Package 'dtwclust'

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Description Time series clustering using different techniques related to the Dynamic Time Warping distance and its corresponding lower bounds. Additionally, an implementation of k-Shape clustering is available.							
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Description

Perform time series clustering using different techniques related to the DTW distance and its corresponding lower bounds (LB). Additionally, an implementation of k-Shape clustering is available.

Details

This package tries to consolidate the different procedures available to perform clustering of time series under DTW. Right now only univariate time series are supported. Similarly, time series should have equal lengths for partitional methods.

Please see the documentation for dtwclust, which serves as the main entry point.

Other packages that are particularly leveraged here are the flexclust package for partitional clustering, the proxy package for distance matrix calculations, and the dtw package for the core DTW calculations.

Four distances are registered via pr_DB: "LB_Keogh", "LB_Improved", "SBD" and "DTW2". See lb_keogh, lb_improved and SBD for more details on the first 3. The last one is done with dtw using L2 norm, but it differs from the result you would obtain if you specify L2 as dist.method: with DTW2, pointwise distances (the local cost matrix) are calculated with L1 norm, *each* element of the matrix is squared and the result is fed into dtw, which finds the optimum warping path. The square root of the resulting distance is *then* computed.

Please note that the dist function in the proxy package accepts one or two arguments for data objects. Users should usually use the two-input version, even if there is just one dataset (i.e. proxy::dist(x=data, y=data, ...)), because the one-input version sometimes fails to detect a whole time series as a single object and, instead, calculates distances between each observation of each time series.

Author(s)

Alexis Sarda-Espinosa

References

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See Also

dtwclust, kcca, dist, dtw

DBA

DTW Barycenter Averaging

Description

A global averaging method for time series under DTW (Petitjean, Ketterlin and Gancarski, 2011).

Usage

```
DBA(X, center = NULL, max.iter = 25, error.check = TRUE, trace = FALSE)
```

DBA

Arguments

X	A data matrix where each row is a time series. Optionally, a list where each element is a time series.
center	Optionally, a time series to use as reference. It must be a numeric vector. Defaults to a random series of X if NULL.
max.iter	Maximum number of iterations allowed.
error.check	Should inconsistencies in the data be checked?
trace	If TRUE, the current iteration is printed to screen.

Details

This function tries to find the optimum average series between a group time series in DTW space. Refer to the cited article for specific details on the algorithm.

If a given series reference is provided in center, the algorithm should always converge to the same result provided the rows X keep the same values, although their order may change.

Value

The average time series.

References

Petitjean F, Ketterlin A and Gancarski P (2011). "A global averaging method for dynamic time warping, with applications to clustering." *Pattern Recognition*, **44**(3), pp. 678 - 693. ISSN 0031-3203, http://dx.doi.org/10.1016/j.patcog.2010.09.013, http://www.sciencedirect.com/science/article/pii/S003132031000453X.

Examples

```
# Sample data
data(uciCT)

# Obtain an average for the first 5 time series
dtw.avg <- DBA(CharTraj[1:5], CharTraj[[1]], trace = TRUE)
plot(dtw.avg, type="1")

# Change the provided order
dtw.avg2 <- DBA(CharTraj[5:1], CharTraj[[1]], trace = TRUE)
all(dtw.avg == dtw.avg2)</pre>
```

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dtwclust	Time series clustering under DTW	

Description

This function uses the DTW distance and related lower bounds to cluster time series. For now, all series must be univariate and, in the case of partitional methods, have equal lengths.

Usage

```
dtwclust(data = NULL, type = "partitional", k = 2, method = "average",
  distance = "dtw", centroid = "pam", window.size = NULL, norm = "L1",
  dc = NULL, control = NULL, save.data = FALSE, seed = NULL,
  trace = FALSE, ...)
```

Arguments

data	A list where each element is a time series, or a numerical matrix where each row is a time series. Only the latter is supported in case of type = "partitional".
type	$What \ type \ of \ clustering \ method \ to \ use, partitional, hierarchical \ or \ tadpole.$
k	Numer of desired clusters in partitional methods.
method	Which linkage method to use in hierarchical methods. See hclust.
distance	One of the supported distance definitions (see Distance section). Ignored for type = "tadpole".
centroid	Either a supported string or an appropriate function to calculate centroids when using partitional methods (see Centroid section).
window.size	Window constraint for DTW and LB calculations. See Sakoe-Chiba section.
norm	Pointwise distance for DTW and LB. Either L1 for Manhattan distance or L2 for Euclidean. Ignored for distance = "DTW" (which always uses L1) and distance = "DTW2" (which always uses L2).
dc	Cutoff distance for TADPole algorithm.
control	Parameters for partitional clustering algorithms. See flexclustControl.
save.data	Return a copy of the data in the returned object? Ignored for hierarchical clustering.
seed	Random seed for reproducibility of partitional algorithms.
trace	Boolean flag. If true, more output regarding the progress is printed to screen.
• • •	Additional arguments to pass to dist or a custom distance function.

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Details

Partitional algorithms are implemented via kcca. Hierarchical algorithms use the hclust function. The tadpole algorithm uses the TADPole function.

In case of partitional algorithms, data should be in the form of a matrix. In the other cases, it may be a matrix or a list, but the matrix will be coerced to a list. A matrix input requires that all time series have equal lengths. If the lengths vary slightly between time series, reinterpolating them to a common length is most likely an acceptable approach (Ratanamahatana and Keogh, 2004). If this is not the case, then clustering them directly is probably ill-advised. See the examples.

Value

An object with formal class dtwclust-class if type = "partitional" | "tadpole". Otherwise an object with class helust as returned by helust.

Distance

If a custom distance function is provided, it will receive the data as the first argument. For partitional algorithms, the second argument will be the cluster centers (i.e. other time series) in the form of a matrix where each row is a center series. If hierarchical algorithms are used, the function will also receive the elements of

For partitional algorithms, the function *could* make use of the window.size and norm parameters, which *should* be detected thanks to R's lexical scoping, however this cannot be guaranteed.

The function should return a distance matrix, ideally of class crossdist. In case of partitional algorithms, the time series in the data should be along the rows, and the cluster centers along the columns of the distance matrix.

The other option is to provide a string. For partitional algorithms, it can be a supported distance of kccaFamily. For hierarchical, it can be any distance function registered in dist. In the latter case, all extra parameters should be provided in

Additionally, with either type of algorithm, it can be one of the following custom implementations:

- "dtw": DTW with L1 norm and optionally a Sakoe-Chiba constraint.
- "dtw2": DTW with L2 norm and optionally a Sakoe-Chiba constraint.
- "dtw_lb": DTW with L1 or L2 norm and optionally a Sakoe-Chiba constraint. Some computations are avoided by first estimating the distance matrix with Lemire's lower bound and then iteratively refining with DTW. See dtw_lb.
- "lbk": Keogh's lower bound with either L1 or L2 norm for the Sakoe-Chiba constraint.
- "lbi": Lemire's lower bound with either L1 or L2 norm for the Sakoe-Chiba constraint.
- "sbd": Shape-based distance. Each series is z-normalized in this case. As a result, the cluster centers (for partitional methods) are also z-normalized. See SBD for more details.

Centroid

In the case of partitional algorithms, a suitable function should calculate the cluster centers. In this case, the centers are themselves time series.

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If a custom function is provided, it will receive a matrix as only argument. Each row will be a time series that belongs to a given cluster. The function should return a numeric vector with the center time series.

The other option is to provide a character string. The following options are available:

- "mean": The average along each dimension. In other words, the average of all x_i^j among the j series that belong to the same cluster for all time points t_i .
- "median": The median along each dimension. Similar to mean.
- "shape": Shape averaging. See shape_extraction for more details.
- "dba": DTW Barycenter Averaging. See DBA for more details.
- "pam": Partition around medoids. This basically means that the cluster centers are always one of the time series in the data. In this case, the distance matrix is pre-computed once using all time series in the data and then re-used at each iteration.

Sakoe-Chiba Constraint

A global constraint to speed up the DTW calculation is the Sakoe-Chiba band (Sakoe and Chiba, 1978). To use it, a window width must be defined via window.size.

The windowing constraint uses a centered window. The calculations expect a value in window. size that represents the distance between the point considered and one of the edges of the window. Therefore, if, for example, window.size = 10, the warping for an observation x_i considers the points between x_{i-10} and x_{i+10} , resulting in 10*2 + 1 = 21 observations falling within the window.

Note

Notice that the lower bounds are defined only for time series of equal lengths. DTW and DTW2 don't require this, but they are much slower to compute.

The lower bounds are **not** symmetrical, and DTW is only symmetrical if series are of equal lengths. Specifying distance = "sbd" and centroid = "shape" is equivalent to the k-Shape algorithm (Papparizos and Gravano, 2015). See SBD and shape_extraction for more info.

Author(s)

Alexis Sarda-Espinosa

References

Sakoe H and Chiba S (1978). "Dynamic programming algorithm optimization for spoken word recognition." *Acoustics, Speech and Signal Processing, IEEE Transactions on*, **26**(1), pp. 43-49. ISSN 0096-3518, http://doi.org/10.1109/TASSP.1978.1163055.

Ratanamahatana A and Keogh E (2004). "Everything you know about dynamic time warping is wrong." In 3rd Workshop on Mining Temporal and Sequential Data, in conjunction with 10th ACM SIGKDD Int. Conf. Knowledge Discovery and Data Mining (KDD-2004), Seattle, WA.

Paparrizos J and Gravano L (2015). "k-Shape: Efficient and Accurate Clustering of Time Series." In *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*, series SIGMOD '15, pp. 1855-1870. ISBN 978-1-4503-2758-9, http://doi.org/10.1145/2723372. 2737793.

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Examples

```
# Load data
data(uciCT)
# Reinterpolate to same length and coerce as matrix
data <- t(sapply(CharTraj, reinterpolate, newLength = 205))</pre>
# Simple partitional clustering with L2 distance and PAM
kc.12 <- dtwclust(data, k = 20, distance = "kmeans", centroid = "pam", seed = 3247, trace = TRUE)
cat("Rand index for L2+PAM:", randIndex(kc.l2, CharTrajLabels), "\n\n")
# TADPole clustering (takes around 5 seconds)
kc.tadp <- dtwclust(data, type = "tadpole", k = 20, window.size = 20, dc = 1.5, save.data = TRUE)
cat("Rand index for TADPole:", randIndex(kc.tadp, CharTrajLabels), "\n\n")
plot(kc.tadp)
# Hierarchical clustering based on shabe-based distance
hc.sbd <- dtwclust(data, type = "hierarchical", distance = "sbd")</pre>
cl.sbd <- cutree(hc.sbd, 20)</pre>
cat("Rand index for HC+SBD:", randIndex(cl.sbd, CharTrajLabels), "\n\n")
## Not run:
# Use full DTW and PAM (takes around two minutes)
kc.dtw <- dtwclust(data, k = 20, seed = 3251, trace = TRUE)</pre>
# Use full DTW with DBA centroids (takes around five minutes)
kc.dba <- dtwclust(data, k = 20, centroid = "dba", seed = 3251, trace = TRUE)
## End(Not run)
```

dtwclust-class

Class definition for dtwclust

Description

Formal S4 class to know how to handle data for plotting.

Details

It contains the following specific slots:

- type: A string indicating one of the supported clustering types of dtwclust.
- distance: A string indicating one of the supported distances of dtwclust.
- centroid: A string indicating one of the supported centroids of dtwclust.

Additionally, the class inherits from kccasimple-class, so all related slots and methods are also supported.

dtw_lb

dtw_lb

DTW calculation guided by Lemire's lower bound (LB_Improved)

Description

Calculation of a distance matrix with the Dynamic Time Warping (DTW) distance guided by Lemire's lower bound (LB).

Usage

```
dtw_lb(x, y = NULL, window.size = NULL, norm = "L1", error.check = TRUE)
```

Arguments

A matrix where rows are time series, or a list of time series.

y An object similar to x.

window.size Window size to use with the LB and DTW calculation. See details.

norm Pointwise distance. Either L1 for Manhattan distance or L2 for Euclidean.

error.check Should inconsistencies in the data be checked?

Details

This function first calculates an initial estimate of a distance matrix between two sets of time series using Lemire's improved lower bound. Afterwards, it uses the estimate to calculate the true DTW distances between *only* the nearest neighbors of each series in x found in y. If only x is provided, the distance matrix is calculated between all its time series. This could be useful in case one is interested in only the nearest neighbor of one or more series among a dataset.

The windowing constraint uses a centered window. The calculations expect a value in window. size that represents the distance between the point considered and one of the edges of the window. Therefore, if, for example, window. size = 10, the warping for an observation x_i considers the points between x_{i-10} and x_{i+10} , resulting in 10*2 + 1 = 21 observations falling within the window.

Value

The distance matrix with class crossdist.

Note

This function uses a lower bound that is only defined for time series of equal lengths.

References

Lemire D (2009). "Faster retrieval with a two-pass dynamic-time-warping lower bound." *Pattern Recognition*, **42**(9), pp. 2169 - 2180. ISSN 0031-3203, http://dx.doi.org/10.1016/j.patcog. 2008.11.030, http://www.sciencedirect.com/science/article/pii/S0031320308004925.

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See Also

```
lb_improved
```

Examples

```
# Load data
data(uciCT)

# Reinterpolate to same length
data <- lapply(CharTraj, reinterpolate, newLength = 205)

# Calculate the DTW distance between a certain subset aided with the lower bound system.time(d <- dtw_lb(data[1:5], data[6:100], window.size = 20))

# Nearest neighbors
NN1 <- apply(d, 1, which.min)

# Calculate the DTW distances between all elements (about seven times slower) system.time(d2 <- proxy::dist(data[1:5], data[6:100], method = "DTW", window.type = "slantedband", window.size = 20))

# Nearest neighbors
NN2 <- apply(d2, 1, which.min)

all(NN1 == NN2)</pre>
```

lb_improved

Lemire's improved DTW lower bound

Description

This function calculates a lower bound (LB) on the Dynamic Time Warp (DTW) distance between two time series. It uses a Sakoe-Chiba constraint.

Usage

```
lb_improved(x, y, window.size = NULL, norm = "L1")
```

Arguments

x A time series.

y A time series with the same length as x.

window.size Window size for envelope calculation. See details.

norm Pointwise distance. Either L1 for Manhattan distance or L2 for Euclidean.

lb_keogh

Details

The lower bound is defined for time series of equal length only.

The windowing constraint uses a centered window. The calculations expect a value in window. size that represents the distance between the point considered and one of the edges of the window. Therefore, if, for example, window. size = 10, the warping for an observation x_i considers the points between x_{i-10} and x_{i+10} , resulting in 10*2 + 1 = 21 observations falling within the window.

Value

The improved lower bound for the DTW distance.

References

Lemire D (2009). "Faster retrieval with a two-pass dynamic-time-warping lower bound." *Pattern Recognition*, **42**(9), pp. 2169 - 2180. ISSN 0031-3203, http://dx.doi.org/10.1016/j.patcog. 2008.11.030, http://www.sciencedirect.com/science/article/pii/S0031320308004925.

Examples

```
# Sample data
data(uciCT)

# Lower bound distance between two series
d.lbi <- lb_improved(CharTraj[[1]], CharTraj[[2]], window.size = 20)

# Corresponding true DTW distance
d.dtw <- dtw(CharTraj[[1]], CharTraj[[2]], window.type = "slantedband", window.size = 20)$distance
d.lbi <= d.dtw</pre>
```

1b_keogh

Keogh's DTW lower bound

Description

This function calculates a lower bound (LB) on the Dynamic Time Warp (DTW) distance between two time series. It uses a Sakoe-Chiba constraint.

Usage

```
lb_keogh(x, y, window.size = NULL, norm = "L1")
```

Arguments

x A time series.

y A time series with the same length as x.

window.size Window size for envelope calculation. See details.

norm Pointwise distance. Either L1 for Manhattan distance or L2 for Euclidean.

NCCc NCCc

Details

The lower bound is defined for time series of equal length only.

The windowing constraint uses a centered window. The calculations expect a value in window. size that represents the distance between the point considered and one of the edges of the window. Therefore, if, for example, window. size = 10, the warping for an observation x_i considers the points between x_{i-10} and x_{i+10} , resulting in 10*2 + 1 = 21 observations falling within the window.

Value

A list with:

- d: The lower bound of the DTW distance.
- upper.env: The time series of the upper envelope.
- lower.env: The time series of the lower envelope.

References

Keogh E and Ratanamahatana CA (2005). "Exact indexing of dynamic time warping." *Knowledge and information systems*, **7**(3), pp. 358-386.

Examples

```
# Sample data
data(uciCT)

# Lower bound distance between two series
d.lbk <- lb_keogh(CharTraj[[1]], CharTraj[[2]], window.size = 20)$d

# Corresponding true DTW distance
d.dtw <- dtw(CharTraj[[1]], CharTraj[[2]], window.type = "slantedband", window.size = 20)$distance
d.lbk <= d.dtw</pre>
```

NCCc

Cross-correlation with coefficient normalization

Description

This function uses FFT to compute the cross-correlation sequence between two series. They need not be of equal length.

Usage

```
NCCc(x, y)
```

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Arguments

x A time series.

y Another time series.

Value

The cross-correlation sequence with length length(x) + length(y) - 1.

References

Paparrizos J and Gravano L (2015). "k-Shape: Efficient and Accurate Clustering of Time Series." In *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*, series SIGMOD '15, pp. 1855-1870. ISBN 978-1-4503-2758-9, http://doi.org/10.1145/2723372. 2737793.

See Also

SBD

plot-dtwclust

Plot the result of dtwclust

Description

Plots the time series of each cluster along with the obtained centroid. It uses ggplot2 plotting system.

Usage

Arguments

x An object of class dtwclust-class as returned by dtwclust.

y Ignored.

clus Which clusters to plot.

data The data in the same format as it was provided to dtwclust.

.. Further arguments to pass to geom_line for the plotting of the *cluster centers*.

Default values are: linetype = "dashed", size = 1.5, colour = "black", alpha = 0.5.

Details

The flag save.data must be set to TRUE when running dtwclust to be able to use this.

Optionally, you can manually provide the clustering result as well as the data in data.

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See Also

dtwclust-class, dtwclust

reinterpolate

Wrapper for simple linear reinterpolation

Description

This function is just a wrapper for the native function approx to do simple linear reinterpolation.

Usage

```
reinterpolate(ts, newLength)
```

Arguments

ts A time series.

newLength Desired length of the output series.

Value

Reinterpolated time series

SBD

Shape-based distance

Description

Distance based on coefficient-normalized cross-correlation as proposed by Papparizos and Gravano, 2015, for the k-Shape clustering algorithm.

Usage

```
SBD(x, y, znorm = TRUE)
```

Arguments

x A time series.

y Another time series.

znorm Should each series be z-normalized before calculating the distance?

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Details

This function works best if the series are *z-normalized*. If not, at least they should have corresponding amplitudes, since the values of the signal **do** affect the outcome.

If x and y do **not** have the same length, it would be best if the longer sequence is provided in y, because it will be shifted to match x. Anything before the matching point is discarded and the series is padded with trailing zeros as needed.

The output values lie between 0 and 2, with 0 indicating perfect similarity.

Value

A list with:

- dist: The distance between x and y.
- yshift: A shifted version of y so that it optimally mathces x.

References

Paparrizos J and Gravano L (2015). "k-Shape: Efficient and Accurate Clustering of Time Series." In *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*, series SIGMOD '15, pp. 1855-1870. ISBN 978-1-4503-2758-9, http://doi.org/10.1145/2723372. 2737793.

See Also

NCCc, shape_extraction

shape_extraction

Shape average of several time series

Description

Time-series shape extraction based on optimal alignments as proposed by Papparizos and Gravano, 2015, for the k-Shape clustering algorithm.

Usage

```
shape_extraction(X, cz = NULL, znorm = TRUE)
```

Arguments

Χ	Numeric matrix where each row is a time series.
CZ	Center to use as basis. Should already be $normalized$. Calculation uses all X if $cz = NULL$.
znorm	Boolean flag. Should z-scores be calculated for X before processing?

TADPole

Details

This works only if the signals are *z-normalized*, since the output will also have this normalization.

This centroid computation is casted as an optimization problem called maximization of Rayleigh Quotient. See the cited article for more details.

Value

Centroid time series.

References

Paparrizos J and Gravano L (2015). "k-Shape: Efficient and Accurate Clustering of Time Series." In *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*, series SIGMOD '15, pp. 1855-1870. ISBN 978-1-4503-2758-9, http://doi.org/10.1145/2723372. 2737793.

See Also

```
SBD, zscore
```

Examples

```
# Sample data
data(uciCT)

# Subset of interest, normalized
X <- t(sapply(CharTraj[1:5], zscore))

# Obtain centroid series
C <- shape_extraction(X, znorm = FALSE)

# Result
matplot(t(X), type = "1", col = 1:5)
points(C)</pre>
```

TADPole

TADPole clustering

Description

Time-series Anytime Density Peaks Clustering as proposed by Begum et al., 2015.

Usage

```
TADPole(data, window.size = NULL, k = 2, dc, error.check = TRUE)
```

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Arguments

data The data matrix where each row is a time series. Optionally a list with each time

series.

window.size Window size constraint for DTW. See details.

k The number of desired clusters.

dc The cutoff distance.

error.check Should the data be checked for inconsistencies?

Details

This function can be called either directly or through dtwclust.

TADPole clustering adopts a relatively new clustering framework and adapts it to time series clustering with DTW. See the cited article for the details of the algorithm.

Because of the way the algorithm works, it can be considered a kind of Partitioning Around Medoids (PAM). This means that the cluster centers are always elements of the data.

The algorithm first uses the DTW's upper and lower bounds to find series with many close neighbors (in DTW space). Anything below the cutoff distance (dc) is considered a neighbor. Aided with this information, the algorithm then tries to prune as many DTW calculations as possible in order to accelerate the clustering procedure. The series that lie in dense areas (i.e. that have lots of neighbors) are taken as cluster centers.

The algorithm relies on the DTW bounds, which are only defined for time series of equal lengths.

The windowing constraint uses a centered window. The calculations expect a value in window. size that represents the distance between the point considered and one of the edges of the window. Therefore, if, for example, window.size = 10, the warping for an observation x_i considers the points between x_{i-10} and x_{i+10} , resulting in 10*2 + 1 = 21 observations falling within the window.

Value

A list with:

- cl: Cluster indices.
- centers: Indices of the centers.
- distCalcPercentage: Percentage of distance calculations that were actually performed.

References

Begum N, Ulanova L, Wang J and Keogh E (2015). "Accelerating Dynamic Time Warping Clustering with a Novel Admissible Pruning Strategy." In *Conference on Knowledge Discovery and Data Mining*, series KDD '15. ISBN 978-1-4503-3664-2/15/08, http://www.cs.ucr.edu/~eamonn/Speeded%20Clustering%20Paper%20Camera%20Ready.pdf.

18 zscore

uciCT

Subset of character trajectories data set

Description

Subset: only 5 examples of X velocity. See details.

Format

A list with 100 elements. Each element is a time series. Labels included as factor vector.

Details

Quoting the source:

"Multiple, labelled samples of pen tip trajectories recorded whilst writing individual characters. All samples are from the same writer, for the purposes of primitive extraction. Only characters with a single pen-down segment were considered."

The subset included here (CharTraj) has only 5 examples of the X velocity for each character. A vector with labels is also loaded in CharTrajLabels.

Source

https://archive.ics.uci.edu/ml/datasets/Character+Trajectories

zscore

Wrapper for z-normalization

Description

Wrapper for function scale that returns zeros instead of NaN.

Usage

```
zscore(x, ...)
```

Arguments

x Data to normalize.

... Further arguments to pass to scale.

Value

Normalized data.

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