

# Package ‘Spectrum’

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**Title** Fast Adaptive Spectral Clustering for Single and Multi-View Data

**Version** 1.1

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**Description** A self-tuning spectral clustering method for single or multi-view data. 'Spectrum' uses a new type of adaptive density aware kernel that strengthens connections in the graph based on common nearest neighbours. It uses a tensor product graph data integration and diffusion procedure to integrate different data sources and reduce noise. 'Spectrum' uses either the eigengap or multimodality gap heuristics to determine the number of clusters. The method is sufficiently flexible so that a wide range of Gaussian and non-Gaussian structures can be clustered with automatic selection of K.

**Depends** R (>= 3.5.0)

**License** AGPL-3

**Encoding** UTF-8

**LazyData** true

**Imports** ggplot2, ClusterR, Rfast, diptest

**Suggests** knitr

**VignetteBuilder** knitr

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blobs	<i>8 blob like structures</i>
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### Description

A simulated dataset of 8 Gaussian blobs. Simulated using the 'clusterlab' CRAN package.

### Usage

blobs

### Format

A data frame with 10 rows and 800 variables

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brain	<i>A brain cancer dataset</i>
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### Description

A dataset containing The Cancer Genome Atlas expression data. From this publication [https://tcga-data.nci.nih.gov/docs/publications/lgggbm\\_2016/](https://tcga-data.nci.nih.gov/docs/publications/lgggbm_2016/). The first data frame is a 5133X150 RNA-seq data matrix, the second is a 262X150 miRNA-seq data matrix, the third is 45X150 protein array data matrix. The data was all pre-normalised then subject to log transform.

### Usage

brain

### Format

A list of data frames

**Source**

<https://gdac.broadinstitute.org/>

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circles	<i>Three concentric circles</i>
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**Description**

Simulated data using the 'clusterSim' CRAN package.

**Usage**

```
circles
```

**Format**

A data frame with 2 rows and 540 variables

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cluster_similarity	<i>cluster_similarity: cluster a similarity matrix using the Ng method</i>
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**Description**

This function performs clustering of a similarity matrix following the method of Ng or of Melia. We recommend using the Ng method with GMM to cluster the eigenvectors instead of k-means.

**Usage**

```
cluster_similarity(A2, k = k, clusteralg = "GMM", specalg = "Ng")
```

**Arguments**

A2	Data frame or matrix: a similarity matrix
k	Numerical value: the number of clusters
clusteralg	Character value: GMM or km clustering algorithm (suggested=GMM)
specalg	Character value: Ng or Melia variant of spectral clustering (default=Ng)

**Value**

A numeric vector of cluster assignments

**References**

Ng, Andrew Y., Michael I. Jordan, and Yair Weiss. "On spectral clustering: Analysis and an algorithm." Advances in neural information processing systems. 2002.

Meila, Marina, et al. "Spectral Clustering: a Tutorial for the 2010's." Handbook of Cluster Analysis. CRC Press, 2016. 1-23.

**Examples**

```
ng_similarity <- cluster_similarity(missl[[1]],k=8)
```

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CNN\_kernel

*CNN\_kernel: fast adaptive density-aware kernel*

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**Description**

CNN\_kernel: fast adaptive density-aware kernel

**Usage**

```
CNN_kernel(mat, NN = 3, NN2 = 7)
```

**Arguments**

mat	Matrix: matrix should have samples as columns and rows as features
NN	Numerical value: the number of nearest neighbours to use when calculating local sigma
NN2	Numerical value: the number of nearest neighbours to use when calculating common nearest neighbours

**Value**

A kernel matrix

**Examples**

```
CNN_kern <- CNN_kernel(blobs[,1:50])
```

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estimate_k	<i>estimate_k: estimate K using the eigengap or multimodality gap heuristics</i>
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### Description

This function will try to estimate K given a similarity matrix. Generally the maximum eigengap is preferred, but on some data examining the distribution of the eigenvectors as in the multimodality gap heuristic may be beneficial.

### Usage

```
estimate_k(A2, maxk = 10, showplots = TRUE)
```

### Arguments

A2	Data frame or matrix: a similarity matrix
maxk	Numerical value: maximum number of K to be considered
showplots	Character value: whether to show the plot on the screen

### Value

A data frame containing the eigenvalues and dip-test statistics of the eigenvectors of the graph Laplacian

### Examples

```
k_test <- estimate_k(missl[[1]])
```

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harmonise_ids	<i>harmonise_ids: works on a list of similarity matrices to add entries of NA where there are missing observations between views</i>
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### Description

Simply adds a column and row of NA with the missing ID for data imputation. The similarity matrix requires row and column IDs present for this to work.

### Usage

```
harmonise_ids(l)
```

### Arguments

l	A list of similarity matrices: those to be harmonised.
---	--

**Value**

A list of harmonised similarity matrices.

**Examples**

```
h_test <- harmonise_ids(miss1)
```

---

integrate\_similarity\_matrices

*integrate\_similarity\_matrices: integrate similarity matrices using a tensor product graph linear combination and diffusion technique*

---

**Description**

Given a list of similarity matrices this function will integrate them running the Shu algorithm, also can reduce noise if the input is a list consisting of a single matrix.

**Usage**

```
integrate_similarity_matrices(kernellist, KNNs_p = 10,  
diffusion_iters = 4, method = "TPG")
```

**Arguments**

kernellist	A list of similarity matrices: those to be integrated
KNNs_p	Numerical value: number of nearest neighbours for KNN graph (default=10, suggested=10-20)
diffusion_iters	Numerical value: number of iterations for graph diffusion (default=4, suggested=2-6)
method	Character: either TPG (see reference below) or mean (default=TPG)

**Value**

An integrated similarity matrix

**References**

Shu, Le, and Longin Jan Latecki. "Integration of single-view graphs with diffusion of tensor product graphs for multi-view spectral clustering." Asian Conference on Machine Learning. 2016.

**Examples**

```
i_test <- integrate_similarity_matrices(miss1filled,method='mean')
```

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kernel_pca	<i>kernel_pca: A kernel pca function</i>
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**Description**

kernel\_pca: A kernel pca function

**Usage**

```
kernel_pca(datam, labels = FALSE, axistextsize = 18,
           legendtextsize = 18, dotsize = 3, similarity = TRUE)
```

**Arguments**

datam	Dataframe or matrix: a data frame with samples as columns, rows as features, or a kernel matrix
labels	Factor: to label the plot with colours
axistextsize	Numerical value: axis text size
legendtextsize	Numerical value: legend text size
dotsize	Numerical value: dot size
similarity	Logical flag: whether the input is a similarity matrix or not

**Value**

A kernel PCA plot

**Examples**

```
ex_kernel_pca <- kernel_pca(blobs[,1:50], similarity=FALSE)
```

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mean_imputation	<i>mean_imputation: mean imputation function for multi-view spectral clustering with missing data</i>
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**Description**

Works on a list of similarity matrices to impute missing values using the mean from the other views.

**Usage**

```
mean_imputation(l)
```

**Arguments**

l	A list of data frames: all those to be included in the imputation.
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**Value**

A list of completed data frames.

**Examples**

```
m_test <- mean_imputation(misslfilled)
```

---

missl	<i>A list of the blob data as similarity matrices with a missing entry in one</i>
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**Description**

Two copies of a simulated dataset of 8 Gaussian blobs in a list converted to a similarity matrix, but one has a missing observation.

**Usage**

```
missl
```

**Format**

A list of two data frames

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misslfilled	<i>A list of the blob data as similarity matrices with a missing entry in one filled with NAs</i>
-------------	---

---

**Description**

Two copies of a simulated dataset of 8 Gaussian blobs in a list converted to a similarity matrix, but one has a missing observation filled with NAs.

**Usage**

```
misslfilled
```

**Format**

A list of two data frames



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ng_kernel	<i>ng_kernel: Kernel from the Ng spectral clustering algorithm</i>
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**Description**

This is the kernel from the Ng spectral clustering algorithm. It takes a global sigma which requires tuning for new datasets in most cases. It is possible to use the `sigma_finder` function to find a sigma for a dataset. Sigma is assumed to be squared already.

**Usage**

```
ng_kernel(data, sigma = 0.1)
```

**Arguments**

data	Data frame or matrix: with points as columns, features as rows
sigma	Numerical value: a global sigma that controls the drop off in affinity

**Value**

A similarity matrix of the input data

**References**

Ng, Andrew Y., Michael I. Jordan, and Yair Weiss. "On spectral clustering: Analysis and an algorithm." *Advances in neural information processing systems*. 2002.

**Examples**

```
ng_similarity <- ng_kernel(brain[[1]])
```

---

pca	<i>pca: A pca function</i>
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**Description**

pca: A pca function

**Usage**

```
pca(mydata, labels = FALSE, dotsize = 3, axistextsize = 18,  
    legendtextsize = 18)
```

**Arguments**

mydata	Data frame or matrix: matrix or data frame with samples as columns, features as rows
labels	Factor: to label the plot with colours
dotsize	Numerical value: dot size
axistextsize	Numerical value: axis text size
legendtextsize	Numerical value: legend text size

**Value**

A pca plot object

**Examples**

```
ex_pca <- pca(blobs[,1:50])
```

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rbfkernel_b	<i>rbfkernel_b: fast self-tuning kernel</i>
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**Description**

rbfkernel\_b: fast self-tuning kernel

**Usage**

```
rbfkernel_b(mat, K = 3, sigma = 1)
```

**Arguments**

mat	Matrix: matrix should have samples as columns and rows as features
K	Numerical value: the number of nearest neighbours to use when calculating local sigma
sigma	Numerical value: a global sigma, usually left to 1 which has no effect

**Value**

A kernel matrix

**Examples**

```
stsc_kern <- rbfkernel_b(blobs[,1:50])
```

---

sigma_finder	<i>sigma_finder: heuristic to find sigma for the Ng kernel</i>
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**Description**

This is a heuristic to find the sigma for the kernel from the Ng spectral clustering algorithm. It returns a global sigma. It uses the mean K nearest neighbour distances of all samples to determine sigma.

**Usage**

```
sigma_finder(mat, NN = 3)
```

**Arguments**

mat	Data frame or matrix: with points as columns, features as rows
NN	Numerical value: the number of nearest neighbours to use (default=3)

**Value**

A global sigma

**Examples**

```
sig <- sigma_finder(blobs)
```

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Spectrum	<i>Spectrum: Fast Adaptive Spectral Clustering for Single and Multi-view Data</i>
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**Description**

Spectrum is a self-tuning spectral clustering method for single or multi-view data. Spectrum uses a new type of adaptive density-aware kernel that strengthens connections between points that share common nearest neighbours in the graph. For integrating multi-view data and reducing noise a tensor product graph data integration and diffusion procedure is used. Spectrum analyses eigenvector variance or distribution to determine the number of clusters. Spectrum is well suited for a wide range of data, including both Gaussian and non-Gaussian structures.

**Usage**

```
Spectrum(data, method = 1, silent = FALSE, showres = TRUE,
diffusion = TRUE, kerneltype = c("density", "stsc"), maxk = 10,
NN = 3, NN2 = 7, showpca = FALSE, frac = 2, thresh = 7,
fontsize = 18, dotsize = 3, tunekernel = FALSE,
clusteralg = "GMM", FASP = FALSE, FASPk = NULL, fixk = NULL,
krangemax = 10, runrange = FALSE, diffusion_iters = 4,
KNNs_p = 10, missing = FALSE)
```

**Arguments**

data	Data frame or list of data frames: contains the data with points to cluster as columns and rows as features. For multi-view data a list of dataframes is to be supplied with the samples in the same order.
method	Numerical value: 1 = default eigengap method (Gaussian clusters), 2 = multimodality gap method (Gaussian/ non-Gaussian clusters), 3 = no automatic method (see fixk param)
silent	Logical flag: whether to turn off messages
showres	Logical flag: whether to show the results on the screen
diffusion	Logical flag: whether to perform graph diffusion to reduce noise (default=TRUE)
kerneltype	Character string: 'density' (default) = adaptive density aware kernel, 'stsc' = Zelnik-Manor self-tuning kernel
maxk	Numerical value: the maximum number of expected clusters (default=10). This is data dependent, do not set excessively high.
NN	Numerical value: kernel param, the number of nearest neighbours to use sigma parameters (default=3)
NN2	Numerical value: kernel param, the number of nearest neighbours to use for the common nearest neighbours (default = 7)
showpca	Logical flag: whether to show pca when running on one view
frac	Numerical value: optk search param, fraction to find the last substantial drop (multimodality gap method param)
thresh	Numerical value: optk search param, how many points ahead to keep searching (multimodality gap method param)
fontsize	Numerical value: controls font size of the ggplot2 plots
dotsize	Numerical value: controls the dot size of the ggplot2 plots
tunekernel	Logical flag: whether to tune the kernel, only applies for method 2 (default=FALSE)
clusteralg	Character string: clustering algorithm for eigenvector matrix (GMM or km)
FASP	Logical flag: whether to use Fast Approximate Spectral Clustering (for v. high sample numbers)
FASPk	Numerical value: the number of centroids to compute when doing FASP
fixk	Numerical value: if we are just performing spectral clustering without automatic selection of K, set this parameter and method to 3
krangemax	Numerical value: the maximum K value to iterate towards when running a range of K
runrange	Logical flag: whether to run a range of K or not (default=FALSE), puts Kth results into Kth element of list
diffusion_iters	Numerical value: number of diffusion iterations for the graph (default=4)
KNNs_p	Numerical value: number of KNNs when making KNN graph (default=10, suggested=10-20)
missing	Logical flag: whether to impute missing data in multi-view analysis (default=FALSE)

**Value**

A list, containing: 1) cluster assignments, in the same order as input data columns 2) eigenvector analysis results (either eigenvalues or dip test statistics) 3) optimal K 4) final similarity matrix 5) eigenvectors and eigenvalues of graph Laplacian

**Examples**

```
res <- Spectrum(brain[[1]][,1:50])
```

---

spirals

*Two spirals wrapped around one another*

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**Description**

Simulated data using the 'mlbench' CRAN package.

**Usage**

```
spirals
```

**Format**

A data frame with 2 rows and 180 variables

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