

# Package ‘MPSEM’

September 25, 2017

**Version** 0.3-3

**Date** 2017-09-25

**Type** Package

**Title** Modeling Phylogenetic Signals using Eigenvector Maps

**Author** Guillaume Guenard, with contribution from Pierre Legendre

**Maintainer** Guillaume Guenard <guillaume.guenard@gmail.com>

**Description** Computational tools to represent phylogenetic signals using adapted eigenvector maps.

**Depends** R (>= 3.0.0), ape, MASS

**Suggests** knitr, caper, xtable

**VignetteBuilder** knitr

**License** GPL (>= 2)

**LazyLoad** yes

**NeedsCompilation** yes

**Repository** CRAN

**Date/Publication** 2017-09-25 18:23:06 UTC

## R topics documented:

MPSEM-package . . . . .	2
graph-class . . . . .	3
GraphFunctions . . . . .	4
lmutils . . . . .	6
PEM . . . . .	7
PEM-class . . . . .	11
TraitOUsimTree . . . . .	13

<b>Index</b>	<b>16</b>
--------------	-----------

---

MPSEM-package

*Modeling Phylogenetic Signals using Eigenvector Maps*

---

## Description

Computational tools to represent phylogenetic signals using adapted eigenvector maps.

## Details

Package:	MPSEM
Type:	Package
Version:	0.1-2
Date:	2013-08-29
License:	Copyleft
LazyLoad:	yes

Phylogenetic eigenvector maps (PEM) is a method for using phylogeny to model features of organism, most notably quantitative traits. It consists in calculating sets of explanatory variables (eigenvectors) that are meant to represent different patterns in trait values that are likely to have been induced by evolution. These patterns are used to model the data (using a linear model for instance).

If one gets a ‘target’ species (i.e. a species for which the trait value is unknown), and providing that we know the phylogenetic relationships between that species and those of the model, the method allows to obtain the scores of that new species on the phylogenetic eigenfunctions underlying a PEM. These scores are used to make empirical predictions of trait values for the target species on the basis of those observed for the species of the model.

Functions [PEM.build](#), [PEM.updater](#), [PEM.fitSimple](#), and [PEM.forcedSimple](#) allows one to build, update (i.e. recalculate with alternate weighting parameters) as well as to estimate or force arbitrary values for the weighting function parameters.

Functions [getGraphLocations](#) and [Locations2PEMscores](#) allows one to make predictions using method [predict.PEM](#) and a linear model. To obtain these linear model, user can use function [lm](#) or auxiliary functions [lmforwardsequentialsidak](#) or [lmforwardsequentialAICc](#), which perform forward-stepwise variable addition on the basis of either familywise type I error rate or the Akaike Information Criterion (AIC), respectively.

The package provides low-level utility function for performing operation on graphs (see [graph-functions](#)), calculate influence matrix ([PEMInfluence](#)), and simulate trait values (see [trait-simulator](#)).

A phylogenetic modeling tutorial using MPSEM is available as a vignette (see example below).

## Author(s)

Guillaume Guénard, Département des sciences biologiques, Université de Montréal, Montréal, Québec, Canada.

**References**

Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.

**See Also**

Makarenkov, V., Legendre, L. & Desdevisse, Y. 2004. Modelling phylogenetic relationships using reticulated networks. *Zool. Scr.* 33: 89-96

Blanchet, F. G., Legendre, P. & Borcard, D. 2008. Modelling directional spatial processes in ecological data. *Ecol. Model.* 215: 325-336

**Examples**

```
### To view MPSEM tutorial
vignette("MPSEM")
```

---

graph-class

*Graph class and methods*


---

**Description**

Class and methods to handle graphs.

**Usage**

```
## S3 method for class 'graph'
print(x, ...)
```

**Arguments**

x	An object of <a href="#">graph-class</a>
...	Additional parameters to be passed to the method. Currently ignored.

**Details**

Prints user-relevant information about the graph: number of edges and vertices, edge and vertex labels, addition edge properties and vertex properties.

**Value**

A [graph-class](#) object contains:

edge	a list whose first two unnamed members are the indices of the origin and destination vertices. Additional members must be named and are additional edge properties (e.g. length), and
vertex	a list that optionally contain vertex properties, if any (or an empty list if none).

**Author(s)**

Guillaume Guénard, Département de sciences biologiques, Université de Montréal, Montréal, Québec, Canada.

**References**

Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.

**See Also**

[PEM.build PEM-class](#)

---

GraphFunctions

*Graph creation and manipulation functions*

---

**Description**

A set of primitive functions for creating and manipulating graphs.

**Usage**

```
pop.graph(n, vertex=list(), label=NULL)
add.vertex(x, n, vertex=list(), label=NULL)
add.edge(x, from, to, edge=list(), label=NULL)
rm.edge(x, id)
rm.vertex(x, id)
collapse.vertex(x, id)
Phylo2DirectedGraph(tp)
```

**Arguments**

x	A graph-class object.
n	Number of vertex to populate a new graph ( <a href="#">pop.graph</a> ) or to add to an existing graph ( <a href="#">add.vertex</a> ).
vertex	List of vertex properties.
edge	List of edge properties.
label	Labels to be given to edges or vertices.
from	Origin of the edge to be added (vertex labels or indices).
to	Destination of the edge to be added (vertex labels or indices).
id	Label or index of vertex or edge to be removed.
tp	Phylogenetic tree object of class 'phylo', as defined in <a href="#">ape-package</a> .

## Details

A new graph can be populated with  $n$  vertices using function `pop.graph` and vertices can be added later with function `add.vertex`. The graphs so created contain no edges; the latter are added using function `add.edge`. Vertices and edges are removed using functions `rm.vertex` and `rm.edge`, respectively.

Function `collapse.vertex` allows one to remove a vertex while reestablishing the connections between the vertices located above and below that vertex using a new set of edges.

Function `Phylo2DirectedGraph` uses the graph functions to convert a rooted phylogenetic tree of class 'phylo' (see `ape-package`) to a directed graph object of `graph-class`. It recycles tip labels and creates default node labels, if they were absent from the phylo object, and uses them as vertex labels. The resulting acyclic graph (i.e. a mono-phylogeny) can then be edited to represent cases that do not have a tree topology (poly-phylogenies).

## Value

A `graph-class` object. Objects returned by `Phylo2DirectedGraph` have a `numeric` edge property called 'distance' featuring branch lengths and a `link{logical}` vertex property called 'species' specifying whether a vertex is a tree tip or an internal node.

## Author(s)

Guillaume Guénard, Département de sciences biologiques, Université de Montréal, Montréal, QC, Canada.

## References

- Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.
- Makarenkov, V., Legendre, L. & Desdevisse, Y. 2004. Modelling phylogenetic relationships using reticulated networks. *Zool. Scr.* 33: 89-96
- Blanchet, F. G., Legendre, P. & Borcard, D. 2008. Modelling directional spatial processes in ecological data. *Ecol. Model.* 215: 325-336

## See Also

`graph-class`.

## Examples

```
## Populate a graph with 7 vertices labeled A-G having properties x and y:
gr <- pop.graph(n=7,
               vertex=list(x=rnorm(7,0,1),y=rnorm(7,0,1)),
               label=c("A","B","C","D","E","F","G"))

gr
## Adding 3 vertices H, I, and J with property x (y is absent) and a new
## property z (type character), which is unknown for A-G:
gr <- add.vertex(x=gr,
                 n=3,
                 label=c("H","I","J")),
```

```

        vertex=list(x=rnorm(3,0,1),z=c("A","B","C")))
gr
gr$vertex
### Adding 10 edges, labeled E1-E10 and with properties a and b, to the graph:
gr <- add.edge(x=gr,
              from=c("A","B","B","C","C","D","D","E","E","F"),
              to=c("A","C","D","E","F","F","G","H","I","J"),
              edge=list(a=rnorm(10,0,1),b=rnorm(10,0,1)),
              label=paste("E",1:10,sep=""))
gr
gr$edge
### Removing edges 2, 4, and 7 from the graph:
print(rm.edge(gr,id=c(2,4,7)))
### Removing vertices 1, 3, 7, and 10 from the graph:
print(rm.vertex(gr,id=c(1,3,7,10)))
# Notice that the edges that had one of the removed vertex as their
# origin or destination are also removed:
print.default(rm.vertex(gr,id=c(1,3,7,10)))
### Vertex collapsing.
x <- pop.graph(n=9,label=c("A","B","C","D","E","F","G","H","I"))
x <- add.edge(x,from=c("A","A","B","B","C","C","D","D","E","E"),
             to=c("B","C","D","E","E","I","F","G","G","H"),
             label=paste("E",1:10,sep=""),edge=list(length=c(1,2,3,2,1,3,2,2,1,3)))
print.default(x)
for(i in c("A","B","C","D","E","F","G","H","I"))
  print(collapse.vertex(x,id=i))
#
if(require(ape)) {
  tree1 <- read.tree(text=paste("((A:0.15,B:0.2)N4:0.15,C:0.35)N2:0.25,((D:0.25,E:0.1)N5:0.3,",
                                "(F:0.15,G:0.2)N6:0.3)N3:0.1)N1;",sep=""))
  x <- Phylo2DirectedGraph(tree1)
  print(x)
}

```

---

Imutils

*Linear modelling utility functions*


---

## Description

Utility functions to build linear models using Phylogenetic Eigenvector Maps as their features.

## Usage

```

lmforwardsequentialsidak(y, x, object, alpha=0.05)
lmforwardsequentialAICc(y, x, object)

```

## Arguments

y	a response variable
x	descriptors to be used as auxiliary traits

object	a PEM class object
alpha	the threshold above which to stop adding variables

### Details

Function `lmforwardsequentialsidak`, performs a forward stepwise selection of the PEM eigenvectors until the familywise test of significance of the new variable to be included exceeds the threshold `alpha`. The familywise type I error probability is obtained using the Holm-Sidak correction of the testwise probabilities, thereby correcting for type I error rate inflation due to multiple testing. `lmforwardsequentialAICc` carries out forward stepwise selection of the eigenvectors as long as the candidate model features a lower sample-size-corrected Akaike information criterion than the previous model. The final model should be regarded as overfit from the Neyman-Pearson (*i.e.* frequentist) point of view, but it is the model that minimizes information loss from the standpoint of information theory.

### Value

Both functions return a `lm` class object.

### Author(s)

Guillaume Guénard, Département de sciences biologiques Université de Montréal, Montréal, QC, Canada.

### References

- Burnham, K. P. & Anderson, D. R. 2002. Model selection and multimodel inference: a practical information-theoretic approach, 2nd ed. Springer-Verlag. xxvi + 488 pp.
- Holm, S. 1979. A simple sequentially rejective multiple test procedure. *Scand. J. Statist.* 6: 65-70.
- Sidak, Z. 1967. Rectangular confidence regions for means of multivariate normal distributions. *J. Am. Stat. Ass.* 62, 626-633.

### Examples

```
## No example has yet been produced.
```

---

PEM

*Phylogenetic Eigenvector Map*

---

### Description

Functions to calculate and manipulate Phylogenetic Eigenvector Maps (PEM).

**Usage**

```

PEMinfluence(x, mroot = TRUE)
PEMweights(d, a = 0, psi = 1)
PEM.build(x, d = "distance", sp = "species", a = 0, psi = 1,
tol=.Machine$double.eps^0.5)
PEM.updater(object, a, psi = 1, tol = .Machine$double.eps^0.5)
PEM.fitSimple(y, x, w, d = "distance", sp = "species", lower = 0,
upper = 1, tol = .Machine$double.eps^0.5)
PEM.forcedSimple(y, x, w, d = "distance", sp = "species", a = 0, psi = 1,
tol = .Machine$double.eps^0.5)
getGraphLocations(tpall, targets)
getAncGraphLocations(x, tpall)
Locations2PEMscores(object, gsc)

```

**Arguments**

x	A <a href="#">graph-class</a> object containing a phylogenetic graph.
w	A <a href="#">graph-class</a> object containing a phylogenetic graph.
object	A <a href="#">PEM-class</a> object containing a Phylogenetic Eigenvector Map.
y	One or many response variable(s) in the form of a numeric vector or a <a href="#">matrix</a> , respectively.
mroot	Boolean (TRUE or FALSE) specifying whether multiple rooting is allowed.
d	The name of the member of x\$edge where the phylogenetic distances (edge lengths) can be found.
a	The steepness parameter describing whether changes occur, on average, progressively long edges (a close to 0) or abruptly at vertices (a close to 1).
psi	Relative evolution rate along the edges (default: 1). This parameter is only relevant when multiple values are assigned to different portions of the phylogeny.
sp	Name of the member of x\$vertex where a <a href="#">logical</a> vertex property specifying which vertices are species can be found. (see <a href="#">graph-class</a> ).
tol	Eigenvalue threshold to regard eigenvectors as usable.
lower	Lower limit for the L-BFGS-B optimization algorithm as implemented in <a href="#">optim</a> .
upper	Upper limit for the L-BFGS-B optimization algorithm as implemented in <a href="#">optim</a> .
tpall	Parameter of function <code>getGraphLocations</code> : Phylogenetic tree object of class 'phylo' (package <a href="#">ape</a> ) containing all species (model and target) used in the study.
targets	Name of the target species to extract using the <code>tpall</code> .
gsc	The output of <code>getGraphLocations</code> .

**Details**

Functions [PEMinfluence](#) and [PEMweights](#) are used internally by [PEM.build](#) to create a binary matrix referred to as an 'influence matrix' and weight its columns. That matrix has a row for each vertex of graph 'x' and a column for each of its edges. The elements of the influence matrix are 1 whenever the vertex associated with a row is located in the tree either directly or indirectly



downward the edge associated with a column. That function is implemented in C language using recursive function calls. Although `PEMInfluence` allows one to use multiple roots as its default parameter, it is called within `PEM.build` with `mroot = FALSE`. User must therefore ensure that the graph provided to `PEM` is single-rooted.

Function `PEM.build` is used to produce a phylogenetic eigenvector map, while function `PEM.updater` allows one to re-calculate a `PEM-class` object with new weighting function parameters. Function `PEM.fitSimple` performs a maximum likelihood estimation of  $\alpha$  and  $\psi$  assuming single values for the whole tree whereas function `PEM.forcedSimple` allows one to force parameters  $\alpha$  and  $\psi$  to a `PEM-class` object while adding the same computational details as those `PEM.fitSimple` would have produced (and which are necessary to make predictions).

Functions `getGraphLocations` returns the coordinates of a species in terms of its position with respect to the influence matrix while function `Locations2PEMscores` transforms these coordinates into sets of scores that can be used to make predictions. Function `getAncGraphLocations` produce the same output as `getGraphLocations`, but of the ancestral species (i.e. the nodes of the phylogeny) in order to estimate ancestral trait values.

## Value

Function `PEMInfluence` returns the influence matrix of graph  $x$  and function `PEMweights` returns weights corresponding to the distances. Functions `PEM.build`, `PEM.fitSimple`, `PEM.forcedSimple` returns a `PEM-class` object. Function `getGraphLocations` returns a list whose first member is an influence coordinates matrix whose rows refer to the target species and columns refer to the edges and second member is the lengths of the terminal edges connecting each target species to the rest of the phylogeny. Function `Locations2PEMscores` returns a list whose first member is a PEM score matrix whose rows refer to the target species and columns refer to the eigenvectors and second member is the variance associated with the terminal edges connecting the target species to the phylogeny.

## Author(s)

Guillaume Guénard, Département de sciences biologiques Université de Montréal, Montréal, QC, Canada.

## References

Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.

## Examples

```
t1 <- read.tree(text=paste("((A:0.15,B:0.2)N4:0.15,C:0.35)N2:0.25,((D:0.25,E:0.1)N5:0.3",
                           "(F:0.15,G:0.2)N6:0.3)N3:0.1)N1;", sep=""))
x <- Phylo2DirectedGraph(t1)
#
## Calculates the (binary) influence matrix
PEMInfluence(x)
PEMInfluence(x)[x$vertex$species,]
#
## Building phylogenetic eigenvector maps
PEM1 <- PEM.build(x)
```

```

print(PEM1)
PEM2 <- PEM.build(x, a = 0.2)
PEM3 <- PEM.build(x, a = 1)
PEM4 <- PEM.updater(PEM3,a=0.5)
#
## Extracts the eigenvectors
as.data.frame(PEM4)
#
### Example of an hypothetical set of trait values
y <- c(A=-1.1436265,B=-0.3186166,C=1.9364105,D=1.7164079,E=1.0013993,
      F=-1.8586351,G=-2.0236371)
#
## Estimate single steepness parameter for the whole tree.
PEMfs1 <- PEM.fitSimple(y=y,x=NULL,w=x,d="distance",sp="species",lower=0,upper=1)
PEMfs1$optim      # Results of the optimization.
#
## Force neutral evolution for the whole tree.
PEMfrc1 <- PEM.forcedSimple(y=y,x=NULL,w=x,d="distance",sp="species",a=0)
PEMfrc1$x$edge$a  # Steepness parameter forced for each individual edge.
#
## Get graph locations for target species X, Y, and Z
tpAll <- read.tree(text=paste("((X:0.45,((A:0.15,B:0.2)N4:0.15,",
                              "(C:0.25,Z:0.2)NZ:0.1)N2:0.05)NX:0.2,",
                              "(((D:0.25,E:0.1)N5:0.05,Y:0.25)NY:0.25,",
                              "(F:0.15,G:0.2)N6:0.3)N3:0.1)N1;","sep="))
grloc <- getGraphLocations(tpAll, c("X","Y","Z"))
#
PEMfs2 <- PEM.fitSimple(y=y,x=NULL,w=grloc$x,d="distance",sp="species",lower=0,upper=1)
PEMfs2$optim      # Same as for PEMfs1$optim
#
PEMsc1 <- Locations2PEMscores(PEMfs2, grloc)
lm1 <- lm(y~V_2+V_3+V_5,data=PEMfs2)
#
ypred <- predict(object=PEMfs2,targets=grloc,lmobject=lm1,interval="none")
#
tpModel <- drop.tip(tpAll,c("X","Y","Z"))
#
## Plotting the results:
layout(t(c(1,1,2)))
par(mar=c(6,2,2,0.5)+0.1)
plot(tpModel,show.tip.label=TRUE,show.node.label=TRUE,root.edge = TRUE,
     srt = 0,adj=0.5,label.offset=0.08,font=1,cex=1.5,xpd=TRUE)
edgelabels(paste("E",1:nrow(tpModel$edge),sep=""),
           edge=1:nrow(tpModel$edge),bg="white",font=1,cex=1)
points(x=0.20,y=2.25,pch=21,bg="black")
lines(x=c(0.20,0.20,0.65),y=c(2.25,0.55,0.55),xpd=TRUE,lty=2)
text("X",x=0.69,y=0.55,xpd=TRUE,font=1,cex=1.5)
points(x=0.35,y=4.5,pch=21,bg="black")
lines(x=c(0.35,0.35,0.6),y=c(4.5,5.47,5.47),xpd=TRUE,lty=2)
text("Y",x=0.64,y=5.47,xpd=TRUE,font=1,cex=1.5)
points(x=0.35,y=3,pch=21,bg="black")
lines(x=c(0.35,0.35,0.55),y=c(3,3.5,3.5),xpd=TRUE,lty=2)
text("Z",x=0.59,y=3.5,xpd=TRUE,font=1,cex=1.5)

```

```

text(c("NX", "NY", "NZ"), x=c(0.20, 0.35, 0.35), y=c(2.25, 4.5, 3)+0.3*c(1, -1, -1), font=1, cex=1)
add.scale.bar(length=0.1, cex=1.25)
par(mar=c(3.75, 0, 2, 2)+0.1)
plot(x=y, y=1:7, ylim=c(0.45, 7), xlim=c(-4, 4), axes=FALSE, type="n", xlab="")
axis(1, label=c("-4", "-2", "0", "2", "4"), at=c(-4, -2, 0, 2, 4)) ; abline(v=0)
points(x=y, y=1:7, xlim=c(-2, 2), pch=21, bg="black") # Observed values
text("B", x=-3.5, y=7, cex=1.5, xpd=TRUE) ; text("Trait value", x=0, y=-0.5, cex=1.25, xpd=TRUE)
points(x=y, y=c(0.5, 5.5, 3.5), pch=23, bg="white", cex=1.25) # Predicted values
#
## Estimating ancestral trait values:
ANCloc <- getAncGraphLocations(x)
PEMfsAnc <- PEM.fitSimple(y=y, x=NULL, w=ANCloc$x, d="distance", sp="species", lower=0, upper=1)
PEMfsAnc$optim
#
PEManc1 <- Locations2PEMscores(PEMfsAnc, ANCloc)
y_anc <- predict(object=PEMfsAnc, targets=ANCloc, lobject=lm1, interval="confidence")
#

```

PEM-class

*Class and methods for Phylogenetic Eigenvector Maps (PEM)***Description**

Class and methods to handle Phylogenetic Eigenvector Maps (PEM).

**Usage**

```

## S3 method for class 'PEM'
print(x, ...)
## S3 method for class 'PEM'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
## S3 method for class 'PEM'
predict(object, targets, lobject, newdata,
        interval = c("none", "confidence", "prediction"), level = 0.95, ...)

```

**Arguments**

x	A <a href="#">PEM-class</a> object containing a Phylogenetic Eigenvector Map.
row.names	Included for method consistency reason; ignored.
optional	Included for method consistency reason; ignored.
object	A <a href="#">PEM-class</a> object.
targets	Output of <a href="#">getGraphLocations</a> .
lobject	An object of class 'lm' (see <a href="#">lm</a> for details).
newdata	auxiliary trait values
interval	The kind of limits (confidence or prediction) to return with the predictions. interval="none": do not return a confidence interval.

level	Probability of the confidence of prediction interval.
...	Further parameters to be passed to other functions or methods (currently ignored).

### Details

The `print` method provides the number of eigenvectors, the number of observations these vectors are spanning, and their associated eigenvalues.

The `as.data.frame` method extracts the eigenvectors from the object and allows one to use `PEM-class` objects as data parameter in function such as `lm` and `glm`.

The `predict` object is a barebone interface meant to make predictions. It must be given species locations with respect to the phylogenetic graph (`target`), which are provided by function `getGraphLocations` and a linear model in the form of an object from `lm`. The user must provide auxiliary trait values if `lmobject` involves such trait.

### Value

A `PEM-class` object contains:

<code>x</code>	the <code>graph-class</code> object that was used to build the PEM (see <code>PEM.build</code> ),
<code>sp</code>	a <code>logical</code> vector specifying which vertex is a tip,
<code>B</code>	the influence matrix for those vertices that are tips,
<code>ne</code>	the number of edges,
<code>nsp</code>	the number of tips,
<code>Bc</code>	the column-centred influence matrix,
<code>means</code>	the column means of <code>B</code>
<code>dist</code>	edge lengths,
<code>a</code>	the steepness parameter (see <code>PEM.build</code> for details),
<code>psi</code>	the relative evolution rate along the edges (see <code>PEM.build</code> for details),
<code>w</code>	edge weights,
<code>BcW</code>	the weighted and column-centred influence matrix,
<code>d</code>	the singular values of <code>BcW</code> ,
<code>u</code>	the eigenvectors (left singular vectors) of <code>BcW</code> , and
<code>vt</code>	the right singular vectors of <code>BcW</code> .

In addition to these standard component, function, `PEM.fitSimple` and `PEM.forcedSimple` add the following members, which are necessary to make predictions:

<code>S2</code>	the variance(s) of the response(s),
<code>y</code>	a copy of the response(s), and
<code>opt</code>	the list returned by <code>optim</code> ,

as well as a copy of the estimated weighting parameters as edge properties.

**Author(s)**

Guillaume Guénard, Département des sciences biologiques, Université de Montréal, Montréal, Québec, Canada.

**References**

Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.

---

TraitOUsimTree	<i>Simulates the evolution of a quantitative trait.</i>
----------------	---

---

**Description**

Functions to simulate the evolution of a quantitative trait along a phylogenetic tree inputted as an object of class ‘phylo’ (package [ape](#)) or [graph-class](#) object.

**Usage**

```
EvolveOptimMarkovTree(tp, tw, anc, p=1, root=tp$edge[1,1])
TraitOUsimTree(tp, a, sigma, opt, p=1, root=tp$edge[1,1])
OUvar(d, a=0, theta=1, sigma=1)
PEMvar(d, a=0, psi=1)
TraitVarGraphSim(x, variance, distance="distance", p=1, ...)
```

**Arguments**

tp	A rooted phylogenetic tree of class ‘phylo’ (see package <a href="#">ape</a> ),
tw	Transition matrix giving the probability that the optimum trait value changes from one state to another at vertices. All rows must sum to 1.
anc	Ancestral state of a trait (at root).
p	Number of variates to generate.
root	Root node of the tree.
d	Phylogenetic distances (edge lengths).
a	Selection rate ( <a href="#">OUvar</a> ) or steepness ( <a href="#">PEMvar</a> ).
theta	Adaptive evolution rate, i.e. mean trait shift by natural selection.
sigma	Neutral evolution rate, i.e. mean trait shift by drift.
psi	Mean evolution rate.
opt	An index vector of optima at the nodes.
x	A <a href="#">graph-class</a> object.
variance	Variance function ( <a href="#">OUvar</a> , <a href="#">PEMvar</a> , or any suitable user-defined function).
distance	The name of the member of ‘x\$edge’ where edge lengths can be found.
...	Additional parameters for the specified variance function.

## Details

Function `EvolveOptimMarkovTree` allows one to simulate the changes of optimum trait values as a Markov process. The index whereby the process starts, at the tree root, is set by parameter `anc`; this is the ancestral character state. From the root onwards to the tips, the optimum is given the opportunity to change following a multinomial random draw with transition probabilities given by the rows of matrix `tw`. The integers thus obtained can be used as indices of a vector featuring the actual optimum trait values corresponding to the simulated selection regimes. The resulting optimum trait values at the nodes are used by `TraitOUsimTree` as its parameters `opt` to simulate trait values at nodes and tips. Function `TraitVarGraphSim` uses a graph variance function (either `OUvar` or `PEMvar`) to reconstruct a covariance matrix that is used to generate covariates drawn from a multi-normal distribution.

## Value

Functions `EvolveOptimMarkovTree` and `TraitOUsimTree` return a matrix whose rows represent the vertices (nodes and tips) of the phylogenetic tree and whose columns stand for the  $n$  different trials the function was asked to perform. For `EvolveQTraitTree`, the elements of the matrix are integers, representing the selection regimes prevailing at the nodes and tips, whereas for `TraitOUsimTree`, the elements are simulated quantitative trait values at the nodes and tips. These functions are implemented in C language and therefore run swiftly even for large (10000+ species) trees.

Function `TraitVarGraphSim` returns  $p$  phylogenetic signals and is implemented using a rotation of a matrix of standard normal random (mean=0, variance=1) deviates. The rotation matrix is itself obtained by Choleski factorization of the trait covariance matrix expected for a given set of trees, variance function, and variance function parameters.

## Author(s)

Guillaume Guénard, Département de sciences biologiques Université de Montréal, Montréal, QC, Canada.

## References

- Butler, M. A. & King, A. A. 2004. Phylogenetic comparative analysis: a modeling approach for adaptive evolution. *Am. Nat.* 164: 683-695.
- Guénard, G., Legendre, P., and Peres-Neto, P. 2013. Phylogenetic eigenvector maps (PEM): a framework to model and predict species traits. *Meth. Ecol. Evol.* In press.

## Examples

```
opt <- c(-2,0,2) # Three trait optima: -2, 0, and 2
### Transition probabilities:
transit <- matrix(c(0.7,0.2,0.2,0.2,0.7,0.1,0.1,0.1,0.7),
                 length(opt),length(opt),dimnames=list(from=opt,to=opt))

# In this example, the trait has a probability of 0.7 to stay at a given
# optimum, a probability of 0.2 for the optimum to change from -2 to 0,
# from 0 to -2, and from 2 to -2, and a probability of 0.1 for the
# optimum to change from -2 to 2, from 0 to 2, and from 2 to 0.
```

```

nsp <- 25 # A random tree for 25 species.
tree2 <- rtree(nsp,tip.label=paste("Species",1:nsp,sep=""))
tree2$node.label=paste("N",1:tree2$Nnode,sep="") # Node labels.

## Simulate 10 trials of optimum change.
reg <- EvolveOptimMarkovTree(tp=tree2,tw=transit,p=10,anc=2)
y1 <- TraitOUsimTree(tp=tree2,a=0,sigma=1,
                    opt=opt[reg[,1]],p=10) # Neutral
y2 <- TraitOUsimTree(tp=tree2,a=1,sigma=1,
                    opt=opt[reg[,1]],p=10) # Few selection.
y3 <- TraitOUsimTree(tp=tree2,a=10,sigma=1,
                    opt=opt[reg[,1]],p=10) # Strong selection.

### Display optimum change with colours.
displayOUprocess <- function(tp,trait,regime,mvalue) {
  layout(matrix(1:2,1,2))
  n <- length(tp$tip.label)
  ape::plot.phylo(tp,show.tip.label=TRUE,show.node.label=TRUE,root.edge=FALSE,
                 direction="rightwards",adj=0,
                 edge.color=rainbow(length(trait))[regime[tp$edge[,2]]])
  plot(y=1:n,x=mvalue[1:n],type="b",xlim=c(-5,5),ylab="",xlab="Trait value",yaxt="n",
       bg=rainbow(length(trait))[regime[1:n]],pch=21)
  text(trait[regime[1:n]],y=1:n,x=5,col=rainbow(length(trait))[regime[1:n]])
  abline(v=0)
}

displayOUprocess(tree2,opt,reg[,1],y1[,1]) # Trait evolve neutrally,
displayOUprocess(tree2,opt,reg[,1],y2[,1]) # under weak selection,
displayOUprocess(tree2,opt,reg[,1],y3[,1]) # under strong selection.

#
x <- Phylo2DirectedGraph(tree2)
y4 <- TraitVarGraphSim(x, variance = MPSEM::OUvar, p=10, a=5)
#
DisplayTreeEvol <- function(tp,mvalue) {
  layout(matrix(1:2,1,2))
  n <- length(tp$tip.label)
  ape::plot.phylo(tp,show.tip.label = TRUE, show.node.label = TRUE, root.edge = FALSE,
                 direction = "rightwards", adj = 0)
  plot(y=1:n,x=mvalue[1:n],type="b",xlim=c(-5,5),ylab="",xlab="Trait value",yaxt="n",pch=21)
  abline(v=0)
}
## Recursively displays the simulated traits.
for(i in 1:10) {
  DisplayTreeEvol(tree2,y4[i,])
  if(is.null(locator(1)))
    break # Stops recursive display on a mouse right-click.
}

```

# Index

add.edge (GraphFunctions), 4  
add.vertex (GraphFunctions), 4  
as.data.frame.PEM (PEM-class), 11  
collapse.vertex (GraphFunctions), 4  
EvolveOptimMarkovTree  
    (TraitOUsimTree), 13  
getAncGraphLocations (PEM), 7  
getGraphLocations (PEM), 7  
graph-class (graph-class), 3  
graph-functions (GraphFunctions), 4  
lmforwardsequentialAICc (lmutils), 6  
lmforwardsequentialsidak (lmutils), 6  
Locations2PEMscores (PEM), 7  
OUvar (TraitOUsimTree), 13  
PEM-class (PEM-class), 11  
PEM.build (PEM), 7  
PEM.fitSimple (PEM), 7  
PEM.forcedSimple (PEM), 7  
PEM.updater (PEM), 7  
PEMinfluence (PEM), 7  
PEMvar (TraitOUsimTree), 13  
PEMweights (PEM), 7  
Phylo2DirectedGraph (GraphFunctions),  
    4  
pop.graph (GraphFunctions), 4  
predict.PEM (PEM-class), 11  
print.graph (graph-class), 3  
print.PEM (PEM-class), 11  
rm.edge (GraphFunctions), 4  
rm.vertex (GraphFunctions), 4  
trait-simulator (TraitOUsimTree), 13  
TraitOUsimTree (TraitOUsimTree), 13  
TraitVarGraphSim (TraitOUsimTree), 13  
  
add.edge, 5  
add.vertex, 4, 5  
ape, 8, 13  
as.data.frame, 12  
  
collapse.vertex, 5  
  
EvolveOptimMarkovTree, 14  
  
getAncGraphLocations, 9  
getGraphLocations, 2, 9, 11, 12  
glm, 12  
graph-class, 3  
graph-functions, 2  
GraphFunctions, 4  
  
lm, 2, 11, 12  
lmforwardsequentialAICc, 2  
lmforwardsequentialsidak, 2, 7  
lmutils, 6  
Locations2PEMscores, 2, 9  
logical, 8, 12  
  
matrix, 8  
MPSEM (MPSEM-package), 2  
MPSEM-package, 2  
  
numeric, 5  
  
optim, 8, 12  
OUvar, 13  
  
PEM, 7  
PEM-class, 11  
PEM.build, 2, 4, 8, 9, 12  
PEM.fitSimple, 2, 9, 12  
PEM.forcedSimple, 2, 9, 12  
PEM.updater, 2, 9  
PEMinfluence, 2, 8, 9  
PEMvar, 13  
PEMweights, 8, 9  
Phylo2DirectedGraph, 5  
pop.graph, 4, 5  
predict, 12  
predict.PEM, 2  
print, 12  
  
rm.edge, 5



rm.vertex, [5](#)

trait-simulator, [2](#)

TraitUUsimTree, [13](#), [14](#)

TraitVarGraphSim, [14](#)