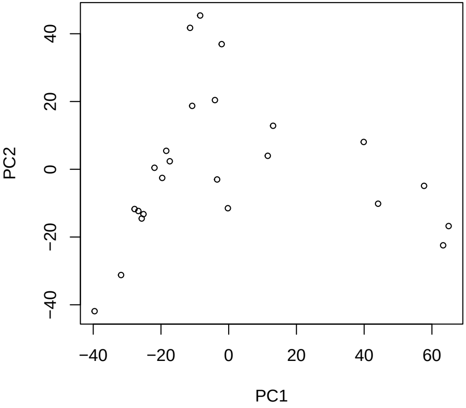
Second challenge

- Let's try some *community* data (counts of different species)!
- Here) (`bugDat.csv`) is a dataset I collected during my Master's degree, which I spent catching a lot of bugs
- I collected bugs using a couple kinds of collection methods across the season
- Was there a large difference in collection methods?

Part 3: NMDS (nonlinear decompositions)

Problems with linear transformations

- Recall: PCA and other decomposition methods use a *linear mapping* onto a new coordinates system
- This doesn't always work well: especially if you have non-normally distributed (e.g. community) data
- Individual species are often normally distributed along a gradient, creating an **arch** in PCA space (see here for more details)
- Because of this, the y-axis (2nd PCA) isn't really a useful gradient to compare across



The arch effect (seen at ESC 2023 poster session!)

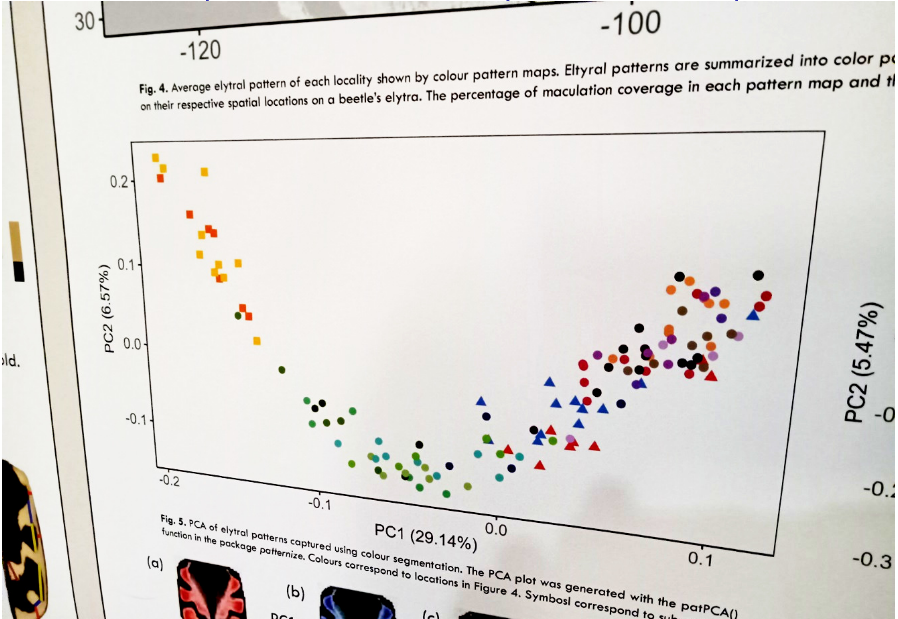
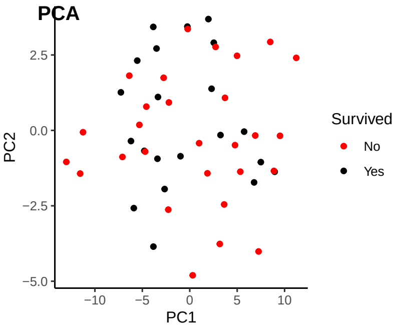


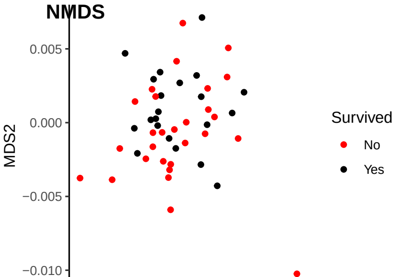
Fig. 4. Average elytral pattern of each locality shown by colour pattern maps. Eltyral patterns are summarized into color p
on their respective spatial locations on a beetle's elytra. The percentage of maculation coverage in each pattern map and th

Fig. 5. PCA of elytral patterns captured using colour segmentation. The PCA plot was generated with the patPCA()
function in the package patternize. Colours correspond to locations in Figure 4. Symbosl correspond to sub

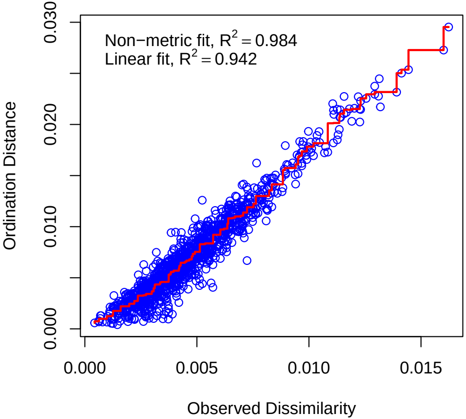
Non-metric dimensional scaling

- **Non-metric multidimensional scaling** is another way of decomposing multidimensional data
- Uses rank-order of data: *order* matters, but not magnitude
- Uses Bray-Curtis distance, not Euclidean (better for community studies)





Nonlinear “stress” mapping



- Instead of using a linear transformation
- ”

2-column