dispRity manual

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Chapter 1

dispRity

This is a package for measuring disparity in R. It allows users to summarise matrices as representations as multidimensional spaces into a single value or distribution describing a specific aspect of this multidimensional space (the disparity). Multidimensional spaces can be ordinated matrices from MDS, PCA, PCO, PCoA but the package is *not* restricted to any type of matrices! This manual is based on the version 0.4.2.

1.1 What is dispRity?

This is a modular package for measuring disparity in R. It allows users to summarise ordinated matrices (e.g. MDS, PCA, PCO, PCoA) to perform some multidimensional analysis. Typically, these analysis are used in palaeobiology and evolutionary biology to study the changes in morphology through time. However, there are many more applications in ecology, evolution and beyond.

1.1.1 Modular?

Because their exist a multitude of ways to measure disparity, each adapted to every specific question, this package uses an easy to modify modular architecture. In coding, each module is simply a function or a modification of a function that can be passed to the main functions of the package to tweak it to your proper needs! In practice, you will notice throughout this manual that some function can take other functions as arguments: the modular architecture of this package allows you to use any function for these arguments (with some restrictions explained for each specific cases). This will allow you to finely tune your multidimensional analysis to the needs of your specific question!

1.2 Installing and running the package

You can install this package easily if you use the latest version of R > 3.4.0 and devtools.

```
## Checking if devtools is already installed
if(!require(devtools)) install.packages("devtools")

## Installing the latest released version directly from GitHub
install_github("TGuillerme/dispRity", ref = "release")

## Loading the package
library(dispRity)
```

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Note this uses the release branch (version0.4). For the piping-hot (but potentially unstable) version, you can change the argument ref = release to ref = master. dispRity depends mainly on the ape package and uses functions from several other packages (ade4, geometry, grDevices, hypervolume, paleotree, snow, Claddis, geomorph and RCurl).

1.3 Why not CRAN?

This package is not available on CRAN. This is mainly because some parts are still in development and that the reactivity of GitHub is better for implementing new suggestions from users. However, the package follows the strict (and useful!) CRAN standards via Travis.

1.4 Help

If you need help with the package, hopefully the following manual will be useful. However, parts of this package are still in development and some other parts are probably not covered. Thus if you have suggestions or comments on on what has already been developed or will be developed, please send me an email (guillert@tcd.ie) or if you are a GitHub user, directly create an issue on the GitHub page.

1.5 Citations

You can cite both the package or this manual with the following citation:

Guillerme, T. (2016). disp Rity: a package for measuring disparity in R. Zenodo. $10.5281/\mathrm{zenodo}.55646$

Note that this citation is only temporary (but can still be used!). A proper description of the package is currently in review in Methods in Ecology and Evolution and should be re-submitted this winter. Upon acceptance (hopefully!), a proper DOI will be released for this manual and the package description.

Chapter 2

Glossary

- Multidimensional space. The mathematical multidimensional object that will be analysed with this package. In morphometrics, this is often referred to as the morphospace. However it may also be referred to as the cladisto-space for cladistic data or the eco-space for ecological data etc. In practice, this term designates a matrix where the columns represent the dimensions of the space (often but not necessarily > 3!) and the rows represent the elements within this space.
- Elements. The rows of the multidimensional space matrix. Elements can be taxa, field sites, countries etc.
- **Dimensions**. The columns of the multidimensional space matrix. The dimensions can be referred to as axes of variation, or principal components, for ordinated spaces obtained from a PCA for example.
- Subsets. Subsets of the multidimensional space. A subset (or subsets) contains the same number of dimensions as the space but may contain a smaller subset of elements. For example, if our space is composed of birds and mammals (the elements) and 50 principal components of variation (the dimensions), we can create two subsets containing just mammals or birds, but with the same 50 dimensions, to compare disparity in the two clades.

Chapter 3

Getting started with dispRity

3.1 What sort of data does dispRity work with?

Disparity can be estimated from pretty much any matrix. Classically, however, it is measured from ordinated matrices. These matrices can be from any type of ordination (PCO, PCA, PCoA, MDS, etc.) as long as they have your element names as rows (taxa, experiments, countries etc.) and your ordination axes as columns (the dimensions of your dataset).

3.1.1 Ordination matrices from Claddis

dispRity package can easily take data from Claddis using the Claddis.ordination function. For this, simply input a matrix in the Claddis format to the function and it will automatically calculate and ordinate the distances among taxa:

```
require(Claddis)

## Ordinating the example data from Claddis
Claddis.ordination(Michaux1989)

## [.1] [.2] [.3]
```

```
## [,1] [,2] [,3]

## Ancilla 7.252259e-17 4.154578e-01 0.2534942

## Turrancilla -5.106645e-01 -4.566150e-16 -0.2534942

## Ancillista 5.106645e-01 -8.153839e-16 -0.2534942

## Amalda -3.207162e-16 -4.154578e-01 0.2534942
```

Note that several options are available, namely which type of distance should be computed. See more info in the function manual (?Claddis.ordination). Alternatively, it is of course also possible to manual calculate the ordination matrix using the functions Claddis::MorphDistMatrix and stats::cmdscale.

3.1.2 Ordination matrices from geomorph

You can also easily use data from geomorph using the geomorph.ordination function. This function simply takes Procrustes aligned data and performs an ordination:

```
require(geomorph)
## Loading the plethodon dataset
data(plethodon)
```

##

```
## Performing a Procrustes transform on the landmarks
procrustes <- gpagen(plethodon$land, PrinAxes = FALSE, print.progress = FALSE)

## Ordinating this data
geomorph.ordination(procrustes)[1:5,1:5]

## PC1 PC2 PC3 PC4 PC5

## [1,] -0.0369931363 0.05118247 -0.0016971082 -0.003128809 -0.010936371

## [2,] -0.0007493738 0.05942082 0.0001371715 -0.002768680 -0.008117383

## [3,] 0.0056004654 0.07419599 -0.0052612103 -0.005034566 -0.002746592

## [4,] -0.0134808572 0.06463959 -0.0458436015 -0.007887369 0.009816827

## [5,] -0.0334696244 0.06863518 0.0136292041 0.007359409 0.022347225</pre>
```

Options for the ordination (from ?prcomp) can be directly passed to this function to perform customised ordinations. Additionally you can give the function a geomorph.data.frame object. If the latter contains sorting information (i.e. factors), they can be directly used to make a customised dispRity object customised dispRity object!

3.1.3 Other kinds of ordination matrices

If you are not using the packages mentioned above (Claddis and geomorph) you can easily make your own ordination matrices by using the following functions from the stats package. Here is how to do it for the following types of matrices:

• Multivariate matrices (principal components analysis; PCA)

PC2

PC1

```
## A multivariate matrix
head(USArrests)
```

```
##
              Murder Assault UrbanPop Rape
## Alabama
                13.2
                          236
                                    58 21.2
## Alaska
                10.0
                          263
                                     48 44.5
## Arizona
                 8.1
                          294
                                    80 31.0
                 8.8
                          190
                                     50 19.5
## Arkansas
                          276
                                    91 40.6
## California
                 9.0
## Colorado
                 7.9
                          204
                                    78 38.7
## Ordinating the matrix using `prcomp`
ordination <- prcomp(USArrests)</pre>
## Selecting the ordinated matrix
ordinated matrix <- ordination$x
head(ordinated_matrix)
```

PC3

PC4

```
## Alabama
               64.80216 -11.448007 -2.4949328 -2.4079009
## Alaska
              92.82745 -17.982943 20.1265749 4.0940470
## Arizona
              124.06822
                          8.830403 -1.6874484
                                              4.3536852
## Arkansas
               18.34004 -16.703911
                                   0.2101894
                                              0.5209936
## California 107.42295
                        22.520070 6.7458730
## Colorado
              34.97599 13.719584 12.2793628 1.7214637
```

This results in a ordinated matrix with US states as elements and four dimensions (PC 1 to 4). For an alternative method, see the ?princomp function.

• Distance matrices (classical multidimensional scaling; MDS)

```
## A matrix of distances between cities
str(eurodist)
## Class 'dist' atomic [1:210] 3313 2963 3175 3339 2762 ...
     ..- attr(*, "Size")= num 21
##
     ..- attr(*, "Labels")= chr [1:21] "Athens" "Barcelona" "Brussels" "Calais" ...
## Ordinating the matrix using cmdscale() with k = 5 dimensions
ordinated_matrix <- cmdscale(eurodist, k = 5)</pre>
head(ordinated_matrix)
##
                              [,2]
                                         [,3]
                                                    [,4]
                                                                [,5]
                   [,1]
## Athens
             2290.27468 1798.8029
                                     53.79314 -103.82696 -156.95511
                                                84.58583
## Barcelona -825.38279 546.8115 -113.85842
                                                          291.44076
## Brussels
               59.18334 -367.0814
                                   177.55291
                                                38.79751
                                                          -95.62045
## Calais
              -82.84597 -429.9147
                                    300.19274
                                               106.35369 -180.44614
## Cherbourg -352.49943 -290.9084 457.35294
                                               111.44915 -417.49668
              293.68963 -405.3119
                                   360.09323 -636.20238 159.39266
## Cologne
```

This results in a ordinated matrix with European cities as elements and five dimensions.

Of course any other method for creating the ordination matrix is totally valid, you can also not use any ordination at all! The only requirements for the dispRity functions is that the input is a matrix with elements as rows and dimensions as columns.

3.2 Performing a simple dispRity analysis

Two dispRity functions allow users to run an analysis pipeline simply by inputting an ordination matrix. These functions allow users to either calculate the disparity through time (dispRity.through.time) or the disparity of user-defined groups (dispRity.per.group).

IMPORTANT

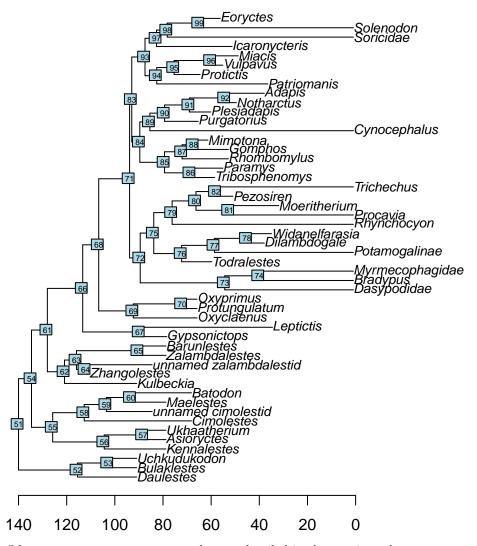
Note that disparity.through.time and disparity.per.group are wrapper functions (i.e. they incorporate lots of other functions) that allow users to run a basic disparity-through-time, or disparity among groups, analysis without too much effort. As such they use a lot of default options. These are described in the help files for the functions that are used to make the wrapper functions, and not described in the help files for disparity.through.time and disparity.per.group. These defaults are good enough for data exploration, but for a proper analysis you should consider the best parameters for your question and data. For example, which metric should you use? How many bootstraps do you require? What model of evolution is most appropriate if you are time slicing? Should you rarefy the data? See time.subsets, custom.subsets, boot.matrix and dispRity.metric for more details of the defaults used in each of these functions. Note that any of these default arguments can be changed within the disparity.through.time or disparity.per.group functions.

3.2.1 Example data

To illustrate these functions, we will use data from Beck and Lee [2014]. This dataset contains an ordinated matrix of 50 discrete characters from mammals (BeckLee_mat50), another matrix of the same 50 mammals and the estimated discrete data characters of their descendants (thus 50 + 49 rows, BeckLee_mat99), a dataframe containing the ages of each taxon in the dataset (BeckLee_ages) and finally a phylogenetic tree with the relationships among the 50 mammals (BeckLee_tree).

```
## Loading the ordinated matrices
data(BeckLee_mat50)
data(BeckLee_mat99)
## The first five taxa and dimensions of the 50 taxa matrix
head(BeckLee_mat50[, 1:5])
##
                   [,1]
                               [,2]
                                         [,3]
                                                  [,4]
                                                           [,5]
## Cimolestes
             -0.4087147 0.0139690317 0.26268300 0.2297096 0.1310953
## Maelestes
## Batodon
             ## Bulaklestes -0.6802291 -0.0134872777 0.11018009 -0.4103588 0.4326298
## Daulestes
             -0.7386111 0.0009001369 0.12006449 -0.4978191 0.4741342
## Uchkudukodon -0.5105254 -0.2420633915 0.44170317 -0.1172972 0.3602273
## The first five taxa and dimensions of the 99 taxa + ancestors matrix
BeckLee_mat99[c(1, 2, 98, 99), 1:5]
                  [,1]
                           [,2]
##
                                     [,3]
                                               [,4]
                                                         [,5]
## Cimolestes -0.60824375 -0.0323683 0.08458885 -0.43384481 -0.30536875
## Maelestes -0.57302058 -0.2840361 0.01308847 -0.12588477 0.06123611
## n48
           -0.05529018 0.4799330 0.04118477 0.04944912 -0.35588301
## n49
           ## Loading a list of first and last occurrence dates for the fossils
data(BeckLee_ages)
head(BeckLee_ages)
```

```
##
               FAD LAD
## Adapis
              37.2 36.8
## Asioryctes 83.6 72.1
## Leptictis 33.9 33.3
## Miacis
              49.0 46.7
## Mimotona
              61.6 59.2
## Notharctus 50.2 47.0
## Loading and plotting the phylogeny
data(BeckLee_tree)
plot(BeckLee_tree, cex = 0.8)
axisPhylo(root = 140)
nodelabels(cex = 0.5)
```



Of course you can use your own data as detailed in the previous chapter.

3.2.2 Disparity through time

The dispRity.through.time function calculates disparity through time, a common analysis in palaeontology. This function (and the following one) uses an analysis pipeline with a lot of default parameters to make the analysis as simple as possible. Of course all the defaults can be changed if required, more on this later.

For a disparity through time analysis, you will need:

- An ordinated matrix (we covered that above)
- A phylogenetic tree: this must be a phylo object (from the ape package) and needs a root.time element. To give your tree a root time (i.e. an age for the root), you can simply do\my_tree\$root.time <- my_age.
- The required number of time subsets (here time = 3)
- Your favourite disparity metric (here the sum of variances)

Using the Beck and Lee (2014) data described above:

This generates a dispRity object (see here for technical details). When displayed, these dispRity objects provide us with information on the operations done to the matrix:

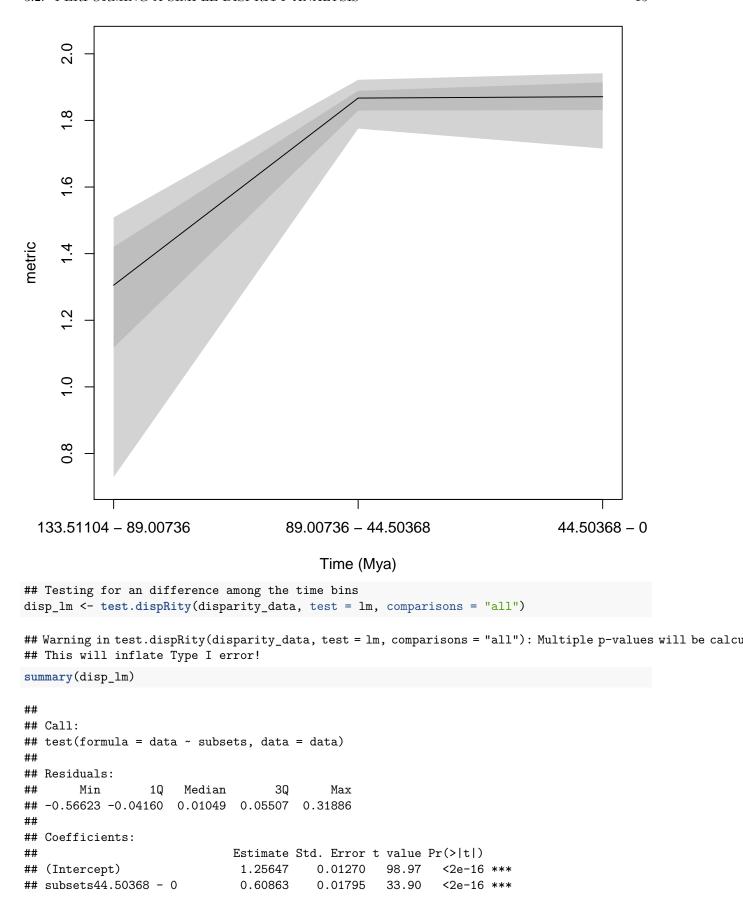
```
## Print the disparity_data object
disparity_data
```

```
## ---- dispRity object ----
## 3 discrete time subsets for 50 elements with 48 dimensions:
## 133.51104 - 89.00736, 89.00736 - 44.50368, 44.50368 - 0.
## Data was bootstrapped 100 times (method:"full").
## Disparity was calculated as: metric.
```

We asked for three subsets (evenly spread across the age of the tree), the data was bootstrapped 100 times (default) and the metric used was the sum of variances.

We can now summarise or plot the disparity_data object, or perform statistical tests on it (e.g. a simple lm):

```
## Summarising disparity through time
summary(disparity_data)
```



```
## subsets89.00736 - 44.50368  0.60169   0.01795  33.51   <2e-16 ***
## ---
## Signif. codes:   0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error:  0.127 on 297 degrees of freedom
## Multiple R-squared:  0.8361, Adjusted R-squared:  0.835
## F-statistic: 757.5 on 2 and 297 DF, p-value: < 2.2e-16</pre>
```

Please refer to the specific tutorials for (much!) more information on the nuts and bolts of the package. You can also directly explore the specific function help files within R and navigate to related functions.

3.2.3 Disparity among groups

The dispRity.per.group function is used if you are interested in looking at disparity among groups rather than through time. For example, you could ask if there is a difference in disparity between two groups?

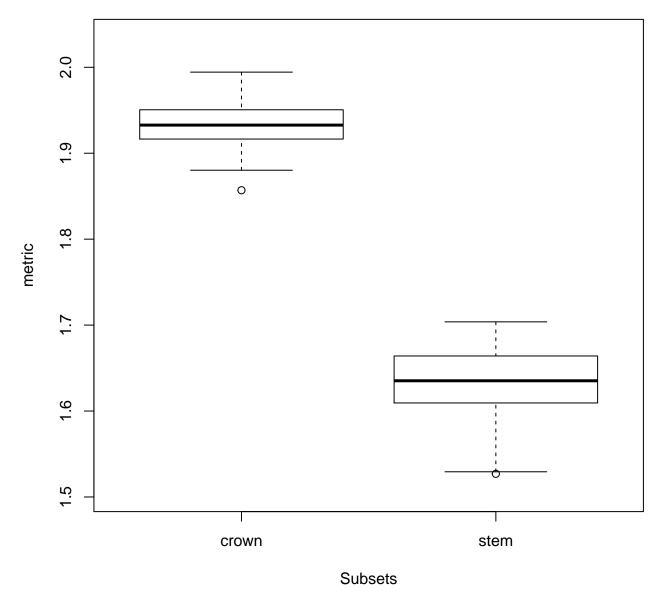
To perform such an analysis, you will need:

- An matrix with rows as elements and columns as dimensions (always!)
- A list of group members: this list should be a list of numeric vectors or names corresponding to the row names in the matrix. For example list("a" = c(1,2), "b" = c(3,4)) will create a group a containing elements 1 and 2 from the matrix and a group b containing elements 3 and 4. Note that elements can be present in multiple groups at once.
- Your favourite disparity metric (here the sum of variances)

Using the Beck and Lee [2014] data described above:

We can display the disparity of both groups by simply looking at the output variable (disparity_data) and then summarising the disparity_data object and plotting it, and/or by performing a statistical test to compare disparity across the groups (here a Wilcoxon test).

```
## Print the disparity_data object
disparity data
## ---- dispRity object ----
## 2 customised subsets for 50 elements with 48 dimensions:
##
       crown, stem.
## Data was bootstrapped 100 times (method:"full").
## Disparity was calculated as: metric.
## Summarising disparity in the different groups
summary(disparity_data)
##
     subsets n
                  obs bs.median 2.5%
                                        25%
                                              75% 97.5%
## 1
       crown 30 1.995
                          1.933 1.883 1.917 1.951 1.983
        stem 20 1.715
                          1.635 1.535 1.610 1.664 1.691
## Plotting the results
plot(disparity_data)
```



```
## Testing for a difference between the groups
test.dispRity(disparity_data, test = wilcox.test, details = TRUE)
```

```
## $`crown : stem`
## $`crown : stem`[[1]]
##
## Wilcoxon rank sum test with continuity correction
##
## data: dots[[1L]][[1L]] and dots[[2L]][[1L]]
## W = 10000, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0</pre>
```

Chapter 4

Details of specific functions

The following section contains information specific to some functions. If any of your questions are not covered in these sections, please refer to the function help files in R, send me an email (guillert@tcd.ie), or raise an issue on GitHub. The several tutorials below describe specific functionalities of certain functions; please always refer to the function help files for the full function documentation!

Before each section, make sure you loaded the Beck and Lee [2014] data (see example data for more details).

```
## Loading the data
data(BeckLee_mat50) ; data(BeckLee_mat99)
data(BeckLee_tree) ; data(BeckLee_ages)
```

4.1 Time slicing

The function time.subsets allows users to divide the matrix into different time subsets or slices given a dated phylogeny that contains all the elements (i.e. taxa) from the matrix. Each subset generated by this function will then contain all the elements present at a specific point in time or during a specific period in time.

Two types of time subsets can be performed by using the method option:

- Discrete time subsets (or time-binning) using method = discrete
- Continuous time subsets (or time-slicing) using method = continuous

For the time-slicing method details see Cooper and Guillerme (in prep.). For both methods, the function takes the time argument which can be a vector of numeric values for:

- Defining the boundaries of the time bins (when method = discrete)
- Defining the time slices (when method = continuous)

Otherwise, the time argument can be set as a single numeric value for automatically generating a given number of equidistant time-bins/slices. Additionally, it is also possible to input a dataframe containing the first and last occurrence data (FAD/LAD) for taxa that span over a longer time than the given tips/nodes age, so taxa can appear in more than one time bin/slice.

Here is an example for method = discrete:

```
## 120 - 80, 80 - 40, 40 - 0.
```

Note that we can also generate equivalent results by just telling the function that we want three time-bins as follow:

In this example, the taxa were split inside each time-bin according to their age. However, the taxa here are considered as single points in time. It is totally possible that some taxa could have had longer longevity and that they exist in multiple time bins. In this case, it is possible to include them in more than one bin by providing a table of first and last occurrence dates (FAD/LAD). This table should have the taxa names as row names and two columns for respectively the first and last occurrence age:

Displaying the table of first and last occurrence dates for each taxa
head(BeckLee_ages)

```
## 3 discrete time subsets for 50 elements:

## 120 - 80, 80 - 40, 40 - 0.

When using this method, the oldest boundary of the first bin (or the first slice, see below) is automatically generated as the root are plus 1% of the tree length, as long as at least three elements (tays are present at
```

When using this method, the oldest boundary of the first bin (or the first slice, see below) is automatically generated as the root age plus 1% of the tree length, as long as at least three elements/taxa are present at that point in time. The algorithm adds an extra 1% tree length until reaching the required minimum of three elements. It is also possible to include nodes in each bin by using inc.nodes = TRUE and providing a matrix that contains the ordinated distance among tips and nodes.

For the time-slicing method (method = continuous), the idea is fairly similar. This option, however, requires a matrix that contains the ordinated distance among taxa and nodes and an extra argument describing the assumed evolutionary model (via the model argument). This model argument is used when the time slice occurs along a branch of the tree rather than on a tip or a node, meaning that a decision must be made about what the value for the branch should be. The model can be one of the following:

• Punctuated models

- acctran where the data chosen along the branch is always the one of the descendant
- deltran where the data chosen along the branch is always the one of the ancestor
- random where the data chosen along the branch is randomly chosen between the descendant or the
 ancestor
- proximity where the data chosen along the branch is either the descendant or the ancestor depending on branch length

• Gradual models

- equal.split where the data chosen along the branch is both the descendant and the ancestor with an even probability
- gradual.split where the data chosen along the branch is both the descendant and the ancestor with a probability depending on branch length

Note that the four first models are a proxy for punctuated evolution: the selected data is always either the one of the descendant or the ancestor. In other words, changes along the branches always occur at either ends of it. The two last models are a proxy for gradual evolution: the data from both the descendant and the ancestor is used with an associate probability. These later models perform better when bootstrapped, effectively approximating the "intermediate" state between and the ancestor and the descendants.

```
## Generating four time slices every 40 million years under a model of proximity evolution
time.subsets(data = BeckLee_mat99, tree = BeckLee_tree,
    method = "continuous", model = "proximity", time = c(120, 80, 40, 0),
    FADLAD = BeckLee_ages)

## ---- dispRity object ----
## 4 continuous (proximity) time subsets for 99 elements:
## 120, 80, 40, 0.

## Generating four time slices automatically
time.subsets(data = BeckLee_mat99, tree = BeckLee_tree,
    method = "continuous", model = "proximity", time = 4, FADLAD = BeckLee_ages)

## ---- dispRity object ----
## 4 continuous (proximity) time subsets for 99 elements:
## 133.51104, 89.00736, 44.50368, 0.
```

4.2 Customised subsets

Another way of separating elements into different categories is to use customised subsets as briefly explained above. This function simply takes the list of elements to put in each group (whether they are the actual element names or their position in the matrix).

4.3 Bootstraps and rarefactions

One important step in analysing ordinated matrices is to pseudo-replicate the data to see how robust the results are, and how sensitive they are to outliers in the dataset. This can be achieved using the function boot.matrix to bootstrap and/or rarefy the data. The default options will bootstrap the matrix 100 times without rarefaction using the "full" bootstrap method (see below):

```
## Default bootstrapping
boot.matrix(data = BeckLee_mat50)

## ---- dispRity object ----
## 50 elements with 48 dimensions.
## Data was bootstrapped 100 times (method:"full").
```

The number of bootstrap replicates can be defined using the bootstraps option. The method can be modified by controlling which bootstrap algorithm to use through the boot.type argument. Currently two algorithms are implemented:

- full where the bootstrapping is entirely stochastic (n elements are replaced by any m elements drawn from the data)
- single where only one random element is replaced by one other random element for each pseudo-replicate

```
## Bootstrapping with the single bootstrap method
boot.matrix(BeckLee_mat50, boot.type = "single")

## ---- dispRity object ----
## 50 elements with 48 dimensions.
## Data was bootstrapped 100 times (method:"single").
```

This function also allows users to rarefy the data using the rarefaction argument. Rarefaction allows users to limit the number of elements to be drawn at each bootstrap replication. This is useful if, for example, one is interested in looking at the effect of reducing the number of elements on the results of an analysis.

This can be achieved by using the rarefaction option that draws only n-x at each bootstrap replicate (where x is the number of elements not sampled). The default argument is FALSE but it can be set to TRUE to fully rarefy the data (i.e. remove x elements for the number of pseudo-replicates, where x varies from the maximum number of elements present in each subset to a minimum of three elements). It can also be set to one or more numeric values to only rarefy to the corresponding number of elements.

```
## Bootstrapping with the full rarefaction
boot.matrix(BeckLee_mat50, bootstraps = 20, rarefaction = TRUE)

## ---- dispRity object ----
## 50 elements with 48 dimensions.
## Data was bootstrapped 20 times (method:"full") and fully rarefied.

## Or with a set number of rarefaction levels
boot.matrix(BeckLee_mat50, bootstraps = 20, rarefaction = c(6:8, 3))

## ---- dispRity object ----
## 50 elements with 48 dimensions.
## Data was bootstrapped 20 times (method:"full") and rarefied to 6, 7, 8, 3 elements.
```

One additional important argument is dimensions that specifies how many dimensions from the matrix should be used for further analysis. When missing, all dimensions from the ordinated matrix are used.

```
## Using the first 50% of the dimensions
boot.matrix(BeckLee_mat50, dimensions = 0.5)
## ---- dispRity object ----
```

```
## 50 elements with 24 dimensions.
## Data was bootstrapped 100 times (method:"full").
## Using the first 10 dimensions
boot.matrix(BeckLee_mat50, dimensions = 10)
## ---- dispRity object ----
## 50 elements with 10 dimensions.
## Data was bootstrapped 100 times (method:"full").
Of course, one could directly supply the subsets generated above (using time.subsets or custom.subsets)
to this function.
## Creating subsets of crown and stem mammals
crown_stem <- custom.subsets(BeckLee_mat50,</pre>
                                 group = list("crown" = c(16, 19:41, 45:50),
                                              "stem" = c(1:15, 17:18, 42:44)))
## Bootstrapping and rarefying these groups
boot.matrix(crown_stem, bootstraps = 200, rarefaction = TRUE)
## ---- dispRity object ----
## 2 customised subsets for 50 elements with 48 dimensions:
       crown, stem.
## Data was bootstrapped 200 times (method: "full") and fully rarefied.
## Creating time slice subsets
time_slices <- time.subsets(data = BeckLee_mat99, tree = BeckLee_tree,
                               method = "continuous", model = "proximity",
                                time = c(120, 80, 40, 0),
                                FADLAD = BeckLee_ages)
## Bootstrapping the time slice subsets
boot.matrix(time_slices, bootstraps = 100)
## ---- dispRity object ----
## 4 continuous (proximity) time subsets for 99 elements with 97 dimensions:
       120, 80, 40, 0.
## Data was bootstrapped 100 times (method:"full").
```

4.4 Disparity metrics

There are many ways of measuring disparity! In brief, disparity is a summary metric that will represent an aspect of an ordinated space (e.g. a MDS, PCA, PCO, PCoA). For example, one can look at ellipsoid hyper-volume of the ordinated space (Donohue *et al.* 2013), the sum and the product of the ranges and variances (Wills *et al.* 1994) or the median position of the elements relative to their centroid (Wills *et al.* 1994). Of course, there are many more examples of metrics one can use for describing some aspect of the ordinated space, with some performing better than other ones at particular descriptive tasks, and some being more generalist.

Because of this great diversity of metrics, the package dispRity does not have one way to measure disparity but rather proposes to facilitate users in defining their own disparity metric that will best suit their particular analysis. In fact, the core function of the package, dispRity, allows the user to define any metric with the metric argument. However the metric argument has to follow certain rules:

- 1. It must be composed from one to three function objects;
- 2. The function(s) must take as a first argument a matrix or a vector;
- 3. The function(s) must be of one of the three dimension-levels described below;

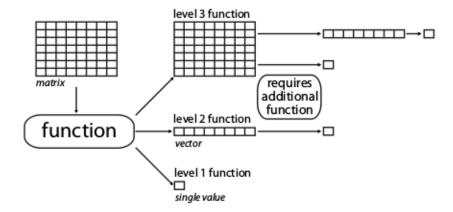


Figure 4.1: Illustration of the different dimension-levels of functions with an input matrix

4. At least one of the functions must be of dimension-level 1 or 2 (see below).

4.4.1 The function dimension-levels

The metric function dimension-levels determine the "dimensionality of decomposition" of the input matrix. In other words, each dimension-level designates the dimensions of the output, i.e. either three (a matrix); two (a vector); or one (a single numeric value) dimension.

4.4.1.1 Dimension-level 1 functions

A dimension-level 1 function will decompose a matrix or a vector into a single value:

```
## Creating a dummy matrix
dummy_matrix <- matrix(rnorm(12), 4, 3)

## Example of dimension-level 1 functions
mean(dummy_matrix)</pre>
```

```
## [1] -0.3227241
median(dummy_matrix)
```

```
## [1] -0.2690165
```

Any summary metric such as mean or median are good examples of dimension-level 1 functions as they reduce the matrix to a single dimension (i.e. one value).

4.4.1.2 Dimension-level 2 functions

A dimension-level 2 function will decompose a matrix into a vector.

```
## Defining the function as the product of rows
prod.rows <- function(matrix) apply(matrix, 1, prod)

## A dimension-level 2 metric
prod.rows(dummy_matrix)</pre>
```

```
## [1] -1.2630799 0.2148864 -0.1797556 -0.2421790
```

Several dimension-level 2 functions are implemented in dispRity (see ?dispRity.metric) such as the variances or ranges functions that calculate the variance or the range of each dimension of the ordinated matrix respectively.

4.4.1.3 Dimension-level 3 functions

Finally a dimension-level 3 function will transform the matrix into another matrix. Note that the dimension of the output matrix doesn't need to match the the input matrix:

```
## A dimension-level 3 metric
var(dummy_matrix)
                      [,2]
            [,1]
                                [.3]
## [1,] 1.916420 1.9501955 0.2907060
## [2,] 1.950196 3.2948635 0.3958234
## [3,] 0.290706 0.3958234 0.6704976
## A dimension-level 3 metric with a forced matrix output
as.matrix(dist(dummy_matrix))
##
            1
                     2
                              3
## 1 0.000000 5.140790 4.005068 3.120827
## 2 5.140790 0.000000 2.179318 2.982267
## 3 4.005068 2.179318 0.000000 2.174896
## 4 3.120827 2.982267 2.174896 0.000000
```

4.4.2 make.metric

Of course, functions can be more complex and involve multiple operations such as the centroids function (see ?dispRity.metric) that calculates the Euclidean distance between each element and the centroid of the ordinated space. The make.metric function implemented in dispRity is designed to help test and find the dimension-level of the functions. This function tests:

- 1. If your function can deal with a matrix or a vector as an input;
- 2. Your function's dimension-level according to its output (dimension-level 1, 2 or 3, see above);
- 3. Whether the function can be implemented in the dispRity function (the function is fed into a lapply loop).

For example, let's see if the functions described above are the right dimension-levels:

Additional dimension-level 2 and/or 1 function(s) will be needed.

```
## Which dimension-level is the mean function? And can it be used in dispRity?
make.metric(mean)

## mean outputs a single value.
## mean is detected as being a dimension-level 1 function.

## Which dimension-level is the prod.rows function? And can it be used in dispRity?
make.metric(prod.rows)

## prod.rows outputs a matrix object.
## prod.rows is detected as being a dimension-level 2 function.

## Which dimension-level is the var function? And can it be used in dispRity?
make.metric(var)

## var outputs a matrix object.

## var is detected as being a dimension-level 3 function.
```

A non verbose version of the function is also available. This can be done using the option silent = TRUE and will simply output the dimension-level of the metric.

```
## Testing whether mean is dimension-level 1
if(make.metric(mean, silent = TRUE) != "level1") {
    message("The metric is not dimension-level 1.")
}
## Testing whether var is dimension-level 1
if(make.metric(var, silent = TRUE) != "level1") {
    message("The metric is not dimension-level 1.")
}
```

The metric is not dimension-level 1.

4.4.3 Metrics in the dispRity function

Using this metric structure, we can easily use any disparity metric in the dispRity function as follows:

```
## Measuring disparity as the standard deviation of all the values of the
## ordinated matrix (dimension-level 1 function).
summary(dispRity(BeckLee_mat50, metric = sd))
##
     subsets n
                 obs
## 1
           1 50 0.201
## Measuring disparity as the standard deviation of the variance of each axis of
## the ordinated matrix (dimension-level 1 and 2 functions).
summary(dispRity(BeckLee_mat50, metric = c(sd, variances)))
     subsets n
                 obs
## 1
           1 50 0.028
## Measuring disparity as the standard deviation of the variance of each axis of
```

```
## subsets n obs
## 1 1 50 0.0001025857
```

Note that the order of each function in the metric argument does not matter, the dispRity function will automatically detect the function dimension-levels (using make.metric) and apply them to the data in decreasing order (dimension-level 3 > 2 > 1).

the variance covariance matrix (dimension-level 1, 2 and 3 functions).
summary(dispRity(BeckLee_mat50, metric = c(sd, variances, var)), round = 10)

```
## subsets n obs
## [1,] TRUE TRUE TRUE
```

In these examples, we considered disparity to be a single value. For example, in the previous example, we defined disparity as the standard deviation of the variances of each column of the variance/covariance matrix (metric = c(variances, sd, var)). It is, however, possible to calculate disparity as a distribution.

4.4.4 Metrics implemented in dispRity

Several disparity metrics are implemented in the dispRity package. The detailed list can be found in ?dispRity.metric along with some description of each metric.

Level	Name	Description	Source
2	ancestra	al. Elistlistance between an element and its ancestor	dispRity
2	centroi	ds The distance between each element and the centroid of the ordinated space	dispRity
1	convhul	1. Slime sueface of the convex hull formed by all the elements	geometry::convhull
1	convhul	1. vBhamelume of the convex hull formed by all the elements	geometry::convhull
1	diagona	The longest distance in the ordinated space (like the diagonal in two dimensions)	dispRity
1	ellipse	.volume/blume of the ellipsoid of the space	Donohue et al. (2013)
1	mode.val	1 The modal value	dispRity
1	n.ball.	volime hyper-spherical (n-ball) volume	dispRity
2	pairwise	e.dfist pairwise distances between elements	stats::dist
2	radius	The radius of each dimensions	dispRity
2	ranges	The range of each dimension	dispRity
1	span.tre	ee. Thangth imal spanning tree length	vegan::spantree
2	variance	es The variance of each dimension	dispRity

1: Note that by default, the centroid is the centroid of the elements. It can, however, be fixed to a different value by using the centroid argument centroids(space, centroid = rep(0, ncol(space))), for example the origin of the ordinated space.

2: This function uses an estimation of the eigenvalue that only works for MDS or PCoA ordinations (not PCA).

4.4.5 Equations and implementations

Some of the functions described below are implemented in the dispRity package and do not require any other packages to calculate (see implementation here).

$$ancestral.dist = \sqrt{\sum_{i=1}^{n} (k_n - Ancestor_n)^2}$$
(4.1)

$$centroids = \sqrt{\sum_{i=1}^{n} (k_n - Centroid_k)^2}$$
(4.2)

$$diagonal = \sqrt{\sum_{i=1}^{k} |max(k_i) - min(k_i)|}$$
(4.3)

$$ellipse.volume = \frac{\pi^{k/2}}{\Gamma(\frac{k}{2}+1)} \prod_{i=1}^{k} (\lambda_i^{0.5})$$

$$\tag{4.4}$$

$$n.ball.volume = \frac{\pi^{k/2}}{\Gamma(\frac{k}{2}+1)} \prod_{i=1}^{k} R$$
 (4.5)

$$radius = \left| \frac{\sum_{i=1}^{n} k_i}{n} - f(\mathbf{v}k) \right| \tag{4.6}$$

$$ranges = |max(k_i) - min(k_i)| \tag{4.7}$$

$$variances = \sigma^2 k_i \tag{4.8}$$

$$span.tree.length = \sum (branch length)$$
 (4.9)

Where k is the number of dimensions, n the number of elements, Γ is the Gamma distribution, λ_i is the eigenvalue of each dimensions, σ^2 is their variance and $Centroid_k$ is their mean, $Ancestor_n$ is the coordinates of the ancestor of element n, $f(\mathbf{v}k)$ is function to select one value from the vector \mathbf{v} of the dimension k (e.g. it's maximum, minimum, mean, etc.), R is the radius of the sphere or the product of the radii of each dimensions

$$(\prod_{i=1}^k R_i$$
 - for a hyper-ellipsoid).

4.4.6 Using the different disparity metrics

Here is a brief demonstration of the main metrics implemented in dispRity. First, we will create a dummy/simulated ordinated space using the space.maker utility function (more about that here:

```
## Creating a 10*5 normal space
set.seed(1)
dummy_space <- space.maker(10, 5, rnorm)</pre>
```

We will use this simulated space to demonstrate the different metrics.

4.4.6.1 Volumes and surface metrics

The functions ellipse.volume, convhull.surface, convhull.volume and n.ball.volume all measure the surface or the volume of the ordinated space occupied:

Because there is only one subset (i.e. one matrix) in the dispRity object, this operation is the equivalent of ellipse.volume(dummy_space) (with rounding).

```
## Calculating the convex hull surface
summary(dispRity(dummy_space, metric = convhull.surface))
```

1 10

1

```
##
     subsets n
## 1
          1 10 11.91
## Calculating the convex hull volume
summary(dispRity(dummy_space, metric = convhull.volume))
     subsets n
                 obs
## 1
          1 10 1.031
## Calculating the convex hull volume
summary(dispRity(dummy_space, metric = n.ball.volume))
##
     subsets n obs
          1 10 4.43
## 1
```

The convex hull functions make a (good) estimation of the multidimensional properties of the ordinated space.

Cautionary note: measuring volumes in a high number of dimensions can be strongly affected by the curse of dimensionality that often results in near 0 disparity values.

4.4.6.2 Ranges, variances, radius, pairwise distance, modal value and diagonal

The functions ranges, variances radius, pairwise.dist, mode.val and diagonal all measure properties of the ordinated space based on its dimensional properties (they are also less affected by the "curse of dimensionality"):

ranges, variances and radius work on the same principle and measure the range/variance/radius of each dimension:

```
## Calculating the ranges of each dimension in the ordinated space
ranges(dummy_space)
## [1] 2.430909 3.726481 2.908329 2.735739 1.588603
## Calculating disparity as the distribution of these ranges
summary(dispRity(dummy_space, metric = ranges))
     subsets n obs.median 2.5%
##
                                   25%
                                         75% 97.5%
## 1
          1 10
                     2.431 1.673 2.431 2.908 3.645
## Calculating disparity as the sum and the product of these ranges
summary(dispRity(dummy_space, metric = c(sum, ranges)))
     subsets n obs
## 1
          1 10 13.39
summary(dispRity(dummy_space, metric = c(prod, ranges)))
##
     subsets n
                  obs
          1 10 114.5
## 1
## Calculating the variances of each dimension in the ordinated space
variances(dummy_space)
## [1] 0.6093144 1.1438620 0.9131859 0.6537768 0.3549372
## Calculating disparity as the distribution of these variances
summary(dispRity(dummy_space, metric = variances))
     subsets n obs.median 2.5%
                                  25%
                                        75% 97.5%
```

0.609 0.38 0.609 0.913 1.121

```
## Calculating disparity as the sum and the product of these variances
summary(dispRity(dummy_space, metric = c(sum, variances)))
##
     subsets n
                  obs
## 1
           1 10 3.675
summary(dispRity(dummy_space, metric = c(prod, variances)))
##
     subsets n
                  obs
## 1
           1 10 0.148
## Calculating the radius of each dimension in the ordinated space
radius(dummy_space)
## [1] 1.4630780 2.4635449 1.8556785 1.4977898 0.8416318
## By default the radius is the maximum distance from the centre of
## the dimension. It can however be changed to any function:
radius(dummy_space, type = min)
## [1] 0.05144054 0.14099827 0.02212226 0.17453525 0.23044528
radius(dummy_space, type = mean)
## [1] 0.6233501 0.7784888 0.7118713 0.6253263 0.5194332
## Calculating disparity as the mean average radius
summary(dispRity(dummy_space, metric = c(mean, radius), type = mean))
##
     subsets n
                  obs
## 1
           1 10 0.652
The pairwise distances uses the function stats::dist and can take the normal dist options:
## The average pairwise euclidean distance
summary(dispRity(dummy_space, metric = c(mean, pairwise.dist)))
##
     subsets n
                  obs
           1 10 2.539
## The distribution of the Manhattan distances
summary(dispRity(dummy_space, metric = pairwise.dist, method = "manhattan"))
##
     subsets n obs.median 2.5%
                                    25%
                                          75% 97.5%
## 1
                     3.619 2.566 3.335 5.672 9.63
The diagonal function measures the multidimensional diagonal of the whole space (i.e. in our case the
longest Euclidean distance in our five dimensional space). The mode.val function measures the modal value
of the matrix:
## Calculating the ordinated space's diagonal
summary(dispRity(dummy space, metric = diagonal))
##
     subsets n
                  obs
## 1
           1 10 3.659
## Calculating the modal value of the matrix
summary(dispRity(dummy_space, metric = mode.val))
     subsets n
                  obs
           1 10 -2.21
## 1
```

This metric is only a Euclidean diagonal (mathematically valid) if the dimensions within the space are all orthogonal!

4.4.6.3 Centroids and ancestral distance metrics

The **centroids** metric allows users to measure the position of the different elements compared to a fixed point in the ordinated space. By default, this function measures the distance between each element and their centroid (centre point):

```
## The distribution of the distances between each element and their centroid
summary(dispRity(dummy_space, metric = centroids))

## subsets n obs.median 2.5% 25% 75% 97.5%
## 1 1 10 2.214 0.788 1.267 1.993 3.167

## Disparity as the median value of these distances
summary(dispRity(dummy_space, metric = c(median, centroids)))

## subsets n obs
## 1 1 10 1.435
```

It is however possible to fix the coordinates of the centroid to a specific point in the ordinated space, as long as it has the correct number of dimensions:

```
## The distance between each element and the origin of the ordinated space
summary(dispRity(dummy_space, metric = centroids, centroid = c(0,0,0,0,0)))

## subsets n obs.median 2.5% 25% 75% 97.5%

## 1 1 10 2.323 0.785 1.2 2.044 3.176

## Disparity as the distance between each element and a specific point in space
summary(dispRity(dummy_space, metric = centroids, centroid = c(0,1,2,3,4)))

## subsets n obs.median 2.5% 25% 75% 97.5%
```

The ancestral.dist metric works on a similar principle as the centroids function but changes the centroid to be the coordinates of each element's ancestor. Therefore this functions needs a tree and node coordinates as additional arguments:

4.675 4.293 5.032 6.155 6.957

```
## subsets n obs
## 1 1 9 36.56
```

1

1 10

4.4.6.4 Minimal spanning tree length

The span.tree.length uses the vegan::spantree function to heuristically calculate the minimum spanning tree (the shortest multidimensional tree connecting each elements) and calculates its length as the sum of every branch lengths.

Note that because the solution is heuristic, this metric can take a long time to compute for big matrices.

4.5 Summarising dispRity data (plots)

Because of its architecture, printing dispRity objects only summarises their content but does not print the disparity value measured or associated analysis (more about this here). To actually see what is in a dispRity object, one can either use the summary function for visualising the data in a table or plot to have a graphical representation of the results.

4.5.1 Summarising dispRity data

This function is an S3 function (summary.dispRity) allowing users to summarise the content of dispRity objects that contain disparity calculations.

```
## Example data from previous sections
crown_stem <- custom.subsets(BeckLee_mat50,</pre>
                                 group = list("crown" = c(16, 19:41, 45:50),
                                               "stem" = c(1:15, 17:18, 42:44)))
## Bootstrapping and rarefying these groups
boot_crown_stem <- boot.matrix(crown_stem, bootstraps = 100, rarefaction = TRUE)</pre>
## Calculate disparity
disparity_crown_stem <- dispRity(boot_crown_stem, metric = c(sum, variances))</pre>
## Creating time slice subsets
time_slices <- time.subsets(data = BeckLee_mat99, tree = BeckLee_tree,</pre>
    method = "continuous", model = "proximity", time = c(120, 80, 40, 0),
    FADLAD = BeckLee_ages)
## Bootstrapping the time slice subsets
boot_time_slices <- boot.matrix(time_slices, bootstraps = 100)</pre>
## Calculate disparity
disparity_time_slices <- dispRity(boot_time_slices, metric = c(sum, variances))</pre>
## Creating time bin subsets
time_bins <- time.subsets(data = BeckLee_mat99, tree = BeckLee_tree,
    method = "discrete", time = c(120, 80, 40, 0), FADLAD = BeckLee_ages,
    inc.nodes = TRUE)
## Bootstrapping the time bin subsets
boot_time_bins <- boot.matrix(time_bins, bootstraps = 100)</pre>
## Calculate disparity
disparity_time_bins <- dispRity(boot_time_bins, metric = c(sum, variances))</pre>
```

These objects are easy to summarise as follows:

```
## Default summary
summary(disparity_time_slices)
```

```
subsets n
                  obs bs.median 2.5%
                                         25%
                                               75% 97.5%
## 1
         120 5 2.823
                          2.295 1.398 2.037 2.563 2.767
## 2
          80 19 3.233
                          3.065 2.785 2.973 3.133 3.266
## 3
          40 15 3.359
                          3.149 2.764 2.996 3.285 3.443
## 4
           0 10 4.055
                          3.685 3.169 3.453 3.760 3.961
```

Information about the number of elements in each subset and the observed (i.e. non-bootstrapped) disparity are also calculated. This is specifically handy when rarefying the data for example:

head(summary(disparity_crown_stem))

```
obs bs.median 2.5%
                                         25%
                                               75% 97.5%
##
     subsets n
## 1
       crown 30 1.995
                          1.933 1.873 1.915 1.943 1.972
       crown 29
                           1.935 1.861 1.906 1.953 1.976
## 2
                   NA
## 3
       crown 28
                   NA
                          1.929 1.872 1.910 1.945 1.970
## 4
      crown 27
                   NA
                          1.933 1.852 1.905 1.947 1.981
## 5
      crown 26
                          1.932 1.867 1.910 1.948 1.971
                   NA
## 6
       crown 25
                   NA
                           1.929 1.847 1.913 1.949 1.975
```

The summary functions can also take various options such as:

- quantile values for the confidence interval levels (by default, the 50 and 95 quantiles are calculated)
- cent.tend for the central tendency to use for summarising the results (default is median)
- roundingoption corresponding to the number of decimal places to print (default is2')
- recall option for printing the call of the dispRity object as well (default is FALSE)

These options can easily be changed from the defaults as follows:

Same as above but using the 88th quantile and the standard deviation as the summary
summary(disparity_time_slices, quantile = 88, cent.tend = sd)

```
## subsets n obs bs.sd 6% 94%
## 1 120 5 2.823 0.380 1.489 2.654
## 2 80 19 3.233 0.127 2.869 3.224
## 3 40 15 3.359 0.189 2.815 3.394
## 4 0 10 4.055 0.205 3.291 3.885
## Printing the details of the object and rounding the values to the 5th decimal place
summary(disparity_time_slices, recall = TRUE, rounding = 5)
```

```
---- dispRity object ----
## 4 continuous (proximity) time subsets for 99 elements with 97 dimensions:
       120, 80, 40, 0.
## Data was bootstrapped 100 times (method:"full").
## Disparity was calculated as: c(sum, variances).
##
     subsets n
                    obs bs.median
                                     2.5%
                                              25%
                                                      75%
## 1
         120 5 2.82292
                          2.29516 1.39758 2.03734 2.56317 2.76690
## 2
          80 19 3.23312
                          3.06472 2.78542 2.97332 3.13308 3.26617
## 3
          40 15 3.35947
                          3.14918 2.76395 2.99563 3.28541 3.44267
           0 10 4.05457
                          3.68545 3.16864 3.45263 3.76034 3.96114
```

Note that the summary table is a data.frame, hence it is as easy to modify as any dataframe using dplyr. You can also export it in csv format using write.csv or write_csv or even directly export into LaTeX format using the following;

```
## Loading the xtable package
require(xtable)
## Converting the table in LaTeX
xtable(summary(disparity_time_slices))
```

4.5.2 Plotting dispRity data

An alternative (and more fun!) way to display the calculated disparity is to plot the results using the S3 method plot.dispRity. This function takes the same options as summary.dispRity along with various graphical options described in the function help files (see ?plot.dispRity).

The plots can be of four different types:

- continuous for displaying continuous disparity curves
- box, lines, and polygons to display discrete disparity results in respectively a boxplot, confidence interval lines, and confidence interval polygons.

This argument can be left empty. In this case, the algorithm will automatically detect the type of subsets from the dispRity object and plot accordingly.

It is also possible to display the number of elements in each subset (as a horizontal dotted line) using the option elements = TRUE. Additionally, when the data is rarefied, one can indicate which level of rarefaction to display (i.e. only display the results for a certain number of elements) by using the rarefaction argument.

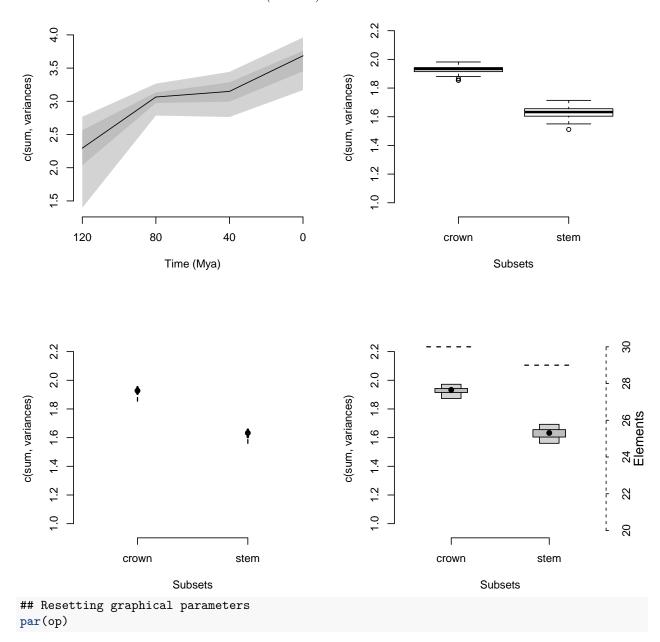
```
## Graphical parameters
op <- par(mfrow = c(2, 2), bty = "n")

## Plotting continuous disparity results
plot(disparity_time_slices, type = "continuous")

## Plotting discrete disparity results
plot(disparity_crown_stem, type = "box")

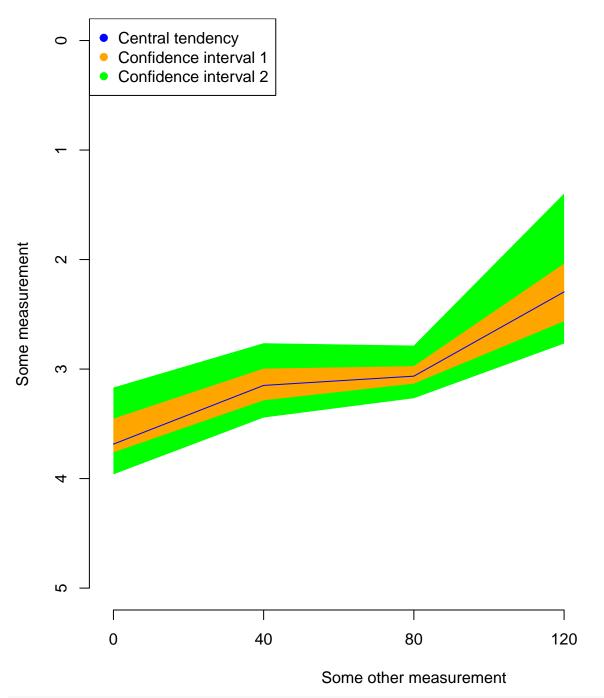
## As above but using lines for the rarefaction level of 20 elements only
plot(disparity_crown_stem, type = "line", rarefaction = 20)

## As above but using polygons while also displaying the number of elements
plot(disparity_crown_stem, type = "polygon", elements = TRUE)</pre>
```



Since plot.dispRity uses the arguments from the generic plot method, it is of course possible to change pretty much everything using the regular plot arguments:





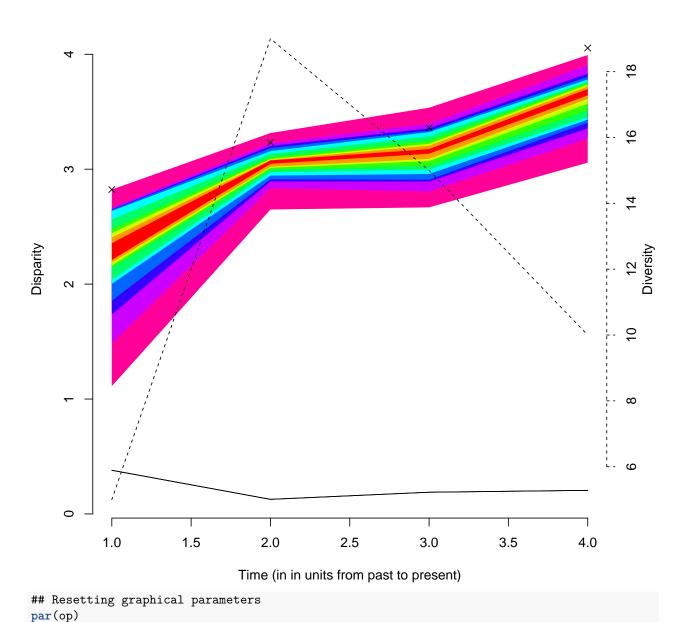
Resetting graphical parameters
par(op)

In addition to the classic plot arguments, the function can also take arguments that are specific to plot.dispRity like adding the number of elements or rarefaction level (as described above), and also changing the values of the quantiles to plot as well as the central tendency.

```
## Graphical options
op <- par(bty = "n")

## Plotting the results with some plot.dispRity arguments
plot(disparity_time_slices, quantile = c(seq(from = 10, to = 100, by = 10)),
    cent.tend = sd, type = "c", elements = TRUE, col = c("black", rainbow(10)),
    ylab = c("Disparity", "Diversity"), time.subsets = FALSE,
    xlab = "Time (in in units from past to present)", observed = TRUE,
    main = "Many more options...")</pre>
```

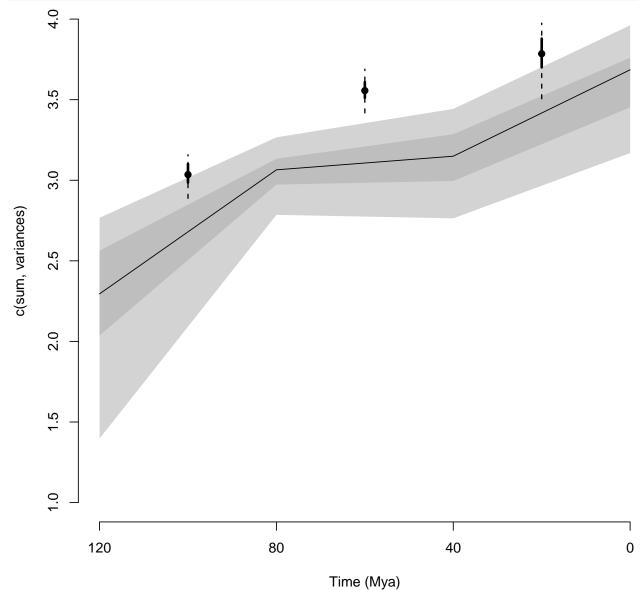
Many more options...



Note that the argument observed = TRUE allows to plot the disparity values calculated from the

non-bootstrapped data as crosses on the plot.

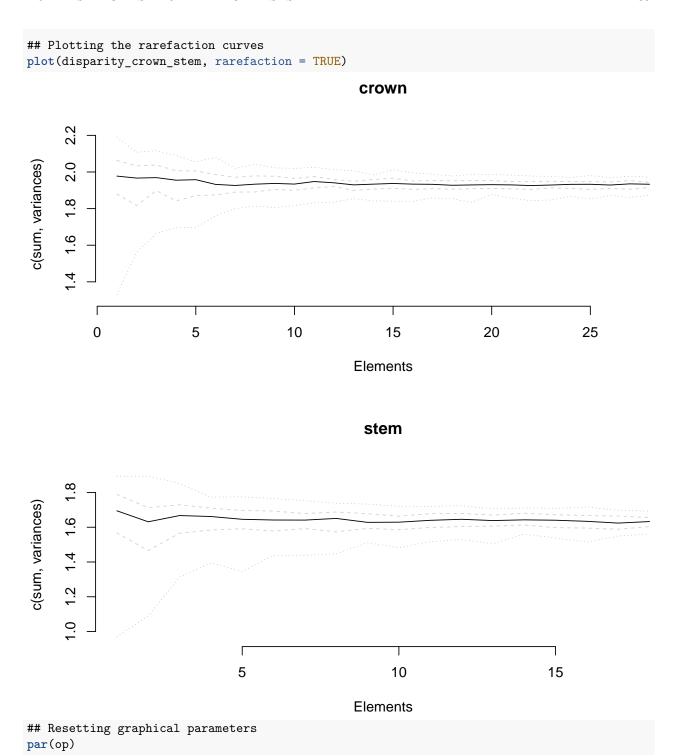
For comparing results, it is also possible to add a plot to the existent plot by using add = TRUE:



```
## Resetting graphical parameters
par(op)
```

Finally, if your data has been fully rarefied, it is also possible to easily look at rarefaction curves by using the rarefaction = TRUE argument:

```
## Graphical options
op <- par(bty = "n")</pre>
```



4.6 Testing disparity hypotheses

The dispRity package allows users to apply statistical tests to the calculated disparity to test various hypotheses. The function test.dispRity works in a similar way to the dispRity function: it takes a dispRity object, a test and a comparisons argument.

The comparisons argument indicates the way the test should be applied to the data:

- pairwise (default): to compare each subset in a pairwise manner
- referential: to compare each subset to the first subset
- sequential: to compare each subset to the following subset
- all: to compare all the subsets together (like in analysis of variance)

It is also possible to input a list of pairs of numeric values or characters matching the subset names to create personalised tests. Some other tests implemented in dispRity such as the dispRity::null.test have a specific way they are applied to the data and therefore ignore the comparisons argument.

The test argument can be any statistical or non-statistical test to apply to the disparity object. It can be a common statistical test function (e.g. stats::t.test), a function implemented in dispRity (e.g. see ?null.test) or any function defined by the user.

This function also allows users to correct for Type I error inflation (false positives) when using multiple comparisons via the correction argument. This argument can be empty (no correction applied) or can contain one of the corrections from the stats::p.adjust function (see ?p.adjust).

Note that the test.dispRity algorithm deals with some classical test outputs (h.test, lm and numeric vector) and summarises the test output. It is, however, possible to get the full detailed output by using the options details = TRUE.

Here we are using the variables generated in the section above:

with Bonferroni correction

```
## T-test to test for a difference in disparity between crown and stem mammals
test.dispRity(disparity_crown_stem, test = t.test)
## [[1]]
##
                statistic: t
## crown : stem
                    66.67693
##
## [[2]]
##
                parameter: df
                     169.1446
## crown : stem
##
## [[3]]
                      p.value
## crown : stem 2.275095e-123
## Performing the same test but with the detailed t.test output
test.dispRity(disparity crown stem, test = t.test, details = TRUE)
## $`crown : stem`
## $`crown : stem`[[1]]
##
   Welch Two Sample t-test
##
##
## data: dots[[1L]][[1L]] and dots[[2L]][[1L]]
## t = 66.677, df = 169.14, p-value < 2.2e-16
\#\# alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## 0.2894967 0.3071619
## sample estimates:
## mean of x mean of y
## 1.928128 1.629799
## Wilcoxon test applied to time sliced disparity with sequential comparisons,
```

```
test.dispRity(disparity_time_slices, test = wilcox.test,
              comparisons = "sequential", correction = "bonferroni")
## [[1]]
##
            statistic: W
## 120 : 80
                      27
## 80 : 40
                    3466
                      455
## 40 : 0
##
## [[2]]
                 p.value
## 120 : 80 1.720545e-33
## 80 : 40 5.370214e-04
## 40 : 0
            3.599349e-28
## Measuring the overlap between distributions in the time bins (using the
## implemented Bhattacharyya Coefficient function - see ?bhatt.coeff)
test.dispRity(disparity_time_bins, test = bhatt.coeff)
## Warning in test.dispRity(disparity_time_bins, test = bhatt.coeff): Multiple p-values will be calculated
## This will inflate Type I error!
                      bhatt.coeff
## 120 - 80 : 80 - 40
                          0.000000
## 120 - 80 : 40 - 0
                          0.000000
## 80 - 40 : 40 - 0
                          0.490448
It is also possible to apply some more complex tests that have their own output classes (like stats::lm).
The results can then be analysed as usual using the associated summary S3 method:
## Performing and linear model applied to the same data
(slice_lm <- test.dispRity(disparity_time_slices, test = lm,</pre>
                             comparisons = "all"))
## Warning in test.dispRity(disparity_time_slices, test = lm, comparisons = "all"): Multiple p-values will h
## This will inflate Type I error!
##
## Call:
## test(formula = data ~ subsets, data = data)
## Coefficients:
## (Intercept)
                 subsets120
                                subsets40
                                              subsets80
        3.6216
                    -1.3756
                                  -0.4873
                                                -0.5747
## The output is a regular `lm` output
class(slice_lm)
## [1] "lm"
## This output can be summarised using summary
summary(slice_lm)
##
## Call:
## test(formula = data ~ subsets, data = data)
##
## Residuals:
##
        Min
                  1Q
                      Median
                                     3Q
                                              Max
```

```
## -1.13370 -0.13528 0.02831 0.15469 0.57698
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 3.62157 0.02441 148.39
                                           <2e-16 ***
                         0.03451 -39.86 <2e-16 ***
## subsets120 -1.37564
                         0.03451 -14.12 <2e-16 ***
## subsets40 -0.48733
                         0.03451 -16.65 <2e-16 ***
## subsets80 -0.57468
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.2441 on 396 degrees of freedom
## Multiple R-squared: 0.8051, Adjusted R-squared: 0.8037
## F-statistic: 545.4 on 3 and 396 DF, p-value: < 2.2e-16
```

Of course, due to the modular design of the package, tests can always be made by the user (the same way disparity metrics can be user made). The only condition is that the test can be applied to at least two distributions. In practice, the test.dispRity function will pass the calculated disparity data (distributions) to the provided function in either pairs of distributions (if the comparisons argument is set to pairwise, referential or sequential) or a table containing all the distributions (comparisons = all; this should be in the same format as data passed to lm for example).

4.6.1 NPMANOVA in dispRity

One often useful test to apply to multidimensional data is the permutational multivariate analysis of variance based on distance matrices vegan::adonis.

```
library(vegan)
```

```
## Warning: package 'vegan' was built under R version 3.4.3
## Loading required package: permute
##
## Attaching package: 'permute'
## The following object is masked from 'package:devtools':
##
##
       check
## Loading required package: lattice
## This is vegan 2.4-5
data(dune)
data(dune.env)
## Beta diversity distance matrix
betad <- betadiver(dune, "z")</pre>
## Create a pairwise distance matrix
make.pairwise.dist.matrix <- function(matrix) {</pre>
    if(class(matrix) == "matrix" || class(matrix) == "data.frame") {
        ## Simply calculate the distances
        return(dist(matrix))
    } else {
        ## Transform the distances into a matrix
        pair_distances <- matrix</pre>
```

```
pairwise_dist <- matrix(NA, nrow = nrow(matrix), ncol = nrow(matrix))</pre>
        colnames(pairwise_dist) <- rownames(pairwise_dist) <- rownames(matrix)</pre>
        diag(pairwise_dist) <- 0</pre>
        pairwise_dist[lower.tri(pairwise_dist)] <- pair_distances</pre>
        pairwise_dist <- as.dist(pairwise_dist)</pre>
    }
}
pairwise_dist <- make.pairwise.dist.matrix(dune)</pre>
## Create the factor group
factors <- data.frame(factor = dune.env$Management)</pre>
## Testing adonis
test1 <- adonis(betad ~ factor, factors)</pre>
test2 <- adonis(pairwise_dist ~ factor, factors)</pre>
set.seed(1)
## Check if it works for mammals data set
data(BeckLee_mat50)
data(BeckLee_tree)
## Crown stem group
crown_stem <- crown.stem(BeckLee_tree, inc.nodes = FALSE)</pre>
## Dummy group
group_sample <- sample(1:50, 25)</pre>
group1 <- rownames(BeckLee_mat50)[group_sample]</pre>
group2 <- rownames(BeckLee_mat50)[-group_sample]</pre>
dummy_group <- list(group1 = group1, group2 = group2)</pre>
## Equal groups
equal_group <- list(groupA = rownames(BeckLee_mat50), groupB = rownames(BeckLee_mat50))</pre>
## Create the subsets
subset_crown_stem <- custom.subsets(BeckLee_mat50, group = crown_stem)</pre>
subset_dummy_group <- custom.subsets(BeckLee_mat50, group = dummy_group)</pre>
subset_equal_group <- custom.subsets(BeckLee_mat50, group = equal_group)</pre>
## Calculate disparity
disp_crown_stem <- dispRity(subset_crown_stem, metric = c(median, centroids))</pre>
disp_dummy_group <- dispRity(subset_dummy_group, metric = c(median, centroids))</pre>
disp_equal_group <- dispRity(subset_equal_group, metric = c(median, centroids))</pre>
summary(disp_crown_stem)
     subsets n obs
##
## 1 crown 30 1.387
## 2
       stem 20 1.274
summary(disp_dummy_group)
## subsets n obs
## 1 group1 25 1.396
## 2 group2 25 1.373
```

```
summary(disp_equal_group)
     subsets n obs
## 1 groupA 50 1.39
## 2 groupB 50 1.39
## Function for creating the factors table
make.factors <- function(data) {</pre>
    ## Extracting the factors
    factors <- names(sort(unlist(lapply(data$subsets, function(X) return(X$elements)))))</pre>
    ## Trimming the factors names
    group_names <- names(data$subsets)</pre>
    for(group in 1:length(group_names)) {
        factors[grep(group_names[group], factors)] <- group_names[group]</pre>
    }
    return(data.frame(factor = factors, row.names = rownames(data$matrix)))
}
adonis.dispRity <- function(data, ...) {</pre>
  ## Create the factor table
  factors <- make.factors(data)
  ## Run adonis
  return(adonis(make.pairwise.dist.matrix(data$matrix)~factor, factors, ...))
}
```

4.7 Disparity as a distribution

Disparity is often regarded as a summary value of the position of the all elements in the ordinated space. For example, the sum of variances, the product of ranges or the median distance between the elements and their centroid will summarise disparity as a single value. This value can be pseudo-replicated (bootstrapped) to obtain a distribution of the summary metric with estimated error. However, another way to perform disparity analysis is to use the *whole distribution* rather than just a summary metric (e.g. the variances or the ranges).

This is possible in the dispRity package by calculating disparity as a dimension-level 2 metric only! Let's have a look using our previous example of bootstrapped time slices but by measuring the distances between each taxon and their centroid as disparity.

```
## Measuring disparity as a whole distribution
disparity_centroids <- dispRity(boot_time_slices, metric = centroids)</pre>
```

The resulting disparity object is of dimension-level 2, so it can easily be transformed into a dimension-level 1 object by, for example, measuring the median distance of all these distributions:

```
## Measuring median disparity in each time slice
disparity_centroids_median <- dispRity(disparity_centroids, metric = median)</pre>
```

And we can now compare the differences between these methods:

```
## Summarising both disparity measurements:
## The distributions:
summary(disparity_centroids)
```

```
## subsets n obs.median bs.median 2.5% 25% 75% 97.5% ## 1 120 5 1.539 1.287 0.536 1.092 1.553 1.864
```

```
## 2 80 19 1.846 1.688 1.409 1.582 1.814 1.945

## 3 40 15 1.892 1.685 1.327 1.563 1.839 2.062

## 4 0 10 1.855 1.801 1.313 1.680 1.962 2.104
```

```
## The summary of the distributions (as median)
summary(disparity_centroids_median)
```

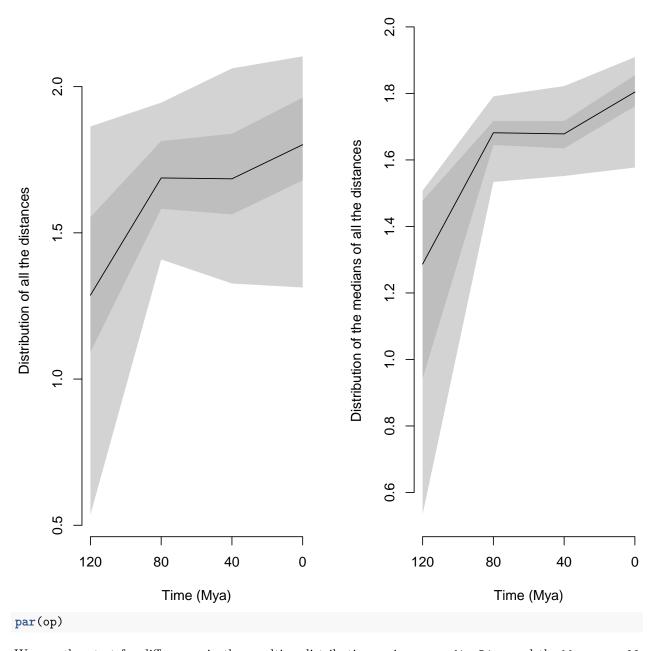
```
obs bs.median 2.5%
                                        25%
                                               75% 97.5%
##
     subsets n
## 1
         120
             5 1.508
                          1.287 0.535 0.943 1.477 1.508
                          1.682 1.534 1.645 1.716 1.791
## 2
          80 19 1.790
## 3
          40 15 1.689
                          1.678 1.552 1.635 1.717 1.822
## 4
           0 10 1.910
                          1.804 1.577 1.761 1.855 1.909
```

We can see that the summary message for the distribution is slightly different than before. Here summary also displays the observed central tendency (i.e. the central tendency of the measured distributions). Note that, as expected, this central tendency is the same in both metrics!

Another, maybe more intuitive way, to compare both approaches for measuring disparity is to plot the distributions:

```
## Graphical parameters
op <- par(bty = "n", mfrow = c(1, 2))

## Plotting both disparity measurements
plot(disparity_centroids, ylab = "Distribution of all the distances")
plot(disparity_centroids_median,
    ylab = "Distribution of the medians of all the distances")</pre>
```



We can then test for differences in the resulting distributions using test.dispRity and the bhatt.coeff test as described above.

```
## Probability of overlap in the distribution of medians
test.dispRity(disparity_centroids_median, test = bhatt.coeff)
```

Warning in test.dispRity(disparity_centroids_median, test = bhatt.coeff): Multiple p-values will be calc
This will inflate Type I error!

In this case, we are looking at the probability of overlap of the distribution of median distances from centroids among each pair of time slices. In other words, we are measuring whether the medians from each bootstrap pseudo-replicate for each time slice overlap. But of course, we might be interested in the actual distribution of the distances from the centroid rather than simply their central tendencies. This can be problematic depending on the research question asked since we are effectively comparing non-independent medians distributions (because of the pseudo-replication).

One solution, therefore, is to look at the full distribution:

```
## Probability of overlap for the full distributions
test.dispRity(disparity_centroids, test = bhatt.coeff)
```

Warning in test.dispRity(disparity_centroids, test = bhatt.coeff): Multiple p-values will be calculated
This will inflate Type I error!

These results show the actual overlap among all the measured distances from centroids concatenated across all the bootstraps. For example, when comparing the slices 120 and 80, we are effectively comparing the 5×100 distances (the distances of the five elements in slice 120 bootstrapped 100 times) to the 19×100 distances from slice 80. However, this can also be problematic for some specific tests since the $n \times 100$ distances are also pseudo-replicates and thus are still not independent.

A second solution is to compare the distributions to each other for each replicate:

```
## Boostrapped probability of overlap for the full distributions
test.dispRity(disparity_centroids, test = bhatt.coeff, concatenate = FALSE)
```

Warning in test.dispRity(disparity_centroids, test = bhatt.coeff, concatenate = FALSE): Multiple p-value
This will inflate Type I error!

```
bhatt.coeff
                             2.5%
                                         25%
                                                   75%
                                                           97.5%
## 120 : 80
              0.2507287 0.0000000 0.1450953 0.3829003 0.5431424
## 120 : 40
              0.3184407 0.0000000 0.2000000 0.4312174 0.7651213
## 120 : 0
              0.2368001 0.0000000 0.0000000 0.3464102 0.5791641
## 80 : 40
              0.5739203 0.2252672 0.4678055 0.6965587 0.8184853
## 80 : 0
              0.4649973 0.1382736 0.3688643 0.5757552 0.7292754
              0.5418625 0.1954287 0.4385665 0.6767986 0.8082483
## 40 : 0
```

These results show the median overlap among pairs of distributions in the first column (bhatt.coeff) and then the distribution of these overlaps among each pair of bootstraps. In other words, when two distributions are compared, they are now compared for each bootstrap pseudo-replicate, thus effectively creating a distribution of probabilities of overlap. For example, when comparing the slices 120 and 80, we have a mean probability of overlap of 0.28 and a probability between 0.18 and 0.43 in 50% of the pseudo-replicates. Note that the quantiles and central tendencies can be modified via the conc.quantiles option.

4.8 Disparity from other matrices

In the example so far, disparity was measured from an ordinated multidimensional space (i.e. a PCO of the distances between taxa based on discrete morphological characters). This is a common approach in palaeobiology, morphometrics or ecology but ordinated matrices are not mandatory for the dispRity package! It

is totally possible to perform the same analysis detailed above using other types of matrices as long as your elements are rows in your matrix.

For example, we can use the data set eurodist, an R inbuilt dataset that contains the distances (in km) between European cities. We can check for example, if Northern European cities are closer to each other than Southern ones:

```
## Making the eurodist data set into a matrix (rather than "dist" object)
eurodist <- as.matrix(eurodist)</pre>
eurodist[1:5, 1:5]
##
             Athens Barcelona Brussels Calais Cherbourg
## Athens
                         3313
                                  2963
               0
                                        3175
## Barcelona 3313
                         0
                                  1318 1326
                                                    1294
                                 0 204
## Brussels 2963
                        1318
                                                    583
## Calais
              3175
                        1326
                                   204
                                           0
                                                     460
## Cherbourg 3339
                                                       0
                         1294
                                   583
                                          460
## The two groups of cities
Northern <- c("Brussels", "Calais", "Cherbourg", "Cologne", "Copenhagen",
              "Hamburg", "Hook of Holland", "Paris", "Stockholm")
Southern <- c("Athens", "Barcelona", "Geneva", "Gibraltar", "Lisbon", "Lyons",
              "Madrid", "Marseilles", "Milan", "Munich", "Rome", "Vienna")
## Creating the subset dispRity object
eurodist_subsets <- custom.subsets(eurodist, group = list("Northern" = Northern,</pre>
                                                         "Southern" = Southern))
## Bootstrapping and rarefying to 9 elements (the number of Northern cities)
eurodist_bs <- boot.matrix(eurodist_subsets, rarefaction = 9)</pre>
## Measuring disparity as the median distance from group's centroid
euro_disp <- dispRity(eurodist_bs, metric = c(median, centroids))</pre>
## Testing the differences using a simple wilcox.test
euro_diff <- test.dispRity(euro_disp, test = wilcox.test)</pre>
euro_diff_rar <- test.dispRity(euro_disp, test = wilcox.test, rarefaction = 9)</pre>
We can compare this approach to an ordination one:
## Ordinating the eurodist matrix
euro_ord <- cmdscale(eurodist, k = nrow(eurodist) - 2)</pre>
## Warning in cmdscale(eurodist, k = nrow(eurodist) - 2): only 11 of the first
## 19 eigenvalues are > 0
## Calculating disparity on the bootstrapped and rarefied subset data
euro_ord_disp <- dispRity(boot.matrix(custom.subsets(euro_ord, group =</pre>
        list("Northern" = Northern, "Southern" = Southern)), rarefaction = 9),
        metric = c(median, centroids))
## Testing the differences using a simple wilcox.test
```

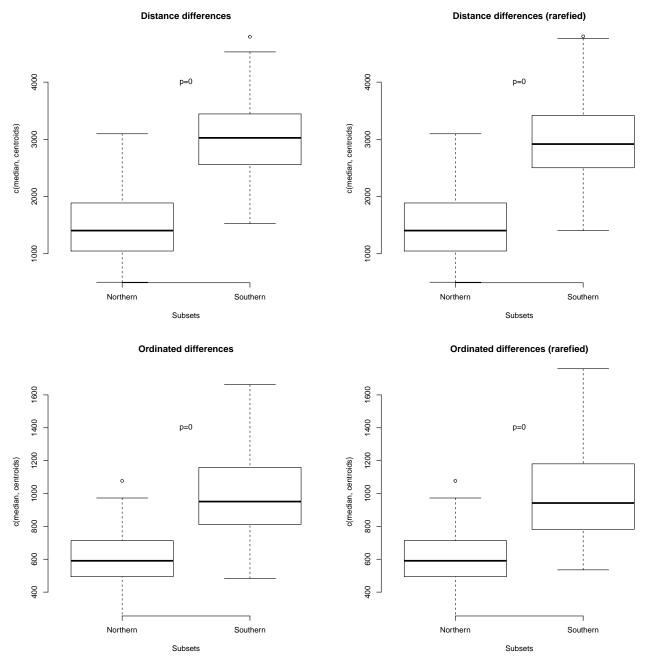
And visualise the differences:

```
## Plotting the differences
par(mfrow = c(2,2), bty = "n")
```

euro_ord_diff_rar <- test.dispRity(euro_ord_disp, test = wilcox.test, rarefaction = 9)</pre>

euro_ord_diff <- test.dispRity(euro_ord_disp, test = wilcox.test)</pre>

```
## Plotting the normal disparity
plot(euro_disp, main = "Distance differences")
## Adding the p-value
text(1.5, 4000, paste0("p=",round(euro_diff[[2]][[1]], digit = 5)))
## Plotting the rarefied disparity
plot(euro_disp, rarefaction = 9, main = "Distance differences (rarefied)")
## Adding the p-value
text(1.5, 4000, paste0("p=",round(euro_diff_rar[[2]][[1]], digit = 5)))
## Plotting the ordinated disparity
plot(euro_ord_disp, main = "Ordinated differences")
## Adding the p-value
text(1.5, 1400, paste0("p=",round(euro_ord_diff[[2]][[1]], digit = 5) ))
## Plotting the rarefied disparity
plot(euro_ord_disp, rarefaction = 9, main = "Ordinated differences (rarefied)")
## Adding the p-value
text(1.5, 1400, paste0("p=",round(euro_ord_diff_rar[[2]][[1]], digit = 5) ))
```



As expected, the results are pretty similar in pattern but different in terms of scale. The median centroids distance is expressed in km in the "Distance differences" plots and in Euclidean units of variation in the "Ordinated differences" plots.

Chapter 5

Making stuff up!

The dispRity package also offers some advanced data simulation features to allow to test hypothesis, explore ordinate-spaces or metrics properties or simply playing around with data! All the following functions are based on the same modular architecture of the package and therefore can be used with most of the functions of the package.

5.1 Simulating discrete morphological data

The function sim.morpho allows to simulate discrete morphological data matrices (sometimes referred to as "cladistic" matrices). It allows to evolve multiple discrete characters on a given phylogenetic trees, given different models, rates, and states. It even allows to include proper inapplicable data to make datasets as messy as in real life!

In brief, the function sim.morpho takes a phylogenetic tree, the number of required characters, the evolutionary model, and a function from which to draw the rates. The package also contains a function for quickly checking the matrix's phylogenetic signal (as defined in systematics not phylogenetic comparative methods) using parsimony. The methods are described in details below

```
[,1] [,2] [,3] [,4] [,5] [,6]
                                         [,7] [,8] [,9]
## t15 "1"
             "1"
                   "0"
                         "1"
                              "1"
                                    "2"
                                          "1"
                                               "1"
## t12 "1"
             "1"
                   "0"
                              "1"
                                    "2"
                                               "1"
                                    "2"
             "1"
                   "0"
                              "1"
                                         "1"
                                               "1"
## t14 "1"
                   "0"
                                    "2"
                                         "1"
                                               "1"
                                                           "0"
## t3
             "0"
                   "1"
                         "0"
                              "1"
                                    "0"
                                         "0"
                                                     "1"
       "0"
```

Checking the matrix properties with a quick Maximum Parsimony tree search
check.morpho(my_matrix, my_tree)

```
## ## Maximum parsimony 139.0000000
## Consistency index 0.7625899
## Retention index 0.8881356
## Robinson-Foulds distance 0.0000000
```

Note that this example produces a tree with a great consistency index and an identical topology to the random coalescent tree! Nearly too good to be true...

5.1.1 A more detailed description

The protocol implemented here to generate discrete morphological matrices is based on the ones developed in [Guillerme and Cooper, 2016, O'Reilly et al., 2016, Puttick et al., 2017, O'Reilly et al., 2017].

- The first tree argument will be the tree on which to "evolve" the characters and therefore requires branch length. You can generate quick and easy random Yule trees using ape::rtree(number_of_taxa) but I would advise to use more realistic trees for more realistic simulations based on more realistic models (really realistic then) using the function tree.bd from the diversitree package [FitzJohn, 2012].
- The second argument, character is the number of characters. Pretty straight forward.
- The third, states is the proportion of characters states above two (yes, the minimum number of states is two). This argument intakes the proportion of *n*-states characters, for example states = c(0.5,0.3,0.2) will generate 50% of binary-state characters, 30% of three-state characters and 20% of four-state characters. There is no limit in the number of state characters proportion as long as the total makes up 100%.
- The forth, model is the evolutionary model for generating the character(s). More about this below.
- The fifth and sixth, rates and substitution are the model parameters described below as well.
- Finally, the two logical arguments, are self explanatory: invariant whether to allow invariant characters (i.e. characters that don't change) and verbose whether to print the simulation progress on your console.

5.1.1.1 Available evolutionary models

There are currently three evolutionary models implemented in sim.morpho but more will come in the future. Note also that they allow fine tuning parameters making them pretty plastic!

- "ER": this model allows any number of character states and is based on the Mk model [Lewis, 2001]. It assumes a unique overall evolutionary rate equal substitution rate between character states. This model is based on the ape::rTraitDisc function.
- "HKY": this is binary state character model based on the molecular HKY model [Hasegawa et al., 1985]. It uses the four molecular states (A,C,G,T) with a unique overall evolutionary rate and a biased substitution rate towards transitions (A <-> G or C <-> T) against transvertions (A <-> C and G <-> T). After evolving the nucleotide, this model transforms them into binary states by converting the purines (A and G) into state 0 and the pyrimidines (C and T) into state 1. This method is based on the phyclust::seq.gen.HKY function and was first proposed by O'Reilly et al. [2016].
- "MIXED": this model uses a random (uniform) mix between both the "ER" and the "HKY" models.

The models can take the following parameters: (1) rates is the evolutionary rate (i.e. the rate of changes along a branch: the evolutionary speed) and (2) substitution is the frequency of changes between one state or another. For example if a character can have high probability of changing (the evolutionary rate) with, each time a change occurs a probability of changing from state X to state Y (the substitution rate).

Note that in the "ER" model, the substitution rate is ignore because... by definition this (substitution) rate is equal!

The parameters arguments rates and substitution takes a distributions from which to draw the parameters values for each character. For example, if you want an "HKY" model with an evolutionary rate (i.e. speed) drawn from a uniform distribution bounded between 0.001 and 0.005, you can define it as rates = c(runif, min = 0.001, max = 0.005), runif being the function for random draws from a uniform distribution and max and min being the distribution parameters. These distributions should always be passed in the format c(random_distribution_function, distribution_parameters) with the names of the distribution parameters arguments.

5.1.1.2 Checking the results

An additional function, check.morpho runs a quick Maximum Parsimony tree search using the phangorn parsimony algorithm. It quickly calculates the parsimony score, the consistency and retention indices and, if a tree is provided (e.g. the tree used to generate the matrix) it calculates the Robinson-Foulds distance between the most parsimonious tree and the provided tree to determine how different they are.

5.1.1.3 Adding inapplicable characters

Once a matrix is generated, it is possible to apply inapplicable characters to it for increasing realism! Inapplicable characters are commonly designated as NA or simply -. They differ from missing characters? in their nature by being inapplicable rather than unknown. For example, considering a binary character defined as "colour of the tail" with the following states "blue" and "red"; on a taxa with no tail, the character should be coded as inapplicable ("-") since the state of the character "colour of tail" is known: it's neither "blue" or "red", it's just not there! It contrasts with coding it as missing ("?" - also called as ambiguous) where the state is unknown, for example, the taxon of interest is a fossil where the tail has no colour preserved or is not present at all due to bad conservation!

This type of characters can be added to the simulated matrices using the apply.NA function/ It takes, as arguments, the matrix, the source of inapplicability (NAs - more below), the tree used to generate the matrix and the two same invariant and verbose arguments as defined above. The NAs argument allows two types of sources of inapplicability:

- "character" where the inapplicability is due to the character (e.g. coding a character tail for species with no tail). In practice, the algorithm chooses a character X as the underlying character (e.g. "presence and absence of tail"), arbitrarily chooses one of the states as "absent" (e.g. 0 = absent) and changes in the next character Y any state next to character X state 0 into an inapplicable token ("-"). This simulates the inapplicability induced by coding the characters (i.e. not always biological).
- "clade" where the inapplicability is due to evolutionary history (e.g. a clade loosing its tail). In practice, the algorithm chooses a random clade in the tree and a random character Z and replaces the state of the taxa present in the clade by the inapplicable token ("-"). This simulates the inapplicability induced by evolutionary biology (e.g. the lose of a feature in a clade).

To apply these sources of inapplicability, simply repeat the number of inapplicable sources for the desired number of characters with inapplicable data.

```
## [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] ## t15 "0" "1" "0" "1" "0" "0" "1" "0" "1" "0"
```

```
"0"
                                   "0"
                                          "0"
                                                "0"
                                                      "1"
                                                                    "1"
                                                                           "0"
               "1"
                             "1"
                                                             "0"
                                                                           "0"
         "0"
               "0"
                      "0"
                             "1"
                                   "0"
                                          "0"
                                                "0"
                                                       "1"
                                                             "0"
                                                                    "1"
## t.14
                                                                    "1"
                                                                           "0"
         "0"
               "0"
                      "0"
                             "1"
                                   "0"
                                          "0"
                                                "0"
                                                       "1"
                                                             "0"
         "0"
               "0"
                      "1"
                             "0"
                                          "0"
                                                "0"
                                                       "0"
                                                                    "0"
                                                                           "1"
## t3
                      "1"
##
         "0"
               "0"
                             "0"
                                   "-"
                                          "0"
                                                "0"
                                                       "0"
                                                                    "0"
                                                                           "1"
   t11 "0"
               "0"
                      "1"
                             "0"
                                          "0"
                                                "0"
                                                       "0"
                                                                    "0"
                                                                            "1"
         "0"
                      "1"
                             "0"
                                          "0"
                                                "0"
                                                       "0"
                                                                           "1"
         "0"
               "0"
                      "0"
                             "0"
                                          "0"
                                                "0"
                                                       "0"
                                                                    "2"
                                                                            "1"
## t1
## t5
                             "0"
                                          "0"
                                                       "0"
```

5.1.2 Parameters for a realistic(ish) matrix

There are many parameters that can create a "realistic" matrix (i.e. not too different from the input tree with a consistency and retention index close to what is seen in the literature) but because of the randomness of the matrix generation not all parameters combination end up creating "good" matrices. The following parameters however, seem to generate fairly "realist" matrices with a starting coalescent tree, equal rates model with 0.85 binary characters and 0.15 three state characters, a gamma distribution with a shape parameter (α) of 5 and no scaling $(\beta = 1)$ with a rate of 100.

5.2 Simulating multidimensional spaces

0.000000

Robinson-Foulds distance

Another way to simulate data is to directly simulate an ordinated space with the space.maker function. This function allows users to simulate multidimensional spaces with a certain number of properties. For example, it is possible to design a multidimensional space with a specific distribution on each axis, a correlation between the axes and a specific cumulative variance per axis. This can be useful for creating ordinated spaces for null hypothesis, for example if you're using the function null.test [Díaz et al., 2016].

This function takes as arguments the number of elements (data points - elements argument) and dimensions (dimensions argument) to create the space and the distribution functions to be used for each axis. The distributions are passed through the distribution argument as... modular functions! You can either pass a single distribution function for all the axes (for example distribution = runif for all the axis being uniform) or a specific distribution function for each specific axis (for example distribution = c(runif, rnorm, rgamma)) for the first axis being uniform, the second normal and the third gamma). You can of course use your very own functions or use the ones implemented in dispRity for more complex ones (see below). Specific optional arguments for each of these distributions can be passed as a list via the arguments argument.

Furthermore, it is possible to add a correlation matrix to add a correlation between the axis via the cor.matrix argument or even a vector of proportion of variance to be bear by each axis via the scree argument to simulate realistic ordinated spaces.

Here is a simple two dimensional example:

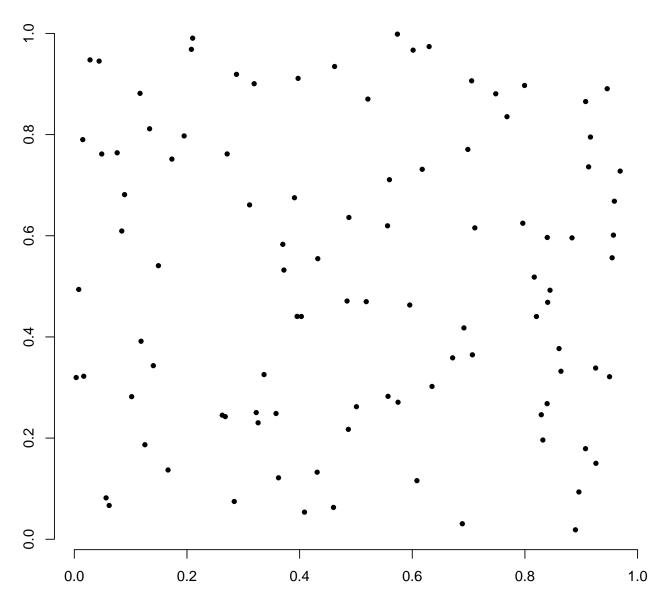
```
## Graphical options
op <- par(bty = "n")

## A square space
square_space <- space.maker(100, 2, runif)

## The resulting 2D matrix
head(square_space)</pre>
```

```
## [,1] [,2]
## [1,] 0.9548679 0.55645395
## [2,] 0.3721235 0.53218069
## [3,] 0.3229877 0.25041834
## [4,] 0.8404244 0.46840450
## [5,] 0.2839796 0.07466592
## [6,] 0.2627652 0.24523019
## Visualising the space
plot(square_space, pch = 20, xlab = "", ylab = "", main = "Uniform 2D space")
```

Uniform 2D space



Of course, more complex spaces can be created by changing the distributions, their arguments or adding a correlation matrix or a cumulative variance vector:

```
## [,1] [,2] [,3]
## [1,] 1.0 0.8 0.2
## [2,] 0.8 1.0 0.7
## [3,] 0.2 0.7 1.0
```

5.2.1 Personalised dimensions distributions

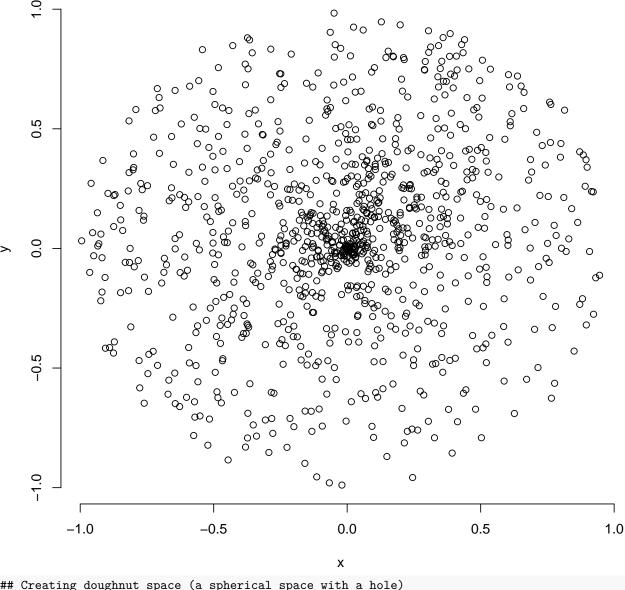
Following the modular architecture of the package, it is of course possible to pass home made distribution functions to the distribution argument. For example, the random.circle function is a personalised one implemented in dispRity. This function allows to create circles based on basic trigonometry allowing to axis to covary to produce circle coordinates. By default, this function generates two sets of coordinates with a distribution argument and a minimum and maximum boundary (inner and outer respectively) to create nice sharp edges to the circle. The maximum boundary is equivalent to the radius of the circle (it removes coordinates beyond the circle radius) and the minimum is equivalent to the radius of a smaller circle with no data (it removes coordinates below this inner circle radius).

```
## Graphical options
op <- par(bty = "n")

## Generating coordinates for a normal circle with a upper boundary of 1
circle <- random.circle(1000, rnorm, inner = 0, outer = 1)

## Plotting the circle
plot(circle, xlab = "x", ylab = "y", main = "A normal circle")</pre>
```

A normal circle



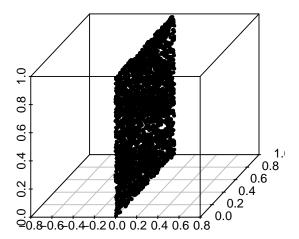
5.2.2 Visualising the space

I suggest using the excellent scatterplot3d package to play around and visualise the simulated spaces:

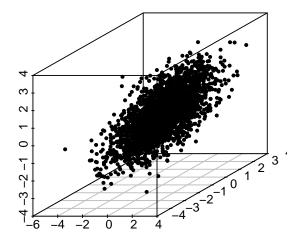
```
## Graphical options
op <- par(mfrow = (c(2, 2)), bty = "n")
## Visualising 3D spaces
require(scatterplot3d)</pre>
```

Loading required package: scatterplot3d

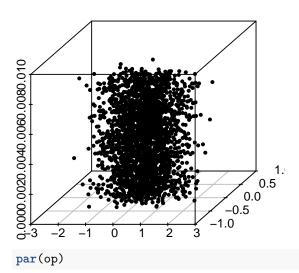
Plane space



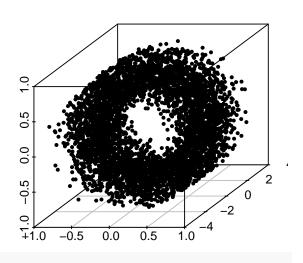
Normal ellipsoid space



Normal cylindrical space



Doughnut space



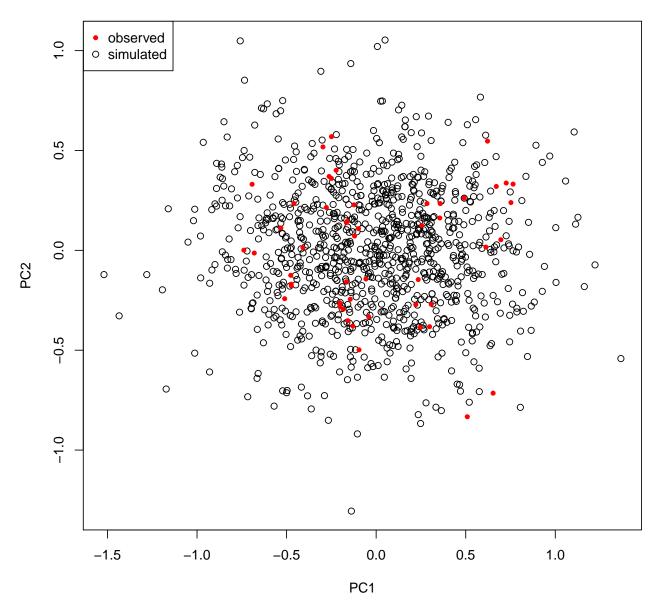
5.2.3 Generating realistic spaces

It is possible to generate "realistic" spaces by simply extracting the parameters of an existing space and scaling it up to the simulated space. For example, we can extract the parameters of the BeckLee_mat50 ordinated space and simulate a similar space.

```
## Loading the data
data(BeckLee_mat50)

## Number of dimensions
obs_dim <- ncol(BeckLee_mat50)</pre>
```

```
## Observed correlation between the dimensions
obs_correlations <- cor(BeckLee_mat50)</pre>
## Observed mean and standard deviation per axis
obs_mu_sd_axis <- mapply(function(x,y) list("mean" = x, "sd" = y),
                         as.list(apply(BeckLee_mat50, 2, mean)),
                         as.list(apply(BeckLee_mat50, 2, sd)), SIMPLIFY = FALSE)
## Observed overall mean and standard deviation
obs_mu_sd_glob <- list("mean" = mean(BeckLee_mat50), "sd" = sd(BeckLee_mat50))
## Scaled observed variance per axis (scree plot)
obs_scree <- variances(BeckLee_mat50)/sum(variances(BeckLee_mat50))</pre>
## Generating our simulated space
simulated_space <- space.maker(1000, dimensions = obs_dim,</pre>
                               distribution = rep(list(rnorm), obs_dim),
                               arguments = obs_mu_sd_axis,
                               cor.matrix = obs_correlations)
## Visualising the fit of our data in the space (in the two first dimensions)
plot(simulated_space[,1:2], xlab = "PC1", ylab = "PC2")
points(BeckLee_mat50[,1:2], col = "red", pch = 20)
legend("topleft", legend = c("observed", "simulated"),
        pch = c(20,21), col = c("red", "black"))
```

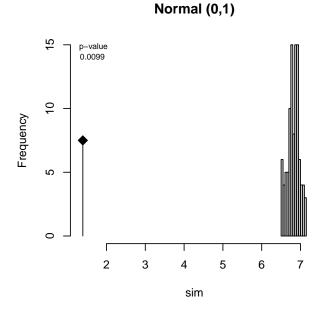


It is now possible to simulate a space using these observed arguments to test several hypothesis:

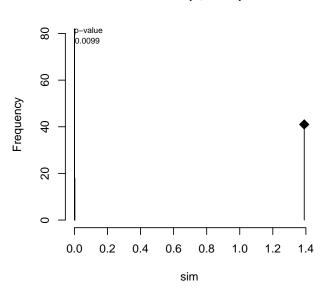
- Is the space uniform or normal?
- If the space is normal, is the mean and variance global or specific for each axis?

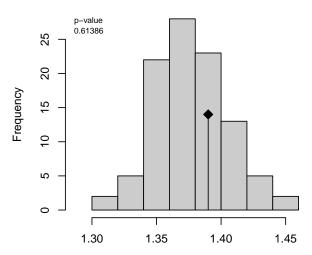
P-value 0.0099 1.4 1.5 1.6 1.7 1.8 1.9 2.0 sim

Uniform (0,1)



Normal (0,0.201)





Normal (variable + correlation)

sim

If we measure disparity as the median distance from the morphospace centroid, we can explain the distribution of the data as normal with the variable observed mean and standard deviation and with a correlation between the dimensions.

Chapter 6

The guts of the dispRity package

6.1 Manipulating dispRity objects

Disparity analysis involves a lot of manipulation of many matrices (especially when bootstrapping) which can be impractical to visualise and will quickly overwhelm your R console. Even the simple Beck and Lee 2014 example above produces an object with > 72 lines of lists of matrices!

Therefore dispRity uses a specific class of object called a dispRity object. These objects allow users to use S3 method functions such as summary.dispRity, plot.dispRity and print.dispRity. dispRity also contains various utility functions that manipulate the dispRity object (e.g. sort.dispRity, extract.dispRity see the full list in the next section). These functions modify the dispRity object without having to delve into its complex structure! The full structure of a dispRity object is detailed here.

```
## Loading the example data
data(disparity)
## What is the class of the median_centroids object?
class(disparity)
## [1] "dispRity"
## What does the object contain?
names(disparity)
## [1] "matrix"
                   "call"
                                "subsets"
                                             "disparity"
## Summarising it using the S3 method print.dispRity
disparity
## ---- dispRity object ----
## 7 continuous (acctran) time subsets for 99 elements with 97 dimensions:
        90, 80, 70, 60, 50 ...
## Data was bootstrapped 100 times (method:"full") and rarefied to 20, 15, 10, 5 elements.
## Disparity was calculated as: c(median, centroids).
Note that it is always possible to recall the full object using the argument all = TRUE in print.dispRity:
## Display the full object
print(disparity, all = TRUE)
## This is more nearly ~ 5000 lines on my 13 inch laptop screen!
```

6.2 dispRity utilities

The package also provides some utility functions to facilitate multidimensional analysis.

6.2.1 dispRity object utilities

The first set of utilities are functions for manipulating dispRity objects:

6.2.1.1 make.dispRity

This function creates empty dispRity objects.

```
## Creating an empty dispRity object
make.dispRity()

## Empty dispRity object.

## Creating an "empty" dispRity object with a matrix
(disparity_obj <- make.dispRity(matrix(rnorm(20), 5, 4)))

## ---- dispRity object ----
## Contains only a matrix 5x4.</pre>
```

6.2.1.2 fill.dispRity

This function initialises a dispRity object and generates its call properties.

```
## The dispRity object's call is indeed empty
disparity_obj$call

## list()

## Filling an empty disparity object (that needs to contain at least a matrix)
(disparity_obj <- fill.dispRity(disparity_obj))

## ---- dispRity object ----

## 5 elements with 4 dimensions.

## The dipRity object has now the correct minimal attributes
disparity_obj$call</pre>
```

```
## $dimensions
## [1] 4
```

6.2.1.3 matrix.dispRity

This function extracts a specific matrix from a disparity object. The matrix can be one of the bootstrapped matrices or/and a rarefied matrix.

```
## Extracting the matrix containing the coordinates of the elements at time 50
str(matrix.dispRity(disparity, "50"))
## num [1:18, 1:97] -0.1038 0.2844 0.2848 0.0927 0.1619 ...
```

```
## num [1:18, 1:97] -0.1038 0.2844 0.2848 0.0927 0.1619 ...
## - attr(*, "dimnames")=List of 2
## ..$ : chr [1:18] "Leptictis" "Dasypodidae" "n24" "Potamogalinae" ...
## ..$ : NULL
```

```
## Extracting the 3rd bootstrapped matrix with the 2nd rarefaction level
## (15 elements) from the second group (80 Mya)
str(matrix.dispRity(disparity, subsets = 1, bootstrap = 3, rarefaction = 2))

## num [1:15, 1:97] -0.7161 0.3496 -0.573 -0.0445 -0.1427 ...
## - attr(*, "dimnames")=List of 2
## ..$ : chr [1:15] "n7" "n34" "Maelestes" "n20" ...
## ..$ : NULL
```

6.2.1.4 get.subsets.dispRity

This function creates a dispRity object that contains only elements from one specific subsets.

```
## Extracting all the data for the crown mammals
(crown_mammals <- get.subsets.dispRity(disp_crown_stemBS, "Group.crown"))

## The object keeps the properties of the parent object but is composed of only one subsets
length(crown_mammals$subsets)</pre>
```

6.2.1.5 extract.dispRity

This function extracts the calculated disparity values of a specific matrix.

```
## Extracting the observed disparity (default)
extract.dispRity(disparity)

## Extracting the disparity from the bootstrapped values from the
## 10th rarefaction level from the second subsets (80 Mya)
extract.dispRity(disparity, observed = FALSE, subsets = 2, rarefaction = 10)
```

6.2.1.6 scale.dispRity

This is the S3 method of scale (scaling and/or centring) that can be applied to the disparity data of a dispRity object.

```
## Getting the disparity values of the time subsets
head(summary(disparity))

## Scaling the same disparity values
head(summary(scale(disparity, scale = TRUE)))

## Scaling and centering:
head(summary(scale(disparity, scale = TRUE, center = TRUE)))
```

6.2.1.7 sort.dispRity

This is the S3 method of sort for sorting the subsets alphabetically (default) or following a specific pattern.

```
## Sorting the disparity subsets in inverse alphabetic order
head(summary(sort(disparity, decreasing = TRUE)))

## Customised sorting
head(summary(sort(disparity, sort = c(7, 1, 3, 4, 5, 2, 6))))
```

6.3 The dispRity object content

The functions above are utilities to easily and safely access different elements in the dispRity object. Alternatively, of course, each elements can be accessed manually. Here is an explanation on how it works. The dispRity object is a list of two to four elements, each of which are detailed below:

- \$matrix: an object of class matrix, the full multidimensional space.
- \$call: an object of class list containing information on the dispRity object content.
- \$subsets: an object of class list containing the subsets of the multidimensional space.
- \$disparity: an object of class list containing the disparity values.

The dispRity object is loosely based on C structure objects. In fact, it is composed of one unique instance of a matrix (the multidimensional space) upon which the metric function is called via "pointers" to only a certain number of elements and/or dimensions of this matrix. This allows for: (1) faster and easily tractable execution time: the metric functions are called through apply family function and can be parallelised; and (2) a really low memory footprint: at any time, only one matrix is present in the R environment rather than multiple copies of it for each subset.

6.3.1 \$matrix

This is the multidimensional space, stored in the R environment as a matrix object. It requires row names but not column names. By default, if the row names are missing, dispRity function will arbitrarily generate them in numeric order (i.e. rownames(matrix) <- 1:nrow(matrix)). This element of the dispRity object is never modified.

6.3.2 \$call

This element contains the information on the dispRity object content. It is a list that can contain the following:

- \$call\$subsets: a vector of character with information on the subsets type (either "continuous", "discrete" or "custom") and their eventual model ("acctran", "deltran", "random", "proximity", "equal.split", "gradual.split"). This element generated only once via time.subsets() and custom.subsets().
- \$call\$dimensions: either a single numeric value indicating how many dimensions to use or a vector of numeric values indicating which specific dimensions to use. This element is by default the number of columns in \$matrix but can be modified through boot.matrix() or dispRity().
- \$call\$bootstrap: this is a list containing three elements:
 - [[1]]: the number of bootstrap replicates (numeric)
 - [[2]]: the bootstrap method (character)
 - [[3]]: the rarefaction levels (numeric vector)
- \$call\$disparity: this is a list containing one element, \$metric, that is a list containing the different functions passed to the metric argument in dispRity. These are call elements and get modified each time the dispRity function is used (the first element is the first metric(s), the second, the second metric(s), etc.).

6.3.3 \$subsets

This element contain the eventual subsets of the multidimensional space. It is a list of subset names. Each subset name is in turn a list of at least one element called elements which is in turn a matrix. This elements matrix is the raw (observed) elements in the subsets. The elements matrix is composed of numeric values in one column and n rows (the number of elements in the subset). Each of these values are

a "pointer" (C inspired) to the element of the \$matrix. For example, lets assume a dispRity object called disparity, composed of at least one subsets called sub1:

disparity\$subsets\$sub1\$elements

[,1] [1,] 5 [2,] 4 [3,] 6 [4,] 7

The values in the matrix "point" to the elements in **\$matrix**: here, the multidimensional space with only the 4th, 5th, 6th and 7th elements. The following elements in **diparity\$subsets\$sub1** will correspond to the same "pointers" but drawn from the bootstrap replicates. The columns will correspond to different bootstrap replicates. For example:

disparity\$subsets\$sub1[[2]]

```
[,1] [,2] [,3] [,4]
[1,]
        57
              43
                    70
[2,]
        43
              44
                     4
                           4
[3,]
        42
              84
                    44
                           1
[4,]
        84
                          10
```

This signifies that we have four bootstrap pseudo-replicates pointing each time to four elements in $\mathtt{$matrix}$. The next element ([[3]]) will be the same for the eventual first rarefaction level (i.e. the resulting bootstrap matrix will have m rows where m is the number of elements for this rarefaction level). The next element after that ([[4]]) will be the same for with an other rarefaction level and so forth...

6.3.4 \$disparity

The \$disparity element is identical to the \$subsets element structure (a list of list(s) containing matrices) but the matrices don't contain "pointers" to \$matrix but the disparity result of the disparity metric applied to the "pointers". For example, in our first example (\$elements) from above, if the disparity metric is of dimensions level 1, we would have:

```
disparity$disparity$sub1$elements
    [,1]
[1,] 1.82
```

This is the observed disparity (1.82) for the subset called **sub1**. If the disparity metric is of dimension level 2 (say the function **range** that outputs two values), we would have:

disparity\$disparity\$sub1\$elements

```
[,1]
[1,] 0.82
[2,] 2.82
```

The following elements in the list follow the same logic as before: rows are disparity values (one row for a dimension level 1 metric, multiple for a dimensions level 2 metric) and columns are the bootstrap replicates (the bootstrap with all elements followed by the eventual rarefaction levels). For example for the bootstrap without rarefaction (second element of the list):

Chapter 7

Palaeobiology demo: disparity-through-time and within groups

This demo aims to give quick overview of the dispRity package (v.0.4) for palaeobiology analyses of disparity, including disparity through time analyses.

This demo showcases a typical disparity-through-time analysis: we are going to test whether the disparity changed through time in a subset of eutherian mammals from the last 100 million years using a dataset from Beck and Lee (2014).

7.1 Before starting

7.1.1 The morphospace

In this example, we are going to use a subset of the data from Beck and Lee [2014]. See the example data description for more details. Briefly, this dataset contains an ordinated matrix of 50 discrete characters from mammals (BeckLee_mat50), another matrix of the same 50 mammals and the estimated discrete data characters of their descendants (thus 50 + 49 rows, BeckLee_mat99), a dataframe containing the ages of each taxon in the dataset (BeckLee_ages) and finally a phylogenetic tree with the relationships among the 50 mammals (BeckLee_tree). The ordinated matrix will represent our full morphospace, i.e. all the mammalian morphologies that ever existed through time (for this dataset).

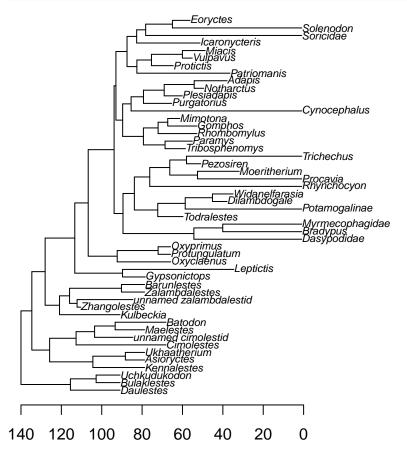
```
## Loading demo and the package data
library(dispRity)

## Setting the random seed for repeatability
set.seed(123)

## Loading the ordinated matrix/morphospace:
data(BeckLee_mat50)
head(BeckLee_mat50[,1:5])
```

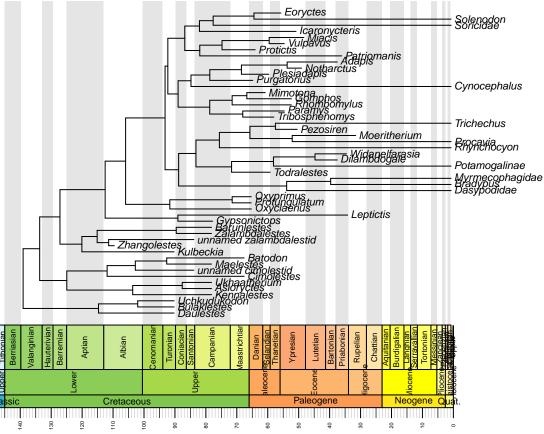
```
## Cimolestes -0.5319679 0.1117759259 0.09865194 -0.1933148 0.2035833 ## Maelestes -0.4087147 0.0139690317 0.26268300 0.2297096 0.1310953 ## Batodon -0.6923194 0.3308625215 -0.10175223 -0.1899656 0.1003108
```

```
## Bulaklestes -0.6802291 -0.0134872777 0.11018009 -0.4103588 0.4326298
## Daulestes
                -0.7386111 \quad 0.0009001369 \quad 0.12006449 \ -0.4978191 \ 0.4741342
## Uchkudukodon -0.5105254 -0.2420633915 0.44170317 -0.1172972 0.3602273
dim(BeckLee_mat50)
## [1] 50 48
## The morphospace contains 50 taxa and has 48 dimensions (or axes)
## Showing a list of first and last occurrences data for some fossils
data(BeckLee_ages)
head(BeckLee_ages)
##
               FAD LAD
              37.2 36.8
## Adapis
## Asioryctes 83.6 72.1
## Leptictis 33.9 33.3
## Miacis
              49.0 46.7
## Mimotona
              61.6 59.2
## Notharctus 50.2 47.0
## Plotting a phylogeny
data(BeckLee_tree)
plot(BeckLee_tree, cex = 0.7)
axisPhylo(root = 140)
```



You can have an even nicer looking tree if you use the strap package!





7.2 A disparity-through-time analysis

7.2.1 Splitting the morphospace through time

One of the crucial steps in disparity-through-time analysis is to split the full morphospace into smaller time subsets that contain the total number of morphologies at certain points in time (time-slicing) or during certain periods in time (time-binning). Basically, the full morphospace represents the total number of morphologies across all time and will be greater than any of the time subsets of the morphospace.

The dispRity package provides a time.subsets function that allows users to split the morphospace into time slices (using method = continuous) or into time bins (using method = discrete). In this example, we are going to split the morphospace into five equal time bins of 20 million years long from 100 million years ago to the present. We will also provide to the function a table containing the first and last occurrences dates for some fossils to take into account that some fossils might occur in several of our different time bins.

```
## Creating the vector of time bins ages
(time_bins <- rev(seq(from = 0, to = 100, by = 20)))

## [1] 100 80 60 40 20 0

## Splitting the morphospace using the time.subsets function
(binned_morphospace <- time.subsets(data = BeckLee_mat50, tree = BeckLee_tree,</pre>
```

method = "discrete", time = time_bins, inc.nodes = FALSE,

```
FADLAD = BeckLee_ages))
## ---- dispRity object ----
## 5 discrete time subsets for 50 elements:
       100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
The output object is a dispRity object (see more about that here. In brief, however, dispRity objects
are lists of different elements (i.e. disparity results, morphospace time subsets, morphospace attributes, etc.)
that display only a summary of the object when calling the object to avoiding filling the R console with
superfluous output.
## Printing the class of the object
class(binned_morphospace)
## [1] "dispRity"
## Printing the content of the object
str(binned_morphospace)
## List of 3
    $ matrix : num [1:50, 1:48] -0.532 -0.409 -0.692 -0.68 -0.739 ...
     ..- attr(*, "dimnames")=List of 2
##
##
     ....$ : chr [1:50] "Cimolestes" "Maelestes" "Batodon" "Bulaklestes" ...
##
     .. ..$ : NULL
##
    $ call
             :List of 1
##
    ..$ subsets: chr "discrete"
   $ subsets:List of 5
##
##
    ..$ 100 - 80:List of 1
     ....$ elements: int [1:8, 1] 5 4 6 8 43 10 11 42
##
##
     ..$ 80 - 60 :List of 1
     ....$ elements: int [1:15, 1] 7 8 9 1 2 3 12 13 14 44 ...
##
     ..$ 60 - 40 :List of 1
     ....$ elements: int [1:13, 1] 41 49 24 25 26 27 28 21 22 19 ...
##
##
     ..$ 40 - 20 :List of 1
##
     ....$ elements: int [1:6, 1] 15 39 40 35 23 47
     ..$ 20 - 0 :List of 1
     ....$ elements: int [1:10, 1] 36 37 38 32 33 34 50 48 29 30
##
    - attr(*, "class")= chr "dispRity"
names(binned_morphospace)
## [1] "matrix" "call"
                            "subsets"
## Printing the object as a dispRity class
binned_morphospace
## ---- dispRity object ----
## 5 discrete time subsets for 50 elements:
       100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
    These objects will gradual splitly contain more information when completing the following steps
```

in the disparity-through-time analysis.

7.2.2 Bootstrapping the data

Once we obtain our different time subsets, we can bootstrap and rarefy them (i.e. pseudo-replicating the data). The bootstrapping allows us to make each subset more robust to outliers and the rarefaction allows

us to compare subsets with the same number of taxa to remove sampling biases (i.e. more taxa in one subset than the others). The boot.matrix function bootstraps the dispRity object and the rarefaction option within performs rarefaction.

```
## Bootstrapping each time subset 100 times (default)
(boot_bin_morphospace <- boot.matrix(binned_morphospace))</pre>
## ---- dispRity object ----
## 5 discrete time subsets for 50 elements with 48 dimensions:
       100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
## Data was bootstrapped 100 times (method:"full").
## Getting the minimum number of rows (i.e. taxa) in the time subsets
min(size.subsets(boot_bin_morphospace))
## [1] 6
## Bootstrapping each time subset 100 times and rarefying them
(rare_bin_morphospace <- boot.matrix(binned_morphospace, bootstraps = 100,</pre>
   rarefaction = 6))
   ---- dispRity object ----
## 5 discrete time subsets for 50 elements with 48 dimensions:
       100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
## Data was bootstrapped 100 times (method:"full") and rarefied to 6 elements.
```

7.2.3 Calculating disparity

We can now calculate the disparity within each time subsets along with some confidence intervals generated by the pseudoreplication step above (bootstraps/rarefaction). Disparity can be calculated in many ways and this package allows users to come up with their own disparity metrics. For more details, please refer to the dispRity metric section.

In this example, we are going to calculate the spread of the data in each time subset by calculating disparity as the sum of the variance of each dimension of the morphospace in each time subset using the dispRity function. Thus, in this example, disparity is defined by the multi-dimensional variance of each time subset (i.e. the spread of the taxa within the morphospace). Note that this metric comes with a caveat (not solved here) since it ignores covariances among the dimensions of the morphospace. We use this here because it is a standard metric used in disparity-through-time analysis [Wills et al., 1994].

```
## Calculating disparity for the bootstrapped data
(boot_disparity <- dispRity(boot_bin_morphospace, metric = c(sum, variances)))

## ---- dispRity object ----
## 5 discrete time subsets for 50 elements with 48 dimensions:
## 100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
## Data was bootstrapped 100 times (method:"full").
## Disparity was calculated as: c(sum, variances).

## Calculating disparity for the rarefied data
(rare_disparity <- dispRity(rare_bin_morphospace, metric = c(sum, variances)))

## ---- dispRity object ----
## 5 discrete time subsets for 50 elements with 48 dimensions:
## 100 - 80, 80 - 60, 60 - 40, 40 - 20, 20 - 0.
## Data was bootstrapped 100 times (method:"full") and rarefied to 6 elements.
## Disparity was calculated as: c(sum, variances).</pre>
```

The dispRity function does not actually display the calculated disparity values but rather only the properties of the disparity object (size, subsets, metric, etc.). To display the actual calculated scores, we need to summarise the disparity object using the S3 method summary that is applied to a dispRity object (see ?summary.dispRity for more details).

As for any R package, you can refer to the help files for each individual function for more details.

```
## Summarising the disparity results
summary(boot_disparity)
                                  25%
                                       75% 97.5%
     subsets n
               obs bs.median 2.5%
## 1 100 - 80 8 1.675
                      1.488 1.087 1.389 1.568 1.648
## 2 80 - 60 15 1.782
                      1.679 1.538 1.631 1.728 1.792
## 4 40 - 20 6 2.022
                     1.707 1.212 1.537 1.822 1.942
     20 - 0 10 1.971
                      1.794 1.598 1.716 1.842 1.890
summary(rare_disparity)
```

```
##
     subsets n obs bs.median 2.5%
                                      25%
                                           75% 97.5%
## 1 100 - 80 8 1.675 1.484 1.194 1.400 1.547 1.636
## 2 100 - 80 6 NA
                       1.477 0.993 1.361 1.569 1.698
                      1.674 1.517 1.600 1.725 1.793
## 3 80 - 60 15 1.782
## 4 80 - 60 6 NA
                     1.655 1.299 1.532 1.754 1.882
## 5 60 - 40 13 1.913
                        1.767 1.601 1.714 1.829 1.861
## 6 60 - 40 6 NA
                        1.787 1.314 1.672 1.879 1.984
## 7 40 - 20 6 2.022
                        1.736 1.281 1.603 1.822 1.948
## 8
     20 - 0 10 1.971
                        1.807 1.595 1.729 1.856 1.917
## 9
    20 - 0 6 NA
                        1.790 1.435 1.718 1.873 1.995
```

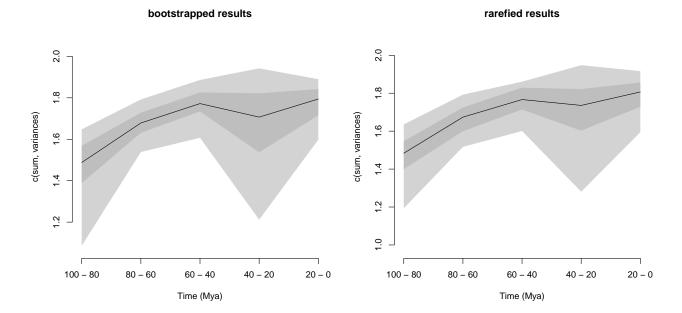
The summary.dispRity function comes with many options on which values to calculate (central tendency and quantiles) and on how many digits to display. Refer to the function's manual for more details.

7.2.4 Plotting the results

It is sometimes easier to visualise the results in a plot than in a table. For that we can use the plot S3 function to plot the dispRity objects (see ?plot.dispRity for more details).

```
## Graphical options
quartz(width = 10, height = 5); par(mfrow = (c(1,2)), bty = "n")

## Plotting the bootstrapped and rarefied results
plot(boot_disparity, type = "continuous", main = "bootstrapped results")
plot(rare_disparity, type = "continuous", main = "rarefied results")
```



7.3 Testing differences

[[1]]

Finally, to draw some valid conclusions from these results, we can apply some statistical tests. We can test, for example, if mammalian disparity changed significantly through time over the last 100 million years. To do so, we can compare the means of each time-bin in a sequential manner to see whether the disparity in bin n + 1, and whether this is in turn equal to the disparity in bin n + 2, etc. Because our data is temporally autocorrelated (i.e. what happens in bin n + 1 depends on what happened in bin n) and pseudoreplicated (i.e. each bootstrap draw creates non-independent time subsets because they are all based on the same time subsets), we apply a non-parametric mean comparison: the wilcox.test. Also, we need to apply a p-value correction (e.g. Bonferroni correction) to correct for multiple testing (see ?p.adjust for more details).

```
## Testing the differences between bins in the bootstrapped dataset.
test.dispRity(boot_disparity, test = wilcox.test, comparison = "sequential",
    correction = "bonferroni")
## [[1]]
##
                      statistic: W
## 100 - 80 : 80 - 60
                               471
## 80 - 60 : 60 - 40
                              1562
  60 - 40 : 40 - 20
                              6250
## 40 - 20 : 20 - 0
                              3725
##
## [[2]]
##
                           p.value
## 100 - 80 : 80 - 60 7.427563e-28
## 80 - 60 : 60 - 40 1.798899e-16
## 60 - 40 : 40 - 20
                     9.061511e-03
## 40 - 20 : 20 - 0
                      7.379715e-03
## Testing the differences between bins in the rarefied dataset.
test.dispRity(rare_disparity, test = wilcox.test, comparison = "sequential",
    correction = "bonferroni")
```

```
##
                      statistic: W
## 100 - 80 : 80 - 60
                               662
                              1814
## 80 - 60 : 60 - 40
## 60 - 40 : 40 - 20
                              5752
## 40 - 20 : 20 - 0
                              3621
##
## [[2]]
##
                           p.value
## 100 - 80 : 80 - 60 1.214988e-25
## 80 - 60 : 60 - 40 2.823697e-14
## 60 - 40 : 40 - 20 2.653018e-01
## 40 - 20 : 20 - 0
                      3.026079e-03
```

Here our results show significant changes in disparity through time between all time bins (all p-values < 0.05). However, when looking at the rarefied results, there is no significant difference between the time bins in the Palaeogene (60-40 to 40-20 Mya), suggesting that the differences detected in the first test might just be due to the differences in number of taxa sampled (13 or 6 taxa) in each time bin.

Chapter 8

Ecology demo

This is an example of typical disparity analysis that can be performed in ecology.

8.1 Data

For this example, we will use the famous iris inbuilt data set

```
data(iris)
```

This data contains petal and sepal length for 150 individual plants sorted into three species.

```
## Separating the species
species <- iris[,5]
## Which species?
unique(species)</pre>
```

```
## [1] setosa versicolor virginica
## Levels: setosa versicolor virginica
## Separating the petal/sepal length
measurements <- iris[,1:4]
head(measurements)</pre>
```

```
Sepal.Length Sepal.Width Petal.Length Petal.Width
##
## 1
               5.1
                            3.5
                                          1.4
                                                       0.2
## 2
               4.9
                            3.0
                                          1.4
                                                       0.2
## 3
               4.7
                            3.2
                                          1.3
                                                       0.2
## 4
               4.6
                            3.1
                                          1.5
                                                       0.2
## 5
               5.0
                            3.6
                                          1.4
                                                       0.2
               5.4
                            3.9
                                          1.7
                                                       0.4
```

We can then ordinate the data using a PCA (prcomp function) thus defining our four dimensional space as the poetically named petal-space.

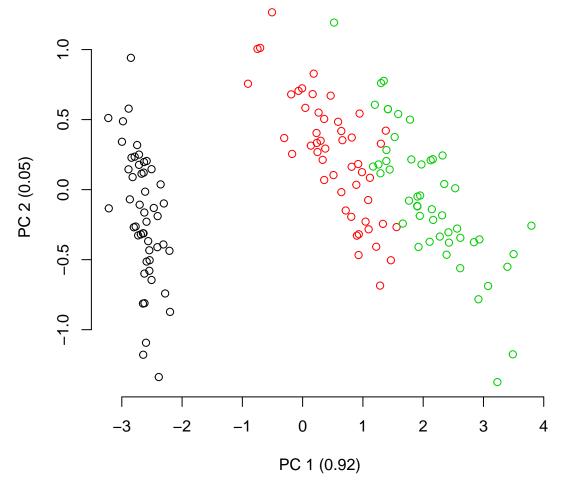
```
## Ordinating the data
ordination <- prcomp(measurements)

## The petal-space
petal_space <- ordination$x</pre>
```

```
## Adding the elements names to the petal-space (the individuals IDs)
rownames(petal_space) <- 1:nrow(petal_space)</pre>
```

8.2 Classic analysis

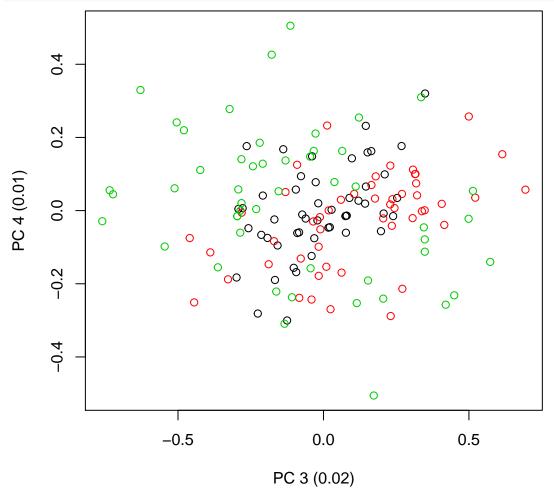
A classical way to represent this ordinated data would be to use two dimensional plots to look at how the different species are distributed in the petal-space.



This shows the distribution of the different species in the petal-space along the two first axis of variation. This is a pretty standard way to visualise the multidimensional space and further analysis might be necessary to test wether the groups are different such as a linear discriminant analysis (LDA). However, in this case

we are ignoring the two other dimensions of the ordination! If we look at the two other axis we see a totally different result:

```
## Plotting the two second axis of the petal-space
plot(petal_space[, 3], petal_space[, 4], col = species,
    xlab = paste0("PC 3 (", round(variances[3], 2), ")"),
    ylab = paste0("PC 4 (", round(variances[4], 2), ")"))
```



Additionally, these two represented dimensions do not represent a biological reality *per se*; i.e. the values on the first dimension do not represent a continuous trait (e.g. petal length), instead they just represent the ordinations of correlations between the data and some factors.

Therefore, we might want to approach this problem without getting stuck in only two dimensions and consider the whole dataset as a n-dimensional object.

8.3 A multidimensional approach with dispRity

The first step is to create different subsets that represent subsets of the ordinated space (i.e. sub-regions within the n-dimensional object). Each of these subsets will contain only the individuals of a specific species.

```
"virginica" = which(species == "virginica")))
## Visualising the dispRity object content
petal_subsets
## ---- dispRity object ----
## 3 customised subsets for 150 elements:
## setosa, versicolor, virginica.
```

This created a dispRity object (more about that here) with three subsets corresponding to each subspecies.

8.3.1 Bootstrapping the data

We can the bootstrap the subsets to be able test the robustness of the measured disparity to outliers. We can do that using the default options of boot.matrix (more about that here):

```
## Bootstrapping the data
(petal_bootstrapped <- boot.matrix(petal_subsets))

## ---- dispRity object ----
## 3 customised subsets for 150 elements with 4 dimensions:
## setosa, versicolor, virginica.
## Data was bootstrapped 100 times (method:"full").</pre>
```

8.3.2 Calculating disparity

Disparity can be calculated in many ways, therefore the dispRity function allows users to define their own measure of disparity. For more details on measuring disparity, see the dispRity metrics section.

In this example, we are going to define disparity as the median distance between the different individuals and the centroid of the ordinated space. High values of disparity will indicate a generally high spread of points from this centroid (i.e. on average, the individuals are far apart in the ordinated space). We can define the metrics easily in the dispRity function by feeding them to the metric argument. Here we are going to feed the functions stats::median and dispRity::centroids which calculates distances between elements and their centroid.

```
## Calculating disparity as the median distance between each elements and
## the centroid of the petal-space
(petal_disparity <- dispRity(petal_bootstrapped, metric = c(median, centroids)))

## ---- dispRity object ----
## 3 customised subsets for 150 elements with 4 dimensions:
## setosa, versicolor, virginica.
## Data was bootstrapped 100 times (method:"full").
## Disparity was calculated as: c(median, centroids).</pre>
```

8.3.3 Summarising the results (plot)

Similarly to the custom.subsets and boot.matrix function, dispRity displays a dispRity object. But we are definitely more interested in actually look at the calculated values.

First we can summarise the data in a table by simply using summary:

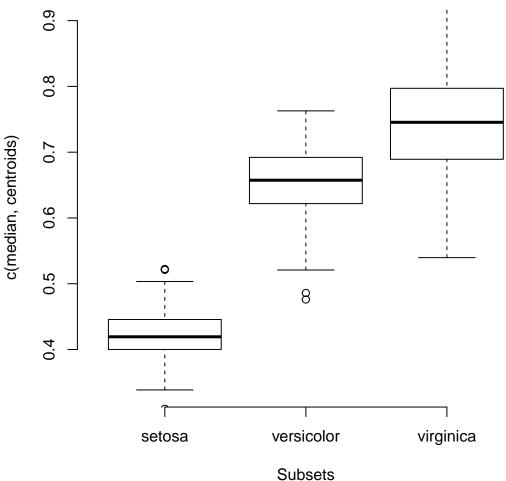
```
## Displaying the summary of the calculated disparity
summary(petal_disparity)
```

```
## subsets n obs bs.median 2.5% 25% 75% 97.5% ## 1 setosa 50 0.421 0.419 0.342 0.401 0.445 0.503 ## 2 versicolor 50 0.693 0.657 0.530 0.622 0.692 0.733 ## 3 virginica 50 0.785 0.745 0.577 0.690 0.797 0.880
```

We can also plot the results in a similar way:

```
## Graphical options
par(bty = "n")

## Plotting the disparity in the petal_space
plot(petal_disparity)
```



Now contrary to simply plotting the two first axis of the PCA where we saw that the species have a different position in the two first petal-space, we can now also see that they occupy this space clearly differently!

8.3.4 Testing hypothesis

Finally we can test our hypothesis that we guessed from the disparity plot (that some groups occupy different volume of the petal-space) by using the test.dispRity option.

```
## Fitting a linear model to our data
disparity_lm <- test.dispRity(petal_disparity, test = lm, comparisons = "all")</pre>
```

Warning in test.dispRity(petal_disparity, test = lm, comparisons = "all"): Multiple p-values will be calc

Post-hoc testing of the differences between species (corrected for multiple tests)
test.dispRity(petal_disparity, test = t.test, correction = "bonferroni")

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1

```
## [[1]]
##
                          statistic: t
## setosa : versicolor
                            -33.714480
## setosa : virginica
                            -34.257797
## versicolor : virginica
                             -8.595829
##
## [[2]]
##
                          parameter: df
## setosa : versicolor
                               189.0217
## setosa : virginica
                               150.1371
## versicolor : virginica
                               171.2387
##
## [[3]]
##
                               p.value
## setosa : versicolor
                          2.107278e-81
## setosa : virginica
                          2.252270e-72
## versicolor : virginica 1.506037e-14
```

This will inflate Type I error!

We can now see that there is a significant difference in petal-space occupancy between all species of iris.

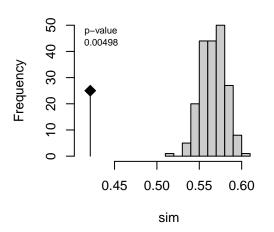
8.3.4.1 Setting up a multidimensional null-hypothesis

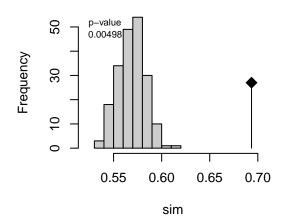
One other series of test can be done on the shape of the petal-space. Using a MCMC permutation test we can simulate a petal-space with specific properties and see if our observed petal-space matches these properties (similarly to Díaz et al. [2016]):

```
## Testing against a uniform distribution
disparity_uniform <- null.test(petal_disparity, replicates = 200,
    null.distrib = runif, scale = FALSE)
plot(disparity_uniform)</pre>
```

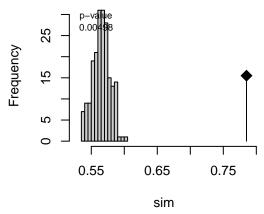
MC test for subsets setosa

MC test for subsets versicolor





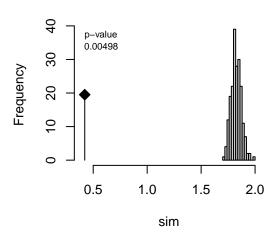
MC test for subsets virginica

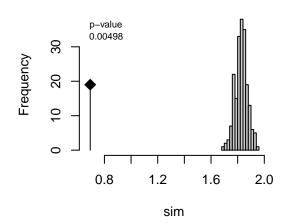


```
## Testing against a normal distribution
disparity_normal <- null.test(petal_disparity, replicates = 200,
    null.distrib = rnorm, scale = TRUE)
plot(disparity_normal)</pre>
```

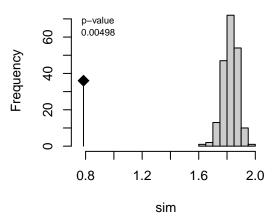
MC test for subsets setosa

MC test for subsets versicolor





MC test for subsets virginica



In both cases we can see that our petal-space is not entirely normal or uniform. This is expected because of the simplicity of these parameters.

Chapter 9

Future directions

9.1 More tests!

Some more tests are being developed such as a sequential.test to run sequential linear models for testing hypothesis in disparity through time or a model.test developed in collaboration with Mark Puttick to fit modes of evolution to disparity curves. Stay tuned!

9.2 More rarefactions!

I am working on including several "clever" bootstrap and rarefaction algorithms for palaeobiology studies based on geological sampling (following:and Butler et al. 2012 *Evolution* and Kotric and Knoll 2015 *Palaeobiology*).

9.3 Faster disparity calculations

I am slowly implementing parallel disparity calculation as well as C implementations of some disparity metrics to increase significantly improve the speed of the dispRity function.

9.4 More modularity

I am equally slowly developing functions to allow more of the options in the package to be modular (in the same way as the metric argument in dispRity). The next arguments to benefit this increased modularity will be time.subsets's model argument and boot.matrix's type argument.

9.5 More suggestions?

More generally, I welcome any suggestions or collaborations for developing some additional specific ideas. Feel free to contact me via email (guillert@tcd.ie) or if you are a GitHub user, directly create an issue on the GitHub page.

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