

Package ‘moRphomenses’

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

Version 1.0.2

Description Mitteroecker & Gunz (2009) <[doi:10.1007/s11692-009-9055-x](https://doi.org/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](https://doi.org/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)

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mm_ArrayData	<i>Array Data</i>
--------------	-------------------

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	An optional vector of midpoints to center each individual's profile. These should be unique to each individual and repeated for each observation of DAYS, VALUE, and IDs. If NULL (default), 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 recommendation is minmax, but Geometric mean, Zscore, natural log and log10 transformations are available, if desired.
impute_missing	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	<i>Build, implement, visualize multivariate linear model.</i>
---------------	---

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 specified in ... Standard lm notation applies.
univ_series	Default (FALSE) will evaluate multiple covariates and their interaction in a single 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	<i>Define Shapespace of aligned dataset.</i>
-------------------	--

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.
max_Shapes	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	<i>Check Imputation</i>
--------------------	-------------------------

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\$shape_data_wNA</code>).
A2	An aligned and imputed array (presumably made with <code>mm_ArrayData\$Shape_data</code>).
Ob0	One-by-One. If TRUE (default, in interactive sessions), individuals will be plotted 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 Ob0=TRUE user input is required to advance or exit the plotting.

mm_ColorLeaves	<i>Color leves of a dendrogram</i>
----------------	------------------------------------

Description

Specify color order appropriately 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.

mm_CompModel	<i>Compare Model Metrics</i>
--------------	------------------------------

Description

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

Usage

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

Arguments

mv_results	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	<i>Compare Complex Model Metrics</i>
-------------------	--------------------------------------

Description

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

Usage

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

Arguments

mv_results	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 \$transformation
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*

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 milliliter

mm_Diagnostics	<i>Run a suite of diagnostic analyses.</i>
----------------	--

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).
max_PC_viz	Maximum number of PCs to include in visualizations (EG Eigenplots, or shape trends).
max_PC_calc	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 cumulative 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	<i>Add confidence ellipses to an active scatterplot.</i>
------------	--

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
)
```

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	<i>Launch mm_Explorer</i>
-------------	---------------------------

Description

Launch mm_Explorer

Usage

```
mm_Explorer()
```

Value

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

mm_FillMissing	<i>Impute Missing Data</i>
----------------	----------------------------

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	<i>Flatten Array</i>
-----------------	----------------------

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

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

Value

Returns a flattened array

mm_get_interval	<i>Create equally spaced intervals.</i>
-----------------	---

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.
```

mm_grps_PlotArray *Plot Arrays of groups*

Description

Attempts to optimally format a grid of arrays by group

Usage

```
mm_grps_PlotArray(A, grps)
```

Arguments

A an array to be plotted
grps a vector defining group IDs to subset along the 3rd dimension of the array

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	<i>Take a color and modify it</i>
--------------	-----------------------------------

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	<i>Generate Phenotypes</i>
--------------	----------------------------

Description

Partition sample into clusters, based on information from

Usage

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

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 clusters 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 [dendextend::cutree](#) for a given height.
- ctk_grps - If `ctk_grps` is specified, a vector defining group membership (as integer); the results of clustering using [dendextend::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
)
```

Arguments

A	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.

Value

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

mm_pretty_pca	<i>Plot Calendar Days</i>
---------------	---------------------------

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
yPC	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 scatterplot only.

Details

A better PCA plot

Value

Returns no object, plots results of PCA

mm_ScreePlot	<i>Scree Plot</i>
--------------	-------------------

Description

Plot total within group sum of squares to evaluate clusters

Usage

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

Arguments

x	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	<i>Silhouette Width Plot</i>
------------	------------------------------

Description

Plot average silhouette widths to evaluate clusters

Usage

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

Arguments

x	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	<i>Geometric Scaling</i>
----------------	--------------------------

Description

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

Usage

```
mm_transf_geom(x)
```

Arguments

x 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	<i>natural log transform</i>
---------------	------------------------------

Description

Transform a vector by the natural log.

Usage

```
mm_transf_log(x)
```

Arguments

x 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	<i>Common log transform</i>
-----------------	-----------------------------

Description

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

Usage

```
mm_transf_log10(x)
```

Arguments

x 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	<i>Min-Max Scaling</i>
------------------	------------------------

Description

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

Usage

```
mm_transf_minmax(x)
```

Arguments

x 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	<i>Z scores</i>
------------------	-----------------

Description

Calculate and return z-scores given a numeric vector.

Usage

```
mm_transf_zscore(x)
```

Arguments

x	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	<i>Visualize Multivariate LM</i>
-------------	----------------------------------

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. Otherwise, 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.

mm_VizShapespace	<i>Visualize PC axes</i>
------------------	--------------------------

Description

Plot a scatterplot and visualize 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.
yPC	The PC to be plotted on the y axis.
yr	The y-axis 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

Geometric Morphometric Analysis of Hormone Cycle Phenotypes

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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