

Package ‘uwot’

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Title The Uniform Manifold Approximation and Projection (UMAP) Method for Dimensionality Reduction

Version 0.1.14

Description An implementation of the Uniform Manifold Approximation and Projection dimensionality reduction by McInnes et al. (2018) <[arXiv:1802.03426](https://arxiv.org/abs/1802.03426)>. It also provides means to transform new data and to carry out supervised dimensionality reduction. An implementation of the related LargeVis method of Tang et al. (2016) <[arXiv:1602.00370](https://arxiv.org/abs/1602.00370)> is also provided. This is a complete re-implementation in R (and C++, via the 'Rcpp' package): no Python installation is required. See the uwot website (<<https://github.com/jlmelville/uwot>>) for more documentation and examples.

License GPL (>= 3)

URL <https://github.com/jlmelville/uwot>

BugReports <https://github.com/jlmelville/uwot/issues>

Encoding UTF-8

Suggests testthat, covr, bigstatsr, RSpectra

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Author James Melville [aut, cre],
Aaron Lun [ctb],
Mohamed Nadhir Djekidel [ctb],
Yuhan Hao [ctb]

Maintainer James Melville <jlmelville@gmail.com>

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load_uwot	<i>Save or Load a Model</i>
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Description

Functions to write a UMAP model to a file, and to restore.

Usage

```
load_uwot(file, verbose = FALSE)
```

Arguments

file	name of the file where the model is to be saved or read from.
verbose	if TRUE, log information to the console.

Value

The model saved at file, for use with [umap_transform](#). Additionally, it contains an extra item: `mod_dir`, which contains the path to the temporary working directory used during loading of the model. This directory cannot be removed until this model has been unloaded by using [unload_uwot](#).

See Also

[save_uwot](#), [unload_uwot](#)

Examples

```
iris_train <- iris[c(1:10, 51:60), ]
iris_test <- iris[100:110, ]

# create model
model <- umap(iris_train, ret_model = TRUE, n_epochs = 20)

# save without unloading: this leaves behind a temporary working directory
model_file <- tempfile("iris_umap")
```

```
model <- save_uwot(model, file = model_file)

# The model can continue to be used
test_embedding <- umap_transform(iris_test, model)

# To manually unload the model from memory when finished and to clean up
# the working directory (this doesn't touch your model file)
unload_uwot(model)

# At this point, model cannot be used with umap_transform, this would fail:
# test_embedding2 <- umap_transform(iris_test, model)

# restore the model: this also creates a temporary working directory
model2 <- load_uwot(file = model_file)
test_embedding2 <- umap_transform(iris_test, model2)

# Unload and clean up the loaded model temp directory
unload_uwot(model2)

# clean up the model file
unlink(model_file)

# save with unloading: this deletes the temporary working directory but
# doesn't allow the model to be re-used
model3 <- umap(iris_train, ret_model = TRUE, n_epochs = 20)
model_file3 <- tempfile("iris_umap")
model3 <- save_uwot(model3, file = model_file3, unload = TRUE)
```

Description

Carry out dimensionality reduction of a dataset using a method similar to LargeVis (Tang et al., 2016).

Usage

```
lvish(  
  X,  
  perplexity = 50,  
  n_neighbors = perplexity * 3,  
  n_components = 2,  
  metric = "euclidean",  
  n_epochs = -1,  
  learning_rate = 1,  
  scale = "maxabs",  
  init = "lvrandom",
```

```

init_sdev = NULL,
repulsion_strength = 7,
negative_sample_rate = 5,
nn_method = NULL,
n_trees = 50,
search_k = 2 * n_neighbors * n_trees,
n_threads = NULL,
n_sgd_threads = 0,
grain_size = 1,
kernel = "gauss",
pca = NULL,
pca_center = TRUE,
pcg_rand = TRUE,
fast_sgd = FALSE,
ret_nn = FALSE,
ret_extra = c(),
tmpdir = tempdir(),
verbose = getOption("verbose", TRUE),
batch = FALSE,
opt_args = NULL,
epoch_callback = NULL,
pca_method = NULL,
binary_edge_weights = FALSE
)

```

Arguments

- | | |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| X | Input data. Can be a data.frame , matrix , dist object or sparseMatrix . Matrix and data frames should contain one observation per row. Data frames will have any non-numeric columns removed, although factor columns will be used if explicitly included via metric (see the help for metric for details). A sparse matrix is interpreted as a distance matrix, and is assumed to be symmetric, so you can also pass in an explicitly upper or lower triangular sparse matrix to save storage. There must be at least <code>n_neighbors</code> non-zero distances for each row. Both implicit and explicit zero entries are ignored. Set zero distances you want to keep to an arbitrarily small non-zero value (e.g. <code>1e-10</code>). X can also be NULL if pre-computed nearest neighbor data is passed to <code>nn_method</code> , and <code>init</code> is not "spca" or "pca". |
| perplexity | Controls the size of the local neighborhood used for manifold approximation. This is the analogous to <code>n_neighbors</code> in umap . Change this, rather than <code>n_neighbors</code> . |
| n_neighbors | The number of neighbors to use when calculating the perplexity. Usually set to three times the value of the perplexity. Must be at least as large as perplexity. |
| n_components | The dimension of the space to embed into. This defaults to 2 to provide easy visualization, but can reasonably be set to any integer value in the range 2 to 100. |
| metric | Type of distance metric to use to find nearest neighbors. One of: |

- "euclidean" (the default)
- "cosine"
- "manhattan"
- "hamming"
- "correlation" (a distance based on the Pearson correlation)
- "categorical" (see below)

Only applies if `nn_method = "annoy"` (for `nn_method = "fnn"`, the distance metric is always "euclidean").

If `X` is a data frame or matrix, then multiple metrics can be specified, by passing a list to this argument, where the name of each item in the list is one of the metric names above. The value of each list item should be a vector giving the names or integer ids of the columns to be included in a calculation, e.g. `metric = list(euclidean = 1:4, manhattan = 5:10)`.

Each metric calculation results in a separate fuzzy simplicial set, which are intersected together to produce the final set. Metric names can be repeated. Because non-numeric columns are removed from the data frame, it is safer to use column names than integer ids.

Factor columns can also be used by specifying the metric name "categorical". Factor columns are treated different from numeric columns and although multiple factor columns can be specified in a vector, each factor column specified is processed individually. If you specify a non-factor column, it will be coerced to a factor.

For a given data block, you may override the `pca` and `pca_center` arguments for that block, by providing a list with one unnamed item containing the column names or ids, and then any of the `pca` or `pca_center` overrides as named items, e.g. `metric = list(euclidean = 1:4, manhattan = list(5:10, pca_center = FALSE))`. This exists to allow mixed binary and real-valued data to be included and to have PCA applied to both, but with centering applied only to the real-valued data (it is typical not to apply centering to binary data before PCA is applied).

<code>n_epochs</code>	Number of epochs to use during the optimization of the embedded coordinates. The default is calculate the number of epochs dynamically based on dataset size, to give the same number of edge samples as the LargeVis defaults. This is usually substantially larger than the UMAP defaults. If <code>n_epochs = 0</code> , then coordinates determined by "init" will be returned.
<code>learning_rate</code>	Initial learning rate used in optimization of the coordinates.
<code>scale</code>	Scaling to apply to <code>X</code> if it is a data frame or matrix: <ul style="list-style-type: none"> • "none" or FALSE or NULL No scaling. • "Z" or "scale" or TRUE Scale each column to zero mean and variance 1. • "maxabs" Center each column to mean 0, then divide each element by the maximum absolute value over the entire matrix. • "range" Range scale the entire matrix, so the smallest element is 0 and the largest is 1. • "colrange" Scale each column in the range (0,1).

For Ivish, the default is "maxabs", for consistency with LargeVis.

<code>init</code>	<p>Type of initialization for the coordinates. Options are:</p> <ul style="list-style-type: none"> • <code>"spectral"</code> Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, with Gaussian noise added. • <code>"normlaplacian"</code>. Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, without noise. • <code>"random"</code>. Coordinates assigned using a uniform random distribution between -10 and 10. • <code>"lvrandom"</code>. Coordinates assigned using a Gaussian distribution with standard deviation $1e-4$, as used in LargeVis (Tang et al., 2016) and t-SNE. • <code>"laplacian"</code>. Spectral embedding using the Laplacian Eigenmap (Belkin and Niyogi, 2002). • <code>"pca"</code>. The first two principal components from PCA of X if X is a data frame, and from a 2-dimensional classical MDS if X is of class <code>"dist"</code>. • <code>"spca"</code>. Like <code>"pca"</code>, but each dimension is then scaled so the standard deviation is $1e-4$, to give a distribution similar to that used in t-SNE and LargeVis. This is an alias for <code>init = "pca"</code>, <code>init_sdev = 1e-4</code>. • <code>"agspectral"</code> An "approximate global" modification of <code>"spectral"</code> which all edges in the graph to a value of 1, and then sets a random number of edges (<code>negative_sample_rate</code> edges per vertex) to 0.1, to approximate the effect of non-local affinities. • A matrix of initial coordinates. <p>For spectral initializations, (<code>"spectral"</code>, <code>"normlaplacian"</code>, <code>"laplacian"</code>), if more than one connected component is identified, each connected component is initialized separately and the results are merged. If <code>verbose = TRUE</code> the number of connected components are logged to the console. The existence of multiple connected components implies that a global view of the data cannot be attained with this initialization. Either a PCA-based initialization or increasing the value of <code>n_neighbors</code> may be more appropriate.</p>
<code>init_sdev</code>	<p>If non-NULL, scales each dimension of the initialized coordinates (including any user-supplied matrix) to this standard deviation. By default no scaling is carried out, except when <code>init = "spca"</code>, in which case the value is 0.0001. Scaling the input may help if the unscaled versions result in initial coordinates with large inter-point distances or outliers. This usually results in small gradients during optimization and very little progress being made to the layout. Shrinking the initial embedding by rescaling can help under these circumstances. Scaling the result of <code>init = "pca"</code> is usually recommended and <code>init = "spca"</code> as an alias for <code>init = "pca"</code>, <code>init_sdev = 1e-4</code> but for the spectral initializations the scaled versions usually aren't necessary unless you are using a large value of <code>n_neighbors</code> (e.g. <code>n_neighbors = 150</code> or higher).</p>
<code>repulsion_strength</code>	<p>Weighting applied to negative samples in low dimensional embedding optimization. Values higher than one will result in greater weight being given to negative samples.</p>
<code>negative_sample_rate</code>	<p>The number of negative edge/1-simplex samples to use per positive edge/1-simplex sample in optimizing the low dimensional embedding.</p>

nn_method	<p>Method for finding nearest neighbors. Options are:</p> <ul style="list-style-type: none"> • "fnn". Use exact nearest neighbors via the FNN package. • "annoy" Use approximate nearest neighbors via the RcppAnnoy package. <p>By default, if X has less than 4,096 vertices, the exact nearest neighbors are found. Otherwise, approximate nearest neighbors are used. You may also pass precalculated nearest neighbor data to this argument. It must be a list consisting of two elements:</p> <ul style="list-style-type: none"> • "idx". A $n_vertices \times n_neighbors$ matrix containing the integer indexes of the nearest neighbors in X. Each vertex is considered to be its own nearest neighbor, i.e. <code>idx[, 1] == 1:n_vertices</code>. • "dist". A $n_vertices \times n_neighbors$ matrix containing the distances of the nearest neighbors. <p>Multiple nearest neighbor data (e.g. from two different precomputed metrics) can be passed by passing a list containing the nearest neighbor data lists as items. The <code>n_neighbors</code> parameter is ignored when using precomputed nearest neighbor data.</p>
n_trees	<p>Number of trees to build when constructing the nearest neighbor index. The more trees specified, the larger the index, but the better the results. With <code>search_k</code>, determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy". Sensible values are between 10 to 100.</p>
search_k	<p>Number of nodes to search during the neighbor retrieval. The larger <code>k</code>, the more the accurate results, but the longer the search takes. With <code>n_trees</code>, determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy".</p>
n_threads	<p>Number of threads to use (except during stochastic gradient descent). Default is half the number of concurrent threads supported by the system. For nearest neighbor search, only applies if <code>nn_method = "annoy"</code>. If <code>n_threads > 1</code>, then the Annoy index will be temporarily written to disk in the location determined by tempfile.</p>
n_sgd_threads	<p>Number of threads to use during stochastic gradient descent. If set to <code>> 1</code>, then be aware that if <code>batch = FALSE</code>, results will <i>not</i> be reproducible, even if <code>set.seed</code> is called with a fixed seed before running. Set to "auto" to use the same value as <code>n_threads</code>.</p>
grain_size	<p>The minimum amount of work to do on each thread. If this value is set high enough, then less than <code>n_threads</code> or <code>n_sgd_threads</code> will be used for processing, which might give a performance improvement if the overhead of thread management and context switching was outweighing the improvement due to concurrent processing. This should be left at default (1) and work will be spread evenly over all the threads specified.</p>
kernel	<p>Type of kernel function to create input probabilities. Can be one of "gauss" (the default) or "knn". "gauss" uses the usual Gaussian weighted similarities. "knn" assigns equal probabilities to every edge in the nearest neighbor graph, and zero otherwise, using perplexity nearest neighbors. The <code>n_neighbors</code> parameter is ignored in this case.</p>

pca	If set to a positive integer value, reduce data to this number of columns using PCA. Doesn't applied if the distance metric is "hamming", or the dimensions of the data is larger than the number specified (i.e. number of rows and columns must be larger than the value of this parameter). If you have > 100 columns in a data frame or matrix, reducing the number of columns in this way may substantially increase the performance of the nearest neighbor search at the cost of a potential decrease in accuracy. In many t-SNE applications, a value of 50 is recommended, although there's no guarantee that this is appropriate for all settings.
pca_center	If TRUE, center the columns of X before carrying out PCA. For binary data, it's recommended to set this to FALSE.
pcg_rand	If TRUE, use the PCG random number generator (O'Neill, 2014) during optimization. Otherwise, use the faster (but probably less statistically good) Tausworthe "taus88" generator. The default is TRUE.
fast_sgd	If TRUE, then the following combination of parameters is set: pcg_rand = TRUE and n_sgd_threads = "auto". The default is FALSE. Setting this to TRUE will speed up the stochastic optimization phase, but give a potentially less accurate embedding, and which will not be exactly reproducible even with a fixed seed. For visualization, fast_sgd = TRUE will give perfectly good results. For more generic dimensionality reduction, it's safer to leave fast_sgd = FALSE. If fast_sgd = TRUE, then user-supplied values of pcg_rand and n_sgd_threads, are ignored.
ret_nn	If TRUE, then in addition to the embedding, also return nearest neighbor data that can be used as input to nn_method to avoid the overhead of repeatedly calculating the nearest neighbors when manipulating unrelated parameters (e.g. min_dist, n_epochs, init). See the "Value" section for the names of the list items. If FALSE, just return the coordinates. Note that the nearest neighbors could be sensitive to data scaling, so be wary of reusing nearest neighbor data if modifying the scale parameter.
ret_extra	A vector indicating what extra data to return. May contain any combination of the following strings: <ul style="list-style-type: none"> • "nn" same as setting ret_nn = TRUE. • "P" the high dimensional probability matrix. The graph is returned as a sparse symmetric N x N matrix of class dgCMatrix-class, where a non-zero entry (i, j) gives the input probability (or similarity or affinity) of the edge connecting vertex i and vertex j. Note that the graph is further sparsified by removing edges with sufficiently low membership strength that they would not be sampled by the probabilistic edge sampling employed for optimization and therefore the number of non-zero elements in the matrix is dependent on n_epochs. If you are only interested in the fuzzy input graph (e.g. for clustering), setting n_epochs = 0 will avoid any further sparsifying. Be aware that setting binary_edge_weights = TRUE will affect this graph (all non-zero edge weights will be 1). • sigma a vector of the bandwidths used to calibrate the input Gaussians to reproduce the target "perplexity".
tmpdir	Temporary directory to store nearest neighbor indexes during nearest neighbor

	search. Default is <code>tempdir</code> . The index is only written to disk if <code>n_threads > 1</code> and <code>nn_method = "annoy"</code> ; otherwise, this parameter is ignored.
<code>verbose</code>	If TRUE, log details to the console.
<code>batch</code>	If TRUE, then embedding coordinates are updated at the end of each epoch rather than during the epoch. In batch mode, results are reproducible with a fixed random seed even with <code>n_sgd_threads > 1</code> , at the cost of a slightly higher memory use. You may also have to modify <code>learning_rate</code> and increase <code>n_epochs</code> , so whether this provides a speed increase over the single-threaded optimization is likely to be dataset and hardware-dependent.
<code>opt_args</code>	A list of optimizer parameters, used when <code>batch = TRUE</code> . The default optimization method used is Adam (Kingma and Ba, 2014). <ul style="list-style-type: none"> • <code>method</code> The optimization method to use. Either "adam" or "sgd" (stochastic gradient descent). Default: "adam". • <code>beta1</code> (Adam only). The weighting parameter for the exponential moving average of the first moment estimator. Effectively the momentum parameter. Should be a floating point value between 0 and 1. Higher values can smooth oscillatory updates in poorly-conditioned situations and may allow for a larger <code>learning_rate</code> to be specified, but too high can cause divergence. Default: 0.5. • <code>beta2</code> (Adam only). The weighting parameter for the exponential moving average of the uncentered second moment estimator. Should be a floating point value between 0 and 1. Controls the degree of adaptivity in the step-size. Higher values put more weight on previous time steps. Default: 0.9. • <code>eps</code> (Adam only). Intended to be a small value to prevent division by zero, but in practice can also affect convergence due to its interaction with <code>beta2</code>. Higher values reduce the effect of the step-size adaptivity and bring the behavior closer to stochastic gradient descent with momentum. Typical values are between 1e-8 and 1e-3. Default: 1e-7. • <code>alpha</code> The initial learning rate. Default: the value of the <code>learning_rate</code> parameter.
<code>epoch_callback</code>	A function which will be invoked at the end of every epoch. Its signature should be: <code>(epoch, n_epochs, coords)</code> , where: <ul style="list-style-type: none"> • <code>epoch</code> The current epoch number (between 1 and <code>n_epochs</code>). • <code>n_epochs</code> Number of epochs to use during the optimization of the embedded coordinates. • <code>coords</code> The embedded coordinates as of the end of the current epoch, as a matrix with dimensions <code>(N, n_components)</code>.
<code>pca_method</code>	Method to carry out any PCA dimensionality reduction when the <code>pca</code> parameter is specified. Allowed values are: <ul style="list-style-type: none"> • "irlba". Uses <code>prcomp_irlba</code> from the <code>irlba</code> package. • "rsvd". Uses 5 iterations of <code>svdr</code> from the <code>irlba</code> package. This is likely to give much faster but potentially less accurate results than using "irlba". For the purposes of nearest neighbor calculation and coordinates initialization, any loss of accuracy doesn't seem to matter much.

- "bigstatsr". Uses `big_randomSVD` from the `bigstatsr` package. The SVD methods used in `bigstatsr` may be faster on systems without access to efficient linear algebra libraries (e.g. Windows). **Note:** `bigstatsr` is *not* a dependency of `uwot`: if you choose to use this package for PCA, you *must* install it yourself.
- "svd". Uses `svd` for the SVD. This is likely to be slow for all but the smallest datasets.
- "auto" (the default). Uses "irlba", unless more than 50 case "svd" is used.

`binary_edge_weights`

If TRUE then edge weights in the input graph are treated as binary (0/1) rather than real valued. This affects the sampling frequency of neighbors and is the strategy used by the PaCMAP method (Wang and co-workers, 2020). Practical (Böhm and co-workers, 2020) and theoretical (Damrich and Hamprecht, 2021) work suggests this has little effect on UMAP's performance.

Details

`lvish` differs from the official `LargeVis` implementation in the following:

- Only the nearest-neighbor index search phase is multi-threaded.
- Matrix input data is not normalized.
- The `n_trees` parameter cannot be dynamically chosen based on data set size.
- Nearest neighbor results are not refined via the neighbor-of-my-neighbor method. The `search_k` parameter is twice as large than default to compensate.
- Gradient values are clipped to 4.0 rather than 5.0 .
- Negative edges are generated by uniform sampling of vertexes rather than their $\text{degree}^{0.75}$.
- The default number of samples is much reduced. The default number of epochs, `n_epochs`, is set to 5000 , much larger than for `umap`, but may need to be increased further depending on your dataset. Using `init = "spectral"` can help.

Value

A matrix of optimized coordinates, or:

- if `ret_nn = TRUE` (or `ret_extra` contains "nn"), returns the nearest neighbor data as a list called `nn`. This contains one list for each `metric` calculated, itself containing a matrix `idx` with the integer ids of the neighbors; and a matrix `dist` with the distances. The `nn` list (or a sub-list) can be used as input to the `nn_method` parameter.
- if `ret_extra` contains "P", returns the high dimensional probability matrix as a sparse matrix called `P`, of type `dgCMatrix-class`.

The returned list contains the combined data from any combination of specifying `ret_nn` and `ret_extra`.

References

Tang, J., Liu, J., Zhang, M., & Mei, Q. (2016, April). Visualizing large-scale and high-dimensional data. In *Proceedings of the 25th International Conference on World Wide Web* (pp. 287-297). International World Wide Web Conferences Steering Committee. <https://arxiv.org/abs/1602.00370>

Examples

```
# Default number of epochs is much larger than for UMAP, assumes random
# initialization. Use perplexity rather than n_neighbors to control the size
# of the local neighborhood 20 epochs may be too small for a random
# initialization
iris_lvish <- lvish(iris,
  perplexity = 50, learning_rate = 0.5,
  init = "random", n_epochs = 20
)
```

save_uwot

Save or Load a Model

Description

Functions to write a UMAP model to a file, and to restore.

Usage

```
save_uwot(model, file, unload = FALSE, verbose = FALSE)
```

Arguments

model	a UMAP model create by umap .
file	name of the file where the model is to be saved or read from.
unload	if TRUE, unload all nearest neighbor indexes for the model. The model will no longer be valid for use in umap_transform and the temporary working directory used during model saving will be deleted. You will need to reload the model with load_uwot to use the model. If FALSE, then the model can be re-used without reloading, but you must manually unload the NN index when you are finished using it if you want to delete the temporary working directory. To unload manually, use unload_uwot . The absolute path of the working directory is found in the <code>mod_dir</code> item of the return value.
verbose	if TRUE, log information to the console.

Value

model with one extra item: `mod_dir`, which contains the path to the working directory. If `unload = FALSE` then this directory still exists after this function returns, and can be cleaned up with [unload_uwot](#). If you don't care about cleaning up this directory, or `unload = TRUE`, then you can ignore the return value.

See Also

[load_uwot](#), [unload_uwot](#)

Examples

```
iris_train <- iris[c(1:10, 51:60), ]
iris_test <- iris[100:110, ]

# create model
model <- umap(iris_train, ret_model = TRUE, n_epochs = 20)

# save without unloading: this leaves behind a temporary working directory
model_file <- tempfile("iris_umap")
model <- save_uwot(model, file = model_file)

# The model can continue to be used
test_embedding <- umap_transform(iris_test, model)

# To manually unload the model from memory when finished and to clean up
# the working directory (this doesn't touch your model file)
unload_uwot(model)

# At this point, model cannot be used with umap_transform, this would fail:
# test_embedding2 <- umap_transform(iris_test, model)

# restore the model: this also creates a temporary working directory
model2 <- load_uwot(file = model_file)
test_embedding2 <- umap_transform(iris_test, model2)

# Unload and clean up the loaded model temp directory
unload_uwot(model2)

# clean up the model file
unlink(model_file)

# save with unloading: this deletes the temporary working directory but
# doesn't allow the model to be re-used
model3 <- umap(iris_train, ret_model = TRUE, n_epochs = 20)
model_file3 <- tempfile("iris_umap")
model3 <- save_uwot(model3, file = model_file3, unload = TRUE)
```

similarity_graph

Similarity Graph

Description

Create a graph (as a sparse symmetric weighted adjacency matrix) representing the similarities between items in a data set. No dimensionality reduction is carried out. By default, the similarities are

calculated using the merged fuzzy simplicial set approach in the Uniform Manifold Approximation and Projection (UMAP) method (McInnes et al., 2018), but the approach from LargeVis (Tang et al., 2016) can also be used.

Usage

```
similarity_graph(
  X = NULL,
  n_neighbors = NULL,
  metric = "euclidean",
  scale = NULL,
  set_op_mix_ratio = 1,
  local_connectivity = 1,
  nn_method = NULL,
  n_trees = 50,
  search_k = 2 * n_neighbors * n_trees,
  perplexity = 50,
  method = "umap",
  y = NULL,
  target_n_neighbors = n_neighbors,
  target_metric = "euclidean",
  target_weight = 0.5,
  pca = NULL,
  pca_center = TRUE,
  ret_extra = c(),
  n_threads = NULL,
  grain_size = 1,
  kernel = "gauss",
  tmpdir = tempdir(),
  verbose = getOption("verbose", TRUE),
  pca_method = NULL,
  binary_edge_weights = FALSE
)
```

Arguments

- | | |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| X | Input data. Can be a data.frame , matrix , dist object or sparseMatrix . Matrix and data frames should contain one observation per row. Data frames will have any non-numeric columns removed, although factor columns will be used if explicitly included via <code>metric</code> (see the help for <code>metric</code> for details). A sparse matrix is interpreted as a distance matrix, and is assumed to be symmetric, so you can also pass in an explicitly upper or lower triangular sparse matrix to save storage. There must be at least <code>n_neighbors</code> non-zero distances for each row. Both implicit and explicit zero entries are ignored. Set zero distances you want to keep to an arbitrarily small non-zero value (e.g. $1e-10$). X can also be NULL if pre-computed nearest neighbor data is passed to <code>nn_method</code> . |
| n_neighbors | The size of local neighborhood (in terms of number of neighboring sample points) used for manifold approximation. Larger values result in more global |

views of the manifold, while smaller values result in more local data being preserved. In general values should be in the range 2 to 100.

metric

Type of distance metric to use to find nearest neighbors. One of:

- "euclidean" (the default)
- "cosine"
- "manhattan"
- "hamming"
- "correlation" (a distance based on the Pearson correlation)
- "categorical" (see below)

Only applies if `nn_method = "annoy"` (for `nn_method = "fnn"`, the distance metric is always "euclidean").

If `X` is a data frame or matrix, then multiple metrics can be specified, by passing a list to this argument, where the name of each item in the list is one of the metric names above. The value of each list item should be a vector giving the names or integer ids of the columns to be included in a calculation, e.g. `metric = list(euclidean = 1:4, manhattan = 5:10)`.

Each metric calculation results in a separate fuzzy simplicial set, which are intersected together to produce the final set. Metric names can be repeated. Because non-numeric columns are removed from the data frame, it is safer to use column names than integer ids.

Factor columns can also be used by specifying the metric name "categorical". Factor columns are treated different from numeric columns and although multiple factor columns can be specified in a vector, each factor column specified is processed individually. If you specify a non-factor column, it will be coerced to a factor.

For a given data block, you may override the `pca` and `pca_center` arguments for that block, by providing a list with one unnamed item containing the column names or ids, and then any of the `pca` or `pca_center` overrides as named items, e.g. `metric = list(euclidean = 1:4, manhattan = list(5:10, pca_center = FALSE))`. This exists to allow mixed binary and real-valued data to be included and to have PCA applied to both, but with centering applied only to the real-valued data (it is typical not to apply centering to binary data before PCA is applied).

scale

Scaling to apply to `X` if it is a data frame or matrix:

- "none" or FALSE or NULL No scaling.
- "Z" or "scale" or TRUE Scale each column to zero mean and variance 1.
- "maxabs" Center each column to mean 0, then divide each element by the maximum absolute value over the entire matrix.
- "range" Range scale the entire matrix, so the smallest element is 0 and the largest is 1.
- "colrange" Scale each column in the range (0,1).

For method "umap", the default is "none". For "largevis", the default is "maxabs".

set_op_mix_ratio	Interpolate between (fuzzy) union and intersection as the set operation used to combine local fuzzy simplicial sets to obtain a global fuzzy simplicial sets. Both fuzzy set operations use the product t-norm. The value of this parameter should be between 0.0 and 1.0; a value of 1.0 will use a pure fuzzy union, while 0.0 will use a pure fuzzy intersection. Ignored if method = "largevis"
local_connectivity	The local connectivity required – i.e. the number of nearest neighbors that should be assumed to be connected at a local level. The higher this value the more connected the manifold becomes locally. In practice this should be not more than the local intrinsic dimension of the manifold. Ignored if method = "largevis".
nn_method	<p>Method for finding nearest neighbors. Options are:</p> <ul style="list-style-type: none"> • "fnn". Use exact nearest neighbors via the FNN package. • "annoy" Use approximate nearest neighbors via the RcppAnnoy package. <p>By default, if X has less than 4,096 vertices, the exact nearest neighbors are found. Otherwise, approximate nearest neighbors are used. You may also pass pre-calculated nearest neighbor data to this argument. It must be one of two formats, either a list consisting of two elements:</p> <ul style="list-style-type: none"> • "idx". A $n_vertices \times n_neighbors$ matrix containing the integer indexes of the nearest neighbors in X. Each vertex is considered to be its own nearest neighbor, i.e. <code>idx[, 1] == 1:n_vertices</code>. • "dist". A $n_vertices \times n_neighbors$ matrix containing the distances of the nearest neighbors. <p>or a sparse distance matrix of type <code>dgCMatrix</code>, with dimensions $n_vertices \times n_vertices$. Distances should be arranged by column, i.e. a non-zero entry in row j of the ith column indicates that the jth observation in X is a nearest neighbor of the ith observation with the distance given by the value of that element. The <code>n_neighbors</code> parameter is ignored when using precomputed nearest neighbor data. If using the sparse distance matrix input, each column can contain a different number of neighbors.</p>
n_trees	Number of trees to build when constructing the nearest neighbor index. The more trees specified, the larger the index, but the better the results. With <code>search_k</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy". Sensible values are between 10 to 100.
search_k	Number of nodes to search during the neighbor retrieval. The larger k , the more the accurate results, but the longer the search takes. With <code>n_trees</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy".
perplexity	Used only if method = "largevis". Controls the size of the local neighborhood used for manifold approximation. Should be a value between 1 and one less than the number of items in X . If specified, you should <i>not</i> specify a value for <code>n_neighbors</code> unless you know what you are doing.
method	<p>How to generate the similarities between items. One of:</p> <ul style="list-style-type: none"> • "umap" The UMAP method of McInnes et al. (2018).

	<ul style="list-style-type: none"> • "largevis" The LargeVis method of Tang et al. (2016).
y	<p>Optional target data to add supervised or semi-supervised weighting to the similarity graph . Can be a vector, matrix or data frame. Use the <code>target_metric</code> parameter to specify the metrics to use, using the same syntax as <code>metric</code>. Usually either a single numeric or factor column is used, but more complex formats are possible. The following types are allowed:</p> <ul style="list-style-type: none"> • Factor columns with the same length as <code>X</code>. NA is allowed for any observation with an unknown level, in which case UMAP operates as a form of semi-supervised learning. Each column is treated separately. • Numeric data. NA is <i>not</i> allowed in this case. Use the parameter <code>target_n_neighbors</code> to set the number of neighbors used with <code>y</code>. If unset, <code>n_neighbors</code> is used. Unlike factors, numeric columns are grouped into one block unless <code>target_metric</code> specifies otherwise. For example, if you wish columns <code>a</code> and <code>b</code> to be treated separately, specify <code>target_metric = list(euclidean = "a", euclidean = "b")</code>. Otherwise, the data will be effectively treated as a matrix with two columns. • Nearest neighbor data, consisting of a list of two matrices, <code>idx</code> and <code>dist</code>. These represent the precalculated nearest neighbor indices and distances, respectively. This is the same format as that expected for precalculated data in <code>nn_method</code>. This format assumes that the underlying data was a numeric vector. Any user-supplied value of the <code>target_n_neighbors</code> parameter is ignored in this case, because the the number of columns in the matrices is used for the value. Multiple nearest neighbor data using different metrics can be supplied by passing a list of these lists. <p>Unlike <code>X</code>, all factor columns included in <code>y</code> are automatically used. This parameter is ignored if <code>method = "largevis"</code>.</p>
target_n_neighbors	<p>Number of nearest neighbors to use to construct the target simplicial set. Default value is <code>n_neighbors</code>. Applies only if <code>y</code> is non-NULL and numeric. This parameter is ignored if <code>method = "largevis"</code>.</p>
target_metric	<p>The metric used to measure distance for <code>y</code> if using supervised dimension reduction. Used only if <code>y</code> is numeric. This parameter is ignored if <code>method = "largevis"</code>.</p>
target_weight	<p>Weighting factor between data topology and target topology. A value of 0.0 weights entirely on data, a value of 1.0 weights entirely on target. The default of 0.5 balances the weighting equally between data and target. Only applies if <code>y</code> is non-NULL. This parameter is ignored if <code>method = "largevis"</code>.</p>
pca	<p>If set to a positive integer value, reduce data to this number of columns using PCA. Doesn't applied if the distance <code>metric</code> is "hamming", or the dimensions of the data is larger than the number specified (i.e. number of rows and columns must be larger than the value of this parameter). If you have > 100 columns in a data frame or matrix, reducing the number of columns in this way may substantially increase the performance of the nearest neighbor search at the cost of a potential decrease in accuracy. In many t-SNE applications, a value of 50 is recommended, although there's no guarantee that this is appropriate for all settings.</p>

pca_center	If TRUE, center the columns of X before carrying out PCA. For binary data, it's recommended to set this to FALSE.
ret_extra	A vector indicating what extra data to return. May contain any combination of the following strings: <ul style="list-style-type: none">• "nn" nearest neighbor data that can be used as input to nn_method to avoid the overhead of repeatedly calculating the nearest neighbors when manipulating unrelated parameters. See the "Value" section for the names of the list items. Note that the nearest neighbors could be sensitive to data scaling, so be wary of reusing nearest neighbor data if modifying the scale parameter.• "sigma" the normalization value for each observation in the dataset when constructing the smoothed distances to each of its neighbors. This gives some sense of the local density of each observation in the high dimensional space: higher values of sigma indicate a higher dispersion or lower density.
n_threads	Number of threads to use. Default is half the number of concurrent threads supported by the system. For nearest neighbor search, only applies if nn_method = "annoy". If n_threads > 1, then the Annoy index will be temporarily written to disk in the location determined by tempfile .
grain_size	The minimum amount of work to do on each thread. If this value is set high enough, then less than n_threads will be used for processing, which might give a performance improvement if the overhead of thread management and context switching was outweighing the improvement due to concurrent processing. This should be left at default (1) and work will be spread evenly over all the threads specified.
kernel	Used only if method = "largevis". Type of kernel function to create input similarities. Can be one of "gauss" (the default) or "knn". "gauss" uses the usual Gaussian weighted similarities. "knn" assigns equal similarities to every edge in the nearest neighbor graph, and zero otherwise, using perplexity nearest neighbors. The n_neighbors parameter is ignored in this case.
tmpdir	Temporary directory to store nearest neighbor indexes during nearest neighbor search. Default is tmpdir . The index is only written to disk if n_threads > 1 and nn_method = "annoy"; otherwise, this parameter is ignored.
verbose	If TRUE, log details to the console.
pca_method	Method to carry out any PCA dimensionality reduction when the pca parameter is specified. Allowed values are: <ul style="list-style-type: none">• "irlba". Uses prcomp_irlba from the irlba package.• "rsvd". Uses 5 iterations of svdr from the irlba package. This is likely to give much faster but potentially less accurate results than using "irlba". For the purposes of nearest neighbor calculation and coordinates initialization, any loss of accuracy doesn't seem to matter much.• "bigstatsr". Uses big_randomSVD from the bigstatsr package. The SVD methods used in bigstatsr may be faster on systems without access to efficient linear algebra libraries (e.g. Windows). Note: bigstatsr is <i>not</i> a dependency of uwot: if you choose to use this package for PCA, you <i>must</i> install it yourself.

- "svd". Uses `svd` for the SVD. This is likely to be slow for all but the smallest datasets.
- "auto" (the default). Uses "irlba", unless more than 50 case "svd" is used.

binary_edge_weights

If TRUE then edge weights of the returned graph are binary (0/1) rather than reflecting the degree of similarity.

Details

This is equivalent to running `umap` with the `ret_extra = c("fgraph")` parameter, but without the overhead of calculating (or returning) the optimized low-dimensional coordinates.

Value

A sparse symmetrized matrix of the similarities between the items in `X` or if `nn_method` contains pre-computed nearest neighbor data, the items in `nn_method`. Because of the symmetrization, there may be more non-zero items in each column than the specified value of `n_neighbors` (or pre-computed neighbors in `nn_method`). If `ret_extra` is specified then the return value will be a list containing:

- `similarity_graph` the similarity graph as a sparse matrix as described above.
- `nn` (if `ret_extra` contained "nn") the nearest neighbor data as a list called `nn`. This contains one list for each metric calculated, itself containing a matrix `idx` with the integer ids of the neighbors; and a matrix `dist` with the distances. The `nn` list (or a sub-list) can be used as input to the `nn_method` parameter.
- `sigma` (if `ret_extra` contains "sigma"), a vector of calibrated parameters, one for each item in the input data, reflecting the local data density for that item. The exact definition of the values depends on the choice of the method parameter.
- `rho` (if `ret_extra` contains "sigma"), a vector containing the largest distance to the locally connected neighbors of each item in the input data. This will exist only if `method = "umap"`.
- `localr` (if `ret_extra` contains "localr") a vector of the estimated local radii, the sum of "sigma" and "rho". This will exist only if `method = "umap"`.

References

McInnes, L., Healy, J., & Melville, J. (2018). UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction *arXiv preprint arXiv:1802.03426*. <https://arxiv.org/abs/1802.03426>

Tang, J., Liu, J., Zhang, M., & Mei, Q. (2016, April). Visualizing large-scale and high-dimensional data. In *Proceedings of the 25th International Conference on World Wide Web* (pp. 287-297). International World Wide Web Conferences Steering Committee. <https://arxiv.org/abs/1602.00370>

Examples

```
iris30 <- iris[c(1:10, 51:60, 101:110), ]
```

```

# return a 30 x 30 sparse matrix with similarity data based on 10 nearest
# neighbors per item
iris30_sim_graph <- similarity_graph(iris30, n_neighbors = 10)

# Default is to use the UMAP method of calculating similarities, but LargeVis
# is also available: for that method, use perplexity instead of n_neighbors
# to control neighborhood size. Use ret_extra = "nn" to return nearest
# neighbor data as well as the similarity graph. Return value is a list
# containing similarity_graph' and 'nn' items.
iris30_lv_graph <- similarity_graph(iris30, perplexity = 10,
                                  method = "largevis", ret_extra = "nn")
# If you have the neighbor information you don't need the original data
iris30_lv_graph_nn <- similarity_graph(nn_method = iris30_lv_graph$nn,
                                      perplexity = 10, method = "largevis")
all(iris30_lv_graph_nn == iris30_lv_graph$similarity_graph)

```

tumap

Dimensionality Reduction Using t-Distributed UMAP (t-UMAP)

Description

A faster (but less flexible) version of the UMAP gradient. For more detail on UMAP, see the [umap](#) function.

Usage

```

tumap(
  X,
  n_neighbors = 15,
  n_components = 2,
  metric = "euclidean",
  n_epochs = NULL,
  learning_rate = 1,
  scale = FALSE,
  init = "spectral",
  init_sdev = NULL,
  set_op_mix_ratio = 1,
  local_connectivity = 1,
  bandwidth = 1,
  repulsion_strength = 1,
  negative_sample_rate = 5,
  nn_method = NULL,
  n_trees = 50,
  search_k = 2 * n_neighbors * n_trees,
  n_threads = NULL,
  n_sgd_threads = 0,

```

```

grain_size = 1,
y = NULL,
target_n_neighbors = n_neighbors,
target_metric = "euclidean",
target_weight = 0.5,
pca = NULL,
pca_center = TRUE,
pcg_rand = TRUE,
fast_sgd = FALSE,
ret_model = FALSE,
ret_nn = FALSE,
ret_extra = c(),
tmpdir = tempdir(),
verbose = getOption("verbose", TRUE),
batch = FALSE,
opt_args = NULL,
epoch_callback = NULL,
pca_method = NULL,
binary_edge_weights = FALSE
)

```

Arguments

- | | |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| X | Input data. Can be a <code>data.frame</code> , <code>matrix</code> , <code>dist</code> object or <code>sparseMatrix</code> . Matrix and data frames should contain one observation per row. Data frames will have any non-numeric columns removed, although factor columns will be used if explicitly included via <code>metric</code> (see the help for <code>metric</code> for details). A sparse matrix is interpreted as a distance matrix, and is assumed to be symmetric, so you can also pass in an explicitly upper or lower triangular sparse matrix to save storage. There must be at least <code>n_neighbors</code> non-zero distances for each row. Both implicit and explicit zero entries are ignored. Set zero distances you want to keep to an arbitrarily small non-zero value (e.g. $1e-10$). X can also be NULL if pre-computed nearest neighbor data is passed to <code>nn_method</code> , and <code>init</code> is not "spca" or "pca". |
| n_neighbors | The size of local neighborhood (in terms of number of neighboring sample points) used for manifold approximation. Larger values result in more global views of the manifold, while smaller values result in more local data being preserved. In general values should be in the range 2 to 100. |
| n_components | The dimension of the space to embed into. This defaults to 2 to provide easy visualization, but can reasonably be set to any integer value in the range 2 to 100. |
| metric | Type of distance metric to use to find nearest neighbors. One of: <ul style="list-style-type: none"> • "euclidean" (the default) • "cosine" • "manhattan" • "hamming" • "correlation" (a distance based on the Pearson correlation) |

- "categorical" (see below)

Only applies if `nn_method = "annoy"` (for `nn_method = "fnn"`, the distance metric is always "euclidean").

If `X` is a data frame or matrix, then multiple metrics can be specified, by passing a list to this argument, where the name of each item in the list is one of the metric names above. The value of each list item should be a vector giving the names or integer ids of the columns to be included in a calculation, e.g. `metric = list(euclidean = 1:4, manhattan = 5:10)`.

Each metric calculation results in a separate fuzzy simplicial set, which are intersected together to produce the final set. Metric names can be repeated. Because non-numeric columns are removed from the data frame, it is safer to use column names than integer ids.

Factor columns can also be used by specifying the metric name "categorical". Factor columns are treated different from numeric columns and although multiple factor columns can be specified in a vector, each factor column specified is processed individually. If you specify a non-factor column, it will be coerced to a factor.

For a given data block, you may override the `pca` and `pca_center` arguments for that block, by providing a list with one unnamed item containing the column names or ids, and then any of the `pca` or `pca_center` overrides as named items, e.g. `metric = list(euclidean = 1:4, manhattan = list(5:10, pca_center = FALSE))`. This exists to allow mixed binary and real-valued data to be included and to have PCA applied to both, but with centering applied only to the real-valued data (it is typical not to apply centering to binary data before PCA is applied).

<code>n_epochs</code>	Number of epochs to use during the optimization of the embedded coordinates. By default, this value is set to 500 for datasets containing 10,000 vertices or less, and 200 otherwise. If <code>n_epochs = 0</code> , then coordinates determined by "init" will be returned.
<code>learning_rate</code>	Initial learning rate used in optimization of the coordinates.
<code>scale</code>	Scaling to apply to <code>X</code> if it is a data frame or matrix: <ul style="list-style-type: none"> • "none" or FALSE or NULL No scaling. • "Z" or "scale" or TRUE Scale each column to zero mean and variance 1. • "maxabs" Center each column to mean 0, then divide each element by the maximum absolute value over the entire matrix. • "range" Range scale the entire matrix, so the smallest element is 0 and the largest is 1. • "colrange" Scale each column in the range (0,1). <p>For t-UMAP, the default is "none".</p>
<code>init</code>	Type of initialization for the coordinates. Options are: <ul style="list-style-type: none"> • "spectral" Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, with Gaussian noise added. • "normlaplacian". Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, without noise.

- "random". Coordinates assigned using a uniform random distribution between -10 and 10.
- "lvrandom". Coordinates assigned using a Gaussian distribution with standard deviation $1e-4$, as used in LargeVis (Tang et al., 2016) and t-SNE.
- "laplacian". Spectral embedding using the Laplacian Eigenmap (Belkin and Niyogi, 2002).
- "pca". The first two principal components from PCA of X if X is a data frame, and from a 2-dimensional classical MDS if X is of class "dist".
- "spca". Like "pca", but each dimension is then scaled so the standard deviation is $1e-4$, to give a distribution similar to that used in t-SNE. This is an alias for `init = "pca"`, `init_sdev = 1e-4`.
- "agspectral" An "approximate global" modification of "spectral" which all edges in the graph to a value of 1, and then sets a random number of edges (`negative_sample_rate` edges per vertex) to 0.1, to approximate the effect of non-local affinities.
- A matrix of initial coordinates.

For spectral initializations, ("spectral", "normlaplacian", "laplacian"), if more than one connected component is identified, each connected component is initialized separately and the results are merged. If `verbose = TRUE` the number of connected components are logged to the console. The existence of multiple connected components implies that a global view of the data cannot be attained with this initialization. Either a PCA-based initialization or increasing the value of `n_neighbors` may be more appropriate.

<code>init_sdev</code>	If non-NULL, scales each dimension of the initialized coordinates (including any user-supplied matrix) to this standard deviation. By default no scaling is carried out, except when <code>init = "spca"</code> , in which case the value is 0.0001 . Scaling the input may help if the unscaled versions result in initial coordinates with large inter-point distances or outliers. This usually results in small gradients during optimization and very little progress being made to the layout. Shrinking the initial embedding by rescaling can help under these circumstances. Scaling the result of <code>init = "pca"</code> is usually recommended and <code>init = "spca"</code> as an alias for <code>init = "pca"</code> , <code>init_sdev = 1e-4</code> but for the spectral initializations the scaled versions usually aren't necessary unless you are using a large value of <code>n_neighbors</code> (e.g. <code>n_neighbors = 150</code> or higher).
<code>set_op_mix_ratio</code>	Interpolate between (fuzzy) union and intersection as the set operation used to combine local fuzzy simplicial sets to obtain a global fuzzy simplicial sets. Both fuzzy set operations use the product t-norm. The value of this parameter should be between 0.0 and 1.0 ; a value of 1.0 will use a pure fuzzy union, while 0.0 will use a pure fuzzy intersection.
<code>local_connectivity</code>	The local connectivity required – i.e. the number of nearest neighbors that should be assumed to be connected at a local level. The higher this value the more connected the manifold becomes locally. In practice this should be not more than the local intrinsic dimension of the manifold.
<code>bandwidth</code>	The effective bandwidth of the kernel if we view the algorithm as similar to

Laplacian Eigenmaps. Larger values induce more connectivity and a more global view of the data, smaller values concentrate more locally.

repulsion_strength	Weighting applied to negative samples in low dimensional embedding optimization. Values higher than one will result in greater weight being given to negative samples.
negative_sample_rate	The number of negative edge/1-simplex samples to use per positive edge/1-simplex sample in optimizing the low dimensional embedding.
nn_method	<p>Method for finding nearest neighbors. Options are:</p> <ul style="list-style-type: none"> • "fnn". Use exact nearest neighbors via the FNN package. • "annoy" Use approximate nearest neighbors via the RcppAnnoy package. <p>By default, if X has less than 4,096 vertices, the exact nearest neighbors are found. Otherwise, approximate nearest neighbors are used. You may also pass pre-calculated nearest neighbor data to this argument. It must be one of two formats, either a list consisting of two elements:</p> <ul style="list-style-type: none"> • "idx". A $n_vertices \times n_neighbors$ matrix containing the integer indexes of the nearest neighbors in X. Each vertex is considered to be its own nearest neighbor, i.e. <code>idx[, 1] == 1:n_vertices</code>. • "dist". A $n_vertices \times n_neighbors$ matrix containing the distances of the nearest neighbors. <p>or a sparse distance matrix of type <code>dgCMatrix</code>, with dimensions $n_vertices \times n_vertices$. Distances should be arranged by column, i.e. a non-zero entry in row j of the ith column indicates that the jth observation in X is a nearest neighbor of the ith observation with the distance given by the value of that element. The <code>n_neighbors</code> parameter is ignored when using precomputed nearest neighbor data. If using the sparse distance matrix input, each column can contain a different number of neighbors.</p>
n_trees	Number of trees to build when constructing the nearest neighbor index. The more trees specified, the larger the index, but the better the results. With <code>search_k</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy". Sensible values are between 10 to 100.
search_k	Number of nodes to search during the neighbor retrieval. The larger k , the more the accurate results, but the longer the search takes. With <code>n_trees</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy".
n_threads	Number of threads to use (except during stochastic gradient descent). Default is half the number of concurrent threads supported by the system. For nearest neighbor search, only applies if <code>nn_method = "annoy"</code> . If <code>n_threads > 1</code> , then the Annoy index will be temporarily written to disk in the location determined by <code>tempfile</code> .
n_sgd_threads	Number of threads to use during stochastic gradient descent. If set to > 1 , then be aware that if <code>batch = FALSE</code> , results will <i>not</i> be reproducible, even if <code>set.seed</code> is called with a fixed seed before running. Set to "auto" to use the same value as <code>n_threads</code> .

grain_size	The minimum amount of work to do on each thread. If this value is set high enough, then less than <code>n_threads</code> or <code>n_sgd_threads</code> will be used for processing, which might give a performance improvement if the overhead of thread management and context switching was outweighing the improvement due to concurrent processing. This should be left at default (1) and work will be spread evenly over all the threads specified.
y	<p>Optional target data for supervised dimension reduction. Can be a vector, matrix or data frame. Use the <code>target_metric</code> parameter to specify the metrics to use, using the same syntax as <code>metric</code>. Usually either a single numeric or factor column is used, but more complex formats are possible. The following types are allowed:</p> <ul style="list-style-type: none"> • Factor columns with the same length as <code>X</code>. NA is allowed for any observation with an unknown level, in which case UMAP operates as a form of semi-supervised learning. Each column is treated separately. • Numeric data. NA is <i>not</i> allowed in this case. Use the parameter <code>target_n_neighbors</code> to set the number of neighbors used with <code>y</code>. If unset, <code>n_neighbors</code> is used. Unlike factors, numeric columns are grouped into one block unless <code>target_metric</code> specifies otherwise. For example, if you wish columns <code>a</code> and <code>b</code> to be treated separately, specify <code>target_metric = list(euclidean = "a", euclidean = "b")</code>. Otherwise, the data will be effectively treated as a matrix with two columns. • Nearest neighbor data, consisting of a list of two matrices, <code>idx</code> and <code>dist</code>. These represent the precalculated nearest neighbor indices and distances, respectively. This is the same format as that expected for precalculated data in <code>nn_method</code>. This format assumes that the underlying data was a numeric vector. Any user-supplied value of the <code>target_n_neighbors</code> parameter is ignored in this case, because the the number of columns in the matrices is used for the value. Multiple nearest neighbor data using different metrics can be supplied by passing a list of these lists. <p>Unlike <code>X</code>, all factor columns included in <code>y</code> are automatically used.</p>
target_n_neighbors	Number of nearest neighbors to use to construct the target simplicial set. Default value is <code>n_neighbors</code> . Applies only if <code>y</code> is non-NULL and numeric.
target_metric	The metric used to measure distance for <code>y</code> if using supervised dimension reduction. Used only if <code>y</code> is numeric.
target_weight	Weighting factor between data topology and target topology. A value of 0.0 weights entirely on data, a value of 1.0 weights entirely on target. The default of 0.5 balances the weighting equally between data and target. Only applies if <code>y</code> is non-NULL.
pca	If set to a positive integer value, reduce data to this number of columns using PCA. Doesn't applied if the distance metric is "hamming", or the dimensions of the data is larger than the number specified (i.e. number of rows and columns must be larger than the value of this parameter). If you have > 100 columns in a data frame or matrix, reducing the number of columns in this way may substantially increase the performance of the nearest neighbor search at the cost of a potential decrease in accuracy. In many t-SNE applications, a value of 50

is recommended, although there's no guarantee that this is appropriate for all settings.

pca_center	If TRUE, center the columns of X before carrying out PCA. For binary data, it's recommended to set this to FALSE.
pcg_rand	If TRUE, use the PCG random number generator (O'Neill, 2014) during optimization. Otherwise, use the faster (but probably less statistically good) Tausworthe "taus88" generator. The default is TRUE.
fast_sgd	If TRUE, then the following combination of parameters is set: pcg_rand = TRUE and n_sgd_threads = "auto". The default is FALSE. Setting this to TRUE will speed up the stochastic optimization phase, but give a potentially less accurate embedding, and which will not be exactly reproducible even with a fixed seed. For visualization, fast_sgd = TRUE will give perfectly good results. For more generic dimensionality reduction, it's safer to leave fast_sgd = FALSE. If fast_sgd = TRUE, then user-supplied values of pcg_rand and n_sgd_threads, are ignored.
ret_model	If TRUE, then return extra data that can be used to add new data to an existing embedding via umap_transform . The embedded coordinates are returned as the list item embedding. If FALSE, just return the coordinates. This parameter can be used in conjunction with ret_nn and ret_extra. Note that some settings are incompatible with the production of a UMAP model: external neighbor data (passed via a list to nn_method), and factor columns that were included via the metric parameter. In the latter case, the model produced is based only on the numeric data. A transformation using new data is possible, but the factor columns in the new data are ignored.
ret_nn	If TRUE, then in addition to the embedding, also return nearest neighbor data that can be used as input to nn_method to avoid the overhead of repeatedly calculating the nearest neighbors when manipulating unrelated parameters (e.g. min_dist, n_epochs, init). See the "Value" section for the names of the list items. If FALSE, just return the coordinates. Note that the nearest neighbors could be sensitive to data scaling, so be wary of reusing nearest neighbor data if modifying the scale parameter. This parameter can be used in conjunction with ret_model and ret_extra.
ret_extra	A vector indicating what extra data to return. May contain any combination of the following strings: <ul style="list-style-type: none"> • "model" Same as setting ret_model = TRUE. • "nn" Same as setting ret_nn = TRUE. • "fgraph" the high dimensional fuzzy graph (i.e. the fuzzy simplicial set of the merged local views of the input data). The graph is returned as a sparse symmetric N x N matrix of class dgCMatrix-class, where a non-zero entry (i, j) gives the membership strength of the edge connecting vertex i and vertex j. This can be considered analogous to the input probability (or similarity or affinity) used in t-SNE and LargeVis. Note that the graph is further sparsified by removing edges with sufficiently low membership strength that they would not be sampled by the probabilistic edge sampling employed for optimization and therefore the number of non-zero elements in the matrix is dependent on n_epochs. If you are only interested in the

fuzzy input graph (e.g. for clustering), setting `n_epochs = 0` will avoid any further sparsifying. Be aware that setting `binary_edge_weights = TRUE` will affect this graph (all non-zero edge weights will be 1).

- "sigma" the normalization value for each observation in the dataset when constructing the smoothed distances to each of its neighbors. This gives some sense of the local density of each observation in the high dimensional space: higher values of sigma indicate a higher dispersion or lower density.

<code>tmpdir</code>	Temporary directory to store nearest neighbor indexes during nearest neighbor search. Default is <code>tmpdir</code> . The index is only written to disk if <code>n_threads > 1</code> and <code>nn_method = "annoy"</code> ; otherwise, this parameter is ignored.
<code>verbose</code>	If TRUE, log details to the console.
<code>batch</code>	If TRUE, then embedding coordinates are updated at the end of each epoch rather than during the epoch. In batch mode, results are reproducible with a fixed random seed even with <code>n_sgd_threads > 1</code> , at the cost of a slightly higher memory use. You may also have to modify <code>learning_rate</code> and increase <code>n_epochs</code> , so whether this provides a speed increase over the single-threaded optimization is likely to be dataset and hardware-dependent.
<code>opt_args</code>	<p>A list of optimizer parameters, used when <code>batch = TRUE</code>. The default optimization method used is Adam (Kingma and Ba, 2014).</p> <ul style="list-style-type: none"> • <code>method</code> The optimization method to use. Either "adam" or "sgd" (stochastic gradient descent). Default: "adam". • <code>beta1</code> (Adam only). The weighting parameter for the exponential moving average of the first moment estimator. Effectively the momentum parameter. Should be a floating point value between 0 and 1. Higher values can smooth oscillatory updates in poorly-conditioned situations and may allow for a larger <code>learning_rate</code> to be specified, but too high can cause divergence. Default: 0.5. • <code>beta2</code> (Adam only). The weighting parameter for the exponential moving average of the uncentered second moment estimator. Should be a floating point value between 0 and 1. Controls the degree of adaptivity in the step-size. Higher values put more weight on previous time steps. Default: 0.9. • <code>eps</code> (Adam only). Intended to be a small value to prevent division by zero, but in practice can also affect convergence due to its interaction with <code>beta2</code>. Higher values reduce the effect of the step-size adaptivity and bring the behavior closer to stochastic gradient descent with momentum. Typical values are between 1e-8 and 1e-3. Default: 1e-7. • <code>alpha</code> The initial learning rate. Default: the value of the <code>learning_rate</code> parameter.
<code>epoch_callback</code>	<p>A function which will be invoked at the end of every epoch. Its signature should be: <code>(epoch, n_epochs, coords)</code>, where:</p> <ul style="list-style-type: none"> • <code>epoch</code> The current epoch number (between 1 and <code>n_epochs</code>). • <code>n_epochs</code> Number of epochs to use during the optimization of the embedded coordinates. • <code>coords</code> The embedded coordinates as of the end of the current epoch, as a matrix with dimensions <code>(N, n_components)</code>.

pca_method	<p>Method to carry out any PCA dimensionality reduction when the <code>pca</code> parameter is specified. Allowed values are:</p> <ul style="list-style-type: none"> • "irlba". Uses <code>prcomp_irlba</code> from the <code>irlba</code> package. • "rsvd". Uses 5 iterations of <code>svdr</code> from the <code>irlba</code> package. This is likely to give much faster but potentially less accurate results than using "irlba". For the purposes of nearest neighbor calculation and coordinates initialization, any loss of accuracy doesn't seem to matter much. • "bigstatsr". Uses <code>big_randomSVD</code> from the <code>bigstatsr</code> package. The SVD methods used in <code>bigstatsr</code> may be faster on systems without access to efficient linear algebra libraries (e.g. Windows). Note: <code>bigstatsr</code> is <i>not</i> a dependency of <code>uwot</code>: if you choose to use this package for PCA, you <i>must</i> install it yourself. • "svd". Uses <code>svd</code> for the SVD. This is likely to be slow for all but the smallest datasets. • "auto" (the default). Uses "irlba", unless more than 50 case "svd" is used.
binary_edge_weights	<p>If TRUE then edge weights in the input graph are treated as binary (0/1) rather than real valued. This affects the sampling frequency of neighbors and is the strategy used by the PaCMAP method (Wang and co-workers, 2020). Practical (Böhm and co-workers, 2020) and theoretical (Damrich and Hamprecht, 2021) work suggests this has little effect on UMAP's performance.</p>

Details

By setting the UMAP curve parameters `a` and `b` to 1, you get back the Cauchy distribution as used in t-SNE and LargeVis. It also results in a substantially simplified gradient expression. This can give a speed improvement of around 50%.

Value

A matrix of optimized coordinates, or:

- if `ret_model = TRUE` (or `ret_extra` contains "model"), returns a list containing extra information that can be used to add new data to an existing embedding via `umap_transform`. In this case, the coordinates are available in the list item `embedding`. **NOTE:** The contents of the `model` list should *not* be considered stable or part of the public API, and are purposely left undocumented.
- if `ret_nn = TRUE` (or `ret_extra` contains "nn"), returns the nearest neighbor data as a list called `nn`. This contains one list for each `metric` calculated, itself containing a matrix `idx` with the integer ids of the neighbors; and a matrix `dist` with the distances. The `nn` list (or a sub-list) can be used as input to the `nn_method` parameter.
- if `ret_extra` contains "fgraph" returns the high dimensional fuzzy graph as a sparse matrix called `fgraph`, of type `dgCMatrix-class`.
- if `ret_extra` contains "sigma", returns a vector of the smooth knn distance normalization terms for each observation as "sigma" and a vector "rho" containing the largest distance to the locally connected neighbors of each observation.

- if `ret_extra` contains "localr", returns a vector of the estimated local radii, the sum of "sigma" and "rho".

The returned list contains the combined data from any combination of specifying `ret_model`, `ret_nn` and `ret_extra`.

Examples

```
iris_tumap <- tumap(iris, n_neighbors = 50, learning_rate = 0.5)
```

umap

Dimensionality Reduction with UMAP

Description

Carry out dimensionality reduction of a dataset using the Uniform Manifold Approximation and Projection (UMAP) method (McInnes & Healy, 2018). Some of the following help text is lifted verbatim from the Python reference implementation at <https://github.com/lmcinnes/umap>.

Usage

```
umap(
  X,
  n_neighbors = 15,
  n_components = 2,
  metric = "euclidean",
  n_epochs = NULL,
  learning_rate = 1,
  scale = FALSE,
  init = "spectral",
  init_sdev = NULL,
  spread = 1,
  min_dist = 0.01,
  set_op_mix_ratio = 1,
  local_connectivity = 1,
  bandwidth = 1,
  repulsion_strength = 1,
  negative_sample_rate = 5,
  a = NULL,
  b = NULL,
  nn_method = NULL,
  n_trees = 50,
  search_k = 2 * n_neighbors * n_trees,
  approx_pow = FALSE,
  y = NULL,
  target_n_neighbors = n_neighbors,
  target_metric = "euclidean",
  target_weight = 0.5,
```

```

pca = NULL,
pca_center = TRUE,
pcg_rand = TRUE,
fast_sgd = FALSE,
ret_model = FALSE,
ret_nn = FALSE,
ret_extra = c(),
n_threads = NULL,
n_sgd_threads = 0,
grain_size = 1,
tmpdir = tempdir(),
verbose = getOption("verbose", TRUE),
batch = FALSE,
opt_args = NULL,
epoch_callback = NULL,
pca_method = NULL,
binary_edge_weights = FALSE,
dens_scale = NULL
)

```

Arguments

- | | |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| X | Input data. Can be a <code>data.frame</code> , <code>matrix</code> , <code>dist</code> object or <code>sparseMatrix</code> . Matrix and data frames should contain one observation per row. Data frames will have any non-numeric columns removed, although factor columns will be used if explicitly included via <code>metric</code> (see the help for <code>metric</code> for details). A sparse matrix is interpreted as a distance matrix, and is assumed to be symmetric, so you can also pass in an explicitly upper or lower triangular sparse matrix to save storage. There must be at least <code>n_neighbors</code> non-zero distances for each row. Both implicit and explicit zero entries are ignored. Set zero distances you want to keep to an arbitrarily small non-zero value (e.g. $1e-10$). X can also be NULL if pre-computed nearest neighbor data is passed to <code>nn_method</code> , and <code>init</code> is not "spca" or "pca". |
| n_neighbors | The size of local neighborhood (in terms of number of neighboring sample points) used for manifold approximation. Larger values result in more global views of the manifold, while smaller values result in more local data being preserved. In general values should be in the range 2 to 100. |
| n_components | The dimension of the space to embed into. This defaults to 2 to provide easy visualization, but can reasonably be set to any integer value in the range 2 to 100. |
| metric | Type of distance metric to use to find nearest neighbors. One of: <ul style="list-style-type: none"> • "euclidean" (the default) • "cosine" • "manhattan" • "hamming" • "correlation" (a distance based on the Pearson correlation) • "categorical" (see below) |

Only applies if `nn_method = "annoy"` (for `nn_method = "fnn"`, the distance metric is always "euclidean").

If `X` is a data frame or matrix, then multiple metrics can be specified, by passing a list to this argument, where the name of each item in the list is one of the metric names above. The value of each list item should be a vector giving the names or integer ids of the columns to be included in a calculation, e.g. `metric = list(euclidean = 1:4, manhattan = 5:10)`.

Each metric calculation results in a separate fuzzy simplicial set, which are intersected together to produce the final set. Metric names can be repeated. Because non-numeric columns are removed from the data frame, it is safer to use column names than integer ids.

Factor columns can also be used by specifying the metric name "categorical". Factor columns are treated different from numeric columns and although multiple factor columns can be specified in a vector, each factor column specified is processed individually. If you specify a non-factor column, it will be coerced to a factor.

For a given data block, you may override the `pca` and `pca_center` arguments for that block, by providing a list with one unnamed item containing the column names or ids, and then any of the `pca` or `pca_center` overrides as named items, e.g. `metric = list(euclidean = 1:4, manhattan = list(5:10, pca_center = FALSE))`. This exists to allow mixed binary and real-valued data to be included and to have PCA applied to both, but with centering applied only to the real-valued data (it is typical not to apply centering to binary data before PCA is applied).

<code>n_epochs</code>	Number of epochs to use during the optimization of the embedded coordinates. By default, this value is set to 500 for datasets containing 10,000 vertices or less, and 200 otherwise. If <code>n_epochs = 0</code> , then coordinates determined by "init" will be returned.
<code>learning_rate</code>	Initial learning rate used in optimization of the coordinates.
<code>scale</code>	Scaling to apply to <code>X</code> if it is a data frame or matrix: <ul style="list-style-type: none"> • "none" or FALSE or NULL No scaling. • "Z" or "scale" or TRUE Scale each column to zero mean and variance 1. • "maxabs" Center each column to mean 0, then divide each element by the maximum absolute value over the entire matrix. • "range" Range scale the entire matrix, so the smallest element is 0 and the largest is 1. • "colrange" Scale each column in the range (0,1). <p>For UMAP, the default is "none".</p>
<code>init</code>	Type of initialization for the coordinates. Options are: <ul style="list-style-type: none"> • "spectral" Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, with Gaussian noise added. • "normlaplacian". Spectral embedding using the normalized Laplacian of the fuzzy 1-skeleton, without noise. • "random". Coordinates assigned using a uniform random distribution between -10 and 10.

- "lvrandom". Coordinates assigned using a Gaussian distribution with standard deviation $1e-4$, as used in LargeVis (Tang et al., 2016) and t-SNE.
- "laplacian". Spectral embedding using the Laplacian Eigenmap (Belkin and Niyogi, 2002).
- "pca". The first two principal components from PCA of X if X is a data frame, and from a 2-dimensional classical MDS if X is of class "dist".
- "spca". Like "pca", but each dimension is then scaled so the standard deviation is $1e-4$, to give a distribution similar to that used in t-SNE. This is an alias for `init = "pca"`, `init_sdev = 1e-4`.
- "agspectral" An "approximate global" modification of "spectral" which all edges in the graph to a value of 1, and then sets a random number of edges (`negative_sample_rate` edges per vertex) to 0.1, to approximate the effect of non-local affinities.
- A matrix of initial coordinates.

For spectral initializations, ("spectral", "normlaplacian", "laplacian"), if more than one connected component is identified, each connected component is initialized separately and the results are merged. If `verbose = TRUE` the number of connected components are logged to the console. The existence of multiple connected components implies that a global view of the data cannot be attained with this initialization. Either a PCA-based initialization or increasing the value of `n_neighbors` may be more appropriate.

<code>init_sdev</code>	If non-NULL, scales each dimension of the initialized coordinates (including any user-supplied matrix) to this standard deviation. By default no scaling is carried out, except when <code>init = "spca"</code> , in which case the value is 0.0001 . Scaling the input may help if the unscaled versions result in initial coordinates with large inter-point distances or outliers. This usually results in small gradients during optimization and very little progress being made to the layout. Shrinking the initial embedding by rescaling can help under these circumstances. Scaling the result of <code>init = "pca"</code> is usually recommended and <code>init = "spca"</code> as an alias for <code>init = "pca"</code> , <code>init_sdev = 1e-4</code> but for the spectral initializations the scaled versions usually aren't necessary unless you are using a large value of <code>n_neighbors</code> (e.g. <code>n_neighbors = 150</code> or higher).
<code>spread</code>	The effective scale of embedded points. In combination with <code>min_dist</code> , this determines how clustered/clumped the embedded points are.
<code>min_dist</code>	The effective minimum distance between embedded points. Smaller values will result in a more clustered/clumped embedding where nearby points on the manifold are drawn closer together, while larger values will result on a more even dispersal of points. The value should be set relative to the <code>spread</code> value, which determines the scale at which embedded points will be spread out.
<code>set_op_mix_ratio</code>	Interpolate between (fuzzy) union and intersection as the set operation used to combine local fuzzy simplicial sets to obtain a global fuzzy simplicial sets. Both fuzzy set operations use the product t-norm. The value of this parameter should be between 0.0 and 1.0 ; a value of 1.0 will use a pure fuzzy union, while 0.0 will use a pure fuzzy intersection.

local_connectivity	The local connectivity required – i.e. the number of nearest neighbors that should be assumed to be connected at a local level. The higher this value the more connected the manifold becomes locally. In practice this should be not more than the local intrinsic dimension of the manifold.
bandwidth	The effective bandwidth of the kernel if we view the algorithm as similar to Laplacian Eigenmaps. Larger values induce more connectivity and a more global view of the data, smaller values concentrate more locally.
repulsion_strength	Weighting applied to negative samples in low dimensional embedding optimization. Values higher than one will result in greater weight being given to negative samples.
negative_sample_rate	The number of negative edge/1-simplex samples to use per positive edge/1-simplex sample in optimizing the low dimensional embedding.
a	More specific parameters controlling the embedding. If NULL these values are set automatically as determined by <code>min_dist</code> and <code>spread</code> .
b	More specific parameters controlling the embedding. If NULL these values are set automatically as determined by <code>min_dist</code> and <code>spread</code> .
nn_method	Method for finding nearest neighbors. Options are: <ul style="list-style-type: none"> • "fnn". Use exact nearest neighbors via the FNN package. • "annoy" Use approximate nearest neighbors via the RcppAnnoy package. <p>By default, if <code>X</code> has less than 4,096 vertices, the exact nearest neighbors are found. Otherwise, approximate nearest neighbors are used. You may also pass pre-calculated nearest neighbor data to this argument. It must be one of two formats, either a list consisting of two elements:</p> <ul style="list-style-type: none"> • "idx". A <code>n_vertices x n_neighbors</code> matrix containing the integer indexes of the nearest neighbors in <code>X</code>. Each vertex is considered to be its own nearest neighbor, i.e. <code>idx[, 1] == 1:n_vertices</code>. • "dist". A <code>n_vertices x n_neighbors</code> matrix containing the distances of the nearest neighbors. <p>or a sparse distance matrix of type <code>dgCMatrix</code>, with dimensions <code>n_vertices x n_vertices</code>. Distances should be arranged by column, i.e. a non-zero entry in row <code>j</code> of the <code>i</code>th column indicates that the <code>j</code>th observation in <code>X</code> is a nearest neighbor of the <code>i</code>th observation with the distance given by the value of that element. The <code>n_neighbors</code> parameter is ignored when using precomputed nearest neighbor data. If using the sparse distance matrix input, each column can contain a different number of neighbors.</p>
n_trees	Number of trees to build when constructing the nearest neighbor index. The more trees specified, the larger the index, but the better the results. With <code>search_k</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy". Sensible values are between 10 to 100.
search_k	Number of nodes to search during the neighbor retrieval. The larger <code>k</code> , the more the accurate results, but the longer the search takes. With <code>n_trees</code> , determines the accuracy of the Annoy nearest neighbor search. Only used if the <code>nn_method</code> is "annoy".

approx_pow	If TRUE, use an approximation to the power function in the UMAP gradient, from https://martin.ankerl.com/2012/01/25/optimized-approximative-pow-in-c-and-cpp/ .
y	Optional target data for supervised dimension reduction. Can be a vector, matrix or data frame. Use the <code>target_metric</code> parameter to specify the metrics to use, using the same syntax as <code>metric</code> . Usually either a single numeric or factor column is used, but more complex formats are possible. The following types are allowed: <ul style="list-style-type: none"> • Factor columns with the same length as <code>X</code>. NA is allowed for any observation with an unknown level, in which case UMAP operates as a form of semi-supervised learning. Each column is treated separately. • Numeric data. NA is <i>not</i> allowed in this case. Use the parameter <code>target_n_neighbors</code> to set the number of neighbors used with <code>y</code>. If unset, <code>n_neighbors</code> is used. Unlike factors, numeric columns are grouped into one block unless <code>target_metric</code> specifies otherwise. For example, if you wish columns <code>a</code> and <code>b</code> to be treated separately, specify <code>target_metric = list(euclidean = "a", euclidean = "b")</code>. Otherwise, the data will be effectively treated as a matrix with two columns. • Nearest neighbor data, consisting of a list of two matrices, <code>idx</code> and <code>dist</code>. These represent the precalculated nearest neighbor indices and distances, respectively. This is the same format as that expected for precalculated data in <code>nn_method</code>. This format assumes that the underlying data was a numeric vector. Any user-supplied value of the <code>target_n_neighbors</code> parameter is ignored in this case, because the the number of columns in the matrices is used for the value. Multiple nearest neighbor data using different metrics can be supplied by passing a list of these lists. <p>Unlike <code>X</code>, all factor columns included in <code>y</code> are automatically used.</p>
target_n_neighbors	Number of nearest neighbors to use to construct the target simplicial set. Default value is <code>n_neighbors</code> . Applies only if <code>y</code> is non-NULL and numeric.
target_metric	The metric used to measure distance for <code>y</code> if using supervised dimension reduction. Used only if <code>y</code> is numeric.
target_weight	Weighting factor between data topology and target topology. A value of 0.0 weights entirely on data, a value of 1.0 weights entirely on target. The default of 0.5 balances the weighting equally between data and target. Only applies if <code>y</code> is non-NULL.
pca	If set to a positive integer value, reduce data to this number of columns using PCA. Doesn't applied if the distance <code>metric</code> is "hamming", or the dimensions of the data is larger than the number specified (i.e. number of rows and columns must be larger than the value of this parameter). If you have > 100 columns in a data frame or matrix, reducing the number of columns in this way may substantially increase the performance of the nearest neighbor search at the cost of a potential decrease in accuracy. In many t-SNE applications, a value of 50 is recommended, although there's no guarantee that this is appropriate for all settings.
pca_center	If TRUE, center the columns of <code>X</code> before carrying out PCA. For binary data, it's recommended to set this to FALSE.

pcg_rand	If TRUE, use the PCG random number generator (O'Neill, 2014) during optimization. Otherwise, use the faster (but probably less statistically good) Tausworthe "taus88" generator. The default is TRUE.
fast_sgd	If TRUE, then the following combination of parameters is set: pcg_rand = TRUE, n_sgd_threads = "auto" and approx_pow = TRUE. The default is FALSE. Setting this to TRUE will speed up the stochastic optimization phase, but give a potentially less accurate embedding, and which will not be exactly reproducible even with a fixed seed. For visualization, fast_sgd = TRUE will give perfectly good results. For more generic dimensionality reduction, it's safer to leave fast_sgd = FALSE. If fast_sgd = TRUE, then user-supplied values of pcg_rand, n_sgd_threads, and approx_pow are ignored.
ret_model	If TRUE, then return extra data that can be used to add new data to an existing embedding via <code>umap_transform</code> . The embedded coordinates are returned as the list item embedding. If FALSE, just return the coordinates. This parameter can be used in conjunction with <code>ret_nn</code> and <code>ret_extra</code> . Note that some settings are incompatible with the production of a UMAP model: external neighbor data (passed via a list to <code>nn_method</code>), and factor columns that were included via the <code>metric</code> parameter. In the latter case, the model produced is based only on the numeric data. A transformation using new data is possible, but the factor columns in the new data are ignored.
ret_nn	If TRUE, then in addition to the embedding, also return nearest neighbor data that can be used as input to <code>nn_method</code> to avoid the overhead of repeatedly calculating the nearest neighbors when manipulating unrelated parameters (e.g. <code>min_dist</code> , <code>n_epochs</code> , <code>init</code>). See the "Value" section for the names of the list items. If FALSE, just return the coordinates. Note that the nearest neighbors could be sensitive to data scaling, so be wary of reusing nearest neighbor data if modifying the <code>scale</code> parameter. This parameter can be used in conjunction with <code>ret_model</code> and <code>ret_extra</code> .
ret_extra	A vector indicating what extra data to return. May contain any combination of the following strings: <ul style="list-style-type: none"> • "model" Same as setting <code>ret_model = TRUE</code>. • "nn" Same as setting <code>ret_nn = TRUE</code>. • "fgraph" the high dimensional fuzzy graph (i.e. the fuzzy simplicial set of the merged local views of the input data). The graph is returned as a sparse symmetric N x N matrix of class <code>dgCMatrix-class</code>, where a non-zero entry (i, j) gives the membership strength of the edge connecting vertex i and vertex j. This can be considered analogous to the input probability (or similarity or affinity) used in t-SNE and LargeVis. Note that the graph is further sparsified by removing edges with sufficiently low membership strength that they would not be sampled by the probabilistic edge sampling employed for optimization and therefore the number of non-zero elements in the matrix is dependent on <code>n_epochs</code>. If you are only interested in the fuzzy input graph (e.g. for clustering), setting <code>n_epochs = 0</code> will avoid any further sparsifying. Be aware that setting <code>'binary_edge_weights = TRUE'</code> will affect this graph (all non-zero edge weights will be 1). • "sigma" the normalization value for each observation in the dataset when constructing the smoothed distances to each of its neighbors. This gives

some sense of the local density of each observation in the high dimensional space: higher values of `sigma` indicate a higher dispersion or lower density.

<code>n_threads</code>	Number of threads to use (except during stochastic gradient descent). Default is half the number of concurrent threads supported by the system. For nearest neighbor search, only applies if <code>nn_method = "annoy"</code> . If <code>n_threads > 1</code> , then the Annoy index will be temporarily written to disk in the location determined by <code>tempfile</code> .
<code>n_sgd_threads</code>	Number of threads to use during stochastic gradient descent. If set to <code>> 1</code> , then be aware that if <code>batch = FALSE</code> , results will <i>not</i> be reproducible, even if <code>set.seed</code> is called with a fixed seed before running. Set to <code>"auto"</code> to use the same value as <code>n_threads</code> .
<code>grain_size</code>	The minimum amount of work to do on each thread. If this value is set high enough, then less than <code>n_threads</code> or <code>n_sgd_threads</code> will be used for processing, which might give a performance improvement if the overhead of thread management and context switching was outweighing the improvement due to concurrent processing. This should be left at default (1) and work will be spread evenly over all the threads specified.
<code>tmpdir</code>	Temporary directory to store nearest neighbor indexes during nearest neighbor search. Default is <code>tempdir</code> . The index is only written to disk if <code>n_threads > 1</code> and <code>nn_method = "annoy"</code> ; otherwise, this parameter is ignored.
<code>verbose</code>	If TRUE, log details to the console.
<code>batch</code>	If TRUE, then embedding coordinates are updated at the end of each epoch rather than during the epoch. In batch mode, results are reproducible with a fixed random seed even with <code>n_sgd_threads > 1</code> , at the cost of a slightly higher memory use. You may also have to modify <code>learning_rate</code> and increase <code>n_epochs</code> , so whether this provides a speed increase over the single-threaded optimization is likely to be dataset and hardware-dependent.
<code>opt_args</code>	A list of optimizer parameters, used when <code>batch = TRUE</code> . The default optimization method used is Adam (Kingma and Ba, 2014). <ul style="list-style-type: none"> • <code>method</code> The optimization method to use. Either <code>"adam"</code> or <code>"sgd"</code> (stochastic gradient descent). Default: <code>"adam"</code>. • <code>beta1</code> (Adam only). The weighting parameter for the exponential moving average of the first moment estimator. Effectively the momentum parameter. Should be a floating point value between 0 and 1. Higher values can smooth oscillatory updates in poorly-conditioned situations and may allow for a larger <code>learning_rate</code> to be specified, but too high can cause divergence. Default: 0.5. • <code>beta2</code> (Adam only). The weighting parameter for the exponential moving average of the uncentered second moment estimator. Should be a floating point value between 0 and 1. Controls the degree of adaptivity in the step-size. Higher values put more weight on previous time steps. Default: 0.9. • <code>eps</code> (Adam only). Intended to be a small value to prevent division by zero, but in practice can also affect convergence due to its interaction with <code>beta2</code>. Higher values reduce the effect of the step-size adaptivity and bring the behavior closer to stochastic gradient descent with momentum. Typical values are between 1e-8 and 1e-3. Default: 1e-7.

	<ul style="list-style-type: none"> • <code>alpha</code> The initial learning rate. Default: the value of the <code>learning_rate</code> parameter.
<code>epoch_callback</code>	<p>A function which will be invoked at the end of every epoch. Its signature should be: <code>(epoch, n_epochs, coords)</code>, where:</p> <ul style="list-style-type: none"> • <code>epoch</code> The current epoch number (between 1 and <code>n_epochs</code>). • <code>n_epochs</code> Number of epochs to use during the optimization of the embedded coordinates. • <code>coords</code> The embedded coordinates as of the end of the current epoch, as a matrix with dimensions $(N, n_components)$.
<code>pca_method</code>	<p>Method to carry out any PCA dimensionality reduction when the <code>pca</code> parameter is specified. Allowed values are:</p> <ul style="list-style-type: none"> • <code>"irlba"</code>. Uses <code>prcomp_irlba</code> from the <code>irlba</code> package. • <code>"rsvd"</code>. Uses 5 iterations of <code>svdr</code> from the <code>irlba</code> package. This is likely to give much faster but potentially less accurate results than using <code>"irlba"</code>. For the purposes of nearest neighbor calculation and coordinates initialization, any loss of accuracy doesn't seem to matter much. • <code>"bigstatsr"</code>. Uses <code>big_randomSVD</code> from the <code>bigstatsr</code> package. The SVD methods used in <code>bigstatsr</code> may be faster on systems without access to efficient linear algebra libraries (e.g. Windows). Note: <code>bigstatsr</code> is <i>not</i> a dependency of <code>uwot</code>: if you choose to use this package for PCA, you <i>must</i> install it yourself. • <code>"svd"</code>. Uses <code>svd</code> for the SVD. This is likely to be slow for all but the smallest datasets. • <code>"auto"</code> (the default). Uses <code>"irlba"</code>, unless more than 50 case <code>"svd"</code> is used.
<code>binary_edge_weights</code>	<p>If <code>TRUE</code> then edge weights in the input graph are treated as binary (0/1) rather than real valued. This affects the sampling frequency of neighbors and is the strategy used by the PaCMAP method (Wang and co-workers, 2020). Practical (Böhm and co-workers, 2020) and theoretical (Damrich and Hamprecht, 2021) work suggests this has little effect on UMAP's performance.</p>
<code>dens_scale</code>	<p>A value between 0 and 1. If > 0 then the output attempts to preserve relative local density around each observation. This uses an approximation to the densMAP method (Narayan and co-workers, 2021). The larger the value of <code>dens_scale</code>, the greater the range of output densities that will be used to map the input densities. This option is ignored if using multiple <code>metric</code> blocks.</p>

Value

A matrix of optimized coordinates, or:

- if `ret_model = TRUE` (or `ret_extra` contains `"model"`), returns a list containing extra information that can be used to add new data to an existing embedding via `umap_transform`. In this case, the coordinates are available in the list item `embedding`. **NOTE:** The contents of the `model` list should *not* be considered stable or part of the public API, and are purposely left undocumented.

- if `ret_nn = TRUE` (or `ret_extra` contains "nn"), returns the nearest neighbor data as a list called `nn`. This contains one list for each metric calculated, itself containing a matrix `idx` with the integer ids of the neighbors; and a matrix `dist` with the distances. The `nn` list (or a sub-list) can be used as input to the `nn_method` parameter.
- if `ret_extra` contains "fgraph", returns the high dimensional fuzzy graph as a sparse matrix called `fgraph`, of type `dgCMatrix-class`.
- if `ret_extra` contains "sigma", returns a vector of the smooth knn distance normalization terms for each observation as "sigma" and a vector "rho" containing the largest distance to the locally connected neighbors of each observation.
- if `ret_extra` contains "localr", returns a vector of the estimated local radii, the sum of "sigma" and "rho".

The returned list contains the combined data from any combination of specifying `ret_model`, `ret_nn` and `ret_extra`.

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Examples

```

iris30 <- iris[c(1:10, 51:60, 101:110), ]

# Non-numeric columns are automatically removed so you can pass data frames
# directly in a lot of cases without pre-processing
iris_umap <- umap(iris30, n_neighbors = 5, learning_rate = 0.5, init = "random", n_epochs = 20)

# Faster approximation to the gradient and return nearest neighbors
iris_umap <- umap(iris30, n_neighbors = 5, approx_pow = TRUE, ret_nn = TRUE, n_epochs = 20)

# Can specify min_dist and spread parameters to control separation and size
# of clusters and reuse nearest neighbors for efficiency
nn <- iris_umap$nn
iris_umap <- umap(iris30, n_neighbors = 5, min_dist = 1, spread = 5, nn_method = nn, n_epochs = 20)

# Supervised dimension reduction using the 'Species' factor column
iris_sumap <- umap(iris30, n_neighbors = 5, min_dist = 0.001, y = iris30$Species,
                  target_weight = 0.5, n_epochs = 20)

# Calculate Petal and Sepal neighbors separately (uses intersection of the resulting sets):
iris_umap <- umap(iris30, metric = list(
  "euclidean" = c("Sepal.Length", "Sepal.Width"),
  "euclidean" = c("Petal.Length", "Petal.Width")
))

```

umap_transform

Add New Points to an Existing Embedding

Description

Carry out an embedding of new data using an existing embedding. Requires using the result of calling `umap` or `tumap` with `ret_model = TRUE`.

Usage

```

umap_transform(
  X = NULL,
  model = NULL,
  nn_method = NULL,
  init_weighted = TRUE,
  search_k = NULL,
  tmpdir = tempdir(),
  n_epochs = NULL,
  n_threads = NULL,
  n_sgd_threads = 0,
  grain_size = 1,

```

```

    verbose = FALSE,
    init = "weighted",
    batch = NULL,
    learning_rate = NULL,
    opt_args = NULL,
    epoch_callback = NULL
)

```

Arguments

<code>X</code>	The new data to be transformed, either a matrix or data frame. Must have the same columns in the same order as the input data used to generate the model.
<code>model</code>	Data associated with an existing embedding.
<code>nn_method</code>	Optional pre-calculated nearest neighbor data. There are two supported formats. The first is a list consisting of two elements: <ul style="list-style-type: none"> "idx". A <code>n_vertices x n_neighbors</code> matrix where <code>n_vertices</code> is the number of observations in <code>X</code>. The contents of the matrix should be the integer indexes of the data used to generate the model, which are the <code>n_neighbors</code>-nearest neighbors of the data to be transformed. "dist". A <code>n_vertices x n_neighbors</code> matrix containing the distances of the nearest neighbors. <p>The second supported format is a sparse distance matrix of type <code>dgCMatrix</code>, with dimensions <code>n_model_vertices x n_vertices</code>. where <code>n_model_vertices</code> is the number of observations in the original data that generated the model. Distances should be arranged by column, i.e. a non-zero entry in row <code>j</code> of the <code>i</code>th column indicates that the <code>j</code>th observation in the original data used to generate the model is a nearest neighbor of the <code>i</code>th observation in the new data, with the distance given by the value of that element. In this format, a different number of neighbors is allowed for each observation, i.e. each column can contain a different number of non-zero values. Multiple nearest neighbor data (e.g. from two different pre-calculated metrics) can be passed by passing a list containing the nearest neighbor data lists as items.</p>
<code>init_weighted</code>	If <code>TRUE</code> , then initialize the embedded coordinates of <code>X</code> using a weighted average of the coordinates of the nearest neighbors from the original embedding in <code>model</code> , where the weights used are the edge weights from the UMAP smoothed knn distances. Otherwise, use an un-weighted average. This parameter will be deprecated and removed at version 1.0 of this package. Use the <code>init</code> parameter as a replacement, replacing <code>init_weighted = TRUE</code> with <code>init = "weighted"</code> and <code>init_weighted = FALSE</code> with <code>init = "average"</code> .
<code>search_k</code>	Number of nodes to search during the neighbor retrieval. The larger <code>k</code> , the more accurate results, but the longer the search takes. Default is the value used in building the model is used.
<code>tmpdir</code>	Temporary directory to store nearest neighbor indexes during nearest neighbor search. Default is <code>tempdir</code> . The index is only written to disk if <code>n_threads > 1</code> ; otherwise, this parameter is ignored.

n_epochs	Number of epochs to use during the optimization of the embedded coordinates. A value between 30 - 100 is a reasonable trade off between speed and thoroughness. By default, this value is set to one third the number of epochs used to build the model.
n_threads	Number of threads to use, (except during stochastic gradient descent). Default is half the number of concurrent threads supported by the system.
n_sgd_threads	Number of threads to use during stochastic gradient descent. If set to > 1, then be aware that if batch = FALSE, results will <i>not</i> be reproducible, even if set.seed is called with a fixed seed before running. Set to "auto" to use the same value as n_threads.
grain_size	Minimum batch size for multithreading. If the number of items to process in a thread falls below this number, then no threads will be used. Used in conjunction with n_threads and n_sgd_threads.
verbose	If TRUE, log details to the console.
init	<p>how to initialize the transformed coordinates. One of:</p> <ul style="list-style-type: none"> • "weighted" (The default). Use a weighted average of the coordinates of the nearest neighbors from the original embedding in model, where the weights used are the edge weights from the UMAP smoothed knn distances. Equivalent to init_weighted = TRUE. • "average". Use the mean average of the coordinates of the nearest neighbors from the original embedding in model. Equivalent to init_weighted = FALSE. • A matrix of user-specified input coordinates, which must have dimensions the same as (nrow(X), ncol(model\$embedding)). <p>This parameter should be used in preference to init_weighted.</p>
batch	If TRUE, then embedding coordinates are updated at the end of each epoch rather than during the epoch. In batch mode, results are reproducible with a fixed random seed even with n_sgd_threads > 1, at the cost of a slightly higher memory use. You may also have to modify learning_rate and increase n_epochs, so whether this provides a speed increase over the single-threaded optimization is likely to be dataset and hardware-dependent. If NULL, the transform will use the value provided in the model, if available. Default: FALSE.
learning_rate	Initial learning rate used in optimization of the coordinates. This overrides the value associated with the model. This should be left unspecified under most circumstances.
opt_args	<p>A list of optimizer parameters, used when batch = TRUE. The default optimization method used is Adam (Kingma and Ba, 2014).</p> <ul style="list-style-type: none"> • method The optimization method to use. Either "adam" or "sgd" (stochastic gradient descent). Default: "adam". • beta1 (Adam only). The weighting parameter for the exponential moving average of the first moment estimator. Effectively the momentum parameter. Should be a floating point value between 0 and 1. Higher values can smooth oscillatory updates in poorly-conditioned situations and may allow for a larger learning_rate to be specified, but too high can cause divergence. Default: 0.5.

- `beta2` (Adam only). The weighting parameter for the exponential moving average of the uncentered second moment estimator. Should be a floating point value between 0 and 1. Controls the degree of adaptivity in the step-size. Higher values put more weight on previous time steps. Default: 0.9.
- `eps` (Adam only). Intended to be a small value to prevent division by zero, but in practice can also affect convergence due to its interaction with `beta2`. Higher values reduce the effect of the step-size adaptivity and bring the behavior closer to stochastic gradient descent with momentum. Typical values are between 1e-8 and 1e-3. Default: 1e-7.
- `alpha` The initial learning rate. Default: the value of the `learning_rate` parameter.

If NULL, the transform will use the value provided in the `model`, if available.

`epoch_callback` A function which will be invoked at the end of every epoch. Its signature should be: `(epoch, n_epochs, coords, fixed_coords)`, where:

- `epoch` The current epoch number (between 1 and `n_epochs`).
- `n_epochs` Number of epochs to use during the optimization of the embedded coordinates.
- `coords` The embedded coordinates as of the end of the current epoch, as a matrix with dimensions `(N, n_components)`.
- `fixed_coords` The originally embedded coordinates from the `model`. These are fixed and do not change. A matrix with dimensions `(Nmodel, n_components)` where `Nmodel` is the number of observations in the original data.

Details

Note that some settings are incompatible with the production of a UMAP model via `umap`: external neighbor data (passed via a list to the argument of the `nn_method` parameter), and factor columns that were included in the UMAP calculation via the `metric` parameter. In the latter case, the model produced is based only on the numeric data. A transformation is possible, but factor columns in the new data are ignored.

Value

A matrix of coordinates for `X` transformed into the space of the `model`.

Examples

```
iris_train <- iris[1:100, ]
iris_test <- iris[101:150, ]

# You must set ret_model = TRUE to return extra data needed
iris_train_umap <- umap(iris_train, ret_model = TRUE)
iris_test_umap <- umap_transform(iris_test, iris_train_umap)
```

`unload_uwot`*Unload a Model*

Description

Unloads the UMAP model. This prevents the model being used with `umap_transform`, but allows the temporary working directory associated with saving or loading the model to be removed.

Usage

```
unload_uwot(model, cleanup = TRUE, verbose = FALSE)
```

Arguments

<code>model</code>	a UMAP model create by <code>umap</code> .
<code>cleanup</code>	if TRUE, attempt to delete the temporary working directory that was used in either the save or load of the model.
<code>verbose</code>	if TRUE, log information to the console.

See Also

[save_uwot](#), [load_uwot](#)

Examples

```
iris_train <- iris[c(1:10, 51:60), ]
iris_test <- iris[100:110, ]

# create model
model <- umap(iris_train, ret_model = TRUE, n_epochs = 20)

# save without unloading: this leaves behind a temporary working directory
model_file <- tempfile("iris_umap")
model <- save_uwot(model, file = model_file)

# The model can continue to be used
test_embedding <- umap_transform(iris_test, model)

# To manually unload the model from memory when finished and to clean up
# the working directory (this doesn't touch your model file)
unload_uwot(model)

# At this point, model cannot be used with umap_transform, this would fail:
# test_embedding2 <- umap_transform(iris_test, model)

# restore the model: this also creates a temporary working directory
model2 <- load_uwot(file = model_file)
test_embedding2 <- umap_transform(iris_test, model2)
```

```
# Unload and clean up the loaded model temp directory
unload_uwot(model2)

# clean up the model file
unlink(model_file)

# save with unloading: this deletes the temporary working directory but
# doesn't allow the model to be re-used
model3 <- umap(iris_train, ret_model = TRUE, n_epochs = 20)
model_file3 <- tempfile("iris_umap")
model3 <- save_uwot(model3, file = model_file3, unload = TRUE)
```

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