Manipulate, Visualize and Compare Dendrograms: The dendextend R Package

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Abstract

A dendrogram is a tree diagram which is often used to visualize an hierarchical clustering of items. Dendrograms are used in many dispelines, ranging from Phylogenetic Trees in computational biology to Lexomic Trees in text analysis.

The **dendextend** package extends the dendrogram objects in the R programming language, allowing for easy manipulation of a dendrogram's shape, color and content. Furthermore, it enable the tools for comparing the similarity of two dendrograms to one another both graphically (using tanglegrems) and statistically (from cophenetic correlations to Bk plots).

The paper gives a detailed exposition of both the internal structure of the package and the provided user interfaces.

Keywords: Dendrogram, helust, hierarchical clustering, visualization, tanglegram, R.

1. Introduction

1.1. The dendrogram object

The dendrogram class provides general functions for handling tree-like structures in R (R Development Core Team 2013). It is intended as a replacement for similar functions in hierarchical clustering and classification/regression trees, such that all of these can use the same engine for plotting or cutting trees.

A dendrogram object represents a tree as a nested list object, with various attributes. Dendrogram has several useful methods bundled with R:

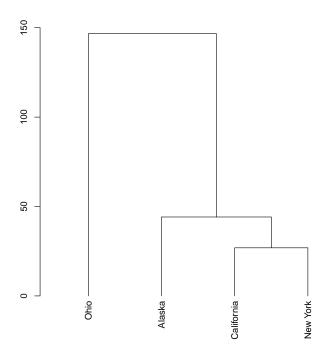
```
methods(class = "dendrogram")
    [1] [[.dendrogram*
                                as.hclust.dendrogram*
                                                       cophenetic.dendrogram*
##
   [4] cut.dendrogram*
                                                       head.dendrogram*
                                cutree.dendrogram
##
   [7] labels.dendrogram*
                                labels<-.dendrogram*
                                                       merge.dendrogram*
## [10] nleaves.dendrogram*
                                nnodes.dendrogram*
                                                       plot.dendrogram*
## [13] print.dendrogram*
                                reorder.dendrogram*
                                                       rev.dendrogram*
## [16] rotate.dendrogram*
                                sort.dendrogram*
                                                       str.dendrogram*
  [19] trim.dendrogram*
                                unroot.dendrogram*
##
      Non-visible functions are asterisked
```

For example, let's create a dendrogram object based on an hierarchical clustering of 4 states in the U.S.:

```
# our data:
data(USArrests)
US_data <- USArrests[c(2, 5, 32, 35), ]
print(US_data)
##
              Murder Assault UrbanPop Rape
                                  48 44.5
## Alaska
                10.0
                         263
                                  91 40.6
## California
                9.0
                         276
## New York
               11.1
                         254
                                   86 26.1
## Ohio
                7.3
                         120
                                  75 21.4
hc <- hclust(dist(US_data), "ave") # create an heirarchical clustering object
dend <- as.dendrogram(hc)</pre>
```

Below are examples for some dendrogram methods:

```
print(dend)
## 'dendrogram' with 2 branches and 4 members total, at height 146.7
labels(dend)
## [1] "Ohio"
                   "Alaska"
                                "California" "New York"
str(dend)
## --[dendrogram w/ 2 branches and 4 members at h = 147]
     |--leaf "Ohio"
##
##
     `--[dendrogram w/2 branches and 3 members at h = 44.1]
##
        |--leaf "Alaska"
        `--[dendrogram w/ 2 branches and 2 members at h = 26.9]
##
           |--leaf "California"
##
##
           `--leaf "New York"
str(dend[[2]]) # looking at one branch of the dendrogram
## --[dendrogram w/ 2 branches and 3 members at h = 44.1]
##
     |--leaf "Alaska"
     `--[dendrogram w/ 2 branches and 2 members at h = 26.9]
##
##
        |--leaf "California"
        `--leaf "New York"
plot(dend)
```



You might notice how the order of the items (leaves/terminal nodes) of the dendrogram is different than their order in the table. In order to re-order the rows in the data-table to have the same order as the items in the dendrogram, we can use the order.dendrogram function:

```
(new_order <- order.dendrogram(dend))</pre>
## [1] 4 1 2 3
# the order of the original items to have them be at the same order as
# they assume in the dendrogram
print(US_data[new_order, ])
##
               Murder Assault UrbanPop Rape
## Ohio
                  7.3
                                     75 21.4
                          120
                 10.0
                                     48 44.5
## Alaska
                          263
## California
                  9.0
                          276
                                     91 40.6
## New York
                 11.1
                          254
                                     86 26.1
```

In order to see what our dendrogram (list) object includes, we need to use the unclass function, which will strip away the class attribute and will allow us to print the list as is, without going through the print.dendrogram method. We can see how each node in the dendrogram/list object has the following (self explaining) attributes:

```
str(unclass(dend))
## List of 2
   $ : atomic [1:1] 4
     ..- attr(*, "members")= int 1
     ..- attr(*, "height")= num 0
##
     ..- attr(*, "label")= chr "Ohio"
##
     ..- attr(*, "leaf")= logi TRUE
##
    $ :List of 2
##
##
     ..$ : atomic [1:1] 1
     .. ..- attr(*, "members")= int 1
##
     .. ..- attr(*, "height")= num 0
##
     .. ..- attr(*, "label")= chr "Alaska"
##
     .. ..- attr(*, "leaf")= logi TRUE
##
##
     ..$ :List of 2
##
     ....$ : atomic [1:1] 2
     ..... attr(*, "label")= chr "California"
##
     ..... attr(*, "members")= int 1
##
     .. .. ..- attr(*, "height")= num 0
##
     .. .. ..- attr(*, "leaf")= logi TRUE
##
     ....$ : atomic [1:1] 3
##
     .. .. - attr(*, "label")= chr "New York"
##
     ..... attr(*, "members")= int 1
##
##
     .. .. ..- attr(*, "height")= num 0
     .. .. ..- attr(*, "leaf")= logi TRUE
##
     .. ..- attr(*, "members")= int 2
##
     ....- attr(*, "midpoint")= num 0.5
##
     .. ..- attr(*, "height")= num 26.9
##
##
     ..- attr(*, "members") = int 3
     ..- attr(*, "midpoint")= num 0.75
##
     ..- attr(*, "height")= num 44.1
   - attr(*, "members")= int 4
   - attr(*, "midpoint")= num 0.875
##
    - attr(*, "height") = num 147
```

Notice how terminal nodes uses the "leaf" attribute (set to TRUE).

```
names(attributes(dend)[-4])
## [1] "members" "midpoint" "height"
```

A very important function is dendrapply. It applies some function recursively to each node of a dendrogram. It is often used for adjusting attributes of the object, or extracting something from it

One current "feature" with this function is that just sending a dendrogram through it will return it with each of its nodes becoming of class "dendrogram". Notice the use of the

unclass_dend function. Example:

```
# dendrapply(dend, unclass) # in case the
itself <- function(x) x
dend_from_dendrapply <- dendrapply(dend, itself)

# here we must first use unclass since '[[]]' inherits its class to the
# output:
class(unclass(dend)[[2]])

## [1] "list"

class(unclass(dend_from_dendrapply)[[2]])

## [1] "dendrogram"

class(unclass_dend(dend_from_dendrapply)[[2]]) # the new uncless_dend solves it.

## [1] "list"</pre>
```

1.2. Motivation for creating dendextend

The dendrogram object has several advantages:

- 1. dendrogram objects are list R objects. This makes their structure very familiar and easy to understand by R users. They are also, relatively, simple to manipulate and extend.
- 2. dendrogram objects has various methods and functions for using them within R base.
- 3. Other tree objects, such as hclust, and objects from the ape package (Paradis et al. 2004), include an as.dendrogram method for converting their objects into a dendrogram. And also as.phylo.dendrogram, as.hclust.dendrogram.
- 4. dendrogram objects are used in various packages as an intermediate step for other purposes (often plotting), such as:
 - (a) The latticeExtra package (Sarkar and Andrews 2012), see the dendrogramGrob function.
 - (b) The labeltodendro package (Nia and Stephens 2011), see the colorplot function.
 - (c) The bclust package (Nia and Davison 2012), see the bclust function.
 - (d) The **ggdendro** package (de Vries and Ripley 2013), see the dendro_data function.
 - (e) The **Heatplus** package (Ploner 2012), see the annHeatmap2 function.
 - (f) The sparcl package (Ploner 2012), see the ColorDendrogram function.

However, even with all of its advantages, the dendrogram class in R still lacks various basic features.

The dendextend package aims at filling some gaps in base R, by extending the available functions for dendrogram manipulation, statistical analysis, and visualization.

This vignettes Provides a step-by-step description of the functionality provided by the **dendextend** package.

1.3. Installing dendextend

To install the stable version from CRAN use:

```
install.packages("dendextend") # not yet available from CRAN
```

To install the GitHub version use:

```
if (!require("devtools")) install.packages("devtools")
require("devtools")
install_github("dendextend", "talgalili")
```

2. Tree attributes (extraction, assignment, length)

2.1. labels in base R

In base R, the labels function is intended to find/extract a suitable set of labels from an object for use in printing or plotting, for example. By default, it uses the names and dimnames functions.

What base R labels function is missing is assignment. In the next few examples we will go through different examples of what the dendextend package offers for various objects.

Credits: These assignment functions were originally written by Gavin Simpson (in a post on (stackoverflow)), and adopted/adjusted to this package by Tal Galili. Some modification were inspired by Gregory Jefferis's code from the **dendroextras** package.

2.2. labels for vectors and matrices

In base R, for vectors, labels gives the names of the object. And if these are missing, then labels will give the vector itself as a character vector:

```
x <- 1:3
names(x) # this vector has no names

## NULL
labels(x) # this vector has no labels

## [1] "1" "2" "3"</pre>
```

Assignment to names is available in base R and works as follows:

```
x <- 1:3
names(x) <- letters[1:3] # assignment for names is in base R
# both names and labels will give the same result:
names(x)

## [1] "a" "b" "c"

labels(x)

## [1] "a" "b" "c"</pre>
```

The new labels assignment function will allow a user to change the labels of the vector just as if it was "names":

```
x <- 1:3
labels(x) <- letters[1:3]
names(x)

## [1] "a" "b" "c"

labels(x)

## [1] "a" "b" "c"</pre>
```

Labels assignment are also available for matrices.

2.3. labels for dendrogram objects

We can get a dendrogram's labels using the labels function from base R. However, in order to assign new values to it, we'll need the assignment function from **dendextend**:

2.4. labels for helust objects

dendextend offers a labels method for hclust objects. It take special care to have the order

of the labels be the same as is with dendrogram object, which is the order of the labels in the plotted tree. This can be turned off when using the order parameter:

2.5. labels assignment and recycling

When the assigned vector has a different length, the **dendextend** assignment functions will recycle the value but also give a warning:

```
x <- 1:3
hc <- hclust(dist(US_data), "ave")
dend <- as.dendrogram(hc)
y <- matrix(1:9, 3, 3)

labels(x) <- "bob"

## Warning: The lengths of the new labels is shorter than the length of the object
- labels are recycled.

labels(x)

## [1] "bob" "bob" "bob"

labels(hc) <- "bob"

## Warning: The lengths of the new labels is shorter than the number of leaves
in the hclust - labels are recycled.

labels(hc)

## [1] "bob" "bob" "bob" "bob" "bob"</pre>
```

```
labels(dend) <- "bob"

## Warning: The lengths of the new labels is shorter than the number of leaves
in the dendrogram - labels are recycled.

labels(dend)

## [1] "bob" "bob" "bob" "bob"

labels(y) <- "bob"

## Warning: The lengths of the new labels is shorter than the length of the object's
colnames - labels are recycled.

labels(y)

## [1] "bob" "bob" "bob"</pre>
```

2.6. Tree size - number of leaves

Getting the size of a tree (e.g. number of leaves/terminal-nodes) is good for validation of functions, and also when we wish to initiate a variable to later fill with data from the leaves. The labels function for dendrogram is expensive, since it uses recursion to get all of the tree's elements. If we are only interested in getting the tree size, it is better to use the nleaves function. It has an S3 method for helust, dendrogram and phylo (from the ape):

```
nleaves(hc)

## [1] 4

nleaves(dend)

## [1] 4
```

For dendrograms the speed improvement is about 10 times using labels, whereas for hclust, there is not any gain made by using nleaves. Here is a quick benchmark:

```
library(microbenchmark)
microbenchmark(nleaves(dend), length(labels(dend)))

## Unit: microseconds
## expr min lq median uq max neval
## nleaves(dend) 23.52 25.76 28.28 30.52 288.4 100
## length(labels(dend)) 374.59 382.15 395.59 421.62 810.2 100
```

```
microbenchmark(nleaves(hc), length(labels(hc)))

## Unit: microseconds

## expr min lq median uq max neval

## nleaves(hc) 16.80 17.36 18.20 19.04 30.8 100

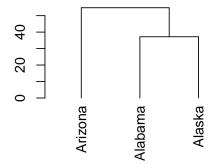
## length(labels(hc)) 29.68 30.80 31.36 31.36 127.7 100
```

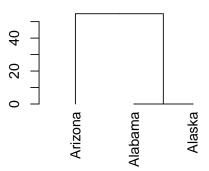
There are border-line cases where the node above some leaves is of height 0. In such a case, we would consider that node as a "terminal node", and in order to count the number of such terminal nodes we would use count_terminal_nodes function. For example:

```
hc <- hclust(dist(USArrests[1:3, ]), "ave")</pre>
dend <- as.dendrogram(hc)</pre>
par(mfrow = c(1, 2))
### Trivial case
count_terminal_nodes(dend) # 3 terminal nodes
## [1] 3
length(labels(dend)) # 3 - the same number
## [1] 3
plot(dend, main = "This is considered a tree \n with THREE terminal nodes/leaves")
### NON-Trivial case
str(dend)
## --[dendrogram w/ 2 branches and 3 members at h = 54.8]
     |--leaf "Arizona"
##
##
     `--[dendrogram w/ 2 branches and 2 members at h = 37.2]
        |--leaf "Alabama"
##
        `--leaf "Alaska"
##
attr(dend[[2]], "height") <- 0</pre>
count_terminal_nodes(dend) # 2 terminal nodes, why? see this plot:
## [1] 2
# while we have 3 leaves, in practice we have only 2 terminal nodes (this
# is a feature, not a bug.)
plot(dend, main = "This is considered a tree \n with TWO terminal nodes only")
```

This is considered a tree with THREE terminal nodes/leaves

This is considered a tree with TWO terminal nodes only





2.7. Tree size - number of nodes

Getting the size of a tree, in terms of the number of nodes can easily be done using:

```
hc <- hclust(dist(USArrests[1:3, ]), "ave")
dend <- as.dendrogram(hc)
nnodes(hc)
## [1] 5
nnodes(dend)
## [1] 5</pre>
```

2.8. Generally getting tree attributes

Getting tree attributes can more generally be achieved using get_nodes_attr, however, the dedicated function are often faster than the general solution. (also, in the future, we might introduce functions based on Rcpp, offering even faster times).

Here are some examples:

```
hc <- hclust(dist(USArrests[1:3, ]), "ave")
dend <- as.dendrogram(hc)

# get_leaves_attr(dend) # error :)
get_leaves_attr(dend, "label")

## [1] "Arizona" "Alabama" "Alaska"

labels(dend, "label")</pre>
```

```
## [1] "Arizona" "Alabama" "Alaska"
get_leaves_attr(dend, "height") # should be 0's
## [1] 0 0 0
get_nodes_attr(dend, "height")
## [1] 54.80 0.00 37.18 0.00 0.00
get_branches_heights(dend, sort = FALSE) # notice the sort=FALSE
## [1] 54.80 37.18
get_leaves_attr(dend, "leaf") # should be TRUE's
## [1] TRUE TRUE TRUE
get_nodes_attr(dend, "leaf") # conatins NA's
## [1] NA TRUE NA TRUE TRUE
get_nodes_attr(dend, "leaf", na.rm = TRUE) #
## [1] TRUE TRUE TRUE
get_leaves_attr(dend, "members") # should be 1's
## [1] 1 1 1
get_nodes_attr(dend, "members", include_branches = FALSE, na.rm = TRUE) #
## [1] 1 1 1
get_nodes_attr(dend, "members") #
## [1] 3 1 2 1 1
get_nodes_attr(dend, "members", include_leaves = FALSE, na.rm = TRUE) #
```

```
## [1] 3 2
hang_dend <- hang.dendrogram(dend)</pre>
get_leaves_attr(hang_dend, "height") # no longer 0!
## [1] 49.32 31.70 31.70
get_nodes_attr(hang_dend, "height") # does not include any 0s!
## [1] 54.80 49.32 37.18 31.70 31.70
# does not include leaves values:
get_nodes_attr(hang_dend, "height", include_leaves = FALSE)
## [1] 54.80
                NA 37.18
                           NA
                                  NA
# remove leaves values all together:
get_nodes_attr(hang_dend, "height", include_leaves = FALSE, na.rm = TRUE)
## [1] 54.80 37.18
get_branches_heights(hang_dend) # notice the sort
## [1] 37.18 54.80
get_branches_heights(hang_dend, sort = FALSE) # notice the sort
## [1] 54.80 37.18
```

Quick comparison on fetching leaves attributes:

```
require(microbenchmark)

## Loading required package: microbenchmark

# get_leaves_attr is twice faster than get_nodes_attr

microbenchmark(get_leaves_attr_4members = get_leaves_attr(dend, "members"),
    get_nodes_attr_4members = get_nodes_attr(dend, "members", include_branches = FALSE,
    na.rm = TRUE))
```

```
## Unit: microseconds

## expr min lq median uq max neval

## get_leaves_attr_4members 282.2 285.8 293.7 318.3 2501.8 100

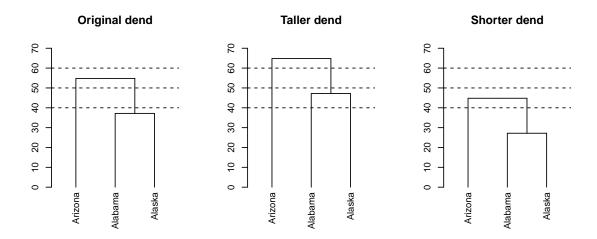
## get_nodes_attr_4members 693.8 707.5 743.3 779.7 984.9 100
```

3. Tree manipulation

3.1. Unrooting and root height

A tree's nodes has various heights. Sometimes we are interested in changing the height of the entire tree. It is useful when This can be accomplished using raise.dendrogram. For example (notice how the entire tree's height is changed):

```
hc <- hclust(dist(USArrests[1:3, ]), "ave")</pre>
dend <- as.dendrogram(hc)</pre>
taller_dend <- raise.dendrogram(dend, 10)
shorter_dend <- raise.dendrogram(dend, -10)
attr(dend, "height") # 54.80041
## [1] 54.8
attr(taller_dend, "height") # 64.80041
## [1] 64.8
attr(shorter_dend, "height") # 44.80041
## [1] 44.8
par(mfrow = c(1, 3))
plot(dend, ylim = c(0, 70), main = "Original dend")
abline(h = c(40, 50, 60), lty = 2)
plot(taller_dend, ylim = c(0, 70), main = "Taller dend")
abline(h = c(40, 50, 60), lty = 2)
plot(shorter_dend, ylim = c(0, 70), main = "Shorter dend")
abline(h = c(40, 50, 60), 1ty = 2)
```

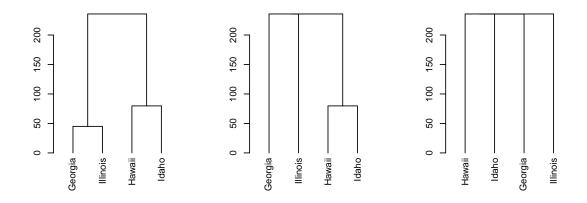


Sometimes we wish to "unroot" the dendrogram, meaning that we merge one of the tree's branches with its root. This is useful, for example, when merging phylogenetic trees from several families, and being unwilling to assume a specific root to the merged trees. Unrooting can be done using the unroot (S3) function (notice the use of the branch_becoming_root parameter):

```
hc <- hclust(dist(USArrests[10:13, ]), "ward")
dend <- as.dendrogram(hc)

unrooted_dend <- unroot(dend, branch_becoming_root = 1)
unrooted_dend_2 <- unroot(unrooted_dend, branch_becoming_root = 3)

par(mfrow = c(1, 3))
plot(dend)
plot(unrooted_dend)
plot(unrooted_dend_2)</pre>
```



While the unroot.hclust method exists, it is not expected to work since hclust objects are

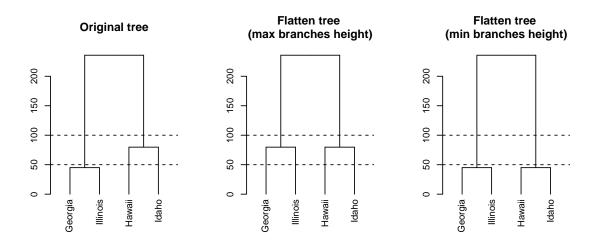
not designed to handle non-binary trees (hence the advantage of using dendrogram objects). For phylo objects (from the ape package), there is also a method that would simply use ape:::unroot(phy = x).

In some rare cases, we might wish to equalize the heights of root's branches. For this we can use the flatten.dendrogram function:

```
hc <- hclust(dist(USArrests[10:13, ]), "ward")
dend <- as.dendrogram(hc)

flatten_dend_1 <- flatten.dendrogram(dend, FUN = max)
flatten_dend_2 <- flatten.dendrogram(dend, FUN = min)

par(mfrow = c(1, 3))
plot(dend, main = "Original tree")
abline(h = c(50, 100), lty = 2)
plot(flatten_dend_1, main = "Flatten tree \n(max branches height)")
abline(h = c(50, 100), lty = 2)
plot(flatten_dend_2, main = "Flatten tree \n(min branches height)")
abline(h = c(50, 100), lty = 2)</pre>
```

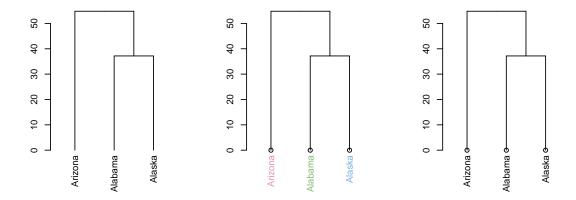


3.2. Coloring labels of leaves

Coloring labels can sometimes be useful, it is done through the labels_colors function (which also has assignemnt). Notice the assignment recycling, as well as the differene in the appearence of a dot when labels' color is black, compared to when it is NULL:

```
par(mfrow = c(1, 3))
hc <- hclust(dist(USArrests[1:3, ]), "ave")
dend <- as.dendrogram(hc)</pre>
```

```
# Defaults:
labels_colors(dend)
## NULL
plot(dend)
# let's add some color:
require(colorspace)
## Loading required package: colorspace
labels_colors(dend) <- rainbow_hcl(3)</pre>
labels_colors(dend)
   Arizona Alabama Alaska
## "#E495A5" "#86B875" "#7DB0DD"
plot(dend)
# changing color to black
labels_colors(dend) <- 1</pre>
## Warning: Length of color vector was shorter then the number of leaves - vector
color recycled
labels_colors(dend)
## Arizona Alabama Alaska
## 1 1 1
plot(dend)
```



```
# removing color (and the nodePar completely - if it has no other
# attributed but lab.col)
labels_colors(dend) <- NULL

## Warning: Length of color vector was shorter then the number of leaves - vector
color recycled

## Warning: 'x' is NULL so the result will be NULL

labels_colors(dend)

## NULL</pre>
```

3.3. Hanging a dendrogram

Hanging a tree means that we change the height of the leaves to be near their parent node. Hanging helps when examining the toplogy of the tree. Currently, hanging of a dendrogram was possible by going through the hclust object, but now you can simply use the hang.dendrogram function. Here is an example:

```
hc <- hclust(dist(USArrests[1:9, ]), "ave")
dend <- as.dendrogram(hc)
hang_dend_1 <- hang.dendrogram(dend, hang = 0.1)
hang_dend_2 <- as.dendrogram(hc, hang = 0.1)  # another way of doing it, if
# we could move from/to hclust
identical(hang_dend_1, hang_dend_2)  # and they are the same :)
## [1] TRUE

require(colorspace)</pre>
```

```
labels_colors(hang_dend_1) <- rainbow_hcl(nleaves(hang_dend_1))

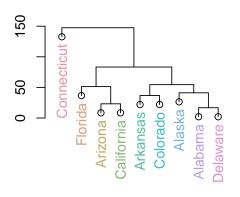
par(mfrow = c(1, 2))
plot(hc, main = "Hanged hclust tree")
plot(hang_dend_1, main = "Hanged dendrogram tree")</pre>
```

Hanged hclust tree

Connecticut Florida Arizona Arkansas Colorado Alaska Alabama Delaware

dist(USArrests[1:9,])
hclust (*, "average")

Hanged dendrogram tree



3.4. Trimming leaves

Trimming a tree from some leaves can be done using the trim (S3 method) function (notice that the attributes of the trimmed tree are updated):

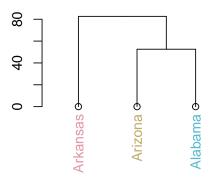
```
hc <- hclust(dist(USArrests[1:5, ]), "ave")</pre>
dend <- as.dendrogram(hc)</pre>
library(colorspace)
labels_colors(dend) <- rainbow_hcl(5)</pre>
trimmed_dend <- trim(dend, c("Alaska", "California"))</pre>
str(unclass(trimmed_dend))
## List of 2
    $ : atomic [1:1] 4
##
     ..- attr(*, "members")= int 1
##
     ..- attr(*, "height")= num 0
##
     ..- attr(*, "label")= chr "Arkansas"
##
     ..- attr(*, "leaf")= logi TRUE
##
##
     ..- attr(*, "nodePar")=List of 1
     .. ..$ lab.col: chr "#E495A5"
##
    $ :List of 2
##
     ..$ : atomic [1:1] 3
##
     ....- attr(*, "label")= chr "Arizona"
```

```
....- attr(*, "members")= int 1
##
     ...- attr(*, "height")= num 0
##
     ....- attr(*, "leaf")= logi TRUE
##
     ... - attr(*, "nodePar")=List of 1
##
     .. ... $\text{lab.col: chr "#BDAB66"}
##
##
     ..$ : atomic [1:1] 1
##
     .. ..- attr(*, "label")= chr "Alabama"
     .. ..- attr(*, "members")= int 1
##
     .. ..- attr(*, "height")= num 0
##
     .. ..- attr(*, "leaf")= logi TRUE
##
     ....- attr(*, "nodePar")=List of 1
##
##
     .. ... $\text{lab.col: chr "#55B8D0"}
     ..- attr(*, "members")= num 2
##
     ..- attr(*, "midpoint")= num 0.5
##
##
    ..- attr(*, "height")= num 52.6
   - attr(*, "members")= num 3
##
   - attr(*, "midpoint")= num 0.75
##
    - attr(*, "height") = num 82.6
par(mfrow = c(1, 2))
plot(dend, main = "Original tree")
plot(trimmed_dend, main = "Tree without Alaska and California")
```

Original tree

Arkansas e Alabama e Alaska e Alaska e

Tree without Alaska and California



If we have two trees, we can use the intersect_trees function to reduce both trees to have the same labels (this will be useful later when we'd like to compare the two trees):

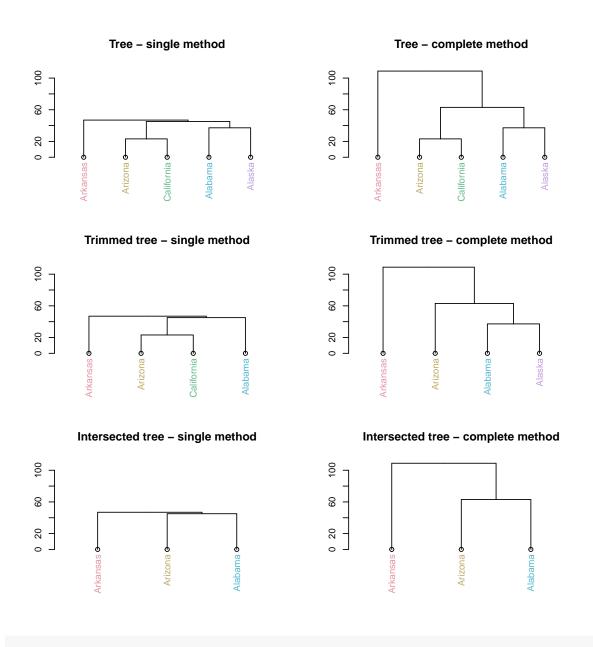
```
hc_1 <- hclust(dist(USArrests[1:5, ]), "single")
hc_2 <- hclust(dist(USArrests[1:5, ]), "complete")
dend_1 <- as.dendrogram(hc_1)
dend_2 <- as.dendrogram(hc_2)</pre>
```

```
library(colorspace)
labels_colors(dend_1) <- rainbow_hcl(5)
labels_colors(dend_2) <- rainbow_hcl(5)

trimmed_dend_1 <- trim(dend_1, c("Alaska"))
trimmed_dend_2 <- trim(dend_2, c("California"))

dends_12 <- intersect_trees(trimmed_dend_1, trimmed_dend_2)

par(mfrow = c(3, 2))
plot(dend_1, main = "Tree - single method", ylim = c(0, 110))
plot(dend_2, main = "Tree - complete method", ylim = c(0, 110))
plot(trimmed_dend_1, main = "Trimmed tree - single method", ylim = c(0, 110))
plot(trimmed_dend_2, main = "Trimmed tree - complete method", ylim = c(0, 110))
plot(dends_12[[1]], main = "Intersected tree - single method", ylim = c(0, 110))
plot(dends_12[[2]], main = "Intersected tree - complete method", ylim = c(0, 110))</pre>
```



Sidenote: a similar function, called plotColoredClusters, is available in the ClassDiscovery package for hclust objects.

3.5. Rotating branches

A dendrogram is an object which can be rotated on its hinges without changing its topological. Rotating a dendrogram in base R can be done using the **reorder** function. The problem with this function is that it is not very intuitive. For this reason we wrote the **rotate** function. It has two main arguments: the object, and the order we wish to rotate it by. The order parameter can be either a numeric vector, used in a similar way we would order a simple

character vector. Or, the order parameter can also be a character vector of the labels of the tree, given in the new desired order of the tree.

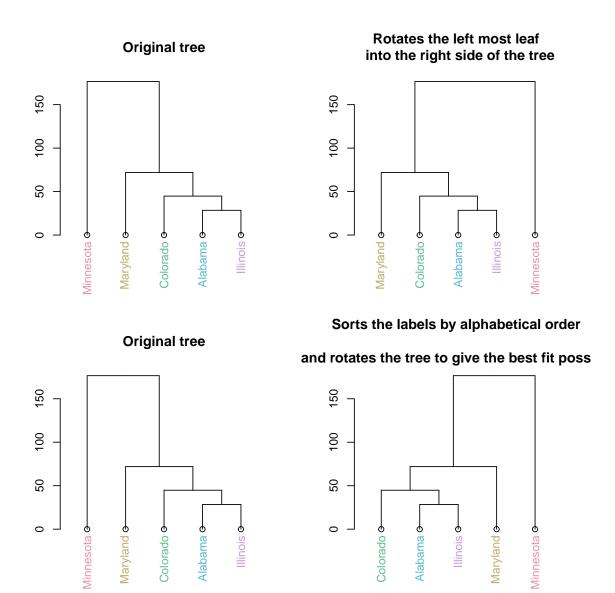
It is also worth noting that some order are impossible to achieve for a given tree's topology. In such a case, the function will do its "best" to get as close as possible.

Here are a few examples:

```
hc <- hclust(dist(USArrests[c(1, 6, 13, 20, 23), ]), "ave")
dend <- as.dendrogram(hc)

# For dendrogram objects:
require(colorspace)
labels_colors(dend) <- rainbow_hcl(nleaves(dend))

# let's color the labels to make the followup of the rotation easier
par(mfrow = c(2, 2))
plot(dend, main = "Original tree")
plot(rotate(dend, c(2:5, 1)), main = "Rotates the left most leaf \n into the right side of
plot(dend, main = "Original tree")
plot(sort(dend), main = "Sorts the labels by alphabetical order \n\nand rotates the tree to</pre>
```



3.6. Cutting trees

The hclust function comes with a very powerfull cutree function, for extracting cluster grouping of the original data based on cutting the heirarchical tree at some height (or setting a predefined k - number of clusters). The limitation of this function is that it is only available for hclust object. Hence, if we are dealing with a tree which is NOT an ultrametric tree (e.g: ultrametric tree = a tree with monotone clustering heights), cutree would not be available for us (since as.hclust would not work on our dendrogram).

In **dendextend**, we extend cutree by turning it into an S3 method, with methods for dendrogram and phylo objects. The phylo method is only turning the phylo object to an helust, and tries to work on it there. However, the dendrogram method (cutree.dendrogram) is a complete re-writing of cutree based on the cut.dendrogram function. cutree.dendrogram fully emulates cutree by default, but at the same time extends it with the type of trees it

can handle, and with some other options.

Since cutree.dendrogram is written in R, it is slower than cutree which is implemented in C. If we can turn the dendrogram into hclust, we will use cutree.hclust, otherwise - cutree.dendrogram will be used.

Here are several examples of how these functions are used:

```
hc <- hclust(dist(USArrests[c(1, 6, 13, 20, 23), ]), "ave")
dend <- as.dendrogram(hc)</pre>
unroot_dend <- unroot(dend, 2)
cutree(hc, k = 2:4) # on hclust
             2 3 4
##
## Alabama
             1 1 1
## Colorado 1 1 2
## Illinois 1 1 1
## Maryland 1 2 3
## Minnesota 2 3 4
cutree(dend, k = 2:4) # on dendrogram
##
             2 3 4
             1 1 1
## Alabama
## Colorado 1 1 2
## Illinois 1 1 1
## Maryland 1 2 3
## Minnesota 2 3 4
cutree(hc, k = 2) # on hclust
     Alabama Colorado Illinois Maryland Minnesota
##
           1
                     1
                               1
                                          1
cutree(dend, k = 2) # on dendrogram
##
     Alabama Colorado Illinois Maryland Minnesota
##
                                         1
           1
                     1
                               1
cutree(dend, h = c(20, 25.5, 50, 170))
             20 25.5 50 170
##
## Alabama
              1
                   1 1
                          1
## Colorado
              2
                   2
## Illinois
              3
                   3
## Maryland
                   4
                      2
                          1
              4
## Minnesota 5
                   5 3
```

```
cutree(hc, h = c(20, 25.5, 50, 170))
##
            20 25.5 50 170
## Alabama
            1 1 1 1
## Colorado 2
                 2 1 1
## Illinois 3 3 1 1
## Maryland 4 4 2 1
## Minnesota 5 5 3 2
# the default (ordered by original data's order)
cutree(dend, k = 2:3, order_clusters_as_data = FALSE)
## [1] 2 1 1 1 1
labels(dend)
## [1] "Minnesota" "Maryland" "Colorado" "Alabama"
                                                     "Illinois"
# cutree now works for unrooted trees! as.hclust(unroot_dend) # ERROR -
# can not do this...
cutree(unroot_dend, k = 2) # all NA's
## Warning: Couldn't cut the tree - returning NA.
## Warning: You (probably) have some branches with equal heights so that there
exist no height(h) that can create 2 clusters
## [1] NA NA NA NA NA
cutree(unroot_dend, k = 1:4)
## Warning: Couldn't cut the tree - returning NA.
## Warning: You (probably) have some branches with equal heights so that there
exist no height(h) that can create 2 clusters
           1 2 3 4
## Alabama 1 NA 2 2
## Colorado 1 NA 2 3
## Illinois 1 NA 2 2
## Maryland 1 NA 3 4
## Minnesota 1 NA 1 1
cutree(unroot_dend, h = c(20, 25.5, 50, 170))
```

```
20 25.5 50 170
##
## Alabama
              1
                   1 2
                   2 2
## Colorado
              2
                          2
## Illinois
              3
                   3 2
                          2
                   4 3
## Maryland
              4
## Minnesota 5
                   5 1
require(microbenchmark)
## this shows how as.hclust is expensive - but still worth it if possible
microbenchmark(cutree(hc, k = 2:4), cutree(as.hclust(dend), k = 2:4), cutree(dend,
    k = 2:4), cutree(dend, k = 2:4, try_cutree_hclust = FALSE))
## Unit: microseconds
##
                                                 expr
                                                                  lq median
                                                         min
##
                                 cutree(hc, k = 2:4)
                                                       95.19 103.6 107.2
##
                    cutree(as.hclust(dend), k = 2:4) 1669.71 1757.6 1841.6
##
                               cutree(dend, k = 2:4) 1755.38 1862.6 1953.0
    cutree(dend, k = 2:4, try_cutree_hclust = FALSE) 8174.42 8529.1 8766.5
##
##
               max neval
##
     155.1
             472.6
                   100
##
   2077.9 5803.7
                     100
   2123.0 4925.1
                   100
##
##
   9478.5 97417.2
                    100
# the dendrogram is MUCH slower...
# and trying to 'hclust' is not expensive (which is nice...)
microbenchmark(cutree_unroot_dend = cutree(unroot_dend, k = 2:4, warn = FALSE),
    cutree_unroot_dend_not_trying_to_hclust = cutree(unroot_dend, k = 2:4, try_cutree_hclu
        warn = FALSE))
## Unit: milliseconds
##
                                              min
                                                     lq median
                                       expr
                                                                   uq
                         cutree_unroot_dend 6.707 6.916 7.039 7.565 12.04
##
    cutree_unroot_dend_not_trying_to_hclust 6.328 6.537 6.724 7.455 15.99
##
##
    neval
      100
##
##
      100
```

Having cutree.dendrogram available to us, we can now gain the ability to color branches for trees which can not be represented as an hclust object.

3.7. Coloring branches

Dendrogram plots with colored branches have been available in R for many years in threads on the mailing lists and through various package. However, until recently, all of the functions in packages have always given the user a new plot function, without seperating the coloring of branches of a dendrogram from its plotting. Often the function for actually plotting the colored branched dendrogram would be hidden from the user. For example, the labeltodendro package (Nia and Stephens 2011) gives a colored branch plot through the colorplot function, but the work horse for this is available in a hidden function called dendroploth or dendroplotv, both take care of the plotting by themselves (instead of modifying the dendrogram object, and then letting the base R function do the work). The same story happens in the Heatplus (Ploner 2012), where the plot.annHeatmap2 function actually uses the hidden function cutplot.dendrogram for doing the plotting.

This was changed in the beginning of 2013 thanks to Gregory Jefferis's **dendroextras** package (Jefferis 2013), which organized this through the colour_clusters function. In the **dendextend** package I will mostly import his code, with some modifications. The biggest limitation in Gregory's code is that he relies on changing the **dendrogram** into hclust in order to use **cutree** on it and get the clusters. This has the advantage of being fast, but the **disadvantage** that it restricts his code to binary trees only. For this reason, I did not use his **slice** function, and made sure to use other functions instead.

4. Tanglegrams - visually comparing two trees side-by-side

- 4.1. Tanglegram visualization
- 4.2. Finding an optimal rotation
 - 5. Comparing two trees statistics and inference
- 5.1. Baker's gamma
- 5.2. Bk method

6. Summary

The **dendextend** package presented in this paper greatly extends the available functionality of the dendrogram objects in R.

Acknowledgments

We are very thankful for code contributions and ideas by the R core team (especially Martin

Maechler and Brian Ripley, but probably also others without our knowledge), Gavin Simpson, Gregory Jefferis ,

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