1 Introduction

This document describes the new phylo4 S4 classes and methods, which are intended to provide a unifying standard for the representation of phylogenetic trees and comparative data in R. The phylobase package was developed to help both end users and package developers by providing a common suite of tools likely to be shared by all packages designed for phylogenetic analysis, facilities for data and tree manipulation, and standardization of formats.

This standardization will benefit end-users by making it easier to move data and compare analyses across packages, and to keep comparative data synchronized with phylogenetic trees. Users will also benefit from a repository of functions for tree manipulation, for example tools for including or excluding subtrees (and associated phenotypic data) or improved tree and data plotting facilities. phylobase will benefit developers by freeing them to put their programming effort into developing new methods rather than into re-coding base tools. We (the phylobase
developers) hope phylobase will also facilitate code validation by providing a repository for benchmark tests, and more generally that it will help catalyze community development of comparative methods in R.

A more abstract motivation for developing phylobase was to improve data checking and abstraction of the tree data formats. phylobase can check that data and trees are associated in the proper fashion, and protects users and developers from accidentally reordering one, but not the other. It also seeks to abstract the data format so that commonly used information (for example, branch length information or the ancestor of a particular node) can be accessed without knowledge of the underlying data structure (i.e., whether the tree is stored as a matrix, or a list, or a parenthesis-based format). This is achieved through generic phylobase functions which retrieve the relevant information from the data structures. The benefits of such abstraction are multiple: (1) easier access to the relevant information via a simple function call (this frees both users and developers from learning details of complex data structures), (2) freedom to optimize data structures in the future without breaking code. Having the generic functions in place to “translate” between the data structures and the rest of the program code allows program and data structure development to proceed somewhat independently. The alternative is code written for specific data structures, in which modifications to the data structure requires rewriting the entire package code (often exacting too high a price, which results in the persistence of less-optimal data structures). (3) providing broader access to the range of tools in phylobase. Developers of specific packages can use these new tools based on S4 objects without knowing the details of S4 programming.

The base phylo4 class is modeled on the the phylo class in ape. phylo4d and multiphylo4 extend the phylo4 class to include data or multiple trees respectively. In addition to describing the classes and methods, this vignette gives examples of how they might be used.

2 Package overview

The phylobase package currently implements the following functions and data structures:

- Data structures for storing a single tree and multiple trees: phylo4 and multiPhylo4?
- A data structure for storing a tree with associated tip and node data: phylo4d
- A data structure for storing multiple trees with one set of tip data: multiPhylo4d
- Functions for reading nexus files into the above data structures
- Functions for converting between the above data structures and ape phylo objects as well as ade4 phylog objects (although the latter are now deprecated ...)
- Functions for editing trees and data (i.e., subsetting and replacing)
- Functions for plotting trees and trees with data

3 Using the S4 help system

The S4 help system works similarly to the S3 help system with some small differences relating to how S4 methods are written. The plot() function is a good example. When we type ?plot we are provided the help for the default plotting function which expects x and y. R also provides a way to smartly dispatch the right type of plotting function. In the case of an ape phylo object
(a S3 class object) R evaluates the class of the object and finds the correct functions, so the following works correctly.

```r
library(ape)
set.seed(1)  ## set random-number seed
rand_tree <- rcoal(10)  ## Make a random tree with 10 tips
plot(rand_tree)
```

However, typing `?plot` still takes us to the default `plot` help. We have to type `?plot.phylo` to find what we are looking for. This is because S3 generics are simply functions with a dot and the class name added.

The S4 generic system is too complicated to describe here, but doesn’t include the same dot notation. As a result `?plot.phylo4` doesn’t work, R still finds the right plotting function.

```r
library(phylobase)

## Attaching package: 'phylobase'
## The following object is masked from 'package:ape':
##
## edges

# convert rand_tree to a phylo4 object
rand_p4_tree <- as(rand_tree, "phylo4")
plot(rand_p4_tree)
```

All fine and good, but how to we find out about all the great features of the `phylobase` plotting function? R has two nifty ways to find it, the first is to simply put a question mark in front of the whole call:

```
`?`(plot(rand_p4_tree))
```

R looks at the class of the `rand_p4_tree` object and takes us to the correct help file (note: this only works with S4 objects). The second ways is handy if you already know the class of your object, or want to compare to generics for different classes:

```
`?`(method, plot("phylo4"))
```

More information about how S4 documentation works can be found in the methods package, by running the following command.

```
help('Documentation', package="methods")
```

### 4 Trees without data

You can start with a tree — an object of class `phylo` from the `ape` package (e.g., read in using the `read.tree()` or `read.nexus()` functions), and convert it to a `phylo4` object.

For example, load the raw `Geospiza` data:
library(phylobase)
data(geospiza_raw)
## what does it contain?
names(geospiza_raw)
## [1] "tree" "data"

Convert the S3 tree to a S4 phylo4 object using the as() function:

```r
g1 <- as(geospiza_raw$tree, "phylo4")
```

<table>
<thead>
<tr>
<th>#</th>
<th>label</th>
<th>node</th>
<th>ancestor</th>
<th>edge.length</th>
<th>node.type</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1</td>
<td>fuliginosa</td>
<td>1</td>
<td>24</td>
<td>0.05500</td>
<td>tip</td>
</tr>
<tr>
<td>#2</td>
<td>fortis</td>
<td>2</td>
<td>24</td>
<td>0.05500</td>
<td>tip</td>
</tr>
<tr>
<td>#3</td>
<td>magnirostris</td>
<td>3</td>
<td>23</td>
<td>0.11000</td>
<td>tip</td>
</tr>
<tr>
<td>#4</td>
<td>conirostris</td>
<td>4</td>
<td>22</td>
<td>0.18333</td>
<td>tip</td>
</tr>
<tr>
<td>#5</td>
<td>scandens</td>
<td>5</td>
<td>21</td>
<td>0.19250</td>
<td>tip</td>
</tr>
<tr>
<td>#6</td>
<td>difficilis</td>
<td>6</td>
<td>20</td>
<td>0.22800</td>
<td>tip</td>
</tr>
<tr>
<td>#7</td>
<td>pallida</td>
<td>7</td>
<td>25</td>
<td>0.08667</td>
<td>tip</td>
</tr>
<tr>
<td>#8</td>
<td>parvulus</td>
<td>8</td>
<td>27</td>
<td>0.02000</td>
<td>tip</td>
</tr>
<tr>
<td>#9</td>
<td>psittacula</td>
<td>9</td>
<td>27</td>
<td>0.02000</td>
<td>tip</td>
</tr>
<tr>
<td>#10</td>
<td>pauper</td>
<td>10</td>
<td>26</td>
<td>0.03500</td>
<td>tip</td>
</tr>
<tr>
<td>#11</td>
<td>Platyspiza</td>
<td>11</td>
<td>18</td>
<td>0.46550</td>
<td>tip</td>
</tr>
<tr>
<td>#12</td>
<td>fusca</td>
<td>12</td>
<td>17</td>
<td>0.53409</td>
<td>tip</td>
</tr>
<tr>
<td>#13</td>
<td>Pinaroloxias</td>
<td>13</td>
<td>16</td>
<td>0.58333</td>
<td>tip</td>
</tr>
<tr>
<td>#14</td>
<td>olivacea</td>
<td>14</td>
<td>15</td>
<td>0.88077</td>
<td>tip</td>
</tr>
<tr>
<td>#15</td>
<td>&lt;NA&gt;</td>
<td>15</td>
<td>0</td>
<td>NA</td>
<td>root</td>
</tr>
<tr>
<td>#16</td>
<td>&lt;NA&gt;</td>
<td>16</td>
<td>15</td>
<td>0.29744</td>
<td>internal</td>
</tr>
<tr>
<td>#17</td>
<td>&lt;NA&gt;</td>
<td>17</td>
<td>16</td>
<td>0.04924</td>
<td>internal</td>
</tr>
<tr>
<td>#18</td>
<td>&lt;NA&gt;</td>
<td>18</td>
<td>17</td>
<td>0.06859</td>
<td>internal</td>
</tr>
<tr>
<td>#19</td>
<td>&lt;NA&gt;</td>
<td>19</td>
<td>18</td>
<td>0.13404</td>
<td>internal</td>
</tr>
<tr>
<td>#20</td>
<td>&lt;NA&gt;</td>
<td>20</td>
<td>19</td>
<td>0.10346</td>
<td>internal</td>
</tr>
<tr>
<td>#21</td>
<td>&lt;NA&gt;</td>
<td>21</td>
<td>20</td>
<td>0.03550</td>
<td>internal</td>
</tr>
<tr>
<td>#22</td>
<td>&lt;NA&gt;</td>
<td>22</td>
<td>21</td>
<td>0.00917</td>
<td>internal</td>
</tr>
<tr>
<td>#23</td>
<td>&lt;NA&gt;</td>
<td>23</td>
<td>22</td>
<td>0.07333</td>
<td>internal</td>
</tr>
<tr>
<td>#24</td>
<td>&lt;NA&gt;</td>
<td>24</td>
<td>23</td>
<td>0.05500</td>
<td>internal</td>
</tr>
<tr>
<td>#25</td>
<td>&lt;NA&gt;</td>
<td>25</td>
<td>19</td>
<td>0.24479</td>
<td>internal</td>
</tr>
<tr>
<td>#26</td>
<td>&lt;NA&gt;</td>
<td>26</td>
<td>25</td>
<td>0.05167</td>
<td>internal</td>
</tr>
<tr>
<td>#27</td>
<td>&lt;NA&gt;</td>
<td>27</td>
<td>26</td>
<td>0.01500</td>
<td>internal</td>
</tr>
</tbody>
</table>

The (internal) nodes appear with labels <NA> because they are not defined:

```r
nodeLabels(g1)
```

```
# 15 16 17 18 19 20 21 22 23 24 25 26 27
# NA NA NA NA NA NA NA NA NA NA NA NA
```

You can also retrieve the node labels with `labels(g1,"internal")`.

A simple way to assign the node numbers as labels (useful for various checks) is
nodeLabels(g1) <- paste("N", nodeId(g1, "internal"), sep="")
head(g1, 5)

##   label node ancestor edge.length node.type
## 1 fuliginosa 1    24 0.055000         tip
## 2    fortis 2    24 0.055000         tip
## 3 magnirostris 3   23 0.110000       tip
## 4 conirostris 4   22 0.183333       tip
## 5   scandens 5    21 0.192500       tip

The `summary` method gives a little extra information, including information on the distribution of branch lengths:

summary(g1)

## Phylogenetic tree: g1
## Number of tips: 14
## Number of nodes: 13
## Branch lengths:
##     mean: 0.1764008
##     variance: 0.04624379
##     distribution:
##         Min. 1st Qu.   Median     Mean 3rd Qu.     Max.
##     0.00917 0.04985 0.08000 0.17640 0.21912 0.88077

Print tip labels:

tipLabels(g1)

##   1     2     3     4     5
## "fuliginosa" "fortis" "magnirostris" "conirostris" "scandens"
##     6     7     8     9    10
## "difficilis" "pallida" "parvulus" "psittacula" "pauper"
##     11    12    13    14
## "Platyspiza" "fusca" "Pinaroloxias" "olivacea"

(labels(g1,"tip") would also work.)

You can modify labels and other aspects of the tree — for example, to convert all the labels to lower case:

tipLabels(g1) <- tolower(tipLabels(g1))

You could also modify selected labels, e.g. to modify the labels in positions 11 and 13 (which happen to be the only labels with uppercase letters):
Note that for a given tree, phylobase always return the tipLabels in the same order.

Print node numbers (in edge matrix order):

```r
tipLabels(g1)[c(11, 13)] <- c("platyspiza", "pinaroloxias")
```

```
Notes that for a given tree, phylobase always return the tipLabels in the same order.
Print node numbers (in edge matrix order):

nodeId(g1, type='all')

## [1] 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
## [24] 24 25 26 27
```

Does it have information on branch lengths?

```r
hasEdgeLength(g1)

## [1] TRUE
```

It does! What do they look like?

```r
edgeLength(g1)

## 0.29744 0.04924 0.06859 0.13404 0.10346 0.03550 0.00917 0.07333 0.05500
## 24-1 24-2 23-3 22-4 21-5 0-15 20-6 19-25 25-7
## 0.05500 0.05500 0.11000 0.18333 0.19250 0.22800 0.24479 0.08667
## 25-26 26-27 27-8 27-9 26-10 25-7 24-1
## 0.05167 0.01500 0.02000 0.03500 0.46550 0.53409 0.58333 0.88077
## 25-26 26-27 27-8 27-9 26-10 19-25 25-7
## 0.05167 0.01500 0.02000 0.03500 0.46550 0.53409 0.58333 0.88077
```

Note that the root has <NA> as its length.

Print edge labels (also empty in this case — therefore all NA):

```r
tipLabels(g1)

## NA NA NA NA NA NA NA NA NA
## 24-1 24-2 23-3 22-4 21-5 0-15 20-6 19-25 25-7
## NA NA NA NA NA NA NA NA NA
## 25-26 26-27 27-8 27-9 26-10 19-25 25-7
## NA NA NA NA NA NA NA NA NA
```

You can also use this function to label specific edges:

```r
tipLabels(g1)["23-24"] <- "an edge"
edgeLabels(g1)

## 15-16 16-17 17-18 18-19 19-20 20-21 21-22
## NA NA NA NA NA NA NA
## 22-23 23-24 24-1 24-2 23-3 22-4 21-5
## NA "an edge" NA NA NA NA NA
## 0-15 20-6 19-25 25-7 25-26 26-27 27-8
## NA NA NA NA NA NA NA
## 27-9 26-10 18-11 17-12 16-13 15-14
## NA NA NA NA NA NA NA
## 15-14 16-13 17-12 18-11 19-20 20-21 21-22
## NA NA NA NA NA NA NA
```

The edge labels are named according to the nodes they connect (ancestor-descendant). You can get the edge(s) associated with a particular node:

```r
getEdge(g1, 24) # default uses descendant node
## 24
## "23-24"

getEdge(g1, 24, type="ancestor") # edges using ancestor node
## 24 24
## "24-1" "24-2"
```

These results can in turn be passed to the function `edgeLength` to retrieve the length of a given set of edges:

```r
edgeLength(g1)[getEdge(g1, 24)]
## 23-24
## 0.055

edgeLength(g1)[getEdge(g1, 24, "ancestor")]
## 24-1 24-2
## 0.055 0.055
```

Is it rooted?

```r
isRooted(g1)
## [1] TRUE
```

Which node is the root?

```r
rootNode(g1)
## N15
## 15
```

Does it contain any polytomies?

```r
hasPoly(g1)
## [1] FALSE
```

Is the tree ultrametric?

```r
isUltrametric(g1)
## [1] TRUE
```
You can also get the depth (distance from the root) of any given node or the tips:

```r
nodeDepth(g1, 23)
## Warning: 'nodeDepth' is deprecated.
## Use 'nodeHeight' instead.
## See help("Deprecated")
## N23
## 0.77077

depthTips(g1)
## Warning: 'depthTips' is deprecated.
## Use 'nodeHeight' instead.
## See help("Deprecated")
## Warning: 'nodeDepth' is deprecated.
## Use 'nodeHeight' instead.
## See help("Deprecated")
## fuliginosa fortis magnirostris conirostris scandens
## 0.88077 0.88077 0.88077 0.88077 0.88077
## difficilis pallida parvulus psittacula pauper
## 0.88077 0.88077 0.88077 0.88077 0.88077
## platyspiza fusca pinaroloxias olivacea
## 0.88077 0.88077 0.88077 0.88077
```

5 Trees with data

The `phylo4d` class matches trees with data, or combines them with a data frame to make a `phylo4d` (tree-with-data) object.

Now we'll take the `Geospiza` data from `geospiza_raw$data` and merge it with the tree. First, let's prepare the data:

```r
g1 <- as(geospiza_raw$tree, "phylo4")
geodata <- geospiza_raw$data
```

However, since *G. olivacea* is included in the tree but not in the data set, we will initially run into some trouble:

```r
g2 <- phylo4d(g1, geodata)
## Error in formatData(phy = x, dt = tip.data, type = "tip", ...): The following nodes are not found in the dataset: olivacea
```

To deal with *G. olivacea* missing from the data, we have a few choices. The easiest is to use `missing.data="warn"` to allow R to create the new object with a warning (you can also use `missing.data="OK"` to proceed without warnings):
```r
g2 <- phylo4d(g1, geodata, missing.data="warn")

## Warning in formatData(phy = x, dt = tip.data, type = "tip", ...): The following
## nodes are not found in the dataset: olivacea

Another way to deal with this would be to use `prune()` to drop the offending tip from the
tree first:

```r
g1sub <- prune(g1, "olivacea")
g1B <- phylo4d(g1sub, geodata)
```n
The difference between the two objects is that the species *G. olivacea* is still present in the
tree but has no data (i.e., NA) associated with it. In the other case, *G. olivacea* is not included
in the tree anymore. The approach you choose depends on the goal of your analysis.

You can summarize the new object with the function `summary`. It breaks down the statistics
about the traits based on whether it is associated with the tips for the internal nodes:

```r
summary(g2)

## Phylogenetic tree: as(x, "phylo4")
## Number of tips: 14
## Number of nodes: 13
## Branch lengths:
##   mean : 0.1764008
##   variance : 0.04624379
##   distribution:
##   Min. 1st Qu. Median  Mean 3rd Qu. Max.
##   0.0232 0.0401 0.0743 0.1209 0.1623 0.8439
## Comparative data:
## Tips: data.frame with 14 taxa and 5 variable(s)
## wingL tarsusL culmenL beakD
## Min. :3.975 Min. :2.807 Min. :1.974 Min. :1.191
## 1st Qu.:4.189 1st Qu.:2.929 1st Qu.:2.187 1st Qu.:1.941
## Median :4.235 Median :2.980 Median :2.311 Median :2.073
## Mean :4.236 Mean :2.991 Mean :2.333 Mean :2.083
## 3rd Qu.:4.265 3rd Qu.:3.039 3rd Qu.:2.430 3rd Qu.:2.347
## Max. :4.420 Max. :3.271 Max. :2.725 Max. :2.824
## NA's :1 NA's :1 NA's :1 NA's :1
gonysW
## Min. :1.401
## 1st Qu.:1.845
## Median :1.962
## Mean :2.014
## 3rd Qu.:2.222
```
Max. : 2.676  
NA's : 1  

Nodes: data.frame with 13 internal nodes and 5 variables  

<table>
<thead>
<tr>
<th>wingL</th>
<th>tarsusL</th>
<th>culmenL</th>
<th>beakD</th>
<th>gonysW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min.</td>
<td>Min.</td>
<td>Min.</td>
<td>Min.</td>
<td>Min.</td>
</tr>
<tr>
<td>1st Qu.</td>
<td>Min.</td>
<td>Min.</td>
<td>Min.</td>
<td>Min.</td>
</tr>
<tr>
<td>Median</td>
<td>Mean</td>
<td>Mean</td>
<td>Mean</td>
<td>Mean</td>
</tr>
<tr>
<td>3rd Qu.</td>
<td>Mean</td>
<td>Mean</td>
<td>Mean</td>
<td>Mean</td>
</tr>
<tr>
<td>NA's</td>
<td>13</td>
<td>13</td>
<td>13</td>
<td>13</td>
</tr>
</tbody>
</table>

Or use `tdata()` to extract the data (i.e., `tdata(g2)`). By default, `tdata()` will retrieve tip data, but you can also get internal node data only (`tdata(tree, "internal")`) or — if the tip and node data have the same format — all the data combined (`tdata(tree, "allnode")`).

If you want to plot the data (e.g. for checking the input), `plot(tdata(g2))` will create the default plot for the data — in this case, since it is a data frame [this may change in future versions but should remain transparent] this will be a pairs plot of the data.

### 6 Subsetting

The `subset` command offers a variety of ways of extracting portions of a phylo4 or phylo4d tree, keeping any tip/node data consistent.

- **tips.include** give a vector of tips (names or numbers) to retain
- **tips.exclude** give a vector of tips (names or numbers) to drop
- **mrca** give a vector of node or tip names or numbers; extract the clade containing these taxa
- **node.subtree** give a node (name or number); extract the subtree starting from this node

Different ways to extract the *fuliginosa*-*scandens* clade:

```r
subset(g2, tips.include=c("fuliginosa", "fortis", "magnirostris", "conirostris", "scandens"))
subset(g2, node.subtree=21)
subset(g2, mrca=c("scandens", "fortis"))
```

One could drop the clade by doing

```r
subset(g2, tips.exclude=c("fuliginosa", "fortis", "magnirostris", "conirostris", "scandens"))
subset(g2, tips.exclude=names(descendants(g2, MRCA(g2, c("difficilis", "fortis"))))))
```
7 Tree-walking

*phylobase* provides many functions that allows users to explore relationships between nodes on a tree (tree-walking and tree traversal). Most functions work by specifying the *phylo4* (or *phylo4d*) object as the first argument, the node numbers/labels as the second argument (followed by some additional arguments).

*getNode* allows you to find a node based on its node number or its label. It returns a vector with node numbers as values and labels as names:

```r
data(geospiza)
getNode(geospiza, 10)
## pauper
## 10

getNode(geospiza, "pauper")
## pauper
## 10
```

If no node is specified, they are all returned, and if a node can’t be found it’s returned as a *NA*. It is possible to control what happens when a node can’t be found:

```r
getNode(geospiza)
## fuliginosa    fortis magnirostris conirostris scandens
## 1    2       3       4       5
## difficilis   pallida parvulus psittacula pauper
## 6    7       8       9      10
## Platyspiza    fusca Pinaroloxias olivacea N15
## 11   12      13      14     15
##   N16 N17 N18 N19 N20
## 16    17     18     19      20
##   N21 N22 N23 N24 N25
## 21    22     23     24      25
##   N26 N27
## 26    27

getNode(geospiza, 10:14)
## pauper Platyspiza fusca Pinaroloxias olivacea
## 10    11    12    13    14

getNode(geospiza, "melanogaster", missing="OK") # no warning
## <NA>
## NA

getNode(geospiza, "melanogaster", missing="warn") # warning!
## Warning in getNode(geospiza, "melanogaster", missing = "warn"): Some nodes not found among all nodes in tree: melanogaster
```
children and ancestor give the immediate neighboring nodes:

children(geospiza, 16)

```
#   N17 Pinaroloxias
#   17  13
```

ancestor(geospiza, 16)

```
#   N15
#   15
```

while descendants and ancestors can traverse the tree up to the tips or root respectively:

descendants(geospiza, 16)  # by default returns only the tips

```
# Pinaroloxias fusca Platyspiza difficilis scandens
# 13 12 11  6  5
# conirostris magnoirostris fuliginosa fortis pallida
#  4  3  1  2  7
# pauper parvulus psittacula
# 10  8  9
```

descendants(geospiza, "all")  # also include the internal nodes

```
# Warning in getNode(phy, node, missing = "warn"): Some nodes not found among all nodes in tree: all

# named list()
```

ancestors(geospiza, 20)

```
#   N19 N18 N17 N16 N15
#   19  18  17  16  15
```

ancestors(geospiza, 20, "ALL")  # uppercase ALL includes self

```
#   N20 N19 N18 N17 N16 N15
#   20  19  18  17  16  15
```

siblings returns the other node(s) associated with the same ancestor:

siblings(geospiza, 20)

```
#   N25
#   25
```

siblings(geospiza, 20, include.self=TRUE)
MRCA returns the most common recent ancestor for a set of tips, and shortest path returns the nodes connecting 2 nodes:

```r
MRCA(geospiza, 1:6)
## N20 N25
## 20  25

shortestPath(geospiza, 4, "pauper")
## N19 N20 N21 N22 N25 N26
## 19  20 21 22 25 26
```

## multiPhylo4 classes

multiPhylo4 classes are not yet implemented but will be coming soon.

## Examples

### Constructing a Brownian motion trait simulator

This section will describe a way of constructing a simulator that generates trait values for extant species (tips) given a tree with branch lengths, assuming a model of Brownian motion.

We can use `as(tree, "phylo4vcov")` to coerce the tree into a variance-covariance matrix form, and then use `mvrnorm` from the MASS package to generate a set of multivariate normally distributed values for the tips. (A benefit of this approach is that we can very quickly generate a very large number of replicates.) This example illustrates a common feature of working with phylobase — combining tools from several different packages to operate on phylogenetic trees with data.

We start with a randomly generated tree using `rcoal()` from ape to generate the tree topology and branch lengths:

```r
set.seed(1001)
library(ape)
tree <- as(rcoal(12), "phylo4")
```

Next we generate the phylogenetic variance-covariance matrix (by coercing the tree to a phylo4vcov object) and pick a single set of normally distributed traits (using MASS:mvrnorm to pick a multivariate normal deviate with a variance-covariance matrix that matches the structure of the tree).

```r
vmat <- as(tree, "phylo4vcov")
vmat <- cov2cor(vmat)
library(MASS)
trvec <- mvrnorm(1, mu=rep(0, 12), Sigma=vmat)
```
The last step (easy) is to convert the phylo4vcov object back to a phylo4d object:

treed <- phylo4d(tree, tip.data=as.data.frame(trvec))
plot(treed)

A Definitions/slots

This section details the internal structure of the phylo4, multiphylo4 (coming soon!), phylo4d, and multiphylo4d (coming soon!) classes. The basic building blocks of these classes are the phylo4 object and a dataframe. The phylo4 tree format is largely similar to the one used by phylo class in the package ape.

We use “edge” for ancestor-descendant relationships in the phylogeny (sometimes called “branches”) and “edge lengths” for their lengths (“branch lengths”). Most generally, “nodes” are all species in the tree; species with descendants are “internal nodes” (we often refer to these just as “nodes”, meaning clear from context); “tips” are species with no descendants. The “root node” is the node with no ancestor (if one exists).

A.1 phylo4

Like phylo, the main components of the phylo4 class are:

edge a 2-column matrix of integers, with \( N \) rows for a rooted tree or \( N - 1 \) rows for an unrooted tree and column names ancestor and descendant. Each row contains information on one edge in the tree. See below for further constraints on the edge matrix.

dge.length numeric list of edge lengths (length \( N \) (rooted) or \( N - 1 \) (unrooted) or empty (length 0))

tip.label character vector of tip labels (required), with length=# of tips. Tip labels need not be unique, but data-tree matching with non-unique labels will cause an error

node.label character vector of node labels, length=# of internal nodes or 0 (if empty). Node labels need not be unique, but data-tree matching with non-unique labels will cause an error

order character: “preorder”, “postorder”, or “unknown” (default), describing the order of rows in the edge matrix. , “pruningwise” and “cladewise” are accepted for compatibility with ape

The edge matrix must not contain NAs, with the exception of the root node, which has an NA for ancestor. phylobase does not enforce an order on the rows of the edge matrix, but it stores information on the current ordering in the @order slot — current allowable values are “unknown” (the default), “preorder” (equivalent to “cladewise” in ape) or “postorder”.

The basic criteria for the edge matrix are similar to those of ape, as documented it’s tree specification. This is a modified version of those rules, for a tree with \( n \) tips and \( m \) internal nodes:

1http://ape.mpl.ird.fr/
2see http://en.wikipedia.org/wiki/Tree_traversal for more information on orderings. (ape’s “pruningwise” is “bottom-up” ordering).
3ape.mpl.ird.fr/misc/FormatTreeR_28July2008.pdf
• Tips (no descendants) are coded $1, \ldots, n$, and internal nodes ($\geq 1$ descendant) are coded $n+1, \ldots, n+m$ ($n+1$ is the root). Both series are numbered with no gaps.

• The first (ancestor) column has only values $> n$ (internal nodes): thus, values $\leq n$ (tips) appear only in the second (descendant) column.

• All internal nodes [not including the root] must appear in the first (ancestor) column at least once [unlike ape, which nominally requires each internal node to have at least two descendants (although it doesn’t absolutely prohibit them and has a collapse.singles function to get rid of them), phylobase does allow these “singleton nodes” and has a method hasSingle for detecting them]. Singleton nodes can be useful as a way of representing changes along a lineage; they are used this way in the ouch package.

• The number of occurrences of a node in the first column is related to the nature of the node: once if it is a singleton, twice if it is dichotomous (i.e., of degree 3 [counting ancestor as well as descendants]), three times if it is trichotomous (degree 4), and so on.

phylobase does not technically prohibit reticulations (nodes or tips that appear more than once in the descendant column), but they will probably break most of the methods.Disconnected trees, cycles, and other exotica are not tested for, but will certainly break the methods.

We have defined basic methods for phylo4:show, print, and a variety of accessor functions (see help files). summary does not seem to be terribly useful in the context of a “raw” tree, because there is not much to compute.

A.2 phylo4d

The phylo4d class extends phylo4 with data. Tip data, and (internal) node data are stored separately, but can be retrieved together or separately with tdata(x,"tip"), tdata(x,"internal") or tdata(x,"all"). There is no separate slot for edge data, but these can be stored as node data associated with the descendant node.