Package 'moRphomenses'

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Title Geometric Morphometric Tools to Align, Scale, and Compare ``Shape" of Menstrual Cycle Hormones

Version 1.0.3

Description Mitteroecker & Gunz (2009) <doi:10.1007/s11692-009-9055-x> describe how geometric morphometric methods allow researchers to quantify the size and shape of physical biological structures. We provide tools to extend geometric morphometric principles to the study of non-physical structures, hormone profiles, as outlined in Ehrlich et al (2021) <doi:10.1002/ajpa.24514>. Easily transform daily measures into multivariate landmark-based data. Includes custom functions to apply multivariate methods for data exploration as well as hypothesis testing. Also includes 'shiny' web app to streamline data exploration. Developed to study menstrual cycle hormones but functions have been generalized and should be applicable to any biomarker over any time period.

License GPL (>= 3.0)

URL <https://github.com/ClancyLabUIUC/moRphomenses>

Depends R (>= 2.10)

Imports stats, graphics, grDevices, utils

Encoding UTF-8

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Suggests dendextend, geomorph, cluster, shiny

NeedsCompilation no

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mm_ArrayData

Array Data

Description

Construct a ragged array (containing missing data) of a specified length (up/down sampling individuals to fit).

Usage

```
mm_ArrayData(
    IDs,
    DAYS,
    VALUE,
    MID = NULL,
```

```
targetLENGTH,
targetMID = NULL,
transformation = c("minmax", "geom", "zscore", "log", "log10"),
impute_missing = 3
```

Arguments

IDs	A vector that contains individual IDs repeated for multiple days of collection.
DAYS	A vector that contains information on time, IE Day 1, Day 2, Day 3. Note: this vector should include integers, continuous data might produce unintended results.
VALUE	A vector containing the variable sampled.
MID	Am optional vector of midpoints to center each individuals profile. These should be unique to each individual and repeated for each observation of DAYS, VALUE, and IDs. If NULL (defualt), data will not be centered on any day.
targetLENGTH	Integer. Number of days to up/down sample observations to using $mm_get_interval$.
targetMID	If NULL (default) data will not be centered and will range from 0 to 1. If specified, data will be centered on 0 ranging from -1 to 1.
transformation	Which (if any) data transformation to apply. Our reccomendation is minmax, but Geometric mean, Zscore, natural log and log10 transformations are available, if desired.
<pre>impute_missing</pre>	Integer. If not null, number of nearest-neighbors to use to impute missing data (Default = 3).

Value

Returns a 3D array of data to be analyzed with individuals in the 3rd dimension.

mm_BuildModel

Build, implement, visualize multivariate linear model.

Description

Easily evaluate simple model sets (one covariate with up to 2 additional classifiers/covariates). Helpful for exploratory analysis. For detailed models or specific combinations of variables, see geomorph::procD.lm for full use of this function.

Usage

```
mm_BuildModel(shape_data, ..., subgrps = NULL, ff1 = NULL, univ_series = FALSE)
```

Arguments

shape_data	This will be the (multivariate) response variable
	Covariate(s)/classifier(s) to build a model set. Individual models are run with interaction effects.
subgrps	Optional. Vector of group membership. Model sets will be run across the whole sample and subgroups. If k is specified, only the full model will be run.
ff1	An explicit model to test in the format: " coords ~". Names must match those specifed in Standard Im notation applies.
univ_series	Default (FALSE) will evaluate multiple covariates and their interaction in a sin- gle model. However, it can be helpful to understand the univariate effects in isolation of interaction/confounding factors. Set univ_series=TRUE to produce a series of model sets, one for each covariate specified (NOTE: ff1 must also be NULL for this to work).

Value

A list containing output of one or more multivariate linear models that can be inspected on their own or interacted with using mm_VizModel or mm_CompModel.

mm_CalcShapespace Define Shapespace of aligned dataset.

Description

Conduct PCA of shape data and visualize major shape trends.

Usage

```
mm_CalcShapespace(dat, max_Shapes = 10)
```

Arguments

dat	A 3D array of shape data to be analyzed.
<pre>max_Shapes</pre>	The maximum amount of PCs to visualize. Default 10.

Value

A list containing the results of shape-pca, including vizualizations of shape extrema for each Principal Component.

mm_CheckImputation CheckImputation

Description

Plot Raw (aligned) data along side by side with imputed data.

Usage

mm_CheckImputation(A1, A2, Ob0 = interactive())

Arguments

A1	An aligned array, containing missing data (presumably made with <code>mm_ArrayData</code> shape_data_wNA).
A2	An aligned and imputed array (presumably made with mm_ArrayData\$Shape_data).
060	One-by-One. If TRUE (default, in interactive sessions), individuals will be plot- ted one at a time, requiring the user to advance/exit the operation. If FALSE, all plots #' will be generated at once to be browsed or exported from the Plots panel.

Value

A series of plots for each individual in the array. If ObO=TRUE user input is required to advance or exit the plotting.

mm_ColorLeaves Color leves of a dendrogram

Description

Specify color order approriately for a dendrogram

Usage

```
mm_ColorLeaves(dendro, cols)
```

Arguments

dendro	A dendrogram or hclust class object
cols	a vector of colors

Details

Leaves of a dendrogram will be re-ordered compared to most input classifiers. This function takes the study-ordered colors and correctly applies them to the dendrogram using dendextend

Value

A dendrogram class object with leaves colored as specified.

e Model Metrics	Compare Model Metric	mm_CompModel
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Description

Compare key figs (Rsq, p-value, etc) across multiple models.

Usage

```
mm_CompModel(mv_results, row_labels = NULL, digits = 4)
```

Arguments

<pre>mv_results</pre>	Input mvlm, created by mm_BuildModel (or by using geomorph::procD.lm)
row_labels	A character vector to use in output. If NULL (default) labels from the input data will be used.
digits	Number of decimal places to round to. Default includes 4 decimal places.

Value

A list containing the results of the mvlm, visualizations of shape trends along the regression line, and the model itself.

mm_CompModel_Full Compare Complex Model Metrics

Description

Compare key figs (Rsq, p-value, etc) across multiple complex models.

Usage

```
mm_CompModel_Full(mv_results, row_labels = NULL, var_labels = NULL, digits = 4)
```

Arguments

<pre>mv_results</pre>	Input mvlm, created by mm_BuildModel (or by using geomorph::procD.lm)
row_labels	A character vector to use in output. If NULL (default) labels from the input data will be used.
var_labels	A character vector to use in output. If NULL (default) labels from the input data will be used.
digits	Number of decimal places to round to. Default includes 4 decimal places.

Value

description

mm_coords_to_shape Visualize shape of target coordinates

Description

Visualize shape of target coordinates

Usage

```
mm_coords_to_shape(A, PCA, target_coords, target_PCs = c(1, 2))
```

Arguments

A	A landmark array used for the pca
PCA	output of prcomp. Should contain \$transormation
target_coords	A single set of X,Y coordinates.
target_PCs	Integer identifying which pc to use on the X and Y axis. Default is $c(1,2)$ for PC1 on x and PC2 on y

Value

A landmark array representing the hypothetical shape of a given set of coordinates.

mm_data	Sample hormone dataset	
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Description

Sample dataset classifiers to be paired with sample array. This table contains 60 rows to match the 60 individuals across the third dimension of the array

Usage

mm_data

Format

A matrix with 2015 obs (rows) and 4 variables (columns).

ID Individual id, each integer represents a different individual.

CYCLEDAY Integer day of cycle. Generally runs from 1 ... (28 on average).

- **MIDPOINT** Single value for each individual, repeated along each CYCLEDAY. In this sample, day of ovulation.
- E1G Daily measure of hormone, in nanograms per mililiter

```
mm_Diagnostics
```

Description

Conduct a set of analyses to make shape-PCA results easier to interpret. Specifically, this will provide a table of eigen values (optional barplot), provide 5-number summary across each PC, conduct a naive Ward's clustering of PC scores (optional dendrogram, along with silhouette plot and scree plot of individual distance to the sample mean

Usage

```
mm_Diagnostics(dat, max_PC_viz = 10, max_PC_calc = NULL, hide_plots = FALSE)
```

Arguments

dat	A 3D array or a mmPCA object (output of mm_CalcShapespace).
<pre>max_PC_viz</pre>	Maximum number of PCs to include in visualizations (EG Eigenplots, or shape trends.
<pre>max_PC_calc</pre>	By default (NULL), all PCs will be included in calculations. However, if fewer PCs are required users may specify an integer, n, to get the first n PCS.
hide_plots	By default (FALSE), helpful visuals are plotted.

Value

Returns a list containing the results of:

- eigs A table containing individual and cumulutive loadings for each PC
- PC_5_num A data.frame containing the fivenum summary for each PC
- TREE A dendrogram representing the results of a naive-Ward's clustering

mm_ellipse Add confidence ellipses to an active scatterplot.

Description

Add confidence ellipses to an active scatterplot.

Usage

```
mm_ellipse(
    dat,
    ci = c(67.5, 90, 95, 99),
    linesCol = "black",
    fillCol = "grey",
    smoothness = 20
)
```

mm_Explorer

Arguments

dat	A matrix of data to draw an ellipses around.
ci	Percentage of data to capture. Must be one of $c(67.5, 90, 95, 99)$.
linesCol	Border color of the shape.
fillCol	Fill color of the shape.
smoothness	Lower values will look jagged, higher value will make smoother lines, but may take a long time to plot. Default value is 20.

Value

No value. Will add an ellipses of a given size to the current plot.

mm_Explorer	Launch mm_Explorer

Description

Launch mm_Explorer

Usage

mm_Explorer()

Value

No value. Will launch shiny app in default web browser.

mm_FillMissing Impute Missing Data

Description

Fill in a ragged away by nearest neighbor imputation

Usage

mm_FillMissing(A, knn = 3)

Arguments

A	A ragged array (IE, contains missing cells), presumably constructed with mm_ArrayData.
knn	Number of nearest neighbors to draw on for imputation (default = 3).

Value

Returns an array of the same dimensions with all missing data filled.

mm_FlattenArray Flatten Array

Description

Convert a 3D array to 2D matrix suitable for PCA, etc. Note, this function is identical to geomorph::two.d.array, reproduced here for convenience.

Usage

mm_FlattenArray(A, sep = ".")

Arguments

А	an array to be flattened
sep	Separator to be used for column names

Value

Returns a flattened array

mm_get_interval	Create equallly spaced intervals.
-----------------	-----------------------------------

Description

Create a sequence from -1:1 of specified length. MIDpoint (day0) can be

Usage

```
mm_get_interval(days, day0 = NULL)
```

Arguments

days	The length of the sequence to return, inclusive of the endpoints (-1,1)
day0	If NULL (default), the median integer will be calculated, centering the range on
	0. Specifying a value will set 0 to that value, creating asymmetric ranges.

Value

Returns a numeric vector of specified length, ranging from -1 to 1

Examples

```
mm_get_interval(15) ## Symmetrical sequence from -1 to 1 with 0 in the middle.
mm_get_interval(15, day0 = 8) ## The same sequence, explicitly specifying the midpoint
mm_get_interval(15, day0 = 3) ## 15 divisions with an asymmetric distribution.
```

Description

Attempts to optimally format a grid of arrays by group

Usage

mm_grps_PlotArray(A, grps, reset_par = TRUE)

Arguments

А	an array to be plotted
grps	a vector defining group IDs to subset along the 3rd dimension of the array
reset_par	Optional, default = TRUE. If false, do not reset graphic parameters in order to create complex plots.

Details

4 Groups will plot as a 2x2 grid, while 9 groups plot in a 3x3. Function is experimental

Value

Returns no values, produces a series of plots.

mm_grp_dists Distance from Centroid

Description

Calculate and plot group distance from centroid (grand mean)

Usage

```
mm_grp_dists(dat, grps, plots = TRUE)
```

Arguments

dat	a 2d matrix of data. Presumably PC scores
grps	a vector defining group IDs
plots	Logical. Should distances be plotted as boxplots? If FALSE, distance calculations are still performed

Value

A list containing individual distances from the sample mean shape. If plots=TRUE, will also visualize results

mm_mute_cols Take a color and modify it

Description

Modify color/transparency using hsv syntax

Usage

mm_mute_cols(cols, s = NULL, v = NULL, alpha = 0.4)

Arguments

cols	a vector of colors, eg: "#0066FF"
S	Either a single value or a vector of same length as cols specifying a new saturation (range 0-1). colors darken to black (0).
v	Either a single value or a vector of same length as cols specifying a new value (range 0-1). colors lighten to white (0)
alpha	Either a single value or a vector of same length as cols specifying a transparency value (range 0-1). colors translucent at 0.

Value

A vector of colors that have been modified in saturation, value, or alpha

mm_Phenotype	Generate Phenotypes	
--------------	---------------------	--

Description

Partition sample into clusters, based on information from

Usage

```
mm_Phenotype(dat, kgrps, cuttree_h = NULL, cuttree_k = NULL, plot_figs = TRUE)
```

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mm_PlotArray

Arguments

dat	Either an Array of shape data, an mmPCA object, or an mmDiag object.
kgrps	A non-negative integer of sub-groups to draw. kgrps=1 will provide results for the whole input dat.
cuttree_h	Optional. Draw clusters by splitting the tree at a given height, h.
cuttree_k	Optional. Draw clsuters by splitting the tree into number of branches, k
plot_figs	Optional. Default = TRUE, plot phenotypes for each set(s) of subgroups.

Value

If plot_figs=TRUE (Default), plot associated graphs and return a list containing:

- ALN an array containing aligned and scaled landmark data, the output of mm_ArrayData
- PCA PC scores, eigenvalues, and shape visualizations, the output of mm_CalcShapespace
- TREE Dendrogram of PC scores, the output of mm_Diagnostics
- k_grps If kgrps is specified, a vector defining group membership (as integer); the results of k-means clustering based on PC scores.
- cth_grps If cth_grps is specified, a vector defining group membership (as integer); the results of clustering using stats::cutree for a given height.
- ctk_grps If ctk_grps is specified, a vector defining group membership (as integer); the results of clustering using stats::cutree for a given number of clusters.

mm_PlotArray

Plot Array Plot individuals and optionally mean form

Description

Plot Array Plot individuals and optionally mean form

Usage

```
mm_PlotArray(
    A,
    MeanShape = TRUE,
    AllCols = NULL,
    MeanCol = NULL,
    plot_type = c("lines", "points"),
    lbl = NULL,
    yr = NULL,
    axis_labels = FALSE,
    reset_par = TRUE
)
```

Arguments

А	An array to be plotted
MeanShape	Logical. Should the Mean Shape be calculated and plotted
AllCols	Either a single color for all individuals, or a vector specifying colors for each individual. If NULL (default) individuals will be plotted in grey
MeanCol	A single color for the mean shape. If Null (default) mean shape will be plotted in black
plot_type	Should the data be plotted as points or lines.
lbl	A title (main =) for the plot. If NULL (default) the name of the array will be used.
yr	Y-range, in the form c(0,100)
axis_labels	Should units be printed along the axis. Defaults to FALSE to maximize the profile shape.
reset_par	Optional, default = TRUE. If false, do not reset graphic parameters in order to create complex plots.

Value

Plot individual(s) profile(s) in the default graphics device.

mm_pretty_pca Plot Calendar Days

Description

Pretty PCA

Usage

```
mm_pretty_pca(PCA, xPC = 1, yPC = 2, clas_col = NULL, legend_cex = 0.8)
```

Arguments

PCA	Input data either prcomp or mmPCA.
xPC	The PC to plot on the x axis
уРС	The PC to plot on the y axis
clas_col	A character vector of groupings. Each level will be plotted as a different color.
legend_cex	A scaling factor to be applied specifically to the legend. Set to NULL for scat- terplot only.

Details

A better PCA plot

mm_ScreePlot

Value

Returns no object, plots results of PCA

```
mm_ScreePlot Scree Plot
```

Description

Plot total within group sum of squares to evalaute clusters

Usage

mm_ScreePlot(x, maxC = 15, ...)

Arguments

х	Input data for cluster analysis (IE, PCA)
maxC	Maximum clusters to evaluate
	Additional arguments to be passed to plot

Value

No value, produces diagnostic plot.

mm_SilPlot Silhouette Width Plot

Description

Plot average silhouete widths to evaluate clusters

Usage

mm_SilPlot(x, maxC = 15, ...)

Arguments

Х	Input data for cluster analysis (IE PCA)
maxC	Maximum clusters to evaluate
	additional arguments passed to plot

Value

No value, produces diagnostic plot.

mm_transf_geom Geometric Scaling

Description

Calculate the geometric mean of a vector and scale all values by it.

Usage

mm_transf_geom(x)

Arguments

Х

A numeric vector to be scaled. Missing values will produce NA, conduct knn imputation using mm_FillMissing first.

Value

Returns a scaled vector

Examples

mm_transf_geom(1:10)

mm_transf_log natural log transform

Description

Transform a vector by the natural log.

Usage

mm_transf_log(x)

Arguments

х

A numeric vector to be scaled. Missing values will produce NA, conduct knn imputation using mm_FillMissing first.

Value

Returns a scaled vector

Examples

mm_transf_log(1:10)

mm_transf_log10 Common log transform

Description

Transform a vector by the common log (base 10).

Usage

```
mm_transf_log10(x)
```

Arguments

```
х
```

A numeric vector to be scaled. Missing values will produce NA, conduct knn imputation using mm_FillMissing first.

Value

Returns a scaled vector

Examples

mm_transf_log10(1:10)

mm_transf_minmax Min-Max Scaling

Description

Scale a vector from 0,1 based on its minimum and maximum values.

Usage

```
mm_transf_minmax(x)
```

Arguments

х

A Numeric vector to be scaled. Missing values are allowed and ignored.

Value

Returns a scaled vector

Examples

mm_transf_minmax(1:10)

mm_transf_zscore Z scores

Description

Calculate and return z-scores given a numeric vector.

Usage

mm_transf_zscore(x)

Arguments

х

A numeric vector to be scaled. Missing values will produce NA, conduct knn imputation using mm_FillMissing first.

Value

Returns a scaled vector

Examples

mm_transf_zscore(1:10)

mm_VizModel Visualize Multivariate LM

Description

Visualize 2D scatterplot of mvlm including predicted shapes.

Usage

mm_VizModel(dat, clas_col = NULL)

Arguments

dat	Input mvlm, created by mm_BuildModel (or by using geomorph::procD.lm)
clas_col	A classifier to color the data by. If null (default) all points will be grey. Other-
	wise, data will be plotted as rainbow(n) colors.

Value

A list containing the results of the mvlm, visualizations of shape trends along the regression line, and the model itself.

Description

Plot a scatterplot and vizualize shape change across the X axis.

Usage

```
mm_VizShapespace(
    mmPCA,
    xPC = 1,
    yPC = 2,
    yr = c(0, 1.1),
    cols = NULL,
    title = "",
    png_dir = NULL
)
```

Arguments

mmPCA	Output of mm_CalcShapespace, containing a PCA object with PC shapes
xPC	The PC to be plotted on the x axis. If yPC is left null, a univariate density distribution will be plotted with min/max shapes.
уРС	The PC to be plotted on the y axis.
yr	The y-xis range, in the format $c(0,1)$
cols	A vector of colors of length n, for use in scatterplot.
title	To be used for the plot
png_dir	A file path to a directory in which to save out PNG figures. Names will be automatically assigned based on input $PC(s)$.

Details

Meant to be a quick diagnostic plot with minimal customization.

Value

Produces a series of plots to visualize PCA analysis. If png_dir is specified, function will save out .png files. Otherwise plots will be displayed in the default plot window.

moRphomenses

Description

Analyze shapes/phenotypes of hormone data using Geometric Morphometric inspired methods.

Author(s)

Daniel E. Ehrlich

print_summary Print basic summary

Description

Print basic summary

Usage

print_summary(aln, grps = NULL)

Arguments

aln	An object created with mm_ArrayData
grps	(Optional) A numeric vector that defines groupings

Value

A character vector with basic descriptive information, to be used with print(). If grps=TRUE, will return a list of character vectors.

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