Biology 559R: Introduction to Phylogenetic Comparative Methods

Topics for this week (Mar 31 & April 2):

- Taxonomic revision in R
  - Principal Component Analyses
- Your Project
• This is probably one the most basic branches of Biology that defines organisms on the basis of shared or common traits, that we humans use to give names to those groups.

• We use these taxonomic groupings to give ranks and organize our understanding of biological diversity (taxonomic hierarchy).

• The process of naming organism includes the description and identification that helps us to create useful classification.

• In last 25 years, the development of phylogenies based on molecular markers has improved the classification by making it less speculative (i.e., expert opinions).
Taxonomy and R

• Make a working directory (e.g., taxonomy_in_R) and select it as your working.

R top menus: Misc>Change Working Directory (select the directory that has our file)

setwd("~/Desktop/R_class_winter_2015_home/0_Bio559R_course_final_files/week_13/data")

• Packages relevant for taxonomy and distribution

#http://ropensci.org/tutorials/rgbif_tutorial.html
#http://ropensci.org/tutorials/taxize_tutorial.html

install.packages("taxize")
install.packages("rgbif")

library("taxize")
library("rgbif")
• Load our data from last class:

```r
birds_traits_data <- read.table("bird_data_pruned.txt", header = TRUE, sep = "\t")
birds_traits_list <- read.table("species_list.txt", header = TRUE, sep = "\t")
```

• Add species list to main data

```r
birds_traits_data_list <- cbind(birds_traits_list, birds_traits_data)
# combine two data frames

birds_traits_data_list$Species_list <- as.character(birds_traits_data_list
$Species_list)
# transform from factor to character

• However, you can also work using only the species list

```r
species <- c(t(birds_traits_list)) # as a vector
species
```
• Taxonomy hierarchy using diverse databases

# We can get full classification using A number of data sources in taxize provide the # capability to retrieve higher taxonomic names, but we will highlight two of the more
classification_sp_ncbi <- lapply(1:2, function(x) {classification(species[x], db = 'ncbi')}) # National Center for Biotechnology Information
classification_sp_ncbi
# [[1]]
# `$Struthio camelus`

<table>
<thead>
<tr>
<th>name</th>
<th>rank</th>
<th>id</th>
</tr>
</thead>
<tbody>
<tr>
<td>cellular organisms</td>
<td>no rank</td>
<td>131567</td>
</tr>
<tr>
<td>Eukaryota superkingdom</td>
<td>kingdom</td>
<td>2759</td>
</tr>
<tr>
<td>Opisthokonta</td>
<td>no rank</td>
<td>33154</td>
</tr>
<tr>
<td>Metazoa</td>
<td>kingdom</td>
<td>33208</td>
</tr>
<tr>
<td>Eumetazoa</td>
<td>no rank</td>
<td>6072</td>
</tr>
<tr>
<td>Bilateria</td>
<td>no rank</td>
<td>33213</td>
</tr>
<tr>
<td>Deuterostomia</td>
<td>no rank</td>
<td>33511</td>
</tr>
<tr>
<td>Chordata</td>
<td>phylum</td>
<td>7711</td>
</tr>
<tr>
<td>Craniata</td>
<td>subphylum</td>
<td>89593</td>
</tr>
<tr>
<td>Vertebrata</td>
<td>no rank</td>
<td>7742</td>
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<tr>
<td>Gnathostomata</td>
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<tr>
<td>Teleostomi</td>
<td>no rank</td>
<td>117570</td>
</tr>
<tr>
<td>Euteleostomi</td>
<td>no rank</td>
<td>117571</td>
</tr>
<tr>
<td>Sarcopterygii</td>
<td>no rank</td>
<td>8287</td>
</tr>
<tr>
<td>Dipnotetrapodomorpha</td>
<td>no rank</td>
<td>1338369</td>
</tr>
<tr>
<td>Tetrapoda</td>
<td>no rank</td>
<td>32523</td>
</tr>
<tr>
<td>Amniota</td>
<td>no rank</td>
<td>32524</td>
</tr>
<tr>
<td>Sauropsida</td>
<td>no rank</td>
<td>8457</td>
</tr>
<tr>
<td>Sauria</td>
<td>no rank</td>
<td>32561</td>
</tr>
<tr>
<td>Archelosauria</td>
<td>no rank</td>
<td>1329799</td>
</tr>
<tr>
<td>Archosaurus</td>
<td>no rank</td>
<td>8492</td>
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<tr>
<td>Dinosauria</td>
<td>no rank</td>
<td>436486</td>
</tr>
<tr>
<td>Saurischia</td>
<td>no rank</td>
<td>436489</td>
</tr>
<tr>
<td>Theropoda</td>
<td>no rank</td>
<td>436491</td>
</tr>
<tr>
<td>Coelurosauria</td>
<td>no rank</td>
<td>436492</td>
</tr>
<tr>
<td>Aves</td>
<td>class</td>
<td>8782</td>
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<tr>
<td>Palaeognathae</td>
<td>superorder</td>
<td>8783</td>
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<tr>
<td>Struthioniformes</td>
<td>order</td>
<td>8798</td>
</tr>
<tr>
<td>Struthionidae</td>
<td>family</td>
<td>8799</td>
</tr>
<tr>
<td>Struthio</td>
<td>genus</td>
<td>8800</td>
</tr>
<tr>
<td>Struthio camelus</td>
<td>species</td>
<td>8801</td>
</tr>
</tbody>
</table>
### Taxonomy and R

- **Taxonomy hierarchy using diverse databases**

  ```r
classification_sp_gbif <- lapply (1:2, function (x) {classification(species[x], db = 'gbif')}) # Global Biodiversity Information Facility
classification_sp_gbif

# [[1]]
# `$`Struthio camelus`
#       name  rank id
# 1 Animalia  kingdom  1
# 2  Chordata  phylum  44
# 3   Aves  class  212
# 4  Struthioniformes  order  725
# 5  Struthionidae  family  9349
# 6        Struthio  genus 2495148
# 7  Struthio camelus  species 2495150
```
• Taxonomy hierarchy using diverse databases

classification_sp_itis <- lapply (1:2, function (x) {classification(species[x], db = 'itis')}) # Integrated Taxonomic Information System

classification_sp_itis

# [[1]]
# $`Struthio camelus`
#
#   name      rank   id
# 1 Animalia  Kingdom 202423
# 2 Bilateria Subkingdom 914154
# 3 Deuterostomia Infrakingdom 914156
# 4 Chordata   Phylum 158852
# 5 Vertebrata Subphylum 331030
# 6 Gnathostomata Infraphylum 914179
# 7 Tetrapoda  Superclass 914181
# 8 Aves       Class 174371
# 9 Struthioniformes Order 174372
# 10 Struthionidae Family 174373
# 11 Struthio   Genus 174374
# 12 Struthio camelus Species 174375
### Taxonomy and R

- Taxonomy hierarchy using diverse databases

```r
classification_sp_col <- lapply(1:2, function (x) {classification(species[x], db = 'col')}) # Catalogue of Life
classification_sp_col
# [[1]]
# $`Struthio camelus`
# name rank id
# 1 Animalia Kingdom 22032961
# 2 Chordata Phylum 22032976
# 3 Aves Class 22033651
# 4 Struthioniformes Order 22041922
# 5 Struthionidae Family 22041927
# 6 Struthio Genus 22044859
# 7 Struthio camelus Species 11908938
```
Georeferencing using GBIF

• Choosing our species of interest

```r
species[1]
# [1] "Struthio camelus"
```

• Find the GBIF ID key and reducing taxonomic redundancy or accounting recent taxonomic changes. We also need to provide 'rank': A taxonomic rank such as species

```r
key1 <- name_suggest(q=species[1], rank='species')$key[1]
key1

# [1] 2495150 ← unique taxonomic number that can be used to search in the gbif website
```

# For example:
# http://www.gbif.org/species/2495150 (you can check this key manually in gbif)
Georeferencing using GBIF

- Get occurrences and records in GBIF to a data frame in R

```r
species_data <- occ_search(taxonKey=key1,
                            hasCoordinate=TRUE,
                            fields=c('name',
                                     'gbifID',
                                     'decimalLatitude',
                                     'decimalLongitude',
                                     'basisOfRecord',
                                     'year',
                                     'country',
                                     'institutionCode',
                                     'collectionCode',
                                     'catalogNumber',
                                     'verbatimLocality',
                                     'verbatimEventDate',
                                     'occurrenceRemarks',
                                     'stateProvince',
                                     'county',
                                     'verbatimElevation',
                                     'locality'),
                            limit=1000,  # get only 1000 records
                            return='data')
```
Georeferencing using GBIF

• Get occurrences and records in GBIF to a data frame in R

```r
head(species_data)
```

<table>
<thead>
<tr>
<th>name</th>
<th>basisOfRecord</th>
<th>decimalLongitude</th>
<th>decimalLatitude</th>
<th>year</th>
<th>country</th>
<th>gbifID</th>
<th>institutionCode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Struthio camelus</td>
<td>HUMAN_OBSERVATION</td>
<td>35.74814</td>
<td>-3.56551</td>
<td>2014</td>
<td>Tanzania, United Republic of</td>
<td>923394342</td>
<td>naturgucker</td>
</tr>
<tr>
<td>Struthio camelus</td>
<td>HUMAN_OBSERVATION</td>
<td>35.56103</td>
<td>-3.17274</td>
<td>2014</td>
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</tr>
<tr>
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<td>HUMAN_OBSERVATION</td>
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<td>-2.93481</td>
<td>2014</td>
<td>Tanzania, United Republic of</td>
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<tr>
<td>Struthio camelus</td>
<td>HUMAN_OBSERVATION</td>
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<td>0.03858</td>
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<td>Struthio camelus</td>
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<td>25.95567</td>
<td>-24.63599</td>
<td>2014</td>
<td>Botswana</td>
<td>1038340462</td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>catalogNumber</th>
<th>locality</th>
<th>collectionCode</th>
<th>verbatimEventDate</th>
<th>verbatimLocality</th>
<th>stateProvince</th>
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<tbody>
<tr>
<td>323828999</td>
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<td>naturgucker</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
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<tr>
<td>-869612390</td>
<td>Ngorongoro-Krater, Kraterboden</td>
<td>naturgucker</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
</tr>
<tr>
<td>-1565621799</td>
<td>Serengeti Plains</td>
<td>naturgucker</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
<td>&lt;NA&gt;</td>
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<tr>
<td>577792</td>
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<td></td>
<td>2014-02-27</td>
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<td>Zimbabwe</td>
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<tr>
<td>844302</td>
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<td></td>
<td>2014-08-26 14:22:18</td>
<td>Ol Pejeta</td>
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<tr>
<td>1038579</td>
<td>Observations</td>
<td></td>
<td>2014-08-26 14:22:18</td>
<td>Gaborone, South-East, Botswana</td>
<td>&lt;NA&gt;</td>
</tr>
</tbody>
</table>

• Prepare and plot distribution data on map

```r
# install.packages("maps")
library(maps)
map("world", xlim = range(species_data$decimalLongitude), ylim = range(species_data$decimalLatitude))
points(species_data$decimalLongitude, species_data$decimalLatitude, col = "blue", cex = 1.5)
```
Georeferencing using GBIF

- Prepare and plot distribution data on map
Multivariate Methods: Principal Component Analyses

There are several methods that are considered under this

- Multivariate regression will have multiple dependent and predictor variables. You can use the methodology implemented in ‘MCMCglmm’ to answer this type of problems.

- Principal components analysis (PCA) is method to reduce the number of original variables to a set of orthogonal (uncorrelated) variables that explain the same amount of variance as the original set.

- However, the PCA results allows you to pick some principal components (PC) that explain most of the variation in your data, so you can use few PCs.

- Finally, you can rotates the axes of variation to give a new set of PCs with the condition to maximize the amount the variance explain for each individual variable. This allows you have PC that better define specific variables over others.
Principal Component Analyses

• We need to install and load some specific packages:

  library(ape)
  library(geiger)
  library(phytools)
  install.packages("psych")
  library(psych)
  install.packages("GPArotation")
  library("GPArotation")
Principal Component Analyses

• We also are going to use a exemplar data set from Darwin's finches

```r
data(geospiza)
finches_phy <- geospiza$phy
finches_data <- geospiza$dat
finches_data
```

```
#                wingL  tarsusL  culmenL  beakD  gonysW
# magnirostris  4.404200 3.038950 2.724667 2.823767 2.675983
# conirostris  4.349867 2.984200 2.654400 2.513800 2.360167
# difficilis   4.224067 2.898917 2.277183 2.011100 1.929983
# scandens    4.261222 2.929033 2.621789 2.144700 2.036944
# fortis      4.244008 2.894717 2.407025 2.362658 2.221867
# fuliginosa  4.132957 2.806514 2.094971 1.941157 1.845379
# pallida    4.265425 3.089450 2.430250 2.016350 1.949125
# fusca      3.975393 2.936536 2.051843 1.191264 1.401186
# parvulus   4.131600 2.973060 1.974420 1.873540 1.813340
# pauper     4.232500 3.035900 2.187000 2.073400 1.962100
# Pinaroloxias 4.188600 2.980200 2.311100 1.547500 1.630100
# Platyspiza  4.419686 3.270543 2.331471 2.347471 2.282443
# psittacula  4.235020 3.049120 2.259640 2.230040 2.073940
```
Principal Component Analyses: Non-phylogenetic

• Non-Rotated Principal Components

finches_non_rotated_pca <- princomp(finches_data, cor=TRUE)

summary(finches_non_rotated_pca) # print components and the variance accounted for

# Importance of components:
#                               Comp.1  Comp.2  Comp.3  Comp.4  Comp.5
# Standard deviation          1.9234840 0.9503424 0.57986608 0.23166735 0.084523804
# Proportion of Variance     0.7399581 0.1806301 0.06724893 0.01073395 0.001428855
# Cumulative Proportion      0.7399581 0.9205883 0.98783719 0.99857115 1.000000000

# Notice: You will have as many components as variables (i.e., 5 components)

loadings(finches_non_rotated_pca) # pc loadings of each variable on the components

# Loadings:
#                               Comp.1  Comp.2  Comp.3  Comp.4  Comp.5
# wingL            -0.505  0.144         0.841  0.129
# tarsusL          -0.261  0.903 -0.131 -0.301
# culmenL          -0.430 -0.322 -0.812 -0.210
# beakD            -0.491 -0.195  0.458 -0.141 -0.701
# gonysW            -0.502 -0.149  0.338 -0.372  0.688

# Notice: Loadings allows you to define the components. For example, tarsusL loads mainly on Comp.2. Most people will define the loadings after axis ‘rotation’
Principal Component Analyses: Non-phylogenetic

- Non-Rotated Principal Components

plot(finches_non_rotated_pca,type="lines")  # scree plot to determine how many components are useful

**Notice:** Use the rule to choose principal component based on the proportion of variance explained ~ 1.0. Similarly, check the “scree plot” and the number of components before the "elbow" are considered those that explain most of the variance (i.e., appears that 2 components are good enough)
Principal Component Analyses: Non-phylogenetic

- Varimax Rotated Principal Components

```r
finches_varimax_pca <- principal(finches_data, n factors=2, rotate="varimax")

# Principal Components Analysis
# Call: principal(r = finches_data, n factors = 2, rotate = "varimax")
# Standardized loadings (pattern matrix) based upon correlation matrix
#                    RC1  RC2   h2    u2
# wingL          0.85 0.49 0.96 0.038
# tarsusL        0.15 0.98 0.99 0.011
# culmenL        0.88 0.02 0.78 0.224
# beakD          0.94 0.18 0.92 0.075
# gonysW         0.95 0.23 0.95 0.049

#                        RC1  RC2
# SS loadings           3.31 1.29
# Proportion Var        0.66 0.26
# Cumulative Var        0.66 0.92
# Proportion Explained  0.72 0.28
# Cumulative Proportion 0.72 1.00

# Test of the hypothesis that 2 components are sufficient.
# The degrees of freedom for the null model are  10  and the objective function was  7.75
# The degrees of freedom for the model are  1  and the objective function was  1.86
# The total number of observations was  13  with MLE Chi Square =  15.2  with prob < 9.7e-05

# Fit based upon off diagonal values = 0.99
```
Principal Component Analyses: Non-phylogenetic

- Varimax Rotated Principal Components. You can get the scores of each species on the two components

```r
finches_varimax_pca$scores
```

<table>
<thead>
<tr>
<th></th>
<th>RC1</th>
<th>RC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnoirostris</td>
<td>1.89987528</td>
<td>0.07182417</td>
</tr>
<tr>
<td>conirostris</td>
<td>1.29886059</td>
<td>-0.29905083</td>
</tr>
<tr>
<td>difficilis</td>
<td>-0.04414877</td>
<td>-0.69844300</td>
</tr>
<tr>
<td>scandens</td>
<td>0.64690615</td>
<td>-0.76496493</td>
</tr>
<tr>
<td>fortis</td>
<td>0.71545604</td>
<td>-0.94622865</td>
</tr>
<tr>
<td>fuliginosa</td>
<td>-0.39439635</td>
<td>-1.43133575</td>
</tr>
<tr>
<td>pallida</td>
<td>-0.12006058</td>
<td>0.79420851</td>
</tr>
<tr>
<td>fusca</td>
<td>-1.94045036</td>
<td>-0.39800242</td>
</tr>
<tr>
<td>parvulus</td>
<td>-0.98365427</td>
<td>0.07426226</td>
</tr>
<tr>
<td>pauper</td>
<td>-0.35808875</td>
<td>0.51428958</td>
</tr>
<tr>
<td>Pinaroloxias</td>
<td>-0.84030741</td>
<td>0.01600282</td>
</tr>
<tr>
<td>Platyspiza</td>
<td>0.17552395</td>
<td>2.56433028</td>
</tr>
<tr>
<td>psittacula</td>
<td>-0.05551553</td>
<td>0.50310795</td>
</tr>
</tbody>
</table>

# Notice: You can use these scores if you want reduce the numbers of variables in your analyses
Principal Component Analyses: Non-phylogenetic

• Varimax Rotated Principal Components. Plot scores in a bivariate scatterplot

```r
finches_varimax_pca_scores <- as.data.frame(finches_varimax_pca$scores)
finches_varimax_pca_scores$names <- row.names(finches_varimax_pca_scores)

plot(finches_varimax_pca_scores$RC1, finches_varimax_pca_scores$RC2,
     main="Scatterplot finches_varimax_pca_scores",
     xlab="PC1",
     ylab="PC2",
     pch=19)
text(finches_varimax_pca_scores$RC1, finches_varimax_pca_scores$RC2+0.1,
     labels=finches_varimax_pca_scores$names, col= "blue", cex= 0.7)
```
Principal Component Analyses: Non-phylogenetic

- Varimax Rotated Principal Components. Plot scores in a bivariate scatterplot
Principal Component Analyses: Phylogenetic

• Non-Rotated Principal Components

```r
## data preparation
finches_phy <- geospiza$phy
finches_data <- geospiza$dat # Has to be a matrix

## analyses
finches_non_rotated_ppca <- phyl.pca(finches Phy,
                                     finches_data,
                                     method="lambda",
                                     mode="cov")
finches_non_rotated_ppca

# Notice: We are selecting a method for estimating the covariance matrix that fits a lambda parameter
```
Principal Component Analyses: Phylogenetic

• Non-Rotated Principal Components

## Results

# Phylogenetic pca
# Standard deviations:
#        PC1        PC2        PC3        PC4        PC5
# 1.05465929 0.28033469 0.13637879 0.06275309 0.03932391
# Loads:
#                PC1         PC2          PC3          PC4          PC5
# wingL -0.9486734 -0.09458879  0.220949927 -0.163218107  0.124950837
# tarsusL -0.7638619 -0.10839839  0.629634425  0.035310984 -0.084133168
# culmenL -0.8694375 -0.49144869 -0.049894201  0.004454391 -0.006877273
# beakD  -0.9869568  0.14929749 -0.039705808 -0.039285967 -0.022507739
# gonysW -0.9905593  0.11456555  0.007906274  0.070172010  0.026083118

# lambda:
# [1] 0.9472762
## Principal Component Analyses: Phylogenetic

- Non-Rotated Principal Components

```r
## get the scores

finches_ppca_scores <- as.data.frame(finches_non_rotated_ppca$S)
finches_ppca_scores$names <- row.names(finches_ppca_scores)
```

<table>
<thead>
<tr>
<th>#</th>
<th>PC1</th>
<th>PC2</th>
<th>PC3</th>
<th>PC4</th>
<th>PC5</th>
<th>names</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnirostris</td>
<td>-1.34885916</td>
<td>0.17473178</td>
<td>-0.167737386</td>
<td>0.01872918</td>
<td>1.856872e-02</td>
<td>magnirostris</td>
</tr>
<tr>
<td>conirostris</td>
<td>-0.91504424</td>
<td>0.04933744</td>
<td>-0.169647804</td>
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Principal Component Analyses: Phylogenetic

• Non-Rotated Principal Components

```r
## plot

plot(finches_ppca_scores$PC1,
     finches_ppca_scores$PC2,
     main="Scatterplot finches_ppca_scores",
     xlab="PPC1",
     ylab="PPC2",
     pch=19)
text(finches_ppca_scores$PC1, finches_ppca_scores$PC2+0.01, labels=finches_ppca_scores $names, col= "blue", cex= 0.7)
```
Principal Component Analyses: Phylogenetic

• Non-Rotated Principal Components