

Package ‘ShiVa’

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Type Package

Title Detection of Evolutionary Shifts in Both Optimal Value and Variance

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Description Implements statistical methods for detecting evolutionary shifts in both the optimal trait value (mean) and evolutionary diffusion variance. The method uses an L1-penalized optimization framework to identify branches where shifts occur, and the shift magnitudes. It also supports the inclusion of measurement error. For more details, see Zhang, Ho, and Kenney (2023) <[doi:10.48550/arXiv.2312.17480](https://doi.org/10.48550/arXiv.2312.17480)>.

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backward_correction *Backward Selection for OU Model Shift Correction*

Description

Performs backward stepwise selection on a given set of candidate shifts in optimal trait values (mean) and evolutionary variance under an Ornstein-Uhlenbeck (OU) model. This function iteratively removes individual shifts to improve model fit based on a specified selection criterion.

Usage

```
backward_correction(
  tree,
  Y,
  alpha,
  shifts_mean,
  shifts_var,
  criterion = "BIC",
  original_model = NULL,
  measurement_error = FALSE,
  max.num.shifts = Inf
)
```

Arguments

tree	A phylogenetic tree of class phylo.
Y	A numeric vector of trait values corresponding to the tips of the tree.
alpha	A non-negative numeric value specifying the strength of selection in the OU process.
shifts_mean	A vector of branch indices with candidate shifts in optimal trait values.
shifts_var	A vector of branch indices with candidate shifts in evolutionary variance.
criterion	A model selection criterion to guide backward elimination. Options include "BIC", "mBIC", or "pBIC". Default is "BIC".
original_model	(Optional) A previously fitted OU model returned by fit_OU_mean_var. If NULL, the model is refit using the provided shifts.

measurement_error

Logical. If TRUE, the model accounts for measurement error by estimating an additional variance term. Default is FALSE.

max.num.shifts An integer specifying the maximum number of total shifts (mean and variance combined) allowed in the model. Default is Inf.

Value

A fitted OU model object (a list), as returned by `fit_OU_mean_var`, with a potentially reduced set of shifts that minimizes the specified criterion.

fit_OU_mean_var	<i>Fit OU Model with Shifts in Mean and Variance</i>
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Description

Fits an Ornstein-Uhlenbeck (OU) model with user-specified shifts in both optimal trait values (mean) and evolutionary variance along a phylogeny. The method uses numerical optimization to estimate shift magnitudes, base variance, and intercept, and can optionally incorporate measurement error in trait values.

Usage

```
fit_OU_mean_var(
  tree,
  Y,
  alpha,
  shifts_mean,
  shifts_var,
  max.steps = 1000,
  t = 0.01,
  thres = 0.01,
  measurement_error = FALSE,
  max.num.shifts = Inf
)
```

Arguments

tree	A phylogenetic tree of class <code>phylo</code> .
Y	A numeric vector of continuous trait values at the tips of the tree.
alpha	A non-negative numeric value specifying the strength of selection in the OU process.
shifts_mean	An integer vector indicating the indices of branches where shifts in the optimal trait value occur.
shifts_var	An integer vector indicating the indices of branches where shifts in evolutionary variance occur.

<code>max.steps</code>	Maximum number of optimization steps. Default is 1000.
<code>t</code>	Step size for the optimizer. Default is 0.01.
<code>thres</code>	Convergence threshold for change in log-likelihood. Default is 0.01.
<code>measurement_error</code>	Logical. If TRUE, a separate measurement error variance is estimated and added to the diagonal of the covariance matrix.
<code>max.num.shifts</code>	Maximum allowed number of shifts (combined for mean and variance). Default is Inf.

Value

A list containing:

<code>tree</code>	The phylogenetic tree.
<code>Y</code>	The trait values.
<code>shifts_mean</code>	Indices of branches with non-zero shifts in optimal trait value.
<code>shifts_var</code>	Indices of branches with non-zero shifts in evolutionary variance.
<code>beta</code>	Estimated shift magnitudes for optima values.
<code>gamma</code>	Estimated shift magnitudes for variance.
<code>sigma2</code>	Estimated base evolutionary variance.
<code>b0</code>	Estimated intercept (ancestral trait value).
<code>sigma2_error</code>	Estimated measurement error variance (only returned if <code>measurement_error = TRUE</code>).
<code>loglik</code>	Log-likelihood of the fitted model.
<code>BIC</code>	BBIC for model selection.
<code>mBIC</code>	mBIC for accounting shift sparsity and shared support.
<code>pBIC</code>	pBIC incorporating determinant of projected design matrix.
<code>fitted.values</code>	Fitted trait values based on the estimated model.
<code>Sigma</code>	Estimated trait covariance matrix under the fitted model.

`generate_design_matrix`

Generate Design Matrix

Description

Constructs a design matrix for a given phylogenetic tree, used in Ornstein-Uhlenbeck modeling.

Usage

```
generate_design_matrix(tree, type = "simpX", alpha = 0)
```

Arguments

tree	A phylogenetic tree of class phylo.
type	A character string specifying the type of design matrix to generate. Options are "simpX" or "orgX".
alpha	The selection strength parameter (only used when type = "orgX").

Value

A design matrix X , where each row corresponds to a tip and each column to an edge in the tree.

get_mean_var_shifts *Estimate Shifts in Optimal Trait Values and Variance*

Description

Estimates shifts in both the optimal trait values (mean) and evolutionary variance along a phylogeny under an Ornstein-Uhlenbeck (OU) process, using an ℓ_1 -penalized optimization procedure. Optionally accounts for measurement error in the observed trait data.

Usage

```
get_mean_var_shifts(
  Y,
  tree,
  alpha,
  lambda1,
  lambda2,
  max.steps = 1000,
  t = 0.01,
  penalty = "L1",
  thres = 0.01,
  sigma2 = NULL,
  measurement_error = FALSE
)
```

Arguments

Y	A numeric vector of continuous trait values for the species at the tips of the tree.
tree	A phylogenetic tree of class phylo.
alpha	The selection strength parameter in the OU process.
lambda1	Non-negative penalty for β (shifts in optimal trait values).
lambda2	Non-negative penalty for γ (shifts in evolutionary variance).
max.steps	Maximum number of optimization steps. Default is 1000.
t	Step size for the gradient-based updates. Default is 0.01.

penalty	Type of penalty to apply. Options are "L1" (default) or "None".
thres	Convergence threshold for the change in loss between steps. Default is 0.01.
sigma2	Optional initial value for the base evolutionary variance. If NULL, it is initialized to 1.
measurement_error	Logical. If TRUE, the method estimates additional measurement error variance.

Value

A list containing:

shifts_mean	Indices of branches with detected shifts in optimal trait values ($\beta \neq 0$).
shifts_var	Indices of branches with detected shifts in evolutionary variance ($\gamma \neq 0$).
beta	Estimated shift coefficients for optimal trait values.
gamma	Estimated shift coefficients for evolutionary variance.
sigma2	Estimated base variance (σ^2) of the OU process.
b0	Estimated intercept (root state).
sigma2_error	Estimated measurement error variance (only returned if measurement_error = TRUE).

`get_mean_var_shifts_model_selection`

Model Selection for OU Shifts in Optimal value and Variance

Description

Performs model selection to estimate the locations and magnitudes of evolutionary shifts in optimal trait values (mean) and diffusion variance under an Ornstein-Uhlenbeck (OU) process. This function searches across user-defined grids of shrinkage parameters for both types of shifts, uses cross-validation for selecting `lambda1`, and applies backward correction to refine top candidate models.

Usage

```
get_mean_var_shifts_model_selection(
  Y,
  tree,
  alpha,
  t = 0.01,
  lambda1_list = NULL,
  lambda2_list = exp(1:10 * 0.4 - 6),
  criterion = "BIC",
  max.steps = 300,
  nfolds = 8,
  top_k = 10,
```

```

    measurement_error = FALSE,
    lambda.type = "lambda.1se",
    max.num.shifts = Inf,
    verbose = TRUE
)

```

Arguments

Y	A numeric vector of trait values for the species at the tips of the phylogenetic tree.
tree	A phylogenetic tree of class phylo.
alpha	A non-negative numeric value representing the selection strength in the OU process.
t	Step size for iterative optimization. Default is 0.01.
lambda1_list	A numeric vector of candidate λ_1 values controlling shrinkage for shifts in optimal values.
lambda2_list	A numeric vector of candidate λ_2 values controlling shrinkage for shifts in variance. Default is $\exp(1:10*0.4-6)$
criterion	Model selection criterion to optimize. Options include "BIC", "mBIC", or "pBIC". Default is "BIC".
max.steps	Maximum number of optimization steps. Default is 300.
nfolds	Number of cross-validation folds for tuning lambda1. Default is 8.
top_k	Number of top candidate models (ranked by criterion) to further refine using backward correction. Default is 10.
measurement_error	Logical. If TRUE, estimates a separate measurement error variance component. Default is FALSE.
lambda.type	A character string specifying the cross-validation rule used to select lambda1 from lambda1_list. Options are "lambda.min" (minimum CV error) and "lambda.1se" (1-SE rule, higher penalty). Default is "lambda.1se".
max.num.shifts	An integer specifying the maximum number of allowed shifts (combined across mean and variance). Default is Inf.
verbose	Logical. If TRUE, prints progress messages to the console. Default is TRUE.

Value

A list containing:

best_model	The final selected OU model object, with estimated shifts and parameters.
score_summary	A data frame summarizing the model selection results, including pre- and post-correction scores and shift locations.

OU.vcv	<i>OU.vcv</i>
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Description

generate covariance matrix for OU process

Usage

```
OU.vcv(tree, alpha)
```

Arguments

tree	phylogenetic tree
alpha	selective force

Value

V	covariance matrix
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plot.ShiftModel	<i>Plot Method for ShiftModel Objects</i>
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Description

Plots a phylogenetic tree with trait values at the tips and highlights branches with detected shifts in optimal value (mean) and variance.

Usage

```
## S3 method for class 'ShiftModel'
plot(x, title = "", ...)
```

Arguments

x	An object of class ShiftModel, typically returned by fit_OU_mean_var() or ShiVa().
title	A character string specifying the plot title.
...	Additional arguments passed to plot.phylo().

Value

No return value. This function is called for its side effect: a plotted tree.

```
print.summary.ShiftModel
```

Print Method for Summary of ShiftModel

Description

Prints a formatted summary of a fitted ShiftModel, including the estimated parameters (alpha, sigma2, log-likelihood, and BIC), as well as details of detected shifts in the optimal trait value (mean) and variance. This method is typically called on the result of summary() applied to an object of class ShiftModel.

Usage

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

Arguments

x An object of class summary.ShiftModel, usually returned by summary(model) where model is a ShiftModel.

... Additional arguments (currently ignored).

Value

No return value. Called for its side effect: printing summary information to the console.

```
ShiVa
```

ShiVa: Automatic Shift Detection in Mean and Variance

Description

Performs automatic detection of evolutionary shifts in both optimal trait values (mean) and diffusion variance under an Ornstein-Uhlenbeck (OU) process. This function serves as a wrapper for get_mean_var_shifts_model_selection, with the added ability to automatically estimate the selection strength parameter alpha if not provided.

Usage

```
ShiVa(
  Y,
  tree,
  alpha = NULL,
  t = 0.01,
  lambda1_list = NULL,
  lambda2_list = exp(1:10 * 0.4 - 6),
```

```

criterion = "BIC",
max.steps = 300,
nfolds = 8,
top_k = 10,
measurement_error = FALSE,
lambda.type = "lambda.1se",
max.num.shifts = Inf
)

```

Arguments

<code>Y</code>	A numeric vector of trait values at the tips of the phylogenetic tree.
<code>tree</code>	A phylogenetic tree of class <code>phylo</code> .
<code>alpha</code>	(Optional) A non-negative numeric value specifying the OU selection strength. If <code>NULL</code> , it is estimated via maximum likelihood using <code>phylo1m()</code> .
<code>t</code>	Step size for optimization. Default is 0.01.
<code>lambda1_list</code>	A numeric vector of candidate λ_1 values for penalizing mean shifts.
<code>lambda2_list</code>	A numeric vector of candidate λ_2 values for penalizing variance shifts. Default is $\exp(1:10 * 0.4 - 6)$.
<code>criterion</code>	Model selection criterion to use. Options are "BIC", "mBIC", or "pBIC". Default is "BIC".
<code>max.steps</code>	Maximum number of optimization steps. Default is 300.
<code>nfolds</code>	Number of folds for cross-validation in tuning <code>lambda1</code> . Default is 8.
<code>top_k</code>	Number of top candidate models (based on criterion) to refine using backward correction. Default is 10.
<code>measurement_error</code>	Logical. If <code>TRUE</code> , estimates a measurement error variance term. Default is <code>FALSE</code> .
<code>lambda.type</code>	Cross-validation rule for selecting <code>lambda1</code> . Options are "lambda.min" or "lambda.1se". Default is "lambda.1se".
<code>max.num.shifts</code>	Maximum number of allowed shifts (in both mean and variance). Default is <code>Inf</code> .

Value

A list with the same structure as `get_mean_var_shifts_model_selection`:

<code>best_model</code>	The final selected OU model object.
<code>score_summary</code>	A data frame summarizing candidate models and backward-corrected scores.

soft_thresholding	<i>Soft Thresholding</i>
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Description

Applies the soft thresholding operation to a numeric input, commonly used in Lasso and sparse modeling to induce shrinkage and sparsity.

Usage

```
soft_thresholding(z, lambda)
```

Arguments

z	A numeric value to be thresholded.
lambda	A non-negative numeric value indicating the threshold level (degree of shrinkage).

Value

A numeric value after applying soft thresholding: $\text{sign}(z) \cdot \max(|z| - \lambda, 0)$.

summary.ShiftModel	<i>Summary of a ShiVa Shift Model</i>
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Description

Generate a summary of a fitted ShiVa model object, including estimated parameters and details of detected shifts in optimal trait value (mean) and evolutionary variance.

Usage

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

Arguments

object	An object of class ShiftModel, typically returned by functions such as fit_OU_mean_var(), or extracted as best_model from get_mean_var_shifts_model_selection() or ShiVa().
...	Additional arguments (currently unused).

Value

An object of class `summary.ShiftModel`, which includes:

- `alpha`: Estimated selection strength parameter.
- `sigma2`: Estimated diffusion variance.
- `loglik`: Log-likelihood of the fitted model.
- `BIC`: Bayesian Information Criterion.
- `mean_shifts`: A data frame of branches with shifts in optimal value.
- `var_shifts`: A data frame of branches with shifts in evolutionary variance.

update_step_gamma	<i>Update Step for Gamma</i>
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Description

Performs one update step for the `gamma_k` parameter in an iterative optimization routine, potentially applying L1 shrinkage.

Usage

```
update_step_gamma(gamma_k, X_k, Sigma, r, lambda2, t, penalty, V, q_k)
```

Arguments

<code>gamma_k</code>	Current value of the <code>gamma_k</code> parameter to be updated.
<code>X_k</code>	The k th column of the design matrix X .
<code>Sigma</code>	Current covariance matrix.
<code>r</code>	Residual vector, typically $Y - X \%*\% \text{beta}$.
<code>lambda2</code>	Non-negative tuning parameter controlling the degree of L1 shrinkage applied to <code>gamma_k</code> .
<code>t</code>	Step size for the gradient update.
<code>penalty</code>	Penalty type; either "L1" for soft thresholding or "None" for unpenalized updates.
<code>V</code>	Baseline covariance matrix when $\sigma^2 = 1$.
<code>q_k</code>	The k th element of the design vector q , used in the update.

Value

A list containing:

<code>gamma_k</code>	The updated value of <code>gamma_k</code> .
<code>Sigma</code>	The updated covariance matrix <code>Sigma</code> .

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