Package 'profrep'

December 4, 2023

Title Profile Repeatability

Version 1.0.0

Description Calculates profile repeatability for replicate stress response curves, or similar time-series data. Profile repeatability is an individual repeatability metric that uses the variances at each timepoint, the maximum variance, the number of crossings (lines that cross over each other), and the number of replicates to compute the repeatability score. For more information see Reed et al. (2019) <doi:10.1016/j.ygcen.2018.09.015>.

Depends R (>= 2.10)

License MIT + file LICENSE

URL https://ubeattie.github.io/profrep/

BugReports https://github.com/ubeattie/profrep/issues

Encoding UTF-8

RoxygenNote 7.2.3

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

Config/testthat/edition 3

Imports stats

LazyData true

VignetteBuilder knitr

NeedsCompilation no

Author Ursula K. Beattie [cre, aut, cph]

(<https://orcid.org/0000-0002-7131-3712>),

David Harris [aut, cph], L. Michael Romero [aut, cph] (<https://orcid.org/0000-0002-8854-8884>), J. Michael Reed [aut, cph] (<https://orcid.org/0000-0002-3571-2652>), Zachary R. Weaver [aut, cph] (<https://orcid.org/0000-0001-6314-0690>)

Maintainer Ursula K. Beattie <ursula.beattie@tufts.edu>

Repository CRAN

Date/Publication 2023-12-04 16:40:08 UTC

R topics documented:

calculate_crossovers	2
clean_data	3
do_ordering	4
example_two_point_data	5
find_next_good_datapoint	6
get_vars	7
profrep	8
retrieve_good_data	9
score_dfs	10
score_individual_df	11
sigmoid	12
sparrow_repeatability_three_point	13
synthetic_data_four_point	14
	15

Index

calculate_crossovers Calculate the Number of Crossovers

Description

Calculate the Number of Crossovers

Usage

```
calculate_crossovers(individual_df, n_trials, n_replicates)
```

Arguments

individual_df	A data frame containing the individual dataset.
n_trials	The total number of trials in the dataset (the number of rows)
n_replicates	The total number of replicates in each trial (the number of columns - 2)

Details

This function calculates the number of crossovers in a dataset by comparing the values of replicates across multiple trials. It assumes that missing values (NAs) have been interpolated using the clean_data function.

Value

The number of crossovers detected in the dataset.

See Also

clean_data for information on data cleaning.

clean_data

Examples

```
data <- matrix(
    c(
        1, 60, 1, 2, 3, 4, 5, # No NA values
        1, 90, 9, NA, 4, NA, 2, # NA Values in row
        1, 120, 3, 6, NA, NA, 9 # Consecutive NA values
    ),
    nrow = 3,
    byrow=TRUE
)
n_trials <- nrow(data)
n_replicates <- ncol(data) - 2
crossovers <- calculate_crossovers(data, n_trials, n_replicates)
cat("Number of crossovers:", crossovers, "\n")</pre>
```

clean_data

Clean Data by Interpolating Missing Values

Description

Clean Data by Interpolating Missing Values

Usage

```
clean_data(data, n_trials, n_replicates)
```

Arguments

data	A data frame containing the dataset to be cleaned.
n_trials	The total number of rows in the dataset.
n_replicates	The total number of replicate columns in each row.

Details

This function cleans a dataset by interpolating missing values in the replicate columns of each row using neighboring values. If the data frame ends in null values (the last columns are nulls), it will extrapolate from the last value. If the first value is null, it will loop around and pull from the last replicate to perform the interpolation between the last replicate and the second replicate.

Value

A cleaned data frame with missing values interpolated.

See Also

find_next_good_datapoint for details on the interpolation process.

Examples

```
my_data <- matrix(
    c(
        1, 60, 1, 2, 3, 4, 5,  # No NA values
        1, 90, 9, NA, 4, NA, 2,  # NA Values in row
        1, 120, 3, 6, NA, NA, 9  # Consecutive NA values
    ),
    nrow = 3,
    byrow=TRUE
   )
cleaned_data <- clean_data(my_data, n_trials = 3, n_replicates = 5)
print(my_data)
print(cleaned_data)</pre>
```

do_ordering

Score and Order Data

Description

Score and Order Data

Usage

```
do_ordering(
  n_trials,
  id_list,
  df_list,
  n_replicates,
  verbose = FALSE,
  sort = TRUE
)
```

Arguments

n_trials	The number of rows an individual sample will have.
id_list	The list of unique individual or sample names
df_list	The list of data frames per unique individual
n_replicates	The number of replicates in the study.
verbose	A boolean parameter the defaults to FALSE. Determines whether messages are printed.
sort	A boolean parameter that defaults to TRUE. If TRUE, sorts the returned data frame by score. If FALSE, returns the data in the individual order it was provided in

4

Details

Performs the ordering of input data by scoring each individual data frame.

The main function of the package, this will send each individuals data out for scoring. Then, when all scores are computed, it will order the result data frame by score and assign a rank.

Ranks are assigned with ties allowed - if N individuals have a tie, their rank is averaged. For example, if the max score is 1, and two individuals have that score, their rank is 1.5

Value

Returns a data frame of the results, in the following form:

```
Column 1: "individual" - the unique identifier of an individual or sample
Column 2: "n_crossings" - the calculated number of crossings.
Column 3: "max_variance" - the maximum of the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurements at a single transmut and the variances of the replicate measurement at a single transmut and the variance of the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the replicate measurement at a single transmut and the variances of the variances of the replicate measurement at a single transmut and transmu
```

Examples

```
df <- data.frame(
    col_a = c('A', 'A', 'B', 'B'),
    col_b = c(5, 15, 5, 15),
    col_c = c(5, 10, 1, 2),
    col_d = c(10, 15, 3, 4)
    )
    id_list <- unique(df[, 1])
    individuals <- list()
    for (i in 1:length(id_list)) {
        individuals[[i]] <- df[df[, 1] == id_list[i], ]
    }
    ret_df <- do_ordering(n_trials=2, id_list=id_list, df_list=individuals, n_replicates=2)
    print(ret_df)
```

example_two_point_data

Example Data: Two Point Data

Description

An example of data that one would perform profile repeatability on. Consists of 9 individual animals, with corticosterone data taken at 2 timepoints ($n_{trials} = 2$), baseline (time = 3) and stressinduced (time = 30). Then, there are 28 replicate columns.

Usage

example_two_point_data

Format

example_two_point_data: A dataframe with 10 rows and 30 columns: Animal The animal name/unique identifier Time The time of the measurement, in days.

SD.DR The name of the replicate column.

Source

This data was extracted from Romero & Rich 2007 (Comp Biochem. Physiol. Part A Mol. Integr. Physiol. 147, 562-568. https://doi.org/10.1016/j.cbpa.2007.02.004)

find_next_good_datapoint

What Is the Next Non-Null Data Point?

Description

What Is the Next Non-Null Data Point?

Usage

```
find_next_good_datapoint(data_row, index, n_replicates)
```

Arguments

data_row	A numeric vector representing the data row.
index	The index of the current data point.
n_replicates	The total number of replicates (length of the row)

Details

Given a data row, an index, and the number of replicates (the number of elements in the row), this function finds the next good data point in the row.

A good data point is a non-missing value (not NA) with a non-empty string.

Value

The next good data point or -999 if none is found.

get_vars

Examples

```
data_row <- c(NA, 3, 2, NA, 5)
index <- 1
n_replicates <- 5
find_next_good_datapoint(data_row, index, n_replicates) # expect 3</pre>
```

```
get_vars
```

Calculate Group Variance

Description

Calculate Group Variance

Usage

get_vars(individual_array, n_replicates)

Arguments

individual_array

	-5
	The array of data for an individual
n_replicates	The number of replicate groups

Details

For the given individual array, for all rows of times, computes the variance in values over replicates. Returns these variances, sum of all values (for all times and replicates), sum of all these values squared, and the number of values.

Value

A list, where the elements are:

1. variances: A vector of the variances of the sample

- 2. total_sum: The sum of all the measurements in the sample
- 3. ssq: The sum of all the squares of the measurements in the sample
- 4. num_measurements: The total number of measurements in the sample that are not null

Examples

```
arr <- data.frame(
    individual=c("a", "a"),
    time=c(5, 15),
    col_a=c(1, 2),
    col_b=c(2, 3)
)
variance_return <- get_vars(individual_array=arr, n_replicates=2)
print(variance_return)</pre>
```

profrep

Description

Perform Profile Repeatability

Usage

profrep(df, n_timepoints, sort = TRUE, verbose = FALSE)

Arguments

0	
df	The input data frame, of minimum shape 3 rows by 4 columns. This can be read in from a csv or another data frame stored in memory. It is assumed that the data frame is of the following structure: Column 1 is the unique identifier of an individual animal or sample Column 2 is the time of the sample Column 3-N are the columns of replicate data. Row 1 is assumed to be header strings for each column.
n_timepoints	The number of rows an individual sample will have. For example, if the repli- cates were collected for individual 1 at times 15 and 30, for replicates A and B, the data frame would look like:
	id time A B :: :: :-: 1 15 1 2 1 30 3 4
sort	A boolean parameter that defaults to TRUE. If TRUE, sorts the returned data frame by score. If FALSE, returns the data in the individual order in which it was provided.
verbose	A boolean parameter that defaults to FALSE. Determines whether messages are printed.

Details

Calculates the profile repeatability measure of the input data according to the method in Reed et al., 2019, J. Gen. Comp. Endocrinol. (270).

Value

Returns a data frame of the results, in the following form:

- Column 1: "individual" the unique identifier of an individual or sample
- Column 2: "n_crossings" the calculated number of crossings.
- Column 3: "max_variance" the maximum of the variances of the replicate measurements at a single time for the individual or sample.

- Column 4: "ave_variance" the average of the variances of the replicate measurements at a single time for the individual or sample.
- Column 5: "base_score" the original, unnormalized profile repeatability score. Smaller numbers rank higher.
- Column 6: "final_score" the base score, normalized by the sigmoid function. Constrained to be between 0 and 1. Scores closer to 1 rank higher.
- Column 7: "rank" the calculated ranking of the individual or sample, against all other individuals or samples in the data set.

See Also

do_ordering for the main data processing function.

calculate_crossovers for how the number of crossings are calculated.

score_individual_df for how the score is calculated for an individual or sample.

clean_data for how missing replicate values are handled.

Examples

```
test_data <- profrep::example_two_point_data
results <- profrep::profrep(df=test_data, n_timepoints=2)
print(results)</pre>
```

retrieve_good_data Retrieve Indices of Non-Missing Data for a Specific Time Point

Description

This function retrieves the indices of non-missing data values at a specific time point from an individual array.

Usage

```
retrieve_good_data(individual_array, t, n_replicates)
```

Arguments

individual_arr	ау
	A data matrix or data frame representing individual data, where rows correspond to time points and columns correspond to replicates and variables.
t	The time point for which you want to retrieve non-missing data indices.
n_replicates	The number of replicates in the data matrix.

Value

A numeric vector containing the indices of non-missing data values at the specified time point t. If there are no non-missing values or only one non-missing value, NULL is returned.

See Also

which function for finding the indices of non-missing values.

Examples

```
# Example usage:
individual_data <- matrix(c(NA, 2, NA, 4, 5, NA), nrow = 1)
retrieve_good_data(individual_data, t = 1, n_replicates = 3)
```

score_dfs

Compute Profile Repeatability Score

Description

Compute Profile Repeatability Score

Usage

```
score_dfs(id_list, df_list, n_replicates, n_trials, verbose = FALSE)
```

Arguments

id_list	The list of the names of the individuals
df_list	A list of data frames, each of which correspond to one of the names in the individual list
n_replicates	The number of replicate columns (number of columns in a df in df_list)
n_trials	The number of trials per individual (number of rows in a df in df_list)
verbose	A boolean parameter the defaults to FALSE. Determines whether messages are printed.

Details

Works on multiple elements of data.

Splits the data into the data frame for a particular individual from the id_list, then calculates metrics to compute the profile repeatability score. Returns a data frame with the individuals name and the score.

Value

A dataframe of the calculated metrics. The column structure is as follows:

- Column 1: "individual" - the unique identifier of an individual or sample

- Column 2: "n_crossings" - the calculated number of crossings.

- Column 3: "max_variance" - the maximum of the variances of the replicate measurements at a single t

- Column 4: "ave_variance" the average of the variances of the replicate measurements at a single t
- Column 5: "base_score" the original, unnormalized profile repeatability score. Smaller numbers r
- Column 6: "final_score" the base score, normalized by the sigmoid function. Constrained to be bet

10

score_individual_df

Examples

```
df <- data.frame(
    col_a = c('A', 'A', 'B', 'B'),
    col_b = c(5, 15, 5, 15),
    col_c = c(5, 10, 1, 2),
    col_d = c(10, 15, 3, 4)
    )
id_list <- unique(df[, 1])
individuals <- list()
for (i in 1:length(id_list)) {
    individuals[[i]] <- df[df[, 1] == id_list[i], ]
}
ret_df <- score_dfs(id_list=id_list, df_list=individuals, n_replicates=2, n_trials=2)
print(ret_df)
```

score_individual_df Score an Individual Data Frame

Description

Score an Individual Data Frame

Usage

```
score_individual_df(
    individual_df,
    n_trials,
    n_replicates,
    max_variance,
    variance_set
)
```

Arguments

individual_df	A data frame containing individual data.
n_trials	The total number of trials in the data frame.
n_replicates	The total number of replicates in each trial.
<pre>max_variance</pre>	The maximum allowed variance value.
variance_set	A vector of variance values.

Details

This function calculates a score for an individual data frame based on various factors, including the number of crossovers, maximum variance, and a set of variances.

The score is computed as follows:

sigmoid

- It factors in the number of crossovers using a scaling factor.
- It considers the maximum variance value in the variance set.
- It adds a component based on the average of variance values.
- It includes a scaled component of the number of crossovers.

Value

A list calculated for the individual data frame. Contains two values:

- 1. n_crossings: The number of crossover events in the data.
- 2. base_score: The un-normalized profile repeatability score for the data.

See Also

calculate_crossovers for information on crossovers calculation.

Examples

```
arr <- data.frame(</pre>
  individual=c("a", "a"),
  time=c(5, 15),
  col_a=c(1, 2),
  col_b=c(2, 3)
)
variance_set <- c(0.5, 0.5)</pre>
max_variance <- 0.5</pre>
score_list <- score_individual_df(</pre>
  individual_df=arr,
  n_trials=2,
  n_replicates=2,
  max_variance=max_variance,
  variance_set=variance_set
)
print(score_list)
```

sigmoid

Calculates the sigmoid function of the input

Description

Calculates the sigmoid function of the input

Usage

sigmoid(float)

Arguments

float A float number

Value

A float number which is the result of the sigmoid function

Examples

sigmoid(0)
sigmoid(2)

Description

An example of data that one would perform profile repeatability on. Consists of 12 individual animals, with corticosterone data taken at 3 times ($n_{trials} = 3$), baseline (time = 0) and two stress-induced (time = 15 and 30). Then, there are 10 replicate columns. This example also shows what happens when there are null data records for some individuals.

Usage

sparrow_repeatability_three_point

Format

sparrow_repeatability_three_point:
A dataframe with 36 rows and 12 columns:

i datariane with 50 10 %5 and 12 columns.

Animal The animal name/unique identifier

TIME The time of the measurement, in days

LD.500 The name of the replicate column

Source

This data was extracted from Rich & Romero 2001 (J. Comp. Physiol. Part B Biochem. Syst. Environ. Physiol. 171, 543-647. https://doi.org/10.1007/s003600100204)

synthetic_data_four_point

Example Data: Synthetic 4-Point Data

Description

An example of data that one would perform profile repeatability on. The data is synthetic data created for testing purposes and is designed to span a range of perceived repeatability scores. Consists of 11 individual animals, with data taken at 4 times (n_trials = 4), baseline (time = 0) and three stress-induced (time = 15, 30, and 45). Then, there are four replicate columns. Replicate column names refer to sample tests performed on the animal.

Usage

synthetic_data_four_point

Format

synthetic_data_four_point:

A dataframe with 44 rows and 6 columns:

Animal The animal name/unique identifier

TIME The time of the measurement (unit not important)

A The (unimportant) name of a replicate column.

B The (unimportant) name of a replicate column.

C The (unimportant) name of a replicate column.

D The (unimportant) name of a replicate column.

Source

Data created for testing purposes by Reed et al., 2019 (Gen. Comp. Endocrinol. 270, 1-9. https://doi.org/10.1016/j.ygcen.2018.09.015)

Index

* datasets example_two_point_data, 5 sparrow_repeatability_three_point, 13 synthetic_data_four_point, 14 * data retrieve_good_data, 9 * manipulation retrieve_good_data, 9 calculate_crossovers, 2, 9, 12 clean_data, 2, 3, 9 do_ordering, 4, 9

 $\texttt{example_two_point_data, 5}$

find_next_good_datapoint, 3, 6

 $\texttt{get_vars}, \textbf{7}$

profrep, 8

retrieve_good_data,9

```
score_dfs, 10
score_individual_df, 9, 11
sigmoid, 12
sparrow_repeatability_three_point, 13
synthetic_data_four_point, 14
```

which, *10*