

Doing More with Dendrograms: The dendextend R Package

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Abstract

The **dendextend** package extends the dendrogram objects in R.
The paper gives a detailed exposition of both the internal structure of the package and the provided user interfaces.

Keywords: Dendrogram, hclust, 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*      labels.dendrogram*
## [7] labels<-.dendrogram* merge.dendrogram*      nleaves.dendrogram*
## [10] plot.dendrogram*      print.dendrogram*      reorder.dendrogram*
## [13] rev.dendrogram*       rotate.dendrogram*     sort.dendrogram*
## [16] str.dendrogram*       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
## Alaska      10.0      263       48 44.5
## California   9.0      276       91 40.6
## 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)
```

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"
```

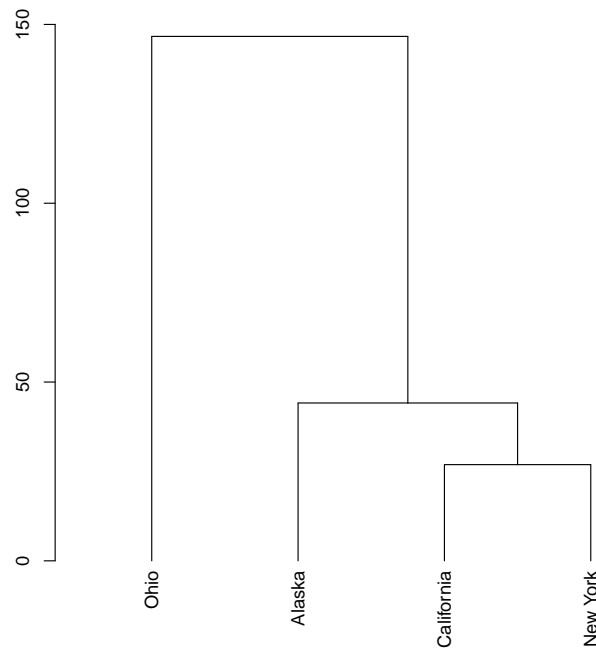
```
str(dend)

## --[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))

## [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    120      75 21.4
## Alaska        10.0    263      48 44.5
## 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 unclass_dend solves it.

## [1] "list"
```

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 labels (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"
```

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"
```

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"
```

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**:

```
labels(dend) # from base R

## [1] "Ohio"      "Alaska"    "California" "New York"

set.seed(2354235)
labels(dend) <- sample(labels(dend)) # labels assingment - thanks to dendextend
labels(dend)

## [1] "New York"  "Ohio"      "Alaska"    "California"
```

2.4. labels for hclust 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:

```
# All are from dendextend
labels(hc)

## [1] "Ohio"      "Alaska"    "California" "New York"

labels(hc, order = FALSE) # this is the order of the rows of the original data.

## [1] "Alaska"    "California" "New York"   "Ohio"

set.seed(229835)
labels(hc) <- sample(labels(hc)) # labels assingment - thanks to dendextend
labels(hc)

## [1] "California" "New York"   "Alaska"    "Ohio"
```

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"
```



```

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"

```

2.6. Tree size

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 `hclust`, `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")
dend <- as.dendrogram(hc)

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)

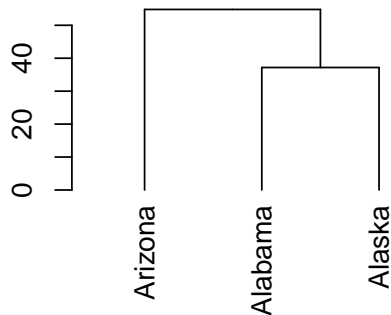
## --[dendrogram w/ 2 branches and 3 members at h = 54.8]
##   |--leaf "Arizona"
##   `--[dendrogram w/ 2 branches and 2 members at h = 37.2]
##     |--leaf "Alabama"
##     `--leaf "Alaska"

attr(dend[[2]], "height") <- 0
count_terminal_nodes(dend) # 2 terminal nodes, why? see this plot:

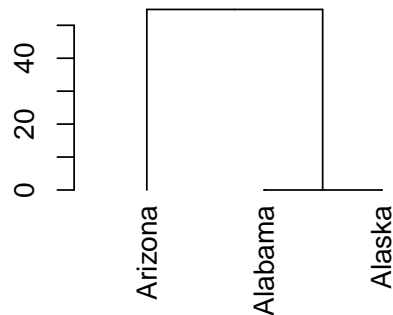
## [1] 2

# 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**



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")
dend <- as.dendrogram(hc)

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

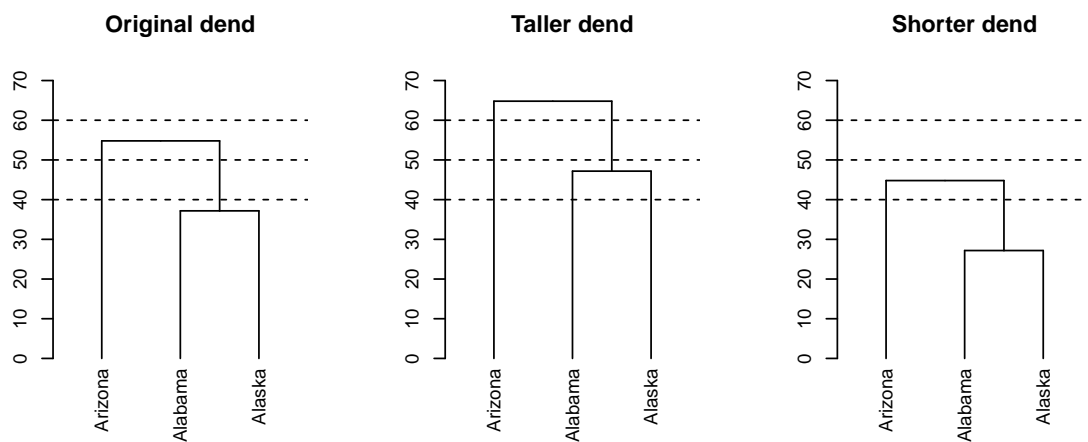
## [1] 44.8

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), lty = 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):

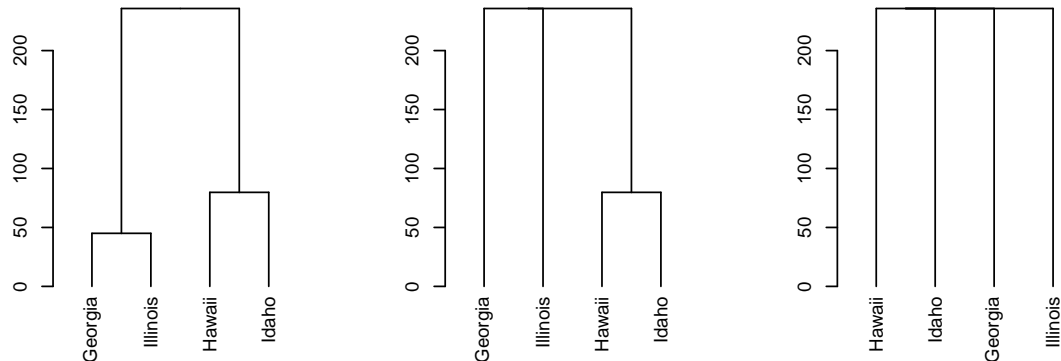
```

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)

```



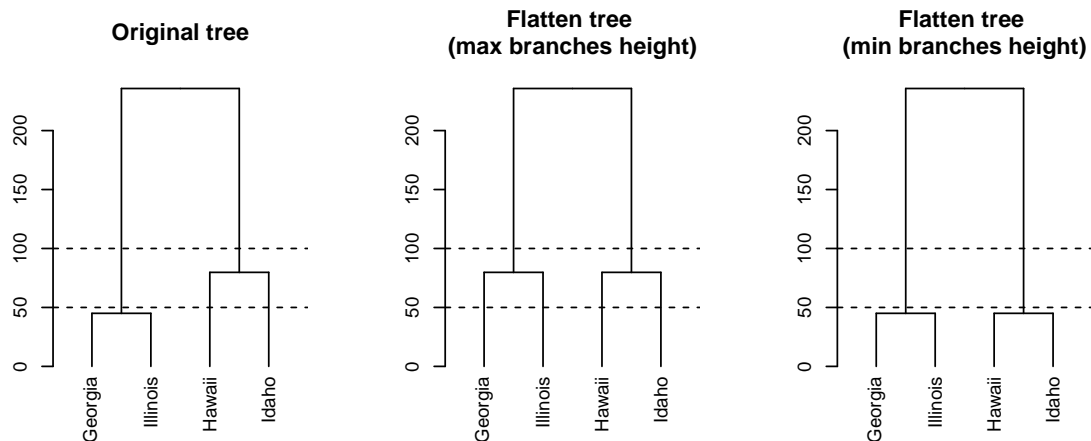
While the `unroot.hclust` method exists, it is not expected to work since `hclust` objects are not designed to handle non-binary trees (hence the advantage of using `dendrogram` objects). For `phylo` objects (from the **ape** package), there is also a method that would simply use `ape::unroot(phy = x)`.

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)
```



3.2. Coloring labels of leaves

Coloring labels can sometimes be useful, it is done through the `labels_colors` function (which also has assignment). Notice the assignment recycling, as well as the difference in the appearance 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)

# Defaults:
labels_colors(dend)

## NULL

plot(dend)

# let's add some color:
require(colorspace)

## Loading required package: colorspace

labels_colors(dend) <- rainbow_hcl(3)
labels_colors(dend)

## Arizona Alabama Alaska
## "#E495A5" "#86B875" "#7DB0DD"

plot(dend)

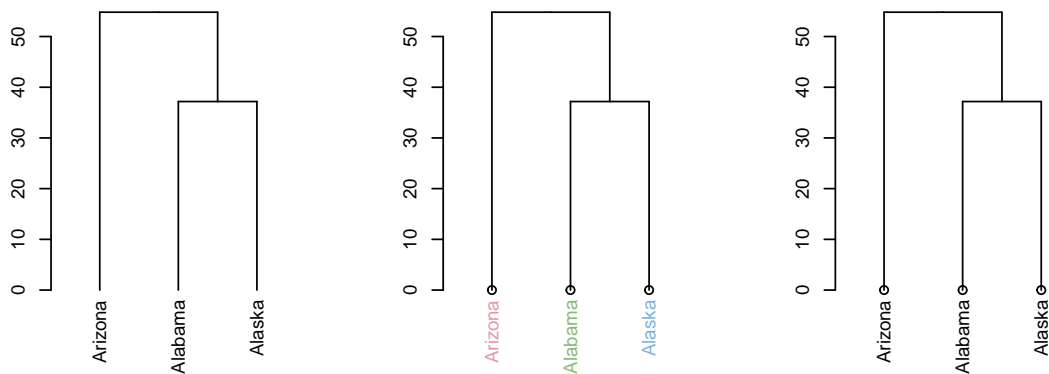
# changing color to black
labels_colors(dend) <- 1
```

```
## 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
```

3.3. 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")
dend <- as.dendrogram(hc)
```

```

library(colorspace)
labels_colors(dend) <- rainbow_hcl(5)

trimmed_dend <- trim(dend, c("Alaska", "California"))

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
## .. .. ..$ 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
## .. .. ..$ 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")

```




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):

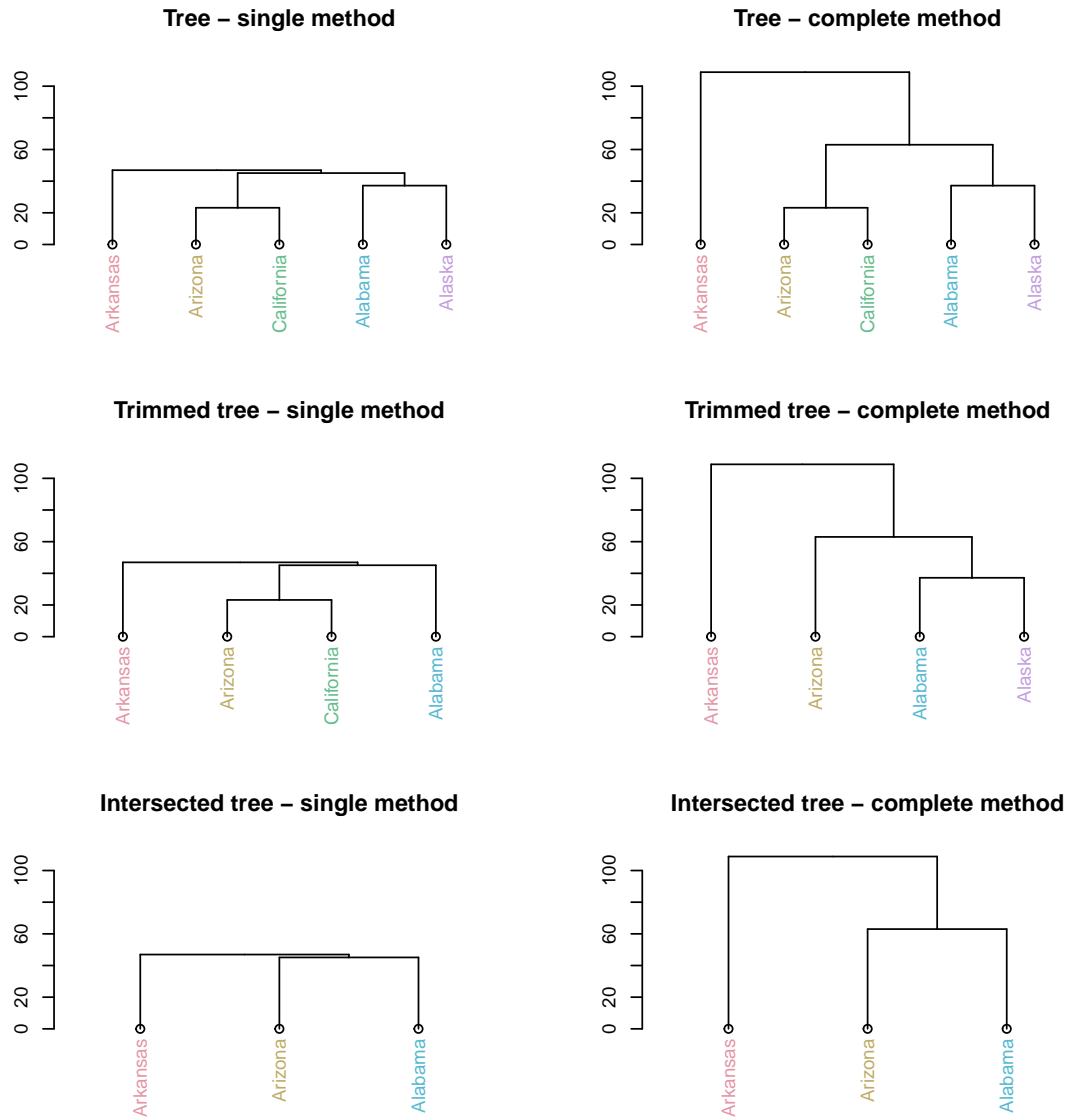
```
hc_1 <- hclust(dist(USArrests[1:5, ]), "single")
hc_2 <- hclust(dist(USArrests[1:5, ]), "complete")
dend_1 <- as.dendrogram(hc_1)
dend_2 <- as.dendrogram(hc_2)

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))
```



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

3.4. 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 separating 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 **labeltoden-****dro** 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 `dendroplot` 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 will not use his `slice` function, and made sure to use other functions instead.

3.5. Rotating branches

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.

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