

Package ‘Rphylopars’

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Title Phylogenetic Comparative Tools for Missing Data and Within-Species Variation

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Description Tools for performing phylogenetic comparative methods for datasets with with multiple observations per species (intraspecific variation or measurement error) and/or missing data. Available functions allow ancestral state reconstruction, missing data imputation, phylogenetic regression (phylogenetic generalized least squares), and phylogenetic principal components analysis (pPCA).

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Rphylopars-package	2
anova.phylopars.lm	3
logLik.phylopars	3
logLik.phylopars.lm	4
phylopars	4
phylopars.crossvalidate	6
phylopars.lm	7
phylopars.pca	9
phylopars.predict	10
phylopars.rerun	11
plot.crossvalidate	12
print.crossvalidate	13
print.phylopars	13
print.phylopars.lm	14
simtraits	14
summary.phylopars	15

summary.phylopars.lm	15
write.phylopars	16

Index	17
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Rphylopars-package	<i>Phylogenetic Comparative Tools for Missing Data and Within-Species Variation</i>
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Description

Tools for performing phylogenetic comparative methods for datasets with with multiple observations per species (intraspecific variation or measurement error) and/or missing data. Available functions allow ancestral state reconstruction, missing data imputation, phylogenetic regression (phylogenetic generalized least squares), and phylogenetic principal components analysis (pPCA).

Details

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Author(s)

Eric W. Goolsby, Jorn Bruggeman, Cecile Ane
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References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.
 Ho, L. S. T. and Ane, C. 2014. "A linear-time algorithm for Gaussian and non-Gaussian trait evolution models". *Systematic Biology* 63(3):397-408.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)
```

```

PPE

# perform phylogenetic PCA
PPE_pca <- phylopars.pca(PPE)
summary(PPE_pca)

# perform phylogenetic regression
p_BM <- phylopars.lm(V3~V1+V2, trait_data = sim_data$trait_data, tree = sim_data$tree, model = "BM")

# perform ancestral state reconstruction / tip prediction
PPP_ace <- phylopars.predict(PPE)

```

anova.phylopars.lm *Phylopars regression ANOVA*

Description

Generic S3 method for phylopars

Usage

```
## S3 method for class 'phylopars.lm'
anova(object, ...)
```

Arguments

object Fitted phylopars.lm object
...

logLik.phylopars *Extract Log_likelihood*

Description

Generic S3 method for phylopars

Usage

```
## S3 method for class 'phylopars'
logLik(object, ...)
```

Arguments

object Fitted phylopars object
...

logLik.phylopars.lm *Extract Log_likelihood*

Description

Generic S3 method for phylopars

Usage

```
## S3 method for class 'phylopars.lm'
logLik(object, ...)
```

Arguments

object	Fitted phylopars.lm object
...	

phylopars *Estimation of phylogenetic and phenotypic covariance parameters*

Description

This function estimates parameters for the phylogenetic and phenotypic variance-covariance matrices for datasets with missing observations and multiple within-species observations. This function is a prerequisite for ancestral state reconstruction and missing tip estimation ([phylopars.predict](#)) and phylogenetic PCA ([phylopars.pca](#)).

Usage

```
phylopars(trait_data, tree, model = "BM", pheno_error = TRUE,
  phylo_correlated = TRUE, pheno_correlated = FALSE, calc_pheno = FALSE,
  calc_pheno_auto_n = 20, calc_pheno_phenocovs, use_means=FALSE,
  species_identifier = "species", verbose = FALSE, phylocov_start,
  phenocov_start, theta_start, model_start, skip_optim = FALSE, REML = TRUE,
  optim_limit = 50, BM_first = TRUE, usezscores = TRUE)
```

Arguments

trait_data	A data frame with one column per trait, as well as a column labeled "species" (with species names matching tips on the phylogeny). Each row corresponds to a single observation, and multiple observation for species are allowed. Missing data should be represented with NA.
tree	An object of class phylo
model	Model of evolution. Default is "BM". Also accepts "lambda", "kappa", "delta", "EB", and "OUrandomRoot", "OUfixedRoot",
pheno_error	If TRUE (default), parameters are estimated assuming within-species variation.
phylo_correlated	If TRUE (default), parameters are estimated assuming traits are correlated.

pheno_correlated	If TRUE, parameters are estimated assuming within-species observations traits are correlated (default is FALSE).
calc_pheno	If TRUE, phenotypic error variance is estimated for each species. If the number of observations for a given species is less than calc_pheno_auto_n (default=20), pooled within-species variance is used, unless phenotypic covariance matrices are supplied in the calc_pheno_phenocovs argument.
calc_pheno_auto_n	The minimum number of within-species observations for a given species for which within-species variance is calculated individually for a given species rather than pooled within-species variance. Only relevant if calc_pheno=TRUE and calc_pheno_phenocovs is not supplied.
calc_pheno_phenocovs	User-supplied phenotypic covariance matrix OR a list of phenotypic covariance matrices for each species.
use_means	Whether to use means (as in Ives et al. 2007) or raw data. Default is raw data (use_means=FALSE).
species_identifier	Optional argument. The name of the column in data where species names are stored. The default value is "species", but can be changed for convenience if data has an alternative species column name.
verbose	Optional argument. Whether or not to print the log-likelihood during optimization (NOTE: constants in the likelihood calculation are dropped from the value reported during optimization.)
phylocov_start	Optional starting value for phylogenetic trait variance-covariance matrix. Must be of dimensions n_traits by n_traits.
phenocov_start	Optional starting value for phenotypic trait variance-covariance matrix. Must be of dimensions n_traits by n_traits.
theta_start	Optional starting parameters for theta.
model_start	Optional starting parameters for the evolutionary model.
skip_optim	Optional argument to skip optimization (NOTE: this will produce the WRONG answer unless BM=TRUE, there is no missing data, and pheno_error=FALSE; generally leave set to FALSE).
REML	If TRUE (default), the algorithm will return REML estimates. If FALSE, maximum likelihood estimates will be returned.
optim_limit	Optional: number of extra optimization attempts allowed if convergence is not achieved. Only necessary if convergence failure is suspected.
BM_first	Whether to estimate covariance assuming Brownian motion prior to estimating alternative evolutionary model parameters.
usezscores	Whether to convert data to z-scores during optimization (recommended).

Value

An object of class phylopars.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>, Cecile Ane, Jorn Bruggeman

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)

PPE

# perform phylogenetic PCA
PPE_pca <- phylopars.pca(PPE)
summary(PPE_pca)

# perform phylogenetic regression
p_BM <- phylopars.lm(V3~V1+V2,trait_data = sim_data$trait_data,tree = sim_data$tree,model = "BM")

# perform ancestral state reconstruction / tip prediction
PPP_ace <- phylopars.predict(PPE)
```

phylopars.crossvalidate

Phylopars cross-validation

Description

This function performs cross-validation of the fitted phylopars object using the leave-one-out method. For each species, all observations for a single trait are temporarily deleted, and the value is phylogenetically imputed using `phylopars.predict()`. A regression between the observed and predicted species means is returned. Also estimated is mean bias and error of the phylopars model, as well as two alternative reference models: mean model and nearest neighbor model.

Usage

```
phylopars.crossvalidate(PPE, plot = FALSE, verbose = FALSE)
```

Arguments

PPE	Fitted phylopars object
plot	Whether or not to plot cross-validation statistics (default is TRUE)
verbose	Whether or not to print progress of cross-validation (default is FALSE)

Value

Returns a summary of cross-validation statistics.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15, ntraits = 4, nreps = 3, nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data, tree = sim_data$tree,
  pheno_error = TRUE, phylo_correlated = TRUE, pheno_correlated = FALSE)

PPE

phylopars.crossvalidate(PPE)
```

phylopars.lm

Phylopars regression

Description

Performs phylogenetic regression.

Usage

```
phylopars.lm(formula, trait_data, tree, model = "BM", pheno_error = TRUE,
  phylo_correlated = TRUE, pheno_correlated = FALSE, calc_pheno = FALSE,
  calc_pheno_auto_n = 20, calc_pheno_phenocovs, use_means = FALSE,
  species_identifier = "species", verbose = FALSE, phylocov_start,
  phenocov_start, theta_start, model_start, skip_optim = FALSE,
  REML = TRUE, optim_limit = 50, BM_first = TRUE, usezscores = TRUE)
```

Arguments

formula	A model formula.
trait_data	A data frame with one column per trait, as well as a column labeled "species" (with species names matching tips on the phylogeny). Each row corresponds to a single observation, and multiple observation for species are allowed. Missing data should be represented with NA.

tree	An object of class phylo
model	Model of evolution. Default is "BM". Also accepts "lambda", "kappa", "delta", "EB", and "OUrandomRoot", "OUfixedRoot",
pheno_error	If TRUE (default), parameters are estimated assuming within-species variation.
phylo_correlated	If TRUE (default), parameters are estimated assuming traits are correlated.
pheno_correlated	If TRUE, parameters are estimated assuming within-species observations traits are correlated (default is FALSE).
calc_pheno	If TRUE, phenotypic error variance is estimated for each species. If the number of observations for a given species is less than calc_pheno_auto_n (default=20), pooled within-species variance is used, unless phenotypic covariance matrices are supplied in the calc_pheno_phenocovs argument.
calc_pheno_auto_n	The minimum number of within-species observations for a given species for which within-species variance is calculated individually for a given species rather than pooled within-species variance. Only relevant if calc_pheno=TRUE and calc_pheno_phenocovs is not supplied.
calc_pheno_phenocovs	User-supplied phenotypic covariance matrix OR a list of phenotypic covariance matrices for each species.
use_means	Whether to use means (as in Ives et al. 2007) or raw data. Default is raw data (use_means=FALSE).
species_identifier	Optional argument. The name of the column in data where species names are stored. The default value is "species", but can be changed for convenience if data has an alternative species column name.
verbose	Optional argument. Whether or not to print the log-likelihood during optimization (NOTE: constants in the likelihood calculation are dropped from the value reported during optimization.)
phylocov_start	Optional starting value for phylogenetic trait variance-covariance matrix. Must be of dimensions n_traits by n_traits.
phenocov_start	Optional starting value for phenotypic trait variance-covariance matrix. Must be of dimensions n_traits by n_traits.
theta_start	Optional starting parameters for theta.
model_start	Optional starting parameters for the evolutionary model.
skip_optim	Optional argument to skip optimization (NOTE: this will produce the WRONG answer unless BM=TRUE, there is no missing data, and pheno_error=FALSE; generally leave set to FALSE).
REML	If TRUE (default), the algorithm will return REML estimates. If FALSE, maximum likelihood estimates will be returned.
optim_limit	Optional: number of extra optimization attempts allowed if convergence is not achieved. Only necessary if convergence failure is suspected.
BM_first	Whether to estimate covariance assuming Brownian motion prior to estimating alternative evolutionary model parameters.
usezscores	Whether to convert data to z-scores during optimization (recommended).

Value

A fitted phylopars.lm object.

Examples

```
# no missing data
s <- simtraits(ntaxa = 50, ntraits = 3, nreps = 1, nmissing = 0)
p_BM <- phylopars.lm(V3~V1+V2, trait_data = s$trait_data, tree = s$tree, model = "BM")
p_lambda <- phylopars.lm(V3~V1+V2, trait_data = s$trait_data, tree = s$tree, model = "lambda")
summary(p_BM)
summary(p_lambda)

# with missing data
# notice that logLik, AIC, and BIC are not reported if data is missing
s <- simtraits(ntaxa = 50, ntraits = 3, nreps = 1, nmissing = 15)
p_BM <- phylopars.lm(V3~V1+V2, trait_data = s$trait_data, tree = s$tree, model = "BM")
p_lambda <- phylopars.lm(V3~V1+V2, trait_data = s$trait_data, tree = s$tree, model = "lambda")
summary(p_BM)
summary(p_lambda)
```

phylopars.pca

Phylogenetic principal components analysis

Description

This function, adapted from [phyl.pca](#) in the **phytools** package, performs phylogenetic principal components analysis on a fitted phylopars object. Additionally, fast algorithms are used to avoid large matrix inversions using the [three.point.compute](#) function in **phylolm**.

Usage

```
phylopars.pca(PPE, mode = "cov", pgl_s_means = FALSE)
```

Arguments

PPE	Fitted phylopars object
mode	Either "cov" (default) or "corr"
pgl_s_means	Whether to use raw species trait means of PGLS species trait means in forming the PCA

Value

Returns an object of class `phyl.pca`.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>, Cecile Ane, Jorn Bruggeman

References

- Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.
- Revell, L. J. (2009) Size-correction and principal components for interspecific comparative studies. *Evolution*, 63, 3258-3268.
- Ho, L. S. T. and Ane, C. (2014) A linear-time algorithm for Gaussian and non-Gaussian trait evolution models. *Systematic Biology*, 63: 397-408.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)

PPE

# perform phylogenetic PCA
PPE_pca <- phylopars.pca(PPE)
summary(PPE_pca)
biplot(PPE_pca)
```

phylopars.predict *Ancestral state reconstruction and missing value tip reconstruction*

Description

This function performs ancestral state reconstruction (and missing value tip reconstruction) given a fitted phylopars object.

Usage

```
phylopars.predict(PPE, nodes, tips, verbose = FALSE)
```

Arguments

PPE	Fitted phylopars object
nodes	Optional argument: vector of which internal nodes to reconstruct.
tips	Optional argument: vector of which species values to predict.
verbose	Whether or not to print progress of node reconstruction / tip prediction (default is FALSE).

Value

Returns a list of reconstructed node and tip means, as well as standard deviations for each mean.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)

phylopars.predict(PPE)
```

phylopars.rerun *Rerun phylopars optimization*

Description

This function reruns parameter optimization for a phylopars object if convergence issues are suspected.

Usage

```
phylopars.rerun(PPE)
```

Arguments

PPE Fitted phylopars object

Value

Returns a fitted object of class phylopars.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)

# suspect convergence failure, so optimize parameters again
PPE <- phylopars.rerun(PPE)
```

plot.crossvalidate *Phylopars cross-validation*

Description

Plots cross-validation results

Usage

```
## S3 method for class 'crossvalidate'
plot(x, ...)
```

Arguments

x Crossvalidate object
...

Value

Returns a summary of cross-validation statistics.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

print.crossvalidate *Phylopars cross-validation*

Description

Generic S3 method for crossvalidate objects

Usage

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

Arguments

x Crossvalidate object
...

Value

Prints cross-validation results.

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

print.phylopars *Print phylopars*

Description

Generic S3 method for phylopars

Usage

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

Arguments

x Fitted phylopars object
...

```
print.phylopars.lm      Print phylopars.lm
```

Description

Generic S3 method for phylopars.lm

Usage

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

Arguments

```
x              Fitted phylopars.lm object
...           ...
```

```
simtraits      Simulate traits for phylopars estimation
```

Description

Simulates traits for codephylopars estimation.

Usage

```
simtraits(ntaxa = 15, ntraits = 4, nreps = 3, nmissing = 10, tree, v, anc, intraspecific)
```

Arguments

```
ntaxa          Either number of taxa (ntaxa) or a tree can be supplied.
ntraits        Number of traits to be simulated.
nreps          Number of replicates per trait per species to simulate.
nmissing       Number of randomly missing trait values.
tree           Either number of taxa (ntaxa) or a tree can be supplied.
v              Trait covariance (v) can be optionally supplied; otherwise off-diagonal elements
               are set to 0.8.
anc            Value for ancestral state at root node for fastBM from the phytools package.
intraspecific Optional value for within-species variance.
```

Value

```
data          Data for phylopars()
tree          Tree for phylopars()
```

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

# estimate parameters under Brownian motion
# pheno_error = TRUE assumes intraspecific variation
# pheno_correlated = FALSE assumes intraspecific variation is not correlated
# phylo_correlated = TRUE assumed traits are correlated

PPE <- phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,
  pheno_error = TRUE,phylo_correlated = TRUE,pheno_correlated = FALSE)

PPE
```

summary.phylopars *Phylopars summary*

Description

Summarizes phylopars

Usage

```
## S3 method for class 'phylopars'
summary(object, ...)
```

Arguments

object Fitted phylopars object
...

summary.phylopars.lm *phylopars.lm summary*

Description

Summarizes phylopars.lm

Usage

```
## S3 method for class 'phylopars.lm'
summary(object, ...)
```

Arguments

object Fitted phylopars.lm object
...

write.phylopars *Write data and tree files for Python phylopars compatibility.*

Description

Writes data and tree files for Python phylopars compatibility.

Usage

```
write.phylopars(trait_data, tree, data_file, tree_file, species_identifier = "species")
```

Arguments

trait_data	A data frame with one column per trait, as well as a column labeled "species" (with species names matching tips on the phylogeny). Each row corresponds to a single observation, and multiple observation for species are allowed. Missing data should be represented with NA.
tree	An object of class phylo
data_file	Desired path to write data file.
tree_file	Desired path to write tree file.
species_identifier	Title of species column in data file. Defaulted to "species"

Author(s)

Eric W. Goolsby <eric.goolsby.evolution@gmail.com>

References

Bruggeman J, Heringa J and Brandt BW. (2009) PhyloPars: estimation of missing parameter values using phylogeny. *Nucleic Acids Research* 37: W179-W184.

Examples

```
# simulate data
sim_data <- simtraits(ntaxa = 15,ntraits = 4,nreps = 3,nmissing = 10)

write.phylopars(trait_data = sim_data$trait_data,tree = sim_data$tree,data_file = "data_path.txt",
tree_file = "tree_path.new")
```


Index

- *Topic **Ancestral state reconstruction**
 - Rphylopars-package, [2](#)
 - *Topic **Intraspecific variation**
 - Rphylopars-package, [2](#)
 - *Topic **Measurement error**
 - Rphylopars-package, [2](#)
 - *Topic **Missing data**
 - Rphylopars-package, [2](#)
 - *Topic **Phylogenetic imputation**
 - Rphylopars-package, [2](#)
 - *Topic **Phylogenetic principle components analysis**
 - Rphylopars-package, [2](#)
 - *Topic **Phylogenetic regression**
 - Rphylopars-package, [2](#)
 - *Topic **Phylogenetic variance-covariance**
 - Rphylopars-package, [2](#)
 - *Topic **Within-species variation**
 - Rphylopars-package, [2](#)
 - *Topic **package**
 - Rphylopars-package, [2](#)
- [anova.phylopars.lm](#), [3](#)
- [fastBM](#), [14](#)
- [logLik.phylopars](#), [3](#)
[logLik.phylopars.lm](#), [4](#)
- [phyl.pca](#), [9](#)
[phylopars](#), [4](#)
[phylopars.crossvalidate](#), [6](#)
[phylopars.lm](#), [7](#)
[phylopars.pca](#), [4](#), [9](#)
[phylopars.predict](#), [4](#), [10](#)
[phylopars.rerun](#), [11](#)
[plot.crossvalidate](#), [12](#)
[print.crossvalidate](#), [13](#)
[print.phylopars](#), [13](#)
[print.phylopars.lm](#), [14](#)
- [Rphylopars-package](#), [2](#)
- [simtraits](#), [14](#)
- [summary.phylopars](#), [15](#)
[summary.phylopars.lm](#), [15](#)
- [three.point.compute](#), [9](#)
- [write.phylopars](#), [16](#)