# Package 'dtwclust'

October 13, 2022

Type Package

**Title** Time Series Clustering Along with Optimizations for the Dynamic Time Warping Distance

**Description** Time series clustering along with optimized techniques related to the Dynamic Time Warping distance and its corresponding lower bounds. Implementations of partitional, hierarchical, fuzzy, k-Shape and TADPole clustering are available. Functionality can be easily extended with custom distance measures and centroid definitions. Implementations of DTW barycenter averaging, a distance based on global alignment kernels, and the soft-DTW distance and centroid routines are also provided. All included distance functions have custom loops optimized for the calculation of cross-distance matrices, including parallelization support. Several cluster validity indices are included.

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LinkingTo Rcpp, RcppArmadillo, RcppParallel, RcppThread

Suggests doParallel, knitr, rmarkdown, testthat

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*Time series clustering along with optimizations for the Dynamic Time Warping distance* 

#### Description

Time series clustering with a wide variety of strategies and a series of optimizations specific to the Dynamic Time Warping (DTW) distance and its corresponding lower bounds (LBs).

## Details

Many of the algorithms implemented in this package are specifically tailored to DTW, hence its name. However, the main clustering function is flexible so that one can test many different clustering approaches, using either the time series directly, or by applying suitable transformations and then clustering in the resulting space. Other implementations included in the package provide some alternatives to DTW.

DTW is a dynamic programming algorithm that tries to find the optimum warping path between two series. Over the years, several variations have appeared in order to make the procedure faster or more efficient. Please refer to the included references for more information, especially Giorgino (2009), which is a good practical introduction.

Most optimizations require equal dimensionality, which means time series should have equal length. DTW itself does not require this, but it is relatively expensive to compute. Other distance definitions may be used, or series could be reinterpolated to a matching length (Ratanamahatana and Keogh 2004).

The main clustering function and entry point for this package is tsclust(), with a convenience wrapper for multiple tests in compare\_clusterings(), and a shiny app in interactive\_clustering(). There is another less-general-purpose shiny app in ssdtwclust().

Please note the random number generator is set to L'Ecuyer-CMRG when **dtwclust** is attached in an attempt to preserve reproducibility. You are free to change this afterwards if you wish (see base::RNGkind()), but **dtwclust** will always use L'Ecuyer-CMRG internally.

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For more information, please read the included package vignettes, which can be accessed by typing browseVignettes("dtwclust").

#### Note

This software package was developed independently of any organization or institution that is or has been associated with the author.

This package can be used without attaching it with base::library() with some caveats:

- The **methods** package must be attached. R usually does this automatically, but utils::Rscript() only does so in R versions 3.5.0 and above.
- If you want to use the **proxy** version of dtw::dtw() (e.g. for clustering), you have to attach the dtw package manually.

Be careful with reproducibility, R's random number generator is only changed session-wide if **dtwclust** is attached.

## Author(s)

Alexis Sarda-Espinosa

## References

Please refer to the package's vignette's references.

as.matrix

### See Also

```
tsclust(), compare_clusterings(), interactive_clustering(), ssdtwclust(), dtw_basic(),
proxy::dist().
```

as.matrix

#### Description

**proxy** exported a non-generic as.matrix function. This is to re-export the base version and add coercion methods for pairdist and crossdist.

#### Usage

as.matrix(x, ...)

#### Arguments

x, ... See base::as.matrix().

## See Also

base::as.matrix()

compare\_clusterings Compare different clustering configurations

## Description

Compare many different clustering algorithms with support for parallelization.

## Usage

```
compare_clusterings(
  series = NULL,
  types = c("p", "h", "f", "t"),
  configs = compare_clusterings_configs(types),
  seed = NULL,
  trace = FALSE,
   ...,
  score.clus = function(...) stop("No scoring"),
  pick.clus = function(...) stop("No picking"),
  shuffle.configs = FALSE,
  return.objects = FALSE,
  packages = character(0L),
  .errorhandling = "stop"
)
```

## Arguments

series	A list of series, a numeric matrix or a data frame. Matrices and data frames are coerced to a list row-wise (see tslist()).
types	Clustering types. It must be any combination of (possibly abbreviated): "partitional", "hierarchical", "fuzzy", "tadpole."
configs	The list of data frames with the desired configurations to run. See pdc_configs() and compare_clusterings_configs().
seed	Seed for random reproducibility.
trace	Logical indicating that more output should be printed to screen.
	Further arguments for tsclust(), score.clus or pick.clus.
score.clus	A function that gets the list of results (and $\ldots$ ) and scores each one. It may also be a named list of functions, one for each type of clustering. See Scoring section.
pick.clus	A function to pick the best result. See Picking section.
shuffle.configs	
	Randomly shuffle the order of configs, which can be useful to balance load when using parallel computation.
return.objects	Logical indicating whether the objects returned by tsclust() should be given in the result.

packages	A character vector with the names of any packages needed for any functions
	used (distance, centroid, preprocessing, etc.). The name "dtwclust" is added
	automatically. Relevant for parallel computation.
.errorhandling	This will be passed to foreach::foreach(). See Parallel section below.

## Details

This function calls tsclust() with different configurations and evaluates the results with the provided functions. Parallel support is included. See the examples.

Parameters specified in configs whose values are NA will be ignored automatically.

The scoring and picking functions are for convenience, if they are not specified, the scores and pick elements of the result will be NULL.

See repeat\_clustering() for when return.objects = FALSE.

#### Value

A list with:

- results: A list of data frames with the flattened configs and the corresponding scores returned by score.clus.
- scores: The scores given by score.clus.
- pick: The object returned by pick.clus.
- proc\_time: The measured execution time, using base::proc.time().
- seeds: A list of lists with the random seeds computed for each configuration.

The cluster objects are also returned if return.objects = TRUE.

#### **Parallel computation**

The configurations for each clustering type can be evaluated in parallel (multi-processing) with the **foreach** package. A parallel backend can be registered, e.g., with **doParallel**.

If the .errorhandling parameter is changed to "pass" and a custom score.clus function is used, said function should be able to deal with possible error objects.

If it is changed to "remove", it might not be possible to attach the scores to the results data frame, or it may be inconsistent. Additionally, if return.objects is TRUE, the names given to the objects might also be inconsistent.

Parallelization can incur a lot of deep copies of data when returning the cluster objects, since each one will contain a copy of datalist. If you want to avoid this, consider specifying score.clus and setting return.objects to FALSE, and then using repeat\_clustering().

#### Scoring

The clustering results are organized in a *list of lists* in the following way (where only applicable types exist; first-level list names in bold):

- partitional list with
  - Clustering results from first partitional config

- etc.

- hierarchical list with
  - Clustering results from first hierarchical config

– etc.

- **fuzzy** list with
  - Clustering results from first fuzzy config
  - etc.
- tadpole list with
  - Clustering results from first tadpole config

– etc.

If score.clus is a function, it will be applied to the available partitional, hierarchical, fuzzy and/or tadpole results via:

```
scores <- lapply(list_of_lists, score.clus, ...)</pre>
```

Otherwise, score.clus should be a list of functions with the same names as the list above, so that score.clus\$partitional is used to score list\_of\_lists\$partitional and so on (via base::Map()).

Therefore, the scores returned shall always be a list of lists with first-level names as above.

#### Picking

If return.objects is TRUE, the results' data frames and the list of TSClusters objects are given to pick.clus as first and second arguments respectively, followed by .... Otherwise, pick.clus will receive only the data frames and the contents of ... (since the objects will not be returned by the preceding step).

## Limitations

Note that the configurations returned by the helper functions assign special names to preprocessing/distance/centroid arguments, and these names are used internally to recognize them.

If some of these arguments are more complex (e.g. matrices) and should *not* be expanded, consider passing them directly via the ellipsis (...) instead of using pdc\_configs(). This assumes that said arguments can be passed to all functions without affecting their results.

The distance matrices (if calculated) are not re-used across configurations. Given the way the configurations are created, this shouldn't matter, because clusterings with arguments that can use the same distance matrix are already grouped together by compare\_clusterings\_configs() and pdc\_configs().

## Author(s)

Alexis Sarda-Espinosa

## See Also

compare\_clusterings\_configs(), tsclust()

## Examples

```
# Fuzzy preprocessing: calculate autocorrelation up to 50th lag
acf_fun <- function(series, ...) {</pre>
    lapply(series, function(x) {
        as.numeric(acf(x, lag.max = 50, plot = FALSE)$acf)
   })
}
# Define overall configuration
cfgs <- compare_clusterings_configs(</pre>
    types = c("p", "h", "f", "t"),
   k = 19L:20L,
   controls = list(
        partitional = partitional_control(
            iter.max = 30L,
            nrep = 1L
        ),
        hierarchical = hierarchical_control(
            method = "all"
        ),
        fuzzy = fuzzy_control(
            # notice the vector
            fuzziness = c(2, 2.5),
            iter.max = 30L
        ),
        tadpole = tadpole_control(
            # notice the vectors
            dc = c(1.5, 2),
            window.size = 19L:20L
       )
   ),
   preprocs = pdc_configs(
       type = "preproc",
        # shared
       none = list(),
        zscore = list(center = c(FALSE)),
        # only for fuzzy
        fuzzy = list(
            acf_fun = list()
       ),
        # only for tadpole
        tadpole = list(
            reinterpolate = list(new.length = 205L)
        ),
        # specify which should consider the shared ones
        share.config = c("p", "h")
   ),
    distances = pdc_configs(
        type = "distance",
        sbd = list(),
        fuzzy = list(
            L2 = list()
```

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```
),
      share.config = c("p", "h")
   ),
   centroids = pdc_configs(
      type = "centroid",
      partitional = list(
         pam = list()
      ),
      # special name 'default'
      hierarchical = list(
         default = list()
      ),
      fuzzy = list(
         fcmdd = list()
      ),
      tadpole = list(
         default = list(),
         shape_extraction = list(znorm = TRUE)
      )
   )
)
# Number of configurations is returned as attribute
num_configs <- sapply(cfgs, attr, which = "num.configs")</pre>
cat("\nTotal number of configurations without considering optimizations:",
   sum(num_configs),
   "\n\n")
# Define evaluation functions based on CVI: Variation of Information (only crisp partition)
vi_evaluators <- cvi_evaluators("VI", ground.truth = CharTrajLabels)</pre>
score_fun <- vi_evaluators$score</pre>
pick_fun <- vi_evaluators$pick</pre>
# Short run with only fuzzy clustering
# ______
comparison_short <- compare_clusterings(CharTraj, types = c("f"), configs = cfgs,</pre>
                                seed = 293L, trace = TRUE,
                                score.clus = score_fun, pick.clus = pick_fun,
                                return.objects = TRUE)
## Not run:
# Parallel run with all comparisons
require(doParallel)
registerDoParallel(cl <- makeCluster(detectCores()))</pre>
comparison_long <- compare_clusterings(CharTraj, types = c("p", "h", "f", "t"),</pre>
                               configs = cfgs,
                                seed = 293L, trace = TRUE,
```

```
score.clus = score_fun,
                                   pick.clus = pick_fun,
                                   return.objects = TRUE)
# Using all external CVIs and majority vote
external_evaluators <- cvi_evaluators("external", ground.truth = CharTrajLabels)</pre>
score_external <- external_evaluators$score</pre>
pick_majority <- external_evaluators$pick</pre>
comparison_majority <- compare_clusterings(CharTraj, types = c("p", "h", "f", "t"),</pre>
                                       configs = cfgs,
                                       seed = 84L, trace = TRUE,
                                       score.clus = score_external,
                                       pick.clus = pick_majority,
                                       return.objects = TRUE)
# best results
plot(comparison_majority$pick$object)
print(comparison_majority$pick$config)
stopCluster(cl); registerDoSEQ()
# A run with only partitional clusterings
# _____
p_cfgs <- compare_clusterings_configs(</pre>
   types = "p", k = 19L:21L,
   controls = list(
       partitional = partitional_control(
          iter.max = 20L,
          nrep = 8L
       )
   ),
   preprocs = pdc_configs(
       "preproc",
       none = list(),
       zscore = list(center = c(FALSE, TRUE))
   ),
   distances = pdc_configs(
       "distance",
       sbd = list(),
       dtw_basic = list(window.size = 19L:20L,
                      norm = c("L1", "L2")),
       gak = list(window.size = 19L:20L,
                 sigma = 100)
   ),
   centroids = pdc_configs(
       "centroid".
       partitional = list(
          pam = list(),
          shape = list()
       )
```

## End(Not run)

 ${\tt compare\_clusterings\_configs}$ 

Create clustering configurations.

## Description

Create configurations for compare\_clusterings()

## Usage

```
compare_clusterings_configs(
  types = c("p", "h", "f"),
  k = 2L,
  controls = NULL,
  preprocs = pdc_configs("preproc", none = list()),
  distances = pdc_configs("distance", dtw_basic = list()),
  centroids = pdc_configs("centroid", default = list()),
  no.expand = character(0L)
)
```

#### Arguments

types	Clustering types. It must be any combination of (possibly abbreviated): parti- tional, hierarchical, fuzzy, tadpole.
k	A numeric vector with one or more elements specifying the number of clusters to test.
controls	A named list of tsclust-controls. NULL means defaults. See details.
preprocs	Preprocessing configurations. See details.

distances	Distance configurations. See details.
centroids	Centroid configurations. See details.
no.expand	A character vector indicating parameters that should <i>not</i> be expanded between pdc_configs() configurations. See examples.

## Details

Preprocessing, distance and centroid configurations are specified with the helper function pdc\_configs(), refer to the examples in compare\_clusterings() to see how this is used.

The controls list may be specified with the usual tsclust-controls functions. The names of the list must correspond to "partitional", "hierarchical", "fuzzy" or "tadpole" clustering. Again, please refer to the examples in compare\_clusterings().

## Value

A list for each clustering type, each of which includes a data frame with the computed and merged configurations. Each data frame has an extra attribute num.configs specifying the number of configurations.

## Examples

```
# compare this with leaving no.expand empty
compare_clusterings_configs(
    distances = pdc_configs("d", dtw_basic = list(window.size = 1L:2L, norm = c("L1", "L2"))),
    centroids = pdc_configs("c", dba = list(window.size = 1L:2L, norm = c("L1", "L2"))),
    no.expand = c("window.size", "norm")
)
```

compute\_envelope Time series warping envelopes

#### Description

This function computes the envelopes for DTW lower bound calculations with a Sakoe-Chiba band for a given univariate time series using the streaming algorithm proposed by Lemire (2009).

#### Usage

```
compute_envelope(x, window.size, error.check = TRUE)
```

## Arguments

Х	A univariate time series.
window.size	Window size for envelope calculation. See details.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

## Details

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 two elements (lower and upper envelopes respectively): lower and upper.

#### Note

This envelope is calculated assuming a Sakoe-Chiba constraint for DTW.

#### 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, doi:10.1016/j.patcog.2008.11.030, https://www.sciencedirect.com/science/article/pii/S0031320308004925.

## Examples

data(uciCT)

H <- compute\_envelope(CharTraj[[1L]], 18L)</pre>

matplot(do.call(cbind, H), type = "1", col = 2:3)
lines(CharTraj[[1L]])

cvi

#### Cluster validity indices

#### Description

Compute different cluster validity indices (CVIs) of a given cluster partition, using the clustering distance measure and centroid function if applicable.

#### Usage

```
cvi(a, b = NULL, type = "valid", ..., log.base = 10)
## S4 method for signature 'matrix'
cvi(a, b = NULL, type = "valid", ..., log.base = 10)
## S4 method for signature 'PartitionalTSClusters'
cvi(a, b = NULL, type = "valid", ..., log.base = 10)
```

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```
## S4 method for signature 'HierarchicalTSClusters'
cvi(a, b = NULL, type = "valid", ..., log.base = 10)
## S4 method for signature 'FuzzyTSClusters'
cvi(a, b = NULL, type = "valid", ..., log.base = 10)
```

#### Arguments

a	An object returned by tsclust(), for crisp partitions a vector that can be co- erced to integers which indicate the cluster memberships, or the membership matrix for soft clustering.
b	If needed, a vector that can be coerced to integers which indicate the cluster memberships. The ground truth (if known) should be provided here.
type	Character vector indicating which indices are to be computed. See supported values below.
	Arguments to pass to and from other methods.
log.base	Base of the logarithm to be used in the calculation of VI (see details).

## Details

Clustering is commonly considered to be an unsupervised procedure, so evaluating its performance can be rather subjective. However, a great amount of effort has been invested in trying to standardize cluster evaluation metrics by using cluster validity indices (CVIs).

In general, CVIs can be either tailored to crisp or fuzzy partitions. CVIs can be classified as internal, external or relative depending on how they are computed. Focusing on the first two, the crucial difference is that internal CVIs only consider the partitioned data and try to define a measure of cluster purity, whereas external CVIs compare the obtained partition to the correct one. Thus, external CVIs can only be used if the ground truth is known.

Note that even though a fuzzy partition can be changed into a crisp one, making it compatible with many of the existing crisp CVIs, there are also fuzzy CVIs tailored specifically to fuzzy clustering, and these may be more suitable in those situations. Fuzzy partitions usually have no ground truth associated with them, but there are exceptions depending on the task's goal.

Each index defines their range of values and whether they are to be minimized or maximized. In many cases, these CVIs can be used to evaluate the result of a clustering algorithm regardless of how the clustering works internally, or how the partition came to be.

Knowing which CVI will work best cannot be determined a priori, so they should be tested for each specific application. Usually, many CVIs are utilized and compared to each other, maybe using a majority vote to decide on a final result. Furthermore, it should be noted that many CVIs perform additional distance calculations when being computed, which can be very considerable if using DTW or GAK.

#### Value

The chosen CVIs.

## **External CVIs**

- Crisp partitions (the first 4 are calculated via flexclust::comPart())
  - "RI": Rand Index (to be maximized).
  - "ARI": Adjusted Rand Index (to be maximized).
  - "J": Jaccard Index (to be maximized).
  - "FM": Fowlkes-Mallows (to be maximized).
  - "VI": Variation of Information (Meila (2003); to be minimized).
- Fuzzy partitions (based on Lei et al. (2017))
  - "RI": Soft Rand Index (to be maximized).
  - "ARI": Soft Adjusted Rand Index (to be maximized).
  - "VI": Soft Variation of Information (to be minimized).
  - "NMIM": Soft Normalized Mutual Information based on Max entropy (to be maximized).

## **Internal CVIs**

The indices marked with an exclamation mark (!) calculate (or re-use if already available) the whole distance matrix between the series in the data. If you were trying to avoid this in the first place, then these CVIs might not be suitable for your application.

The indices marked with a question mark (?) depend on the extracted centroids, so bear that in mind if a hierarchical procedure was used and/or the centroid function has associated randomness (such as shape\_extraction() with series of different length).

The indices marked with a tilde (~) require the calculation of a global centroid. Since DBA() and shape\_extraction() (for series of different length) have some randomness associated, these indices might not be appropriate for those centroids.

- · Crisp partitions
  - "Sil" (!): Silhouette index (Rousseeuw (1987); to be maximized).
  - "D" (!): Dunn index (Arbelaitz et al. (2013); to be maximized).
  - "COP" (!): COP index (Arbelaitz et al. (2013); to be minimized).
  - "DB" (?): Davies-Bouldin index (Arbelaitz et al. (2013); to be minimized).
  - "DBstar" (?): Modified Davies-Bouldin index (DB\*) (Kim and Ramakrishna (2005); to be minimized).
  - "CH" (~): Calinski-Harabasz index (Arbelaitz et al. (2013); to be maximized).
  - "SF" (~): Score Function (Saitta et al. (2007); to be maximized; see notes).
- Fuzzy partitions (using the nomenclature from Wang and Zhang (2007))
  - "MPC": to be maximized.
  - "K" (~): to be minimized.
  - "T": to be minimized.
  - "SC" (~): to be maximized.
  - "PBMF" (~): to be maximized (see notes).

- "valid": Returns all valid indices depending on the type of a and whether b was provided or not.
- "internal": Returns all internal CVIs. Only supported for TSClusters objects.
- "external": Returns all external CVIs. Requires b to be provided.

#### Note

In the original definition of many internal and fuzzy CVIs, the Euclidean distance and a mean centroid was used. **The implementations here change this, making use of whatever distance/centroid was chosen during clustering**. However, some of the CVIs assume that the distances are symmetric, since cross-distance matrices are calculated and only the upper/lower triangulars are considered. A warning will be given if the matrices are not symmetric and the CVI assumes so.

Because of the above, calculating CVIs for clusterings made with TADPole() is a special case. Since TADPole uses 3 distances during its execution (DTW, LB\_Keogh and Euclidean), it is not obvious which one should be used for the calculation of CVIs. Nevertheless, dtw\_basic() is used by default.

The formula for the SF index in Saitta et al. (2007) does not correspond to the one in Arbelaitz et al. (2013). The one specified in the former is used here.

The formulas for the Silhouette index are not entirely correct in Arbelaitz et al. (2013), refer to Rousseeuw (1987) for the correct ones.

The formulas for the PBMF index are not entirely unambiguous in the literature, the ones given in Lin (2013) are used here.

## References

Arbelaitz, O., Gurrutxaga, I., Muguerza, J., Perez, J. M., & Perona, I. (2013). An extensive comparative study of cluster validity indices. Pattern Recognition, 46(1), 243-256.

Kim, M., & Ramakrishna, R. S. (2005). New indices for cluster validity assessment. Pattern Recognition Letters, 26(15), 2353-2363.

Lei, Y., Bezdek, J. C., Chan, J., Vinh, N. X., Romano, S., & Bailey, J. (2017). Extending informationtheoretic validity indices for fuzzy clustering. IEEE Transactions on Fuzzy Systems, 25(4), 1013-1018.

Lin, H. Y. (2013). Effective Feature Selection for Multi-class Classification Models. In Proceedings of the World Congress on Engineering (Vol. 3).

Meila, M. (2003). Comparing clusterings by the variation of information. In Learning theory and kernel machines (pp. 173-187). Springer Berlin Heidelberg.

Rousseeuw, P. J. (1987). Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. Journal of computational and applied mathematics, 20, 53-65.

Saitta, S., Raphael, B., & Smith, I. F. (2007). A bounded index for cluster validity. In International Workshop on Machine Learning and Data Mining in Pattern Recognition (pp. 174-187). Springer Berlin Heidelberg.

Wang, W., & Zhang, Y. (2007). On fuzzy cluster validity indices. Fuzzy sets and systems, 158(19), 2095-2117.

#### cvi\_evaluators

## Examples

```
cvi(CharTrajLabels, sample(CharTrajLabels), type = c("ARI", "VI"))
```

cvi\_evaluators Cluster comparison based on CVIs

#### Description

Create evaluation functions for compare\_clusterings().

## Usage

```
cvi_evaluators(type = "valid", fuzzy = FALSE, ground.truth = NULL)
```

#### Arguments

type	A character vector with options supported by cvi().
fuzzy	Logical indicating whether to use fuzzy CVIs or not.
ground.truth	A vector that can be coerced to integers used for the calculation of external CVIs (passed as b to cvi()).

## Details

Think of this as a factory for compare\_clusterings() that creates functions that can be passed as its score.clus and pick.clus arguments. It is somewhat limited in scope because it depends on the cluster validity indices available in cvi() for scoring and performs *majority voting* for picking. They always assume that no errors occurred.

The scoring function takes the CVIs that are to be minimized and "inverts" them by taking their reciprocal so that maximization can be considered uniformly for the purpose of majority voting. Its ellipsis (...) is passed to cvi().

The picking function returns the best configuration if return.objects is FALSE, or a list with the chosen TSClusters object and the corresponding configuration otherwise.

Refer to the examples in compare\_clusterings().

## Value

A list with two functions: score and pick.

#### Note

To avoid ambiguity, if this function is used, configurations for both fuzzy and crisp clusterings should *not* be provided in the same call to compare\_clusterings(). In such cases the scoring function may fail entirely, e.g. if it was created with type = "valid".

## Description

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

## Usage

```
DBA(
 Χ,
  centroid = NULL,
  ...,
 window.size = NULL,
 norm = "L1",
 max.iter = 20L,
 delta = 0.001,
 error.check = TRUE,
  trace = FALSE,
 mv.ver = "by-variable"
)
dba(
 Χ,
  centroid = NULL,
  ...,
 window.size = NULL,
 norm = "L1",
 max.iter = 20L,
 delta = 0.001,
  error.check = TRUE,
 trace = FALSE,
 mv.ver = "by-variable"
)
```

#### Arguments

Х

X	A matrix or data frame where each row is a time series, or a list where each element is a time series. Multivariate series should be provided as a list of matrices where time spans the rows and the variables span the columns of each matrix.
centroid	Optionally, a time series to use as reference. Defaults to a random series of X if NULL. For multivariate series, this should be a matrix with the same characteristics as the matrices in X.
	Further arguments for dtw_basic(). However, the following are already pre- specified: window.size, norm (passed along), and backtrack.

# DBA

window.size	Window constraint for the DTW calculations. NULL means no constraint. A slanted band is used.
norm	Norm for the local cost matrix of DTW. Either "L1" for Manhattan distance or "L2" for Euclidean distance.
max.iter	Maximum number of iterations allowed.
delta	At iteration i, if all(abs(centroid_{i} - centroid_{i-1}) < delta), convergence is assumed.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.
trace	If TRUE, the current iteration is printed to output.
mv.ver	Multivariate version to use. See below.

#### Details

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

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

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 average time series.

## **Parallel Computing**

Please note that running tasks in parallel does **not** guarantee faster computations. The overhead introduced is sometimes too large, and it's better to run tasks sequentially.

This function uses the RcppParallel package for parallelization. It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when this function is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

This function appears to be very sensitive to numerical inaccuracies if multi-threading is used in a **32 bit** installation. In such systems, consider limiting calculations to 1 thread.

#### **Multivariate series**

There are currently 2 versions of DBA implemented for multivariate series (see examples):

- If mv.ver = "by-variable", then each variable of each series in X and centroid are extracted, and the univariate version of the algorithm is applied to each set of variables, binding the results by column. Therefore, the DTW backtracking is different for each variable.
- If mv.ver = "by-series", then all variables are considered at the same time, so the DTW backtracking is computed based on each multivariate series as a whole. This version was implemented in version 4.0.0 of **dtwclust**, and it is faster, but not necessarily more correct.

#### Note

The indices of the DTW alignment are obtained by calling dtw\_basic() with backtrack = TRUE.

#### 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, doi:10.1016/j.patcog.2010.09.013, https://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)</pre>
# Plot
matplot(do.call(cbind, CharTraj[1:5]), type = "1")
points(dtw_avg)
# Change the provided order
dtw_avg2 <- DBA(CharTraj[5:1], CharTraj[[1]], trace = TRUE)</pre>
# Same result?
all.equal(dtw_avg, dtw_avg2)
## Not run:
# Multivariate versions
# sample centroid reference
cent <- CharTrajMV[[3L]]</pre>
# sample series
x <- CharTrajMV[[1L]]</pre>
# sample set of series
X <- CharTrajMV[1L:5L]</pre>
```

```
# the by-series version does something like this for each series and the centroid
alignment <- dtw_basic(x, cent, backtrack = TRUE)</pre>
# alignment$index1 and alginment$index2 indicate how to map x to cent (row-wise)
# the by-variable version treats each variable separately
alignment1 <- dtw_basic(x[,1L], cent[,1L], backtrack = TRUE)</pre>
alignment2 <- dtw_basic(x[,2L], cent[,2L], backtrack = TRUE)</pre>
alignment3 <- dtw_basic(x[,3L], cent[,3L], backtrack = TRUE)</pre>
# effectively doing:
X1 <- lapply(X, function(x) { x[,1L] })</pre>
X2 <- lapply(X, function(x) { x[,2L] })
X3 <- lapply(X, function(x) { x[,3L] })</pre>
dba1 <- dba(X1, cent[,1L])</pre>
dba2 <- dba(X2, cent[,2L])</pre>
dba3 <- dba(X3, cent[,3L])</pre>
new_cent <- cbind(dba1, dba2, dba3)</pre>
# sanity check
newer_cent <- dba(X, cent, mv.ver = "by-variable")</pre>
all.equal(newer_cent, new_cent, check.attributes = FALSE) # ignore names
```

```
## End(Not run)
```

dtw2

DTW distance with L2 norm

#### Description

Wrapper for the dtw::dtw() function using L2 norm for both the local cost matrix (LCM) creation as well as the final cost aggregation step.

#### Usage

dtw2(x, y, ...)

#### Arguments

х, у	A time series. A multivariate series should have time spanning the rows and variables spanning the columns.
	Further arguments for dtw::dtw().

## Details

The L-norms are used in two different steps by the DTW algorithm. First when creating the LCM, where the element (i, j) of the matrix is computed as the L-norm of  $x_i^v - y_j^v$  for all variables v. Note that this means that, in case of multivariate series, they must have the same number of variables, and that univariate series will produce the same LCM regardless of the L-norm used. After the warping path is found by DTW, the final distance is calculated as the L-norm of all (i, j) elements of the LCM that fall on the warping path.

The dtw::dtw() function allows changing the norm by means of its dist.method parameter, but it only uses it when creating the LCM, and not when calculating the final aggregated cost, i.e. the DTW distance.

This wrapper simply returns the appropriate DTW distance using L2 norm (Euclidean norm). A proxy::dist() version is also registered.

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

An object of class dtw.

dtwclustTimings	Results of timing experiments
-----------------	-------------------------------

#### Description

This is the list with data frames containing the results of the timing experiments vignette included with **dtwclust**. See browseVignettes("dtwclust").

#### Format

The results are organized into different data frames and saved in one list with nested lists. For more details, refer to the included vignette or the scripts available at <a href="https://github.com/asardaes/dtwclust/tree/master/timing-experiments">https://github.com/asardaes/dtwclust/tree/master/timing-experiments</a>.

## Source

Refer to the timing experiments vignette.

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dtw\_basic

#### Description

This is a custom implementation of the DTW algorithm without all the functionality included in dtw::dtw(). Because of that, it should be faster, while still supporting the most common options.

## Usage

```
dtw_basic(
    x,
    y,
    window.size = NULL,
    norm = "L1",
    step.pattern = dtw::symmetric2,
    backtrack = FALSE,
    normalize = FALSE,
    sqrt.dist = TRUE,
    ...,
    error.check = TRUE
)
```

## Arguments

х, у	Time series. Multivariate series must have time spanning the rows and variables spanning the columns.
window.size	Size for slanted band window. NULL means no constraint.
norm	Norm for the LCM calculation, "L1" for Manhattan or "L2" for (squared) Euclidean. See notes.
step.pattern	Step pattern for DTW. Only symmetric1 or symmetric2 supported here. Note that these are <i>not</i> characters. See dtw::stepPattern.
backtrack	Also compute the warping path between series? See details.
normalize	Should the distance be normalized? Only supported for symmetric2.
sqrt.dist	Only relevant for norm = "L2", see notes.
	Currently ignored.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

## Details

If backtrack is TRUE, the mapping of indices between series is returned in a list.

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 DTW distance. For backtrack = TRUE, a list with:

- distance: The DTW distance.
- index1: x indices for the matched elements in the warping path.
- index2: y indices for the matched elements in the warping path.

## **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

It also includes symmetric optimizations to calculate only half a distance matrix when appropriate only one list of series should be provided in x. If you want to avoid this optimization, call dist by giving the same list of series in both x and y.

In order for symmetry to apply here, the following must be true: no window constraint is used (window.size is NULL) or, if one is used, all series have the same length.

#### Note

The elements of the local cost matrix are calculated by using either Manhattan or squared Euclidean distance. This is determined by the norm parameter. When the squared Euclidean version is used, the square root of the resulting DTW distance is calculated at the end (as defined in Ratanamahatana and Keogh 2004; Lemire 2009; see vignette references). This can be avoided by passing FALSE in sqrt.dist.

The DTW algorithm (and the functions that depend on it) might return different values in 32 bit installations compared to 64 bit ones.

An infinite distance value indicates that the constraints could not be fulfilled, probably due to a too small window.size or a very large length difference between the series.

#### Examples

## Not run:

#### dtw\_basic

```
B1 <- CharTrajMV[[6L]] # B character
# Let's extract univariate time series
A1_TipForce <- A1[,1L] # first variable (column)
A1_VelX <- A1[,2L] # second variable (column)
A1_VelY <- A1[,3L] # third variable (column)
B1_TipForce <- B1[,1L] # first variable (column)</pre>
B1_VelX <- B1[,2L] # second variable (column)</pre>
B1_VelY <- B1[,3L] # third variable (column)</pre>
# Looking at each variable independently:
# Just force
dtw_basic(A1_TipForce, B1_TipForce, norm = "L1", step.pattern = symmetric1)
# Corresponding LCM
proxy::dist(A1_TipForce, B1_TipForce, method = "L1")
# Just x velocity
dtw_basic(A1_VelX, B1_VelX, norm = "L1", step.pattern = symmetric1)
# Corresponding LCM
proxy::dist(A1_VelX, B1_VelX, method = "L1")
# Just y velocity
dtw_basic(A1_VelY, B1_VelY, norm = "L1", step.pattern = symmetric1)
# Corresponding LCM
proxy::dist(A1_VelY, B1_VelY, method = "L1")
# NOTES:
# In the previous examples there was one LCM for each *pair* of series.
# Additionally, each LCM has dimensions length(A1_*) x length(B1_*)
# proxy::dist won't return the LCM for multivariate series,
# but we can do it manually:
mv_lcm <- function(mvts1, mvts2) {</pre>
    # Notice how the number of variables (columns) doesn't come into play here
    num_obs1 <- nrow(mvts1)</pre>
    num_obs2 <- nrow(mvts2)</pre>
    lcm <- matrix(0, nrow = num_obs1, ncol = num_obs2)</pre>
    for (i in 1L:num_obs1) {
        for (j in 1L:num_obs2) {
            # L1 norm for ALL variables (columns).
            # Consideration: mvts1 and mvts2 MUST have the same number of variables
            lcm[i, j] <- sum(abs(mvts1[i,] - mvts2[j,]))</pre>
        }
    }
    # return
    lcm
}
```

# Let's say we start with only x velocity and y velocity for each character

```
dtw_basic
```

```
mvts1 <- cbind(A1_VelX, A1_VelY)</pre>
mvts2 <- cbind(B1_VelX, B1_VelY)</pre>
# DTW distance
dtw_d <- dtw_basic(mvts1, mvts2, norm = "L1", step.pattern = symmetric1)</pre>
# Corresponding LCM
lcm <- mv_lcm(mvts1, mvts2) # still 178 x 174</pre>
# Sanity check
all.equal(
    dtw_d,
    dtw::dtw(lcm, step.pattern = symmetric1)$distance # supports LCM as input
)
# Now let's consider all variables for each character
mvts1 <- cbind(mvts1, A1_TipForce)</pre>
mvts2 <- cbind(mvts2, B1_TipForce)</pre>
# Notice how the next code is exactly the same as before,
# even though we have one extra variable now
# DTW distance
dtw_d <- dtw_basic(mvts1, mvts2, norm = "L1", step.pattern = symmetric1)</pre>
# Corresponding LCM
lcm <- mv_lcm(mvts1, mvts2) # still 178 x 174</pre>
# Sanity check
all.equal(
    dtw_d,
    dtw::dtw(lcm, step.pattern = symmetric1)$distance # supports LCM as input
)
# By putting things in a list,
# proxy::dist returns the *cross-distance matrix*, not the LCM
series_list <- list(mvts1, mvts2)</pre>
distmat <- proxy::dist(series_list, method = "dtw_basic",</pre>
                        norm = "L1", step.pattern = symmetric1)
# So this should be TRUE
all.equal(distmat[1L, 2L], dtw_d)
# NOTE: distmat is a 2 x 2 matrix, because there are 2 multivariate series.
# Each *cell* in distmat has a corresponding LCM (not returned by the function).
# Proof:
manual_distmat <- matrix(0, nrow = 2L, ncol = 2L)</pre>
for (i in 1L:nrow(manual_distmat)) {
    for (j in 1L:ncol(manual_distmat)) {
        lcm_cell <- mv_lcm(series_list[[i]], series_list[[j]]) # LCM for this pair</pre>
        manual_distmat[i, j] <- dtw::dtw(lcm_cell, step.pattern = symmetric1)$distance</pre>
    }
}
# TRUE
all.equal(
    as.matrix(distmat),
    manual_distmat
)
```

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## End(Not run)

dtw\_lb

DTW distance matrix guided by Lemire's improved lower bound

# Description

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

## Usage

```
dtw_lb(
    x,
    y = NULL,
    window.size = NULL,
    norm = "L1",
    error.check = TRUE,
    pairwise = FALSE,
    dtw.func = "dtw_basic",
    nn.margin = 1L,
    ...
)
```

## Arguments

х, у	A matrix or data frame where rows are time series, or a list of time series.
window.size	Window size to use with the LB and DTW calculation. See details.
norm	Either "L1" for Manhattan distance or "L2" for Euclidean.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.
pairwise	Calculate pairwise distances?
dtw.func	Which function to use for the core DTW calculations, either "dtw" or "dtw_basic". See dtw::dtw() and dtw_basic().
nn.margin	Either 1 to search for nearest neighbors row-wise, or 2 to search column-wise. Only implemented for dtw.func = "dtw_basic".
	Further arguments for dtw.func or lb_improved().

## Details

This function first calculates an initial estimate of a distance matrix between two sets of time series using lb\_improved() (the proxy::dist() version). Afterwards, it uses the estimate to calculate the corresponding true DTW distance between *only* the nearest neighbors of each series in x found in y, and it continues iteratively until no changes in the nearest neighbors occur.

If only x is provided, the distance matrix is calculated between all its time series, effectively returning a matrix filled with the LB\_Improved values.

This could be useful in case one is interested in only the nearest neighbor of one or more series within 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.

#### **Parallel Computing**

Please note that running tasks in parallel does **not** guarantee faster computations. The overhead introduced is sometimes too large, and it's better to run tasks sequentially.

This function uses the RcppParallel package for parallelization. It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when this function is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

#### Note

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

The proxy::dist() version simply calls this function.

A considerably large dataset is probably necessary before this is faster than using dtw\_basic() with proxy::dist(). Also note that lb\_improved() calculates warping envelopes for the series in y, so be careful with the provided order and nn.margin (see examples).

#### Author(s)

Alexis Sarda-Espinosa

## 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, doi:10.1016/j.patcog.2008.11.030, https://www.sciencedirect.com/science/article/pii/S0031320308004925.

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## GAK

## See Also

lb\_keogh(), lb\_improved()

## Examples

```
# Load data
data(uciCT)
# Reinterpolate to same length
data <- reinterpolate(CharTraj, new.length = max(lengths(CharTraj)))</pre>
# Calculate the DTW distance between a certain subset aided with the lower bound
system.time(d <- dtw_lb(data[1:5], data[6:50], window.size = 20L))</pre>
# Nearest neighbors
NN1 <- apply(d, 1L, which.min)
# Calculate the DTW distances between all elements (slower)
system.time(d2 <- proxy::dist(data[1:5], data[6:50], method = "DTW",</pre>
                               window.type = "sakoechiba", window.size = 20L))
# Nearest neighbors
NN2 <- apply(d2, 1L, which.min)
# Calculate the DTW distances between all elements using dtw_basic
# (might be faster, see notes)
system.time(d3 <- proxy::dist(data[1:5], data[6:50], method = "DTW_BASIC",</pre>
                               window.size = 20L))
# Nearest neighbors
NN3 <- apply(d3, 1L, which.min)
# Change order and margin for nearest neighbor search
# (usually fastest, see notes)
system.time(d4 <- dtw_lb(data[6:50], data[1:5],</pre>
                         window.size = 20L, nn.margin = 2L))
# Nearest neighbors *column-wise*
NN4 <- apply(d4, 2L, which.min)</pre>
# Same results?
identical(NN1, NN2)
identical(NN1, NN3)
identical(NN1, NN4)
```

Fast global alignment kernels

Distance based on (triangular) global alignment kernels.

## Usage

```
GAK(
 х,
 у,
  . . . ,
  sigma = NULL,
 window.size = NULL,
 normalize = TRUE,
  error.check = TRUE
)
gak(
  х,
 у,
  ...,
  sigma = NULL,
 window.size = NULL,
 normalize = TRUE,
  error.check = TRUE
)
```

## Arguments

х, у	Time series. A multivariate series should have time spanning the rows and variables spanning the columns.
	Currently ignored.
sigma	Parameter for the Gaussian kernel's width. See details for the interpretation of NULL.
window.size	Parameterization of the constraining band ( <i>T</i> in Cuturi (2011)). See details.
normalize	Normalize the result by considering diagonal terms.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

## Details

This function uses the Triangular Global Alignment Kernel (TGAK) described in Cuturi (2011). It supports series of different length and multivariate series, so long as the ratio of the series' lengths doesn't differ by more than 2 (or less than 0.5).

The window.size parameter is similar to the one used in DTW, so NULL signifies no constraint, and its value should be greater than 1 if used with series of different length.

The Gaussian kernel is parameterized by sigma. Providing NULL means that the value will be estimated by using the strategy mentioned in Cuturi (2011) with a constant of 1. This estimation

## GAK

For more information, refer to the package vignette and the referenced article.

## Value

The logarithm of the GAK if normalize = FALSE, otherwise 1 minus the normalized GAK. The value of sigma is assigned as an attribute of the result.

## **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

It also includes symmetric optimizations to calculate only half a distance matrix when appropriate only one list of series should be provided in x. If you want to avoid this optimization, call dist by giving the same list of series in both x and y.

#### Note

The estimation of sigma does *not* depend on window.size.

If normalize is set to FALSE, the returned value is **not** a distance, rather a similarity. The proxy::dist() version is thus always normalized. Use proxy::simil() with method set to "uGAK" if you want the unnormalized similarities.

A constrained unnormalized calculation (i.e. with window.size >  $\emptyset$  and normalize = FALSE) will return negative infinity if abs(NROW(x) - NROW(y)) > window.size. Since the function won't perform calculations in that case, it might be faster, but if this behavior is not desired, consider reinterpolating the time series (see reinterpolate()) or increasing the window size.

#### References

Cuturi, M. (2011). Fast global alignment kernels. In *Proceedings of the 28th international conference on machine learning (ICML-11)* (pp. 929-936).

## Examples

# Obtained estimate of sigma

interactive\_clustering

A shiny app for interactive clustering

#### Description

Display a shiny user interface to do clustering based on the provided series.

#### Usage

```
interactive_clustering(series, ...)
```

## Arguments

series	Time series in the formats accepted by tsclust().
	More arguments for shiny::runApp().

#### Explore

This part of the app is simply to see some basic characteristics of the provided series and plot some of them. The field for integer IDs expects a valid R expression that specifies which of the series should be plotted. Multivariate series are plotted with each variable in a different facet.

## Cluster

This part of the app wraps tsclust(), so you should be familiar with it. Some remarks:

- Specifying a custom centroid or hierarchical method expects the name of a function available in the R session (without quotes). Naturally, any required package should be loaded before calling interactive\_clustering. For example, if you want to use cluster::agnes(), you should load cluster beforehand.
- A random seed of 0 means that it will be left as NULL when calling tsclust().

## lb\_improved

- The input fields for Extra parameters (distance, centroid and ellipsis) expect a comma- separated sequence of key-value pairs. For example: window.size = 10L, trace = TRUE. You should be able to pass any variables available in the R session's global environment.
- Regarding plot parameters:
  - The Clusters field is like the integer IDs from the Explore section.
  - The Labels field is passed to the plot method (see TSClusters-methods). You can specify several values like with the Extra parameters, e.g.: nudge\_x = 10, nudge\_y = 1. You can type an empty space to activate them with the defaults, and delete everything to hide them. Note that the location of the labels is random each time.

The plot area reacts to the plot parameters, but the actual clustering with tsclust() won't be executed until you click the Cluster! button. The plot can take a couple of seconds to load! Plotting multivariate series might generate warnings about missing values, they can be safely ignored.

Some of the control parameters are disabled when dtwclust detects them automatically.

The cross-distance matrix is cached so that it can be re-used when appropriate. The cached version is invalidated automatically when necessary.

## Evaluate

This part of the app provides results of the current clustering. External CVIs can be calculated if the name of a variable with the ground truth is provided (see cvi()).

## Note

Tracing is printed to the console.

## Author(s)

Alexis Sarda-Espinosa

#### Examples

## Not run: interactive\_clustering(CharTrajMV)

## End(Not run)

lb\_improved

Lemire's improved DTW lower bound

#### Description

This function calculates an improved 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",
    lower.env = NULL,
    upper.env = NULL,
    force.symmetry = FALSE,
    error.check = TRUE
)
```

#### Arguments

x	A time series (reference).
У	A time series with the same length as x (query).
window.size	Window size for envelope calculation. See details.
norm	Vector norm. Either "L1" for Manhattan distance or "L2" for Euclidean.
lower.env	Optionally, a pre-computed lower envelope for y can be provided (non-proxy version only). See compute_envelope().
upper.env	Optionally, a pre-computed upper envelope for y can be provided (non-proxy version only). See compute_envelope().
force.symmetry	If TRUE, a second lower bound is calculated by swapping x and y, and whichever result has a <i>higher</i> distance value is returned. The proxy version can only work if a square matrix is obtained, but use carefully.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

## Details

The reference time series should go in x, whereas the query time series should go in y.

If the envelopes are provided, they should be provided together. If either one is missing, both will be computed.

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.

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#### lb\_improved

#### **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

#### Note

The lower bound is only defined for time series of equal length and is **not** symmetric.

If you wish to calculate the lower bound between several time series, it would be better to use the version registered with the proxy package, since it includes some small optimizations. The convention mentioned above for references and queries still holds. See the examples.

The proxy version of force.symmetry should only be used when only x is provided or both x and y are identical. It compares the lower and upper triangular of the resulting distance matrix and forces symmetry in such a way that the tightest lower bound is obtained.

## 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, doi:10.1016/j.patcog.2008.11.030, https://www.sciencedirect.com/science/article/pii/S0031320308004925.

## Examples

lb\_keogh

lb\_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",
    lower.env = NULL,
    upper.env = NULL,
    force.symmetry = FALSE,
    error.check = TRUE
)
```

## Arguments

х	A time series (reference).
У	A time series with the same length as x (query).
window.size	Window size for envelope calculation. See details.
norm	Vector norm. Either "L1" for Manhattan distance or "L2" for Euclidean.
lower.env	Optionally, a pre-computed lower envelope for y can be provided (non-proxy version only). See compute_envelope().
upper.env	Optionally, a pre-computed upper envelope for y can be provided (non-proxy version only). See compute_envelope().
force.symmetry	If TRUE, a second lower bound is calculated by swapping x and y, and whichever result has a <i>higher</i> distance value is returned. The proxy version can only work if a square matrix is obtained, but use carefully.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

#### lb\_keogh

## Details

The reference time series should go in x, whereas the query time series should go in y.

If the envelopes are provided, they should be provided together. If either one is missing, both will be computed.

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 y's upper envelope.
- lower.env: The time series of y's lower envelope.

## **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

## Note

The lower bound is only defined for time series of equal length and is not symmetric.

If you wish to calculate the lower bound between several time series, it would be better to use the version registered with the proxy package, since it includes some small optimizations. The convention mentioned above for references and queries still holds. See the examples.

The proxy version of force.symmetry should only be used when only x is provided or both x and y are identical. It compares the lower and upper triangular of the resulting distance matrix and forces symmetry in such a way that the tightest lower bound is obtained.

# 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)

NCCc

Cross-correlation with coefficient normalization

## Description

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

#### Usage

NCCc(x, y, error.check = TRUE)

#### Arguments

x, yUnivariate time series.error.checkLogical indicating whether the function should try to detect inconsistencies and<br/>give more informative errors messages. Also used internally to avoid repeating<br/>checks.

# Value

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

# 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, doi:10.1145/2723372.2737793.

# pam\_cent

# See Also

SBD()

pam\_cent

# Centroid for partition around medoids

# Description

Extract the medoid time series based on a distance measure.

# Usage

```
pam_cent(
   series,
   distance,
   ids = seq_along(series),
   distmat = NULL,
   ...,
   error.check = TRUE
)
```

# Arguments

series	The time series in one of the formats accepted by tslist().
distance	A character indicating which distance to use. Only needed if distmat is NULL. The distance must be registered in proxy::pr_DB().
ids	Integer vector indicating which of the series should be considered.
distmat	Optionally, a pre-computed cross-distance matrix of <i>all</i> series.
	Any extra parameters for the distance function that may be used.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

# Details

The medoid's index is determined by taking the *argmin* of the distmat's row-sums (considering only the rows in ids). The distance matrix is calculated if needed.

# Value

The medoid time series.

# Examples

```
# Computes the distance matrix for all series
pam_cent(CharTraj, "dtw_basic", ids = 6L:10L, window.size = 15L) # series_id = 7L
# Computes the distance matrix for the chosen subset only
pam_cent(CharTraj[6L:10L], "dtw_basic", window.size = 15L) # series_id = 2L
```

pdc\_configs

```
Helper function for preprocessing/distance/centroid configurations
```

# Description

Create preprocessing, distance and centroid configurations for compare\_clusterings\_configs().

# Usage

```
pdc_configs(
  type = c("preproc", "distance", "centroid"),
  ...,
  partitional = NULL,
  hierarchical = NULL,
  fuzzy = NULL,
  tadpole = NULL,
  share.config = c("p", "h", "f", "t")
)
```

# Arguments

type	Which type of function is being targeted by this configuration.
	Any number of named lists with functions and arguments that will be shared by all clusterings. See details.
partitional	A named list of lists with functions and arguments for partitional clusterings.
hierarchical	A named list of lists with functions and arguments for hierarchical clusterings.
fuzzy	A named list of lists with functions and arguments for fuzzy clusterings.
tadpole	A named list of lists with functions and arguments for TADPole clusterings.
share.config	A character vector specifying which clusterings should include the shared lists (the ones specified in $\ldots$ ). It must be any combination of (possibly abbreviated): partitional, hierarchical, fuzzy, tadpole.

## reinterpolate

## Details

The named lists are interpreted in the following way: the name of the list will be considered to be a function name, and the elements of the list will be the possible parameters for the function. Each function must have at least an empty list. The parameters may be vectors that specify different values to be tested.

For preprocessing, the special name none signifies no preprocessing.

For centroids, the special name default leaves the centroid unspecified.

Please see the examples in compare\_clusterings() to see how this is used.

## Value

A list for each clustering, each of which includes a data frame with the computed configurations.

reinterpolate

Wrapper for simple linear reinterpolation

# Description

This function is just a wrapper for the native function stats::approx() to do simple linear reinterpolation. It also supports matrices, data frames, and lists of time series.

#### Usage

reinterpolate(x, new.length, multivariate = FALSE)

# Arguments

x	Data to reinterpolate. Either a vector, a matrix/data.frame where each row is to be reinterpolated, or a list of vectors/matrices.
new.length	Desired length of the output series.
multivariate	Is x a multivariate time series? It will be detected automatically if a list is provided in x.

# Details

Multivariate series must have time spanning the rows and variables spanning the columns.

#### Value

Reinterpolated time series

# Examples

```
data(uciCT)
# list of univariate series
series <- reinterpolate(CharTraj, 205L)
# list of multivariate series
series <- reinterpolate(CharTrajMV, 205L)
# single multivariate series
series <- reinterpolate(CharTrajMV[[1L]], 205L, TRUE)</pre>
```

repeat\_clustering *Repeat a clustering configuration* 

# Description

Repeat a clustering made with compare\_clusterings() in order to obtain the TSClusters object.

# Usage

```
repeat_clustering(series, clusterings, config_id, ...)
```

# Arguments

series	The same time series that were given to compare_clusterings().
clusterings	The list returned by compare_clusterings().
config_id	The character indicating which configuration should be re-computed. Obtained from the clusterings' results' data frames.
• • •	More arguments for tsclust() (e.g. trace).

# Details

Since the purpose of compare\_clusterings() is to test many configurations, it is desirable to set its return.objects parameter to FALSE in order to save RAM. This function can then be used to compute the clustering object for a specific config\_id.

# Value

A TSClusters object.

# SBD

# Limitations

If the preprocessing function is subject to randomness, the clustering will not be correctly recreated by this function, since compare\_clusterings() applies all preprocessing before calling tsclust().

If any parameters were given to compare\_clusterings() through its ellipsis, they should probably be given to this function too.

SBD Shape-based distance	
--------------------------	--

# Description

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

#### Usage

SBD(x, y, znorm = FALSE, error.check = TRUE, return.shifted = TRUE)
sbd(x, y, znorm = FALSE, error.check = TRUE, return.shifted = TRUE)

## Arguments

х, у	Univariate time series.
znorm	Logical. Should each series be z-normalized before calculating the distance?
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.
return.shifted	Logical. Should the shifted version of y be returned? See details.

#### Details

This distance works best if the series are *z*-normalized. If not, at least they should have appropriate amplitudes, since the values of the signals **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. After matching, the series may have to be truncated or extended and padded with zeros if needed.

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

## Value

For return.shifted = FALSE, the numeric distance value, otherwise a list with:

- dist: The shape-based distance between x and y.
- yshift: A shifted version of y so that it optimally matches x (based on NCCc()).

#### **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

It also includes symmetric optimizations to calculate only half a distance matrix when appropriate only one list of series should be provided in x. If you want to avoid this optimization, call dist by giving the same list of series in both x and y.

In some situations, e.g. for relatively small distance matrices, the overhead introduced by the logic that computes only half the distance matrix can be bigger than just calculating the whole matrix.

## Note

If you wish to calculate the distance between several time series, it would be better to use the version registered with the proxy package, since it includes some small optimizations. See the examples.

This distance is calculated with help of the Fast Fourier Transform, so it can be sensitive to numerical precision. Thus, this function (and the functions that depend on it) might return different values in 32 bit installations compared to 64 bit ones.

#### 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, doi:10.1145/2723372.2737793.

# See Also

NCCc(), shape\_extraction()

### Examples

```
# load data
data(uciCT)
# distance between series of different lengths
sbd <- SBD(CharTraj[[1]], CharTraj[[100]], znorm = TRUE)$dist
# cross-distance matrix for series subset (notice the two-list input)
sbD <- proxy::dist(CharTraj[1:10], CharTraj[1:10], method = "SBD", znorm = TRUE)</pre>
```

sdtw

## Description

Soft-DTW distance measure as proposed in Cuturi and Blondel (2017).

# Usage

sdtw(x, y, gamma = 0.01, ..., error.check = TRUE)

#### Arguments

х, у	Time series. Multivariate series must have time spanning the rows and variables spanning the columns.
gamma	Positive regularization parameter, with lower values resulting in less smoothing.
	Currently ignored.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

# Details

Unlike other distances, soft-DTW can return negative values, and sdtw(x, x) is not always equal to zero. Like DTW, soft-DTW does not fulfill the triangle inequality, but it is always symmetric.

# Value

The Soft DTW distance.

## **Proxy version**

The version registered with dist is custom (loop = FALSE in pr\_DB). The custom function handles multi-threaded parallelization directly (with RcppParallel). It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when it is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

It also includes symmetric optimizations to calculate only half a distance matrix when appropriate only one list of series should be provided in x. If you want to avoid this optimization, call dist by giving the same list of series in both x and y.

#### References

Cuturi, M., & Blondel, M. (2017). Soft-DTW: a Differentiable Loss Function for Time-Series. arXiv preprint arXiv:1703.01541.

sdtw\_cent

# Description

Soft-DTW centroid function as proposed in Cuturi and Blondel (2017).

## Usage

```
sdtw_cent(
  series,
  centroid = NULL,
  gamma = 0.01,
  weights = rep(1, length(series)),
   ...,
  error.check = TRUE,
  opts = list(algorithm = "NLOPT_LD_LBFGS", maxeval = 20L)
)
```

# Arguments

series	A matrix or data frame where each row is a time series, or a list where each element is a time series. Multivariate series should be provided as a list of matrices where time spans the rows and the variables span the columns of each matrix.
centroid	Optionally, a time series to use as reference. Defaults to a random series of series if NULL. For multivariate series, this should be a matrix with the same characteristics as the matrices in series.
gamma	Positive regularization parameter, with lower values resulting in less smoothing.
weights	A vector of weights for each element of series.
	Further arguments for the optimization backend (except opts for nloptr, control for optim, and for both).
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.
opts	List of options to pass to nloptr or stats::optim()'s control. The defaults in the function's formals are for nloptr, but the value will be adjusted for optim if needed.

# Details

This function can delegate the optimization to the **nloptr** package. For that to happen, you must load it with either base::library() or base::loadNamespace(). If the aforementioned is not fulfilled, the function will delegate to stats::optim().

#### Value

The resulting centroid, with the optimization results as attributes (except for the returned centroid).

#### **Parallel Computing**

Please note that running tasks in parallel does **not** guarantee faster computations. The overhead introduced is sometimes too large, and it's better to run tasks sequentially.

This function uses the RcppParallel package for parallelization. It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when this function is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

For unknown reasons, this function has returned different results (in the order of 1e-6) when using multi-threading in x64 Windows installations in comparison to other environments (using nloptr v1.0.4). Consider limiting the number of threads if you run into reproducibility problems.

## References

Cuturi, M., & Blondel, M. (2017). Soft-DTW: a Differentiable Loss Function for Time-Series. arXiv preprint arXiv:1703.01541.

shape\_extraction Shape average of several time series

# Description

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

#### Usage

```
shape_extraction(X, centroid = NULL, znorm = FALSE, ..., error.check = TRUE)
```

#### Arguments

Х	A matrix or data frame where each row is a time series, or a list where each element is a time series. Multivariate series should be provided as a list of matrices where time spans the rows and the variables span the columns.
centroid	Optionally, a time series to use as reference. Defaults to a random series of X if NULL. For multivariate series, this should be a matrix with the same characteristics as the matrices in X. <b>It will be z-normalized</b> .
znorm	Logical flag. Should z-scores be calculated for X before processing?
	Further arguments for zscore().

error.check Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

## Details

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

The resulting centroid will have the same length as centroid if provided. Otherwise, there are two possibilities: if all series from X have the same length, all of them will be used as-is, and the output will have the same length as the series; if series have different lengths, a series will be chosen at random and used as reference. The output series will then have the same length as the chosen series.

This centroid computation is cast as an optimization problem called maximization of Rayleigh Quotient. It depends on the SBD() algorithm. See the cited article for more details.

# Value

Centroid time series (z-normalized).

# 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, doi:10.1145/2723372.2737793.

## See Also

SBD(), zscore()

## Examples

ssdtwclust

#### Description

Display a shiny user interface that implements the approach in Dau et al. (2016).

#### Usage

```
ssdtwclust(series, ..., complexity = NULL)
```

# Arguments

series	Time series in the formats accepted by compare_clusterings().
	More arguments for shiny::runApp().
complexity	A function to calculate a constraint's complexity. See details in the Cluster section.

#### Details

The approach developed in Dau et al. (2016) argues that finding a good value of window.size for the DTW distance is very important, and suggests how to find one by using user-provided feedback. After clustering is done, a pair of series is presented at a time, and the user must annotate the pair as:

- Must link: the series should be in the same cluster.
- Cannot link: the series should not be in the same cluster.
- Skip: the choice is unclear.

After each step, a good value of the window size is suggested by evaluating which clusterings fulfill the constraint(s) so far, and how (see Dau et al. (2016) for more information), and performing a majority vote using the window sizes inferred from each constraint. The (main) procedure is thus interactive and can be abandoned at any point.

#### Explore

This part of the app is simply to see some basic characteristics of the provided series and plot some of them. The field for integer IDs expects a valid R expression that specifies which of the series should be plotted. Multivariate series are plotted with each variable in a different facet.

#### Cluster

This part of the app implements the main procedure by leveraging compare\_clusterings(). The interface is similar to interactive\_clustering(), so it's worth checking its documentation too. Since compare\_clusterings() supports parallelization with foreach::foreach(), you can register a parallel backend before opening the shiny app, but you should pre-load the workers with the

necessary packages and/or functions. See parallel::clusterEvalQ() and parallel::clusterExport(), as well as the examples below.

The range of window sizes is specified with a slider, and represents the size as a percentage of the shortest series' length. The step parameter indicates how spaced apart should the sizes be (parameter 'by' in base::seq()). A 0-size window should only be used if all series have the same length. If the series have different lengths, using small window sizes can be problematic if the length differences are very big, see the notes in dtw\_basic().

A window.size should *not* be specified in the extra parameters, it will be replaced with the computed values based on the slider. Using dba() centroid is detected, and will use the same window sizes.

For partitional clusterings with many repetitions, and hierarchical clusterings with many linkage methods, the resulting partitions are aggregated by calling clue::cl\_medoid() with the specified aggregation method.

By default, complexity of a constraint is calculated differently from what is suggested in Dau et al. (2016):

- Allocate a logical flag vector with length equal to the number of tested window sizes.
- For each window size, set the corresponding flag to TRUE if the constraint given by the user is fulfilled.
- Calculate complexity as: (number of sign changes in the vector) / (number of window sizes 1L) / (maximum number of *contiguous* TRUE flags).

You can provide your own function in the complexity parameter. It will receive the flag vector as only input, and a single number is expected as a result.

The complexity threshold can be specified in the app. Any constraint whose complexity is higher than the threshold will not be considered for the majority vote. Constraints with a complexity of 0 are also ignored. An infinite complexity means that the constraint is never fulfilled by any clustering.

# Evaluate

This section provides numerical results for reference. The latest results can be saved in the global environment, which includes clustering results, constraints so far, and the suggested window size. Since this includes everything returned by compare\_clusterings(), you could also use repeat\_clustering() afterwards.

The constraint plots depict if the constraints are fulfilled or not for the given window sizes, where 1 means it was fulfilled and 0 means it wasn't. An error about a zero-dimension viewport indicates the plot height is too small to fit the plots, so please increase the height.

# Note

The optimization mentioned in section 3.4 of Dau et al. (2016) is also implemented here.

Tracing is printed to the console.

# Author(s)

Alexis Sarda-Espinosa

# TADPole

## References

Dau, H. A., Begum, N., & Keogh, E. (2016). Semi-supervision dramatically improves time series clustering under dynamic time warping. In Proceedings of the 25th ACM International on Conference on Information and Knowledge Management (pp. 999-1008). ACM. https://sites.google.com/site/dtwclustering/

# See Also

interactive\_clustering(), compare\_clusterings()

## Examples

```
## Not run:
require(doParallel)
workers <- makeCluster(detectCores())
clusterEvalQ(workers, {
    library(dtwclust)
    RcppParallel::setThreadOptions(1L)
})
registerDoParallel(workers)
ssdtwclust(reinterpolate(CharTraj[1L:20L], 150L))
```

## End(Not run)

TADPole

# TADPole clustering

## Description

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

## Usage

```
TADPole(
   data,
   k = 2L,
   dc,
   window.size,
   error.check = TRUE,
   lb = "lbk",
   trace = FALSE
)
tadpole(
   data,
   k = 2L,
```

```
dc,
window.size,
error.check = TRUE,
lb = "lbk",
trace = FALSE
)
```

## Arguments

data	A matrix or data frame where each row is a time series, or a list where each element is a time series. Multivariate series are <b>not</b> supported.
k	The number of desired clusters. Can be a vector with several values.
dc	The cutoff distance(s). Can be a vector with several values.
window.size	Window size constraint for DTW (Sakoe-Chiba). See details.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.
lb	Which lower bound to use, "lbk" for lb_keogh() or "lbi" for lb_improved().
trace	Logical flag. If TRUE, more output regarding the progress is printed to screen.

## Details

This function can be called either directly or through tsclust().

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 centroids are always elements of the data. However, this algorithm is deterministic, depending on the value of dc.

The algorithm first uses the DTW's upper and lower bounds (Euclidean and LB\_Keogh respectively) 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 centroids.

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

Parallelization is supported in the following way:

- For multiple dc values, multi-processing with foreach::foreach().
- The internal distance calculations use multi-threading with RcppParallel::RcppParallel.

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.
- centroids: Indices of the centroids.
- distCalcPercentage: Percentage of distance calculations that were actually performed.

For multiple k/dc values, a list of lists is returned, each internal list having the aforementioned elements.

#### **Parallel Computing**

Please note that running tasks in parallel does **not** guarantee faster computations. The overhead introduced is sometimes too large, and it's better to run tasks sequentially.

This function uses the RcppParallel package for parallelization. It uses all available threads by default (see RcppParallel::defaultNumThreads()), but this can be changed by the user with RcppParallel::setThreadOptions().

An exception to the above is when this function is called within a **foreach** parallel loop **made by dtwclust**. If the parallel workers do not have the number of threads explicitly specified, this function will default to 1 thread per worker. See the parallelization vignette for more information (browseVignettes("dtwclust")).

## 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, doi:10.1145/2783258.2783286.

tsclust

Time series clustering

#### Description

This is the main function to perform time series clustering. See the details and the examples for more information, as well as the included package vignettes (which can be found by typing browseVignettes("dtwclust")). A convenience wrapper is available in compare\_clusterings(), and a shiny app in interactive\_clustering().

# Usage

```
tsclust(
  series = NULL,
  type = "partitional",
  k = 2L,
  ...,
  preproc = NULL,
```

```
distance = "dtw_basic",
centroid = ifelse(type == "fuzzy", "fcm", "pam"),
control = do.call(paste0(type, "_control"), list()),
args = tsclust_args(),
seed = NULL,
trace = FALSE,
error.check = TRUE
)
```

# Arguments

series	A list of series, a numeric matrix or a data frame. Matrices and data frames are coerced to a list row-wise (see tslist()).
type	What type of clustering method to use: "partitional", "hierarchical", "tadpole" or "fuzzy".
k	Number of desired clusters. It can be a numeric vector with different values.
	Arguments to pass to preprocessing, centroid <b>and</b> distance functions (added to args). Also passed to method from hierarchical_control() if it happens to be a function, and to stats::hclust() if it contains the members parameter.
preproc	Function to preprocess data. Defaults to zscore() <i>only</i> if centroid = "shape", but will be replaced by a custom function if provided.
distance	A registered distance from proxy::dist(). Ignored for type = "tadpole".
centroid	Either a supported string, or an appropriate function to calculate centroids when using partitional/hierarchical/tadpole methods. See Centroids section.
control	An appropriate list of controls. See tsclust-controls.
args	An appropriate list of arguments for preprocessing, distance and centroid func- tions. See tsclust_args() and the examples.
seed	Random seed for reproducibility.
trace	Logical flag. If TRUE, more output regarding the progress is printed to screen.
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

# Details

Partitional and fuzzy clustering procedures use a custom implementation. Hierarchical clustering is done with stats::hclust() by default. TADPole clustering uses the TADPole() function. Specifying type = "partitional", preproc = zscore, distance = "sbd" and centroid = "shape" is equivalent to the k-Shape algorithm (Paparrizos and Gravano 2015).

The series may be provided as a matrix, a data frame or a list. Matrices and data frames are coerced to a list, both row-wise. Only lists can have series with different lengths or multiple dimensions. Most of the optimizations require series to have the same length, so consider reinterpolating them to save some time (see Ratanamahatana and Keogh 2004; reinterpolate()). No missing values are allowed.

In the case of multivariate time series, they should be provided as a list of matrices, where time spans the rows of each matrix and the variables span the columns (see CharTrajMV for an example). All included centroid functions should work with the aforementioned format, although shape is *not* recommended. Note that the plot method will simply append all dimensions (columns) one after the other.

#### Value

An object with an appropriate class from TSClusters.

If controlnrep > 1 and a partitional procedure is used, length(method) > 1 and hierarchical procedures are used, or length(k) > 1, a list of objects is returned.

## **Centroid Calculation**

In the case of partitional/fuzzy algorithms, a suitable function should calculate the cluster centroids at every iteration. In this case, the centroids may also be time series. Fuzzy clustering uses the standard fuzzy c-means centroid by default.

In either case, a custom function can be provided. If one is provided, it will receive the following parameters with the shown names (examples for partitional clustering are shown in parentheses):

- x: The *whole* data list (list(ts1, ts2, ts3))
- cl\_id: An integer vector with length equal to the number of series in data, indicating which cluster a series belongs to (c(1L, 2L, 2L))
- k: The desired number of total clusters (2L)
- cent: The current centroids in order, in a list (list(centroid1, centroid2))
- cl\_old: The membership vector of the *previous* iteration (c(1L, 1L, 2L))
- The elements of . . . that match its formal arguments

In case of fuzzy clustering, the membership vectors (2nd and 5th elements above) are matrices with number of rows equal to amount of elements in the data, and number of columns equal to the number of desired clusters. Each row must sum to 1.

The other option is to provide a character string for the custom implementations. 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. By default, all series are z-normalized in this case, since the resulting centroids will also have this normalization. See shape\_extraction() for more details.
- "dba": DTW Barycenter Averaging. See DBA() for more details.
- "sdtw\_cent": Soft-DTW centroids, See sdtw\_cent() for more details.
- "pam": Partition around medoids (PAM). This basically means that the cluster centroids are always one of the time series in the data. In this case, the distance matrix can be pre-computed once using all time series in the data and then re-used at each iteration. It usually saves overhead overall for small datasets (see tsclust-controls).
- "fcm": Fuzzy c-means. Only supported for fuzzy clustering and used by default in that case.

• "fcmdd": Fuzzy c-medoids. Only supported for fuzzy clustering. It **always** precomputes/uses the whole cross-distance matrix.

The dba, shape and sdtw\_cent implementations check for parallelization. Note that only shape, dba, sdtw\_cent, pam and fcmdd support series of different length. Also note that for shape, dba and sdtw\_cent, this support has a caveat: the final centroids' length will depend on the length of those series that were randomly chosen at the beginning of the clustering algorithm. For example, if the series in the dataset have a length of either 10 or 15, 2 clusters are desired, and the initial choice selects two series with length of 10, the final centroids will have this same length.

As special cases, if hierarchical or tadpole clustering is used, you can provide a centroid function that takes a list of series as first input. It will also receive the contents of args\$cent that match its formal arguments, and should return a single centroid series. These centroids are returned in the centroids slot. By default, the medoid of each cluster is extracted (similar to what pam\_cent() does).

In the following cases, the centroids list will have an attribute series\_id with an integer vector indicating which series were chosen as centroids:

- Partitional clustering using "pam" centroid.
- Fuzzy clustering using "fcmdd" centroid.
- Hierarchical clustering with the default centroid extraction.
- TADPole clustering with the default centroid extraction.

#### **Distance Measures**

The distance measure to be used with partitional, hierarchical and fuzzy clustering can be modified with the distance parameter. The supported option is to provide a string, which must represent a compatible distance registered with proxy's proxy::dist(). Registration is done via proxy::pr\_DB(), and extra parameters can be provided in args\$dist (see the examples).

Note that you are free to create your own distance functions and register them. Optionally, you can use one of the following custom implementations (all registered with proxy):

- "dtw": DTW, optionally with a Sakoe-Chiba/Slanted-band constraint. Done with dtw::dtw().
- "dtw2": DTW with L2 norm and optionally a Sakoe-Chiba/Slanted-band constraint. See dtw2().
- "dtw\_basic": A custom version of DTW with less functionality, but faster. See dtw\_basic().
- "dtw\_lb": DTW with L1 or L2 norm and 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(). Not suitable for pam.precompute = TRUE nor hierarchical clustering.
- "lbk": Keogh's lower bound for DTW with either L1 or L2 norm for the Sakoe-Chiba constraint. See lb\_keogh().
- "lbi": Lemire's lower bound for DTW with either L1 or L2 norm for the Sakoe-Chiba constraint. See lb\_improved().
- "sbd": Shape-based distance. See sbd().
- "gak": Global alignment kernels. See gak().
- "sdtw": Soft-DTW. See sdtw().

Out of the aforementioned, only the distances based on DTW lower bounds *don't* support series of different length. The lower bounds are probably unsuitable for direct clustering unless series are very easily distinguishable.

If you know that the distance function is symmetric, and you use a hierarchical algorithm, or a partitional algorithm with PAM centroids, or fuzzy c-medoids, some time can be saved by calculating only half the distance matrix. Therefore, consider setting the symmetric control parameter to TRUE if this is the case (see tsclust-controls).

# Preprocessing

It is strongly advised to use z-normalization in case of centroid = "shape", because the resulting series have this normalization (see shape\_extraction()). Therefore, zscore() is the default in this case. The user can, however, specify a custom function that performs any transformation on the data, but the user must make sure that the format stays consistent, i.e. a list of time series.

Setting to NULL means no preprocessing (except for centroid = "shape"). A provided function will receive the data as first argument, followed by the contents of args\$preproc that match its formal arguments.

It is convenient to provide this function if you're planning on using the stats::predict() generic (see also TSClusters-methods).

# Repetitions

Due to their stochastic nature, partitional clustering is usually repeated several times with different random seeds to allow for different starting points. This function uses parallel::nextRNGStream() to obtain different seed streams for each repetition, utilizing the seed parameter (if provided) to initialize it. If more than one repetition is made, the streams are returned in an attribute called rng.

Multiple values of k can also be provided to get different partitions using any type of clustering.

Repetitions are greatly optimized when PAM centroids are used and the whole distance matrix is precomputed, since said matrix is reused for every repetition.

## **Parallel Computing**

Please note that running tasks in parallel does **not** guarantee faster computations. The overhead introduced is sometimes too large, and it's better to run tasks sequentially.

The user can register a parallel backend, e.g. with the **doParallel** package, in order to attempt to speed up the calculations (see the examples). This relies on foreach, i.e. it uses multi-processing.

Multi-processing is used in partitional and fuzzy clustering for multiple values of k and/or nrep (in partitional\_control()). See TADPole() to know how it uses parallelization. For cross-distance matrix calculations, the parallelization strategy depends on whether the distance is included with **dtwclust** or not, see the caveats in tsclustFamily.

If you register a parallel backend and special packages must be loaded, provide their names in the packages element of control. Note that "dtwclust" is always loaded in each parallel worker, so that doesn't need to be included. Alternatively, you may want to pre-load **dtwclust** in each worker with parallel::clusterEvalQ().

## Note

The lower bounds are defined only for time series of equal length. They are **not** symmetric, and DTW is not symmetric in general.

# Author(s)

Alexis Sarda-Espinosa

## References

Please refer to the package vignette references (which can be loaded by typing vignette("dtwclust")).

## See Also

TSClusters, TSClusters-methods, tsclustFamily, tsclust-controls, compare\_clusterings(), interactive\_clustering(), ssdtwclust().

#### Examples

```
#' NOTE: More examples are available in the vignette. Here are just some miscellaneous
#' examples that might come in handy. They should all work, but some don't run
#' automatically.
# Load data
data(uciCT)
# Simple partitional clustering with Euclidean distance and PAM centroids
# Reinterpolate to same length
series <- reinterpolate(CharTraj, new.length = max(lengths(CharTraj)))</pre>
# Subset for speed
series <- series[1:20]</pre>
labels <- CharTrajLabels[1:20]</pre>
# Making many repetitions
pc.l2 <- tsclust(series, k = 4L,</pre>
            distance = "L2", centroid = "pam",
            seed = 3247, trace = TRUE,
            control = partitional_control(nrep = 10L))
# Cluster validity indices
sapply(pc.l2, cvi, b = labels)
# Hierarchical clustering with Euclidean distance
# ______
```

 $\ensuremath{\texttt{\#}}$  Re-use the distance matrix from the previous example (all matrices are the same)

# Use all available linkage methods for function hclust

```
hc.l2 <- tsclust(series, type = "hierarchical",</pre>
             k = 4L, trace = TRUE,
             control = hierarchical_control(method = "all",
                                     distmat = pc.l2[[1L]]@distmat))
# Plot the best dendrogram according to variation of information
plot(hc.l2[[which.min(sapply(hc.l2, cvi, b = labels, type = "VI"))]])
# ______
# Multivariate time series
# Multivariate series, provided as a list of matrices
mv <- CharTrajMV[1L:20L]</pre>
# Using GAK distance
mvc <- tsclust(mv, k = 4L, distance = "gak", seed = 390,</pre>
           args = tsclust_args(dist = list(sigma = 100)))
# Note how the variables of each series are appended one after the other in the plot
plot(mvc)
## Not run:
# This function is more verbose but allows for more explicit fine-grained control
# ______
tsc <- tsclust(series, k = 4L,</pre>
           distance = "gak", centroid = "dba",
           preproc = zscore, seed = 382L, trace = TRUE,
           control = partitional_control(iter.max = 30L),
           args = tsclust_args(preproc = list(center = FALSE),
                           dist = list(window.size = 20L,
                                    sigma = 100),
                           cent = list(window.size = 15L,
                                    norm = "L2",
                                    trace = TRUE)))
# Registering a custom distance with the 'proxy' package and using it
# Normalized asymmetric DTW distance
ndtw <- function(x, y, ...) {</pre>
   dtw::dtw(x, y, step.pattern = asymmetric,
          distance.only = TRUE, ...)$normalizedDistance
}
# Registering the function with 'proxy'
if (!pr_DB$entry_exists("nDTW"))
  proxy::pr_DB$set_entry(FUN = ndtw, names=c("nDTW"),
                    loop = TRUE, type = "metric", distance = TRUE,
                    description = "Normalized asymmetric DTW")
```

```
# Subset of (original) data for speed
pc.ndtw <- tsclust(series[-1L], k = 4L,</pre>
              distance = "nDTW",
              seed = 8319,
              trace = TRUE,
              args = tsclust_args(dist = list(window.size = 18L)))
# Which cluster would the first series belong to?
# Notice that newdata is provided as a list
predict(pc.ndtw, newdata = series[1L])
# Custom hierarchical clustering
require(cluster)
hc.diana <- tsclust(series, type = "h", k = 4L,</pre>
               distance = "L2", trace = TRUE,
               control = hierarchical_control(method = diana))
plot(hc.diana, type = "sc")
# _____
# TADPole clustering
pc.tadp <- tsclust(series, type = "tadpole", k = 4L,</pre>
              control = tadpole_control(dc = 1.5,
                                 window.size = 18L))
# Modify plot, show only clusters 3 and 4
plot(pc.tadp, clus = 3:4,
   labs.arg = list(title = "TADPole, clusters 3 and 4",
               x = "time", y = "series"))
# Saving and modifying the ggplot object with custom time labels
require(scales)
t <- seq(Sys.Date(), len = length(series[[1L]]), by = "day")</pre>
gpc <- plot(pc.tadp, time = t, plot = FALSE)</pre>
gpc + ggplot2::scale_x_date(labels = date_format("%b-%Y"),
                     breaks = date_breaks("2 months"))
# Specifying a centroid function for prototype extraction in hierarchical clustering
# Seed is due to possible randomness in shape_extraction when selecting a basis series
hc.sbd <- tsclust(CharTraj, type = "hierarchical",</pre>
             k = 20L, distance = "sbd",
             preproc = zscore, centroid = shape_extraction,
```

```
seed = 320L)
plot(hc.sbd, type = "sc")
# Using parallel computation to optimize several random repetitions
# and distance matrix calculation
_____
require(doParallel)
# Create parallel workers
cl <- makeCluster(detectCores())</pre>
invisible(clusterEvalQ(cl, library(dtwclust)))
registerDoParallel(cl)
## Use constrained DTW and PAM
pc.dtw <- tsclust(CharTraj, k = 20L, seed = 3251, trace = TRUE,</pre>
                args = tsclust_args(dist = list(window.size = 18L)))
## Use constrained DTW with DBA centroids
pc.dba <- tsclust(CharTraj, k = 20L, centroid = "dba",</pre>
                seed = 3251, trace = TRUE,
                args = tsclust_args(dist = list(window.size = 18L),
                                  cent = list(window.size = 18L)))
#' Using distance based on global alignment kernels
pc.gak <- tsclust(CharTraj, k = 20L,</pre>
                distance = "gak",
                centroid = "dba",
                seed = 8319,
                trace = TRUE,
                control = partitional_control(nrep = 8L),
                args = tsclust_args(dist = list(window.size = 18L),
                                  cent = list(window.size = 18L)))
# Stop parallel workers
stopCluster(cl)
# Return to sequential computations. This MUST be done if stopCluster() was called
registerDoSEQ()
## End(Not run)
```

tsclust-controls *Control parameters for clusterings with* tsclust()

#### Description

Control parameters for fine-grained control.

# Usage

```
partitional_control(
  pam.precompute = TRUE,
  iter.max = 100L,
 nrep = 1L,
  symmetric = FALSE,
 packages = character(0L),
 distmat = NULL,
 pam.sparse = FALSE,
 version = 2L
)
hierarchical_control(
 method = "average",
 symmetric = FALSE,
 packages = character(0L),
 distmat = NULL
)
fuzzy_control(
 fuzziness = 2,
 iter.max = 100L,
 delta = 0.001,
 packages = character(0L),
 symmetric = FALSE,
 version = 2L,
 distmat = NULL
)
tadpole_control(dc, window.size, lb = "lbk")
tsclust_args(preproc = list(), dist = list(), cent = list())
```

# Arguments

pam.precompute	Logical flag. Precompute the whole distance matrix once and reuse it on each it- eration if using PAM centroids. Otherwise calculate distances at every iteration. See details.
iter.max	Integer. Maximum number of allowed iterations for partitional/fuzzy clustering.
nrep	Integer. How many times to repeat clustering with different starting points (i.e., different random seeds).
symmetric	Logical flag. Is the distance function symmetric? In other words, is $dist(x,y) == dist(y,x)$ ? If TRUE, only half the distance matrix needs to be computed. Automatically detected and overridden for the distances included in <b>dtwclust</b> .
packages	Character vector with the names of any packages required for custom proxy functions. Relevant for parallel computation, although since the distance entries

	are re-registered in each parallel worker if needed, this is probably useless, but just in case.
distmat	If available, the cross-distance matrix can be provided here. Only relevant for partitional with PAM centroids, fuzzy with FCMdd centroids, or hierarchical clustering.
pam.sparse	Attempt to use a sparse matrix for PAM centroids. See details.
version	Which version of partitional/fuzzy clustering to use. See details.
method	Character vector with one or more linkage methods to use in hierarchical pro- cedures (see stats::hclust()), the character "all" to use all of the available ones, or a function that performs hierarchical clustering based on distance ma- trices (e.g. cluster::diana()). See details.
fuzziness	Numeric. Exponent used for fuzzy clustering. Commonly termed m in the liter- ature.
delta	Numeric. Convergence criterion for fuzzy clustering.
dc	The cutoff distance for the TADPole algorithm.
window.size	The window.size specifically for the TADPole algorithm.
11	
lb	The lower bound to use with TADPole. Either "lbk" or "lbi".
lb preproc	The lower bound to use with TADPole. Either "lbk" or "lbi". A list of arguments for a preprocessing function to be used in tsclust().

# Details

The functions essentially return their function arguments in a classed list, although some checks are performed.

Regarding parameter version: the first version of partitional/fuzzy clustering implemented in the package always performed an extra iteration, which is unnecessary. Use version 1 to mimic this previous behavior.

#### Partitional

When pam.precompute = FALSE, using pam.sparse = TRUE defines a sparse matrix (refer to Matrix::sparseMatrix()) and updates it every iteration (except for "dtw\_lb" distance). For most cases, precomputing the whole distance matrix is still probably faster. See the timing experiments in browseVignettes("dtwclust").

Parallel computations for PAM centroids have the following considerations:

- If pam.precompute is TRUE, both distance matrix calculations and repetitions are done in parallel, regardless of pam.sparse.
- If pam.precompute is FALSE and pam.sparse is TRUE, repetitions are done sequentially, so that the distance calculations can be done in parallel and the sparse matrix updated iteratively.
- If both pam.precompute and pam.sparse are FALSE, repetitions are done in parallel, and each repetition performs distance calculations sequentially, but the distance matrix cannot be updated iteratively.

## Hierarchical

There are some limitations when using a custom hierarchical function in method: it will receive the lower triangular of the distance matrix as first argument (see stats::as.dist()) and the result should support the stats::as.hclust() generic. This functionality was added with the **cluster** package in mind, since its functions follow this convention, but other functions could be used if they are adapted to work similarly.

# **TADPole**

When using TADPole, the dist argument list includes the window.size and specifies norm = "L2".

TSClusters-class Class definition for TSClusters and derived classes

# Description

Formal S4 classes for time-series clusters. See class hierarchy and slot organization at the bottom.

## Details

The base class is TSClusters. The 3 classes that inherit from it are: PartitionalTSClusters, HierarchicalTSClusters and FuzzyTSClusters.

HierarchicalTSClusters also contain stats::hclust() as parent class.

Package clue is supported, but generics from flexclust are not. See also TSClusters-methods.

# Slots

call The function call.

family An object of class tsclustFamily.

control An appropriate control object for tsclust(). See tsclust-controls.

datalist The provided data in the form of a list, where each element is a time series.

type A string indicating one of the supported clustering types of tsclust().

distance A string indicating the distance used.

centroid A string indicating the centroid used.

preproc A string indicating the preprocessing used.

k Integer indicating the number of desired clusters.

cluster Integer vector indicating which cluster a series belongs to (crisp partition). For fuzzy clustering, this is based on **distance**, not on fcluster. For hierarchical, this is obtained by calling stats::cutree() with the given value of k.

centroids A list with the centroid time series.

distmat If computed, the cross-distance matrix.

proctime Time during function execution, as measured with base::proc.time().

- dots The contents of the original call's ellipsis (...).
- args The contents of the original call's args parameter. See tsclust\_args().
- seed The random seed that was used.
- iter The number of iterations used.
- converged A logical indicating whether the function converged.
- clusinfo A data frame with two columns: size indicates the number of series each cluster has, and av\_dist indicates, for each cluster, the average distance between series and their respective centroids (crisp partition).
- cldist A column vector with the distance between each series in the data and its corresponding centroid (crisp partition).
- method A string indicating which hierarchical method was used.
- fcluster Numeric matrix that contains membership of fuzzy clusters. It has one row for each series and one column for each cluster. The rows must sum to 1. Only relevant for fuzzy clustering.

# **TSClusters**

The base class contains the following slots:

- call
- family
- control
- datalist
- type
- distance
- centroid
- preproc
- k
- cluster
- centroids
- distmat
- proctime
- dots
- args
- seed

# PartitionalTSClusters

This class adds the following slots to the base class:

- iter
- converged
- clusinfo
- cldist

# HierarchicalTSClusters

This class adds the following slots to the base class:

- method
- clusinfo
- cldist

# FuzzyTSClusters

This class adds the following slots to the base class:

- iter
- converged
- fcluster

## See Also

**TSClusters-methods** 

tsclusters-methods Methods for TSClusters

# Description

Methods associated with TSClusters and derived objects.

## Usage

```
## S4 method for signature 'TSClusters'
initialize(.Object, ..., override.family = TRUE)
## S4 method for signature 'TSClusters'
show(object)
## S3 method for class 'TSClusters'
update(object, ..., evaluate = TRUE)
## S4 method for signature 'TSClusters'
update(object, ..., evaluate = TRUE)
## S3 method for class 'TSClusters'
predict(object, newdata = NULL, ...)
## S4 method for signature 'TSClusters'
predict(object, newdata = NULL, ...)
```

```
## S3 method for class 'TSClusters'
plot(
 х,
 у,
  · · · ,
 clus = seq_len(x@k),
 labs.arg = NULL,
  series = NULL,
  time = NULL,
 plot = TRUE,
 type = NULL,
 labels = NULL
)
## S4 method for signature 'TSClusters,missing'
plot(
 х,
 у,
  ...,
 clus = seq_len(x@k),
 labs.arg = NULL,
  series = NULL,
 time = NULL,
 plot = TRUE,
 type = NULL,
 labels = NULL
)
```

# Arguments

A TSClusters prototype. You <i>shouldn't</i> use this, see Initialize section and the examples.
For initialize, any valid slots. For plot, passed to ggplot2::geom_line() for the plotting of the <i>cluster centroids</i> , or to stats::plot.hclust(); see Plotting section and the examples. For update, any supported argument. Otherwise ignored.
Logical. Attempt to substitute the default family with one that conforms to the provided elements? See Initialize section.
An object that inherits from TSClusters as returned by tsclust().
Logical. Defaults to TRUE and evaluates the updated call, which will result in a new TSClusters object. Otherwise, it returns the unevaluated call.
New data to be assigned to a cluster. It can take any of the supported formats of tsclust(). Note that for multivariate series, this means that it <b>must</b> be a list of matrices, even if the list has only one matrix.
Ignored.
A numeric vector indicating which clusters to plot.

labs.arg	A list with arguments to change the title and/or axis labels. See the examples and ggplot2::labs() for more information.
series	Optionally, the data in the same format as it was provided to tsclust().
time	Optional values for the time axis. If series have different lengths, provide the time values of the longest series.
plot	Logical flag. You can set this to FALSE in case you want to save the ggplot object without printing anything to screen
type	What to plot. NULL means default. See details.
labels	Whether to include labels in the plot (not for dendrogram plots). See details and note that this is subject to <b>randomness</b> .

#### Details

The update method takes the original function call, replaces any provided argument and optionally evaluates the call again. Use evaluate = FALSE if you want to get the unevaluated call. If no arguments are provided, the object is updated to a new version if necessary (this is due to changes in the internal functions of the package, here for backward compatibility).

## Value

The plot method returns a gg object (or NULL for dendrogram plot) invisibly.

#### Initialize

The initialize method is used when calling methods::new(). The family slot can be substituted with an appropriate one if certain elements are provided by the user. The initialize methods of derived classes also inherit the family and can use it to calculate other slots. In order to get a fully functional object, at least the following slots should be provided:

- type: "partitional", "hierarchical", "fuzzy" or "tadpole".
- datalist: The data in one of the supported formats.
- centroids: The time series centroids in one of the supported formats.
- cluster: The cluster indices for each series in the datalist.
- control\*: A tsclust-controls object with the desired parameters.
- distance\*: A string indicating the distance that should be used.
- centroid\*: A string indicating the centroid to use (only necessary for partitional clustering).

\*Necessary when overriding the default family for the calculation of other slots, CVIs or prediction. Maybe not always needed, e.g. for plotting.

# Prediction

The predict generic can take the usual newdata argument. If NULL, the method simply returns the obtained cluster indices. Otherwise, a nearest-neighbor classification based on the centroids obtained from clustering is performed:

1. newdata is preprocessed with object@family@preproc using the parameters in object@args\$preproc.

- 2. A cross-distance matrix between the processed series and object@centroids is computed with object@family@dist using the parameters in object@args\$dist.
- 3. For non-fuzzy clustering, the series are assigned to their nearest centroid's cluster. For fuzzy clustering, the fuzzy membership matrix for the series is calculated. In both cases, the function in object@family@cluster is used.

#### Plotting

The plot method uses the ggplot2 plotting system (see ggplot2::ggplot()).

The default depends on whether a hierarchical method was used or not. In those cases, the dendrogram is plotted by default; you can pass any extra parameters to stats::plot.hclust() via the ellipsis (...).

Otherwise, the function plots the time series of each cluster along with the obtained centroid. The default values for cluster centroids are: linetype = "dashed", size = 1.5, colour = "black", alpha = 0.5. You can change this by means of the ellipsis (...).

You can choose what to plot with the type parameter. Possible options are:

- "dendrogram": Only available for hierarchical clustering.
- "series": Plot the time series divided into clusters without including centroids.
- "centroids": Plot the obtained centroids only.
- "sc": Plot both series and centroids

In order to enable labels on the (non-dendrogram) plot, you have to select an option that plots the series and at least provide an empty list in the labels argument. This list can contain arguments for ggrepel::geom\_label\_repel() and will be passed along. The following are set by the plot method if they are not provided:

- "mapping": set to aes\_string(x = "t", y = "value", label = "label")
- "data": a data frame with as many rows as series in the datalist and 4 columns:
  - t: x coordinate of the label for each series.
  - value: y coordinate of the label for each series.
  - cl: index of the cluster to which the series belongs (i.e. x@cluster).
  - label: the label for the given series (i.e. names(x@datalist)).

You can provide your own data frame if you want, but it must have those columns and, even if you override mapping, the cl column must have that name. The method will attempt to spread the labels across the plot, but note that this is **subject to randomness**, so be careful if you need reproducibility of any commands used after plotting (see examples).

If created, the function returns the gg object invisibly, in case you want to modify it to your liking. You might want to look at ggplot2::ggplot\_build() if that's the case.

If you want to free the scale of the X axis, you can do the following:

plot(x, plot = FALSE) + facet\_wrap(~cl, scales = "free")

For more complicated changes, you're better off looking at the source code at https://github. com/asardaes/dtwclust/blob/master/R/S4-TSClusters-methods.R and creating your own plotting function.

# Examples

```
data(uciCT)
# Assuming this was generated by some clustering procedure
centroids <- CharTraj[seq(1L, 100L, 5L)]</pre>
cluster <- unclass(CharTrajLabels)</pre>
pc_obj <- new("PartitionalTSClusters",</pre>
              type = "partitional", datalist = CharTraj,
              centroids = centroids, cluster = cluster,
              distance = "sbd", centroid = "dba",
              control = partitional_control(),
              args = tsclust_args(cent = list(window.size = 8L, norm = "L2")))
fc_obj <- new("FuzzyTSClusters",</pre>
              type = "fuzzy", datalist = CharTraj,
              centroids = centroids, cluster = cluster,
              distance = "sbd", centroid = "fcm",
              control = fuzzy_control())
show(fc_obj)
## Not run:
plot(pc_obj, type = "c", linetype = "solid",
     labs.arg = list(title = "Clusters' centroids"))
set.seed(15L)
plot(pc_obj, labels = list(nudge_x = -5, nudge_y = 0.2),
     clus = c(1L, 4L))
## End(Not run)
```

tsclustFamily-class Class definition for tsclustFamily

# Description

Formal S4 class with a family of functions used in tsclust().

#### Details

The custom implementations also handle parallelization.

Since the distance function makes use of **proxy**, it also supports any extra proxy::dist() parameters in ....

The prototype includes the cluster function for partitional methods, as well as a pass-through preproc function. The initializer expects a control from tsclust-controls. See more below.

## Slots

dist The function to calculate the distance matrices.

allcent The function to calculate centroids on each iteration.

cluster The function used to assign a series to a cluster.

preproc The function used to preprocess the data (relevant for stats::predict()).

# **Distance function**

The family's dist() function works like proxy::dist() but supports parallelization and optimized symmetric calculations. If you like, you can use the function more or less directly, but provide a control argument when creating the family (see examples). However, bear in mind the following considerations.

- The second argument is called centroids (inconsistent with proxy::dist()).
- If control\$distmat is *not* NULL, the function will try to subset it.
- If control\$symmetric is TRUE, centroids is NULL, *and* there is no argument pairwise that is TRUE, only half the distance matrix will be computed.
- The function always returns a crossdist matrix.

Note that all distances implemented as part of **dtwclust** have custom proxy loops that use multithreading independently of **foreach**, so see their respective documentation to see what optimizations apply to each one.

For distances *not* included in **dtwclust**, the computation can be in parallel using multi-processing with foreach::foreach(). If you install and load or attach (see base::library() or base::loadNamespace()) the **bigmemory** package, the function will take advantage of said package when all of the following conditions are met, reducing the overhead of data copying across processes:

- control\$symmetric is TRUE
- centroids is NULL
- pairwise is FALSE or NULL
- The distance was registered in proxy::pr\_DB with loop = TRUE
- A parallel backend with more than 1 worker has been registered with foreach

This symmetric, parallel case makes chunks for parallel workers, but they are not perfectly balanced, so some workers might finish before the others.

#### **Centroid function**

The default partitional allcent() function is a closure with the implementations of the included centroids. The ones for DBA(), shape\_extraction() and sdtw\_cent() can use multi-process parallelization with foreach::foreach(). Its formal arguments are described in the Centroid Calculation section from tsclust().

## Note

This class is meant to group together the relevant functions, but they are **not** linked with each other automatically. In other words, neither dist nor allcent apply preproc. They essentially don't know of each other's existence.

# See Also

dtw\_basic(), dtw\_lb(), gak(), lb\_improved(), lb\_keogh(), sbd(), sdtw().

# Examples

## End(Not run)

tslist

Coerce matrices or data frames to a list of time series

#### Description

Change a matrix or data frame to a list of univariate time series

# Usage

tslist(series, simplify = FALSE)

#### Arguments

series	A matrix or data frame where each row is a time series.
simplify	Coerce all series in the resulting list to either matrix (multivariate) or numeric (univariate).

# uciCT

# Details

Almost all functions in **dtwclust** work internally with lists of time series. If you want to avoid constant coercion, create a list of time series once by calling this function.

For matrices and data frames, each **row** is considered as one time series. A list input is simply passed through.

# Value

A list of time series.

### Note

The function assumes that matrix-like objects can be first coerced via base::as.matrix(), so that the result can be indexed with series[i, ].

No consistency checks are performed by this function.

uciCT

Subset of character trajectories data set

#### Description

Subset: only 5 examples of each considered character. See details.

# Format

Lists 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 in CharTraj has only 5 examples of the X velocity for each character. A vector with labels is also loaded in CharTrajLabels.

The subset included in CharTrajMV has 5 examples too, but includes tip force as well as X and Y velocity. Each element of the list is a multivariate series with 3 variables.

Please note that even though both CharTraj and CharTrajMV have the same series names, the actual series in each subset are **not** the same, i.e., CharTraj\$A.V1 is not in CharTrajMV\$A.V1.

## Source

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

# zscore

# Description

Wrapper for function base::scale() that returns zeros instead of NaN. It also supports matrices, data frames, and lists of time series.

# Usage

```
zscore(
    x,
    ...,
    multivariate = FALSE,
    keep.attributes = FALSE,
    error.check = TRUE
)
```

# Arguments

x	Data to normalize. Either a vector, a matrix/data.frame where each row is to be normalized, or a list of vectors/matrices.
	Further arguments to pass to base::scale().
multivariate	Is x a multivariate time series? It will be detected automatically if a list is provided in x.
keep.attributes	
	Should the mean and standard deviation returned by base::scale() be pre- served?
error.check	Logical indicating whether the function should try to detect inconsistencies and give more informative errors messages. Also used internally to avoid repeating checks.

# Details

Multivariate series must have time spanning the rows and variables spanning the columns.

# Value

Normalized data in the same format as provided.

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