Package ‘umap’

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Title Uniform Manifold Approximation and Projection
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Description Uniform manifold approximation and projection is a technique for dimension reduction. The algorithm was described by McInnes and Healy (2018) in <arXiv:1802.03426>. This package provides an interface for two implementations. One is written from scratch, including components for nearest-neighbor search and for embedding. The second implementation is a wrapper for 'python' package 'umap-learn' (requires separate installation, see vignette for more details).

Depends R (>= 3.1.2)
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BugReports https://github.com/tkonopka/umap/issues
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**predict.umap**

**R topics documented:**

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`predict.umap` | *project data points onto an existing umap embedding*

**Description**

`project data points onto an existing umap embedding`

**Usage**

```r
## S3 method for class 'umap'
predict(object, data, ...)
```

**Arguments**

- `object` : trained object of class umap
- `data` : matrix with data
- `...` : additional arguments (not used)

**Value**

new matrix

**Examples**

```r
# embedd iris dataset using default settings
iris.umap = umap(iris[,1:4])

# create a dataset with structure like iris, but with perturbation
iris.perturbed = iris[,1:4] + matrix(rnorm(nrow(iris)*4, 0, 0.1), ncol=4)

# project perturbed dataset
perturbed.embedding = predict(iris.umap, iris.perturbed)

# output is a matrix with embedding coordinates
head(perturbed.embedding)
```
**umap**

*Computes a manifold approximation and projection*

**Description**

Computes a manifold approximation and projection

**Usage**

\[
\text{umap}(d, \text{config} = \text{umap.defaults}, \text{method} = \text{c("naive", "umap-learn")}, \ldots)
\]

**Arguments**

- **d** matrix, input data
- **config** object of class umap.config
- **method** character, implementation. Available methods are 'naive' (an implementation written in pure R) and 'umap-learn' (requires python package 'umap-learn')
- **...** list of settings; overwrite default values from config

**Value**

object of class umap, containing at least a component with an embedding and a component with configuration settings

**Examples**

```r
# embedd iris dataset using default settings
iris.umap = umap(iris[,1:4])

# display object summary
iris.umap

# display embedding coordinates
head(iris.umap$layout)
```

**umap.defaults**

*Default configuration for umap*

**Description**

A list with parameters customizing a UMAP embedding. Each component of the list is an effective argument for umap().
Usage

umap.defaults

Format

An object of class \texttt{umap.config} of length 21.

Details

- \texttt{n_neighbors}: integer; number of nearest neighbors
- \texttt{n_components}: integer; dimension of target (output) space
- \texttt{metric}: character or function; determines how distances between data points are computed. When using a string, available metrics are: euclidean, manhattan. Other available generalized metrics are: cosine, pearson, pearson2. Note the triangle inequality may not be satisfied by some generalized metrics, hence knn search may not be optimal. When using metric.function as a function, the signature must be function(matrix, origin, target) and should compute a distance between the origin column and the target columns
- \texttt{n_epochs}: integer; number of iterations performed during layout optimization
- \texttt{input}: character, use either "data" or "dist"; determines whether the primary input argument to \texttt{umap()} is treated as a data matrix or as a distance matrix
- \texttt{init}: character or matrix. The default string "spectral" computes an initial embedding using eigenvectors of the connectivity graph matrix. An alternative is the string "random", which creates an initial layout based on random coordinates. This setting can also be set to a matrix, in which case layout optimization begins from the provided coordinates.
- \texttt{min_dist}: numeric; determines how close points appear in the final layout
- \texttt{set_op_ratio_mix_ratio}: numeric in range \([0,1]\); determines who the knn-graph is used to create a fuzzy simplicial graph
- \texttt{local_connectivity}: numeric; used during construction of fuzzy simplicial set
- \texttt{bandwidth}: numeric; used during construction of fuzzy simplicial set
- \texttt{alpha}: numeric; initial value of "learning rate" of layout optimization
- \texttt{gamma}: numeric; determines, together with alpha, the learning rate of layout optimization
- \texttt{negative_sample_rate}: integer; determines how many non-neighbor points are used per point and per iteration during layout optimization
- \texttt{a}: numeric; contributes to gradient calculations during layout optimization. When left at NA, a suitable value will be estimated automatically.
- \texttt{b}: numeric; contributes to gradient calculations during layout optimization.
- \texttt{spread}: numeric; used during automatic estimation of \(a/b\) parameters.
- \texttt{random_state}: integer; seed for random number generation used during \texttt{umap()}
- \texttt{transform_state}: integer; seed for random number generation used during \texttt{predict()}
- \texttt{knn.repeat}: number of times to restart knn search
- \texttt{verbose}: logical or integer; determines whether to show progress messages
- \texttt{umap_learn_args}: vector of arguments to python package \texttt{umap-learn}
Examples

# display all default settings
umap.defaults

# create a new settings object with n_neighbors set to 5
custom.settings = umap.defaults
custom.settings$n_neighbors = 5
custom.settings
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