

Package: rSRD (via r-universe)

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Type Package

Title Sum of Ranking Differences Statistical Test

Version 0.2.0

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Description We provide an implementation for Sum of Ranking Differences (SRD), a novel statistical test introduced by Héberger (2010) <[doi:10.1016/j.trac.2009.09.009](https://doi.org/10.1016/j.trac.2009.09.009)>. The test allows the comparison of different solutions through a reference by first performing a rank transformation on the input, then calculating and comparing the distances between the solutions and the reference - the latter is measured in the L1 norm. The reference can be an external benchmark (e.g. an established gold standard) or can be aggregated from the data. The calculated distances, called SRD scores, are validated in two ways, see Héberger and Kollár-Hunek (2011) <[doi:10.1002/cem.1320](https://doi.org/10.1002/cem.1320)>. A randomization test (also called permutation test) compares the SRD scores of the solutions to the SRD scores of randomly generated rankings. The second validation option is cross-validation that checks whether the rankings generated from the solutions come from the same distribution or not. For a detailed analysis about the cross-validation process see Sziklai, Baranyi and Héberger (2021) <[doi:10.48550/arXiv.2105.11939](https://doi.org/10.48550/arXiv.2105.11939)>. The package offers a wide array of features related to SRD including the computation of the SRD scores, validation options, input preprocessing and plotting tools.

License GPL-3

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LinkingTo Rcpp

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Contents

calculateCrossValidation	3
calculateSRDDistribution	4
calculateSRDValues	6
plotCrossValidation	7
plotHeatmapSRD	8
plotPermTest	9
utilsCalculateDistance	10
utilsCalculateRank	11
utilsColorPalette	11
utilsCreateReference	12
utilsDetailedSRD	13
utilsDetailedSRDNoChars	14
utilsMaxSRD	15
utilsPreprocessDF	16
utilsRankingMatrix	16
utilsTieProbability	17

Index 18

```
calculateCrossValidation  
    calculateCrossValidation
```

Description

R interface to test whether the rankings induced by the columns come from the same distribution. If the number of folds and the test method are not specified, the default is the 8-fold Wilcoxon test combined with cross-validation. If the number of rows is less than 8, leave-one-out cross-validation is applied. Columns are ordered based on the SRD values of the different folds, then each consecutive column-pairs are tested. Test statistics for Alpaydin test follows F distribution with $df1=2k$, $df2=k$ degrees of freedom. Dietterich test statistics follow t-distribution with k degrees of freedom (two-tailed). Wilcoxon test statistics is calculated as the absolute value of the difference of the sum of the positive ranks ($W+$) and sum of the negative ranks ($W-$). The distribution for this test statistics can be derived from the Wilcoxon signed rank distribution. For more information about the cross-validation process see Sziklai, Baranyi and Héberger (2021).

Usage

```
calculateCrossValidation(  
  data_matrix,  
  method = "Wilcoxon",  
  number_of_folds = 8,  
  precision = 5,  
  output_to_file = TRUE,  
  seed = NULL  
)
```

Arguments

<code>data_matrix</code>	A data frame. All columns must be numeric and free of NA values. The last column is treated as the reference.
<code>method</code>	A string specifying the method. The methods "Wilcoxon", "Alpaydin" and "Dietterich" are available.
<code>number_of_folds</code>	The number of folds used in the cross validation. Ranges between 5 to 10.
<code>precision</code>	The precision used for the the ranking matrix transformation.
<code>output_to_file</code>	Boolean flag to enable file output.
<code>seed</code>	An optional integer seed for the random number generator in the C++ shuffling routines, enabling reproducible results. When NULL (the default), the random number generator is seeded from the system entropy pool, preserving the original stochastic behaviour.

Value

A List containing

- a new column order sorted by the median of the SRD values computed on the different folds
- a vector of test statistics corresponding to each consecutive column pairs
- a vector indicating the test statistics' statistical significance
- the SRD values of different folds and
- additional data needed for the plotCrossValidation function.

Author(s)

Balázs R. Sziklai <sziklai.balazs@krtk.hu>, Linus Olsson <linusmeol@gmail.com>, Jochen Staudacher <jochen.staudacher@hs-kempten.de>

References

Sziklai, Balázs R., Máté Baranyi, and Károly Héberger (2021). "Testing Cross-Validation Variants in Ranking Environments", arXiv preprint arXiv:2105.11939 (2021).

Examples

```
df <- data.frame(
  Sol_1=c(7, 6, 5, 4, 3, 2, 1),
  Sol_2=c(1, 2, 3, 4, 5, 7, 6),
  Sol_3=c(1, 2, 3, 4, 7, 5, 6),
  Ref=c(1, 2, 3, 4, 5, 6, 7))

calculateCrossValidation(df, output_to_file = FALSE)
calculateCrossValidation(df, output_to_file = FALSE, seed = 42)
```

```
calculateSRDDistribution
```

```
calculateSRDDistribution
```

Description

R interface to calculate the SRD distribution that corresponds to the data. The simulation draws 1,000,000 random rankings; for small n the resulting thresholds (XX1, XX19) can vary slightly between runs. Use the seed parameter for fully reproducible results.

Usage

```
calculateSRDDistribution(
  data_matrix,
  option = "f",
  tie_probability = 0,
  output_to_file = FALSE,
  seed = NULL
)
```

Arguments

<code>data_matrix</code>	A data frame. All columns must be numeric and free of NA values. The last column is treated as the reference.
<code>option</code>	A character to specify how ties are generated in the simulation. The following options are available: <ul style="list-style-type: none"> • 'n': No ties for solution vectors; reference is fixed. • 'r': No ties; both solution and reference are random. • 't': Ties with a fixed user-supplied probability for both solution vectors and reference. • 'p': Ties with a fixed user-supplied probability for solution vectors; reference is fixed. • 'd': Tie distribution reflects the tie frequencies in the solution vectors; reference is fixed. • Default (recommended): Tie distribution reflects tie frequencies in the reference; reference is fixed.
<code>tie_probability</code>	The probability with which ties can occur.
<code>output_to_file</code>	Boolean flag to enable file output. Default FALSE.
<code>seed</code>	An optional integer seed for the random number generator in the C++ simulation, enabling reproducible results. When NULL (the default), the random number generator is seeded from the system entropy pool, preserving the original stochastic behaviour.

Value

A list containing the SRD distribution and related descriptive statistics. `xx1` indicates the 5 percent significance threshold. SRD values between `xx1` and `xx19` are indistinguishable from random rankings; a value above `xx19` indicates reverse ordering (5 percent significance).

Author(s)

Balázs R. Sziklai <sziklai.balazs@krtk.hu>

Linus Olsson <linusmeol@gmail.com>

Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
df <- data.frame(
  A=c(32, 52, 44, 44, 47),
  B=c(73, 75, 65, 76, 70),
  C=c(60, 59, 57, 55, 60),
  D=c(35, 24, 44, 83, 47),
  E=c(41, 52, 46, 50, 65))

calculateSRDDistribution(df, option = 'p', tie_probability = 0.5)

# Reproducible run:
```

```
calculateSRDDistribution(df, seed = 42)
```

```
calculateSRDValues    calculateSRDValues
```

Description

R interface to calculate SRD values. To test the results' significance run `calculateSRDDistribution()`. For more information about SRD scores and their validation see Héberger and Kollár-Hunek (2011).

Usage

```
calculateSRDValues(data_matrix, output_to_file = FALSE)
```

Arguments

`data_matrix` A data frame. All columns must be numeric and free of NA values. The last column is treated as the reference.

`output_to_file` Boolean flag to enable file output. Default FALSE.

Value

A numeric vector containing the normalised SRD values (each in $[0, 1]$) for every non-reference column.

Author(s)

Balázs R. Sziklai <sziklai.balazs@krtk.hu>
Linus Olsson <linusmeol@gmail.com>
Jochen Staudacher <jochen.staudacher@hs-kempten.de>

References

Héberger K., Kollár-Hunek K. (2011) "Sum of ranking differences for method discrimination and its validation: comparison of ranks with random numbers", *Journal of Chemometrics*, 25(4), pp. 151-158.

Examples

```
df <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
  
calculateSRDValues(df)
```

plotCrossValidation *plotCrossValidation*

Description

Plots data generated by the calculateCrossValidation function as a boxplot. Includes max and min as whiskers as well as the average (marked by a crossed circle), median (marked by a horizontal bold line) and the 1st and 3rd quartile of the values. Box geometry (min, Q1, median, Q3, max) is taken directly from the precomputed 'boxplot_values', the single source of truth also reported to the user elsewhere, rather than being re-derived from the fold-wise values. This avoids a second, independent quantile calculation that could drift from the official figures – and, in particular, guarantees that identical reported statistics (whether within one solution, e.g. Q1 equal to the median, or across different solutions sharing the same value) are always drawn at exactly the same height.

Usage

```
plotCrossValidation(cv_results)
```

Arguments

`cv_results` The List of results returned by the calculateCrossValidation function.

Value

None.

Author(s)

Linus Olsson <linusmeol@gmail.com>

Alexander Pothmann

Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
df <- data.frame(
  Sol_1=c(7, 6, 5, 4, 3, 2, 1),
  Sol_2=c(1, 2, 3, 4, 5, 7, 6),
  Sol_3=c(1, 2, 3, 4, 7, 5, 6),
  Ref=c(1, 2, 3, 4, 5, 6, 7))

cv_results <- rSRD::calculateCrossValidation(df, output_to_file = FALSE)
rSRD::plotCrossValidation(cv_results)
```

plotHeatmapSRD	<i>plotHeatmapSRD</i>
----------------	-----------------------

Description

Heatmap is generated based on the pairwise distance - measured in SRD - of the columns. Each column is set as reference once, then SRD values are calculated for the other columns.

Usage

```
plotHeatmapSRD(df, output_to_file = FALSE, color = utilsColorPalette)
```

Arguments

`df` A DataFrame.
`output_to_file` Logical. If true, the distance matrix will be saved to the hard drive.
`color` Vector of colors used for the image. Defaults to colors `utilsColorPalette`.

Value

Returns a heatmap and the corresponding distance matrix.

Author(s)

Attila Gere <gereattilaphd@gmail.com>, Linus Olsson <linusmeol@gmail.com>, Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
srdInput <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
  
plotHeatmapSRD(srdInput)  
  
mycolors<- c("#e3f2fd", "#bbdefb", "#90caf9", "#64b5f6", "#42a5f5",  
             "#2196f3", "#1e88e5", "#1976d2", "#1565c0", "#0d47a1")  
plotHeatmapSRD(srdInput, color=mycolors)
```

`plotPermTest`*plotPermTest*

Description

Plots the permutation test for the given data frame by using the simulation data created by the `calculateSRDDistribution()` function. Vertical lines mark the positions of the solution columns on the simulated SRD distribution. Dashed lines indicate the 5 percent significance thresholds (XX1, XX19) and the median (Med).

Usage

```
plotPermTest(df, simulationData, densityToDistr = FALSE)
```

Arguments

`df` A `DataFrame`.

`simulationData` The output of the `calculateSRDDistribution()` function.

`densityToDistr` Logical. If `FALSE` (default) the y-axis shows relative frequency (probability density). If `TRUE` it shows cumulative relative frequency (CDF).

Value

None.

Author(s)

Linus Olsson <linusmeol@gmail.com>

Examples

```
df <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
  
simulationData <- rSRD::calculateSRDDistribution(df)  
plotPermTest(df, simulationData)
```

`utilsCalculateDistance`*utilsCalculateDistance*

Description

Calculates the distance of two rankings in L_1 norm and inserts the result after the first.

Usage

```
utilsCalculateDistance(df, nameCol, refCol)
```

Arguments

<code>df</code>	A DataFrame.
<code>nameCol</code>	The current Column of the iteration.
<code>refCol</code>	The reference Column of the dataframe.

Value

Returns a new df that has a Distance Column based on the nameCol.

Author(s)

Ali Tugay Sen, Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
SRDInput <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
nameCol <- "A"  
refCol <- "B"  
rSRD::utilsCalculateDistance(SRDInput,nameCol,refCol)
```

utilsCalculateRank *utilsCalculateRank*

Description

Calculates the ranking of a given column.

Usage

```
utilsCalculateRank(df, nameCol)
```

Arguments

df	A DataFrame.
nameCol	The name of the column to be ranked. Note that this parameter needs to be specified as there is no default value.

Value

Returns a new df that has an additional column with the rankings of the column specified by nameCol.

Author(s)

Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
SRDInput <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
columnName <- "A"  
rSRD::utilsCalculateRank(SRDInput, columnName)
```

utilsColorPalette *utilsColorPalette*

Description

Unique color palette for heatmaps.

Usage

```
utilsColorPalette
```

Format

An object of class character of length 250.

Author(s)

Attila Gere <gereattilaphd@uni-mate.hu>

Balázs R. Sziklai <sziklai.balazs@krtk.hu>,

Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
barplot(rep(1,250), col = utilsColorPalette)
```

utilsCreateReference *utilsCreateReference*

Description

Adds a new reference column based on the input DataFrame `df` and the given method. This function iterates over the rows and applies the given method to define the value of the reference. Available options are: max, min, median, mean and mixed. This column is appended to the DataFrame. When "mixed" is specified the function will consider the `refVector` for creating the reference column.

Usage

```
utilsCreateReference(df, method = "max", refVector = c())
```

Arguments

<code>df</code>	A DataFrame.
<code>method</code>	A string value specifying the reference creating method. Available options: max, min, median, mean and mixed.
<code>refVector</code>	A vector of strings that specifies a method for each row. Vector size should be equal to the number of rows in the DataFrame <code>df</code> .

Value

Returns a new DataFrame appended with the reference column created by the method.

Author(s)

Ali Tugay Sen, Linus Olsson <linusmeol@gmail.com>

Examples

```

SRDInput <- data.frame(
  A=c(32, 52, 44, 44, 47),
  B=c(73, 75, 65, 76, 70),
  C=c(60, 59, 57, 55, 60),
  D=c(35, 24, 44, 83, 47),
  E=c(41, 52, 46, 50, 65))
proc_data <- rSRD::utilsPreprocessDF(SRDInput)
ref <- c("min","max","min","max","mean")
rSRD::utilsCreateReference(proc_data, method = "mixed", ref)

```

utilsDetailedSRD *utilsDetailedSRD*

Description

Detailed calculation of the SRD values including the computation of the ranking transformation. Unless there is a column specified with referenceCol the last column will always taken as the reference.

Usage

```

utilsDetailedSRD(
  df,
  referenceCol,
  createRefCol = function() {
  }
)

```

Arguments

df	A DataFrame.
referenceCol	Optional. A string that contains a column of df which will be used as the reference column.
createRefCol	Optional. Can be max, min, median, mean. Creates a new Column based on the existing df and attaches it to df as the reference Column.

Value

Returns a new DataFrame that shows the detailed SRD computation (ranking transformation and distance calculation). A newly added row contains the SRD values (displayed without normalization).

Author(s)

Ali Tugay Sen, Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
SRDInput <- data.frame(
  A=c(32, 52, 44, 44, 47),
  B=c(73, 75, 65, 76, 70),
  C=c(60, 59, 57, 55, 60),
  D=c(35, 24, 44, 83, 47),
  E=c(41, 52, 46, 50, 65))
rSRD::utilsDetailedSRD(SRDInput)
```

```
utilsDetailedSRDNoChars
```

```
utilsDetailedSRDNoChars
```

Description

Detailed calculation of the SRD values including the computation of the ranking transformation. Unless there is a column specified with `referenceCol` the last column will always be taken as the reference. This variant differs from `utilsDetailedSRD` in that non-numeric columns will not be converted to chars, i.e. the data types of non-numeric columns will be preserved in the output.

Usage

```
utilsDetailedSRDNoChars(
  df,
  referenceCol,
  createRefCol = function() {
  }
)
```

Arguments

<code>df</code>	A <code>DataFrame</code> .
<code>referenceCol</code>	Optional. A string that contains a column of <code>df</code> which will be used as the reference column.
<code>createRefCol</code>	Optional. Can be <code>max</code> , <code>min</code> , <code>median</code> , <code>mean</code> . Creates a new Column based on the existing <code>df</code> and attaches it to <code>df</code> as the reference Column.

Value

Returns a new `DataFrame` that shows the detailed SRD computation (ranking transformation and distance calculation). A newly added row contains the SRD values (displayed without normalization).

Author(s)

Ali Tugay Sen, Jochen Staudacher <jochen.staudacher@hs-kempten.de>

Examples

```
SRDInput <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
rSRD::utilsDetailedSRDNoChars(SRDInput)
```

utilsMaxSRD

utilsMaxSRD

Description

Calculates the maximum distance between two rankings of size n. This function is used to normalize SRD values.

Usage

```
utilsMaxSRD(rowsCount)
```

Arguments

rowsCount The number of rows in the SRD calculation.

Value

The maximum achievable SRD value.

Author(s)

Dennis Horn

Examples

```
maxSRD <- rSRD::utilsMaxSRD(5)
```

utilsPreprocessDF *utilsPreprocessDF*

Description

This function preprocesses the DataFrame depending on the method.

Usage

```
utilsPreprocessDF(df, method = "range_scale")
```

Arguments

df	A DataFrame.
method	A string that should contain "scale_to_unit", "standardize", "range_scale" or "scale_to_max".

Value

Returns a new df that has been preprocessed based on the method chosen.

Author(s)

Ali Tugay Sen, Dennis Horn <dennishorn@hotmail.de>, Linus Olsson <linusmeol@gmail.com>

Examples

```
SRDInput <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
method <- "standardize"  
utilsPreprocessDF(SRDInput,method)
```

utilsRankingMatrix *utilsRankingMatrix*

Description

R interface to perform the rank transformation on the columns of the input data frame. Ties are resolved by fractional ranking.

Usage

```
utilsRankingMatrix(data_matrix)
```

Arguments

data_matrix A data frame. All columns must be numeric and free of NA values.

Value

A data frame containing the ranking matrix.

Author(s)

Balázs R. Sziklai <sziklai.balazs@krtk.hu>, Linus Olsson <linusmeol@gmail.com>

Examples

```
df <- data.frame(  
  A=c(32, 52, 44, 44, 47),  
  B=c(73, 75, 65, 76, 70),  
  C=c(60, 59, 57, 55, 60),  
  D=c(35, 24, 44, 83, 47),  
  E=c(41, 52, 46, 50, 65))  
  
utilsRankingMatrix(df)
```

utilsTieProbability *utilsTieProbability*

Description

Calculates the tie probability for a given vector. The tie probability is defined as the number of consecutive tied component-pairs *in the sorted vector* divided by the size of the vector minus 1.

Usage

```
utilsTieProbability(x)
```

Arguments

x A vector.

Value

Returns the tie probability as a numeric value.

Author(s)

Ali Tugay Sen, Linus Olsson <linusmeol@gmail.com>

Examples

```
x <-c(1,2,4,4,5,5,6)  
rSRD::utilsTieProbability(x)
```

Index

* datasets

- utilsColorPalette, [11](#)

- calculateCrossValidation, [3](#)
- calculateSRDDistribution, [4](#)
- calculateSRDValues, [6](#)

- plotCrossValidation, [7](#)
- plotHeatmapSRD, [8](#)
- plotPermTest, [9](#)

- utilsCalculateDistance, [10](#)
- utilsCalculateRank, [11](#)
- utilsColorPalette, [11](#)
- utilsCreateReference, [12](#)
- utilsDetailedSRD, [13](#)
- utilsDetailedSRDNoChars, [14](#)
- utilsMaxSRD, [15](#)
- utilsPreprocessDF, [16](#)
- utilsRankingMatrix, [16](#)
- utilsTieProbability, [17](#)