Package ‘distances’

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Description

The `distances` package provides tools for constructing, manipulating and using distance metrics in R. It calculates distances only as needed (unlike the standard `dist` function which derives the complete distance matrix when called). This saves memory and can increase speed. The package also includes functions for fast nearest and farthest neighbor searching.

Details

See the package's website for more information: [https://github.com/fsavje/distances](https://github.com/fsavje/distances).

Bug reports and suggestions are greatly appreciated. They are best reported here: [https://github.com/fsavje/distances/issues/new](https://github.com/fsavje/distances/issues/new).

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`distances` Constructor for distance metric objects

Description

distances constructs a distance metric for a set of points. Currently, it only creates Euclidean distances. It can, however, create distances in any linear projection of Euclidean space. In other words, Mahalanobis distances or normalized Euclidean distances are both possible. It is also possible to give each dimension of the space different weights.

Usage

```
distances(data, id_variable = NULL, dist_variables = NULL,
          normalize = NULL, weights = NULL)
```

Arguments

- **data**: a matrix or data frame containing the data points between distances should be derived.
- **id_variable**: optional IDs of the data points. If `id_variable` is a single string and `data` is a data frame, the corresponding column in `data` will be taken as IDs. That column will be excluded from `data` when constructing distances (unless it is listed in `dist_variables`). If `id_variable` is `NULL`, the IDs are set to `1:nrow(data)`. Otherwise, `id_variable` must be of length `nrow(data)` and will be used directly as IDs.
**distances**

optional names of the columns in data that should be used when constructing distances. If dist_variables is NULL, all columns will be used (net of eventual column specified by id_variable). If data is a matrix, dist_variables must be NULL.

**normalize**

optional normalization of the data prior to distance construction. If normalize is NULL or "none", no normalization will be done (effectively setting normalize to the identity matrix). If normalize is "mahalanobize", normalization will be done with var(data) (i.e., resulting in Mahalanobis distances). If normalize is "studentize", normalization is done with the diagonal of var(data). If normalize is a matrix, it will be used in the normalization. If normalize is a vector, a diagonal matrix with the supplied vector as its diagonal will be used. The matrix used for normalization must be positive-semidefinite.

**weights**

optional weighting of the data prior to distance construction. If normalize is NULL no weighting will be done (effectively setting weights to the identity matrix). If weights is a matrix, that will be used in the weighting. If normalize is a vector, a diagonal matrix with the supplied vector as its diagonal will be used. The matrix used for weighting must be positive-semidefinite.

**Details**

Let \( x \) and \( y \) be two data points in data described by two vectors. distances uses the following metric to derive the distance between \( x \) and \( y \):

\[
\sqrt{(x - y)^T \left(N^{-0.5}W(N^{-0.5})\right)^T(x - y)}
\]

where \( N^{-0.5} \) is the Cholesky decomposition (lower triangular) of the inverse of the matrix specified by normalize, and \( W \) is the matrix specified by weights.

When normalize is var(data) (i.e., using the "mahalanobize" option), the function gives (weighted) Mahalanobis distances. When normalize is diag(var(data)) (i.e., using the "studentize" option), the function divides each column by its variance leading to (weighted) normalized Euclidean distances. If normalize is the identity matrix (i.e., using the "none" or NULL option), the function derives ordinary Euclidean distances.

**Value**

Returns a distances object.

**Examples**

```r
my_data_points <- data.frame(x = c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10),
                              y = c(10, 9, 8, 7, 6, 6, 7, 8, 9, 10))

# Euclidean distances
my_distances1 <- distances(my_data_points)

# Euclidean distances in only one dimension
my_distances2 <- distances(my_data_points,
                           dist_variables = "x")
```
# Mahalanobis distances
my_distances3 <- distances(my_data_points, 
  normalize = "mahalanobize")

# Custom normalization matrix
my_norm_mat <- matrix(c(3, 1, 1, 3), nrow = 2)
my_distances4 <- distances(my_data_points, 
  normalize = my_norm_mat)

# Give "x" twice the weight compared to "y"
my_distances5 <- distances(my_data_points, 
  weights = c(2, 1))

# Use normalization and weighting
my_distances6 <- distances(my_data_points, 
  normalize = "mahalanobize", 
  weights = c(2, 1))

# Custom ID labels
my_data_points_withID <- data.frame(my_data_points, 
  my_ids = letters[1:10])
my_distances7 <- distances(my_data_points_withID, 
  id_variable = "my_ids")

# Compare to standard R functions
all.equal(as.matrix(my_distances1), as.matrix(dist(my_data_points)))  
# > TRUE
all.equal(as.matrix(my_distances2), as.matrix(dist(my_data_points[, "x"])))  
# > TRUE

tmp_distances <- sqrt(mahalanobis(as.matrix(my_data_points), 
  unlist(my_data_points[1, ]), 
  var(my_data_points)))
names(tmp_distances) <- 1:10
all.equal(as.matrix(my_distances3)[1, ], tmp_distances)  
# > TRUE

tmp_data_points <- as.matrix(my_data_points)
tmp_data_points[, 1] <- sqrt(2) * tmp_data_points[, 1]
all.equal(as.matrix(my_distances5), as.matrix(dist(tmp_data_points)))  
# > TRUE

tmp_data_points <- as.matrix(my_data_points)
tmp_cov_mat <- var(tmp_data_points)
tmp_data_points[, 1] <- sqrt(2) * tmp_data_points[, 1]
tmp_distances <- sqrt(mahalanobis(tmp_data_points, 
  tmp_data_points[1, ], 
  tmp_cov_mat))
names(tmp_distances) <- 1:10
\[
\text{all.equal(as.matrix(my_distances6)[1, ], tmp_distances)}
\]
# > TRUE

tmp_distances <- as.matrix(dist(my_data_points))
colnames(tmp_distances) <- rownames(tmp_distances) <- letters[1:10]
all.equal(as.matrix(my_distances7), tmp_distances)
# > TRUE

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**distance_columns**

*Distance matrix columns*

**Description**

distance_columns extracts columns from the distance matrix.

**Usage**

distance_columns(distances, column_indices, row_indices = NULL)

**Arguments**

- **distances**: A distances object.
- **column_indices**: An integer vector with point indices indicating which columns to be extracted.
- **row_indices**: If NULL, complete rows will be extracted. If integer vector with point indices, only the indicated rows will be extracted.

**Details**

If the complete distance matrix is desired, distance_matrix is faster than distance_columns.

**Value**

Returns a matrix with the requested columns.

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**distance_matrix**

*Distance matrix*

**Description**

distance_matrix makes distance matrices (complete and partial) from distances objects.

**Usage**

distance_matrix(distances, indices = NULL)
Arguments

distances A distances object.
indices If NULL, the complete distance matrix is made. If integer vector with point indices, a partial matrix including only the indicated data points is made.

Value

Returns a distance matrix of class dist.

is.distances Check distances object

Description

is.distances checks whether the provided object is a valid instance of the distances class.

Usage

is.distances(x)

Arguments

x object to check.

Value

Returns TRUE if x is a valid distances object, otherwise FALSE.

max_distance_search Max distance search

Description

max_distance_search searches for the data point furthest from a set of query points.

Usage

max_distance_search(distances, query_indices = NULL, search_indices = NULL)

Arguments

distances A distances object.
query_indices An integer vector with point indices to query. If NULL, all data points in distances are queried.
search_indices An integer vector with point indices to search among. If NULL, all data points in distances are searched over.
nearest_neighbor_search

**Value**

An integer vector with point indices for the data point furthest from each query.

**Description**

*nearest_neighbor_search* searches for the k nearest neighbors of a set of query points.

**Usage**

```r
nearest_neighbor_search(distances, k, query_indices = NULL, search_indices = NULL, radius = NULL)
```

**Arguments**

- **distances**: A `distances` object.
- **k**: The number of neighbors to search for.
- **query_indices**: An integer vector with point indices to query. If `NULL`, all data points in `distances` are queried.
- **search_indices**: An integer vector with point indices to search among. If `NULL`, all data points in `distances` are searched over.
- **radius**: Restrict the search to a fixed radius around each query. If fewer than k search points exist within this radius, no neighbors are reported (indicated by `NA`).

**Value**

A matrix with point indices for the nearest neighbors. Columns in this matrix indicate queries, and rows are ordered by distances from the query.
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