motifcluster

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Motif-Based Spectral Clustering of Weighted Directed Networks

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CLUSTERING METHODS

Functions for spectral clustering are in *motifcluster.clustering*.

cluster_spectrum (spectrum, num_clusts)

Get cluster assignments from spectrum using k-means++.

Get a list of cluster assignments from a spectrum, using k-means++ and num_clusts clusters.

Parameters

- **spectrum** (*dict*) A dictionary containing "*vects*": the matrix of eigenvectors to pass to k-means++.
- **num clusts** (*int*) The number of clusters to find.

Returns cluster_assigns – A list of integers from *I* to *num_clusts*, representing cluster assignments.

Return type list of int

Run motif-based clustering on the adjacency matrix of a (weighted directed) network, using a specified motif, motif type, weighting scheme, embedding dimension, number of clusters and Laplacian type.

Parameters

- adj_mat (matrix) Adjacency matrix to be embedded.
- **motif_name** (*str*) Motif used for the motif adjacency matrix.
- motif type (str) Type of motif adjacency matrix to use. One of "func" or "struc".
- mam_weight_type (str) Weighting scheme for the motif adjacency matrix. One of "un-weighted", "mean" or "product".
- mam_method (*str*) The method to use for building the motif adjacency matrix. One of "*sparse*" or "*dense*".
- **num_eigs** (*int*) Number of eigenvalues and eigenvectors for the embedding.
- type_lap (str) Type of Laplacian for the embedding. One of "comb" or "rw".
- num_clusts (int) The number of clusters to find.

Returns

- adj_mat (*matrix*) The original adjacency matrix.
- **motif_adj_mat** (*matrix*) The motif adjacency matrix.
- comps (list) The indices of the largest connected component of the motif adjacency matrix.

- adj_mat_comps (*matrix*) The original adjacency matrix restricted to the largest connected component of the motif adjacency matrix.
- motif_adj_mat_comps (matrix) The motif adjacency matrix restricted to its largest connected component.
- vals (*list*) A length-*num_eigs* list containing the eigenvalues associated with the Laplace embedding of the restricted motif adjacency matrix.
- **vects** (*matrix*) A matrix containing the eigenvectors associated with the Laplace embedding of the restricted motif adjacency matrix.
- *clusts* A vector containing integers representing the cluster assignment of each vertex.

Examples

```
>>> adj_mat = np.array(range(1, 10)).reshape((3, 3))
>>> run_motif_clustering(adj_mat, "M1", "func",
... "mean", "sparse", 2, "rw", 2)
```

ADJACENCY AND INDICATOR MATRICES

Functions for building adjacency and indicator matrices are in motifcluster.indicators.

_build_G(adj_mat)

Build sparse adjacency matrix.

Build the sparse adjacency matrix G from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns G – The adjacency matrix in sparse form.

Return type sparse matrix

_build_Gd(adj_mat)

Build double-edge adjacency matrix.

Build the sparse double-edge adjacency matrix *Gd* from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Gd – A double-edge adjacency matrix in sparse form.

Return type sparse matrix

_build_Gp (adj_mat)

Build product matrix.

Build the sparse product matrix Gp from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Gp – A product matrix in sparse form.

Return type sparse matrix

_build_Gs(adj_mat)

Build single-edge indicator matrix.

Build the sparse single-edge adjacency matrix Gs from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Gs – A single-edge adjacency matrix in sparse form.

Return type sparse matrix

_build_Id(adj_mat)

Build identity matrix.

Build the sparse identity matrix *Id* from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Id – An identity matrix in sparse form.

Return type sparse matrix

_build_J(adj_mat)

Build directed indicator matrix.

Build the sparse directed indicator matrix J from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns J – A directed indicator matrix in sparse form.

Return type sparse matrix

_build_J0 (adj_mat)

Build missing-edge indicator matrix.

Build the missing-edge indicator matrix J0 from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns J0 – A missing-edge indicator matrix.

Return type sparse matrix

_build_Jd(adj_mat)

Build double-edge indicator matrix.

Build the sparse double-edge indicator matrix *Jd* from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Jd – A double-edge indicator matrix in sparse form.

Return type sparse matrix

_build_Je(adj_mat)

Build edge-and-diagonal matrix.

Build the sparse edge-and-diagonal matrix *Ie* from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Ie – An edge-and-diagonal matrix in sparse form.

Return type sparse matrix

_build_Jn (adj_mat)

Build vertex-distinct indicator matrix.

Build the vertex-distinct indicator matrix Jn from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Jn – A vertex-distinct indicator matrix.

Return type sparse matrix

_build_Js(adj_mat)

Build single-edge indicator matrix.

Build the sparse single-edge indicator matrix *Js* from a graph adjacency matrix.

Parameters adj_mat (*matrix*) – The original adjacency matrix.

Returns Js – A single-edge indicator matrix in sparse form.

MOTIF ADJACENCY MATRICES

Functions for building motif adjacency matrices are in motifcluster.motifadjacency.

```
\begin{tabular}{ll} \textbf{build_motif_adjacency_matrix} (adj\_mat, & motif\_name, & motif\_type='struc', \\ & mam\_weight\_type='unweighted', mam\_method='sparse') \end{tabular}
```

Build a motif adjacency matrix.

Build a motif adjacency matrix from an adjacency matrix. Entry (i, j) of a motif adjacency matrix is the sum of the weights of all motifs containing both nodes i and j.

- The motif is specified by name and the type of motif instance can be one of:
 - Functional: motifs should appear as subgraphs.
 - Structural: motifs should appear as induced subgraphs.
- The weighting scheme can be one of:
 - Unweighted: the weight of any motif instance is one.
 - Mean: the weight of any motif instance is the mean of its edge weights.
 - Product: the weight of any motif instance is the product of its edge weights.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_name** (*str*) Motif used for the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build. One of "func" or "struc".
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse". The sparse formulation avoids generating large dense matrices so tends to be faster for large sparse graphs.

Returns A motif adjacency matrix.

Examples

```
>>> adj_mat = np.array(range(1, 10)).reshape((3, 3))
>>> build_motif_adjacency_matrix(adj_mat, "M1", "func", "mean")
```

mam_M1 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M1.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M10 (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif M10.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M11 (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif M11.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M12 (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif M12.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.

- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M13 (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif M13.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M2 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M2.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M3 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M3.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M4 (adj_mat, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M4.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M5 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M5.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M6 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M6.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- motif_type (str) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M7 (adj_mat, motif_type, mam_weight_type)

Perform the motif adjacency matrix calculations for motif M7.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_M8 (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif M8.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

 ${\tt mam_M9}\ (adj_mat, motif_type, mam_weight_type, mam_method)$

Perform the motif adjacency matrix calculations for motif M9.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

 ${\tt mam_Mcoll} \ (adj_mat, motif_type, mam_weight_type, mam_method)$

Perform the motif adjacency matrix calculations for motif Mcoll.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_Md (adj_mat, mam_weight_type)

Perform the motif adjacency matrix calculations for motif Md.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

Return type sparse matrix

mam_Mexpa (adj_mat, motif_type, mam_weight_type, mam_method)

Perform the motif adjacency matrix calculations for motif Mexpa.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".
- mam_method (str) Which formulation to use. One of "dense" or "sparse".

Returns A motif adjacency matrix.

 $\mathbf{mam_Ms}\;(adj_mat,motif_type,mam_weight_type)$

Perform the motif adjacency matrix calculations for motif Ms.

Parameters

- adj_mat (matrix) Adjacency matrix from which to build the motif adjacency matrix.
- **motif_type** (*str*) Type of motif adjacency matrix to build.
- mam_weight_type (str) The weighting scheme to use. One of "unweighted", "mean" or "product".

Returns A motif adjacency matrix.

NETWORK SAMPLING

Functions for random sampling of weighted directed networks are in motifcluster.sampling.

demonstration_graph()

Generate a small graph for demonstrations.

Generate the sparse and dense adjacency matrices of a small weighted directed graph, for demonstrating methods and running tests.

Returns

- adj_mat_dense (matrix) the adjacency matrix in dense form.
- adj_mat_sparse (sparse matrix) the adjacency matrix in sparse form.

sample_bsbm (source_block_sizes, dest_block_sizes, bipartite_connection_matrix, bipartite_weight_matrix=None, sample_weight_type='unweighted')
Sample a bipartite stochastic block model (BSBM).

Sample the (weighted) adjacency matrix of a (weighted) bipartite stochastic block model (BSBM) with specified parameters.

Parameters

- source block sizes (list of int) A list containing the size of each block of source vertices.
- dest_block_sizes (list of int) A list containing the size of each block of destination vertices.
- **bipartite_connection_matrix** (*matrix*) A matrix containing the source block to destination block connection probabilities.
- **sample_weight_type** (*str*) The type of weighting scheme. One of "*unweighted*", "*constant*" or "*poisson*".
- weight_matrix (matrix) A matrix containing the source block to destination block weight parameters. Unused for sample_weight_type = "constant". Defaults to None.

Returns adj_mat – A randomly sampled (weighted) adjacency matrix of a BSBM.

Examples

sample_dsbm (block_sizes, connection_matrix, weight_matrix=None, sample_weight_type='unweighted') Sample a directed stochastic block model (DSBM).

Sample the (weighted) adjacency matrix of a (weighted) directed stochastic block model (DSBM) with specified parameters.

Parameters

- **block_sizes** (*list of int*) A list containing the size of each block of vertices.
- connection_matrix (matrix) A matrix containing the block-to-block connection probabilities.
- **sample_weight_type** (*str*) The type of weighting scheme. One of "*unweighted*", "*constant*" or "*poisson*".
- weight_matrix (matrix) A matrix containing the block-to-block weight parameters. Unused for sample_weight_type = "constant". Defaults to None.

Returns adj_mat – A randomly sampled (weighted) adjacency matrix of a DSBM.

Return type sparse matrix

Examples

```
>>> block_sizes = [10, 10]
>>> connection_matrix = np.array([0.8, 0.1, 0.1, 0.8]).reshape((2, 2))
>>> weight_matrix = np.array([10, 3, 3, 10]).reshape((2, 2))
>>> sample_dsbm(block_sizes, connection_matrix, weight_matrix, "poisson")
```

UTILITY FUNCTIONS

Assorted utility functions for the motifcluster module are in *motifcluster.utils*.

_a_b_one (*a_mat*, *b_mat*)

Compute a right-multiplication with the ones matrix.

Compute $a * (b @ one_mat)$ where a, b, $ones_mat$ are square matrices of the same size, and $ones_mat$ contains all entries equal to one. The product * is an entry-wise (Hadamard) product, while @ represents matrix multiplication. This method is more efficient than the naive approach when a or b are sparse.

Parameters a, b (*matrix*) – Square matrices of the same size.

Returns The sparse square matrix $a * (b @ one_mat)$.

Return type sparse matrix

_a_one_b (*a_mat*, *b_mat*)

Compute a left-multiplication with the ones matrix.

Compute $a * (one_mat @ b)$ where a, b, $ones_mat$ are square matrices of the same size, and $ones_mat$ contains all entries equal to one. The product * is an entry-wise (Hadamard) product, while @ represents matrix multiplication. This method is more efficient than the naive approach when a or b are sparse.

Parameters a, b (*matrix*) – Square matrices of the same size.

Returns The sparse square matrix $a * (one_mat @ b)$.

Return type sparse matrix

_drop0_killdiag(some_mat)

Set diagonal entries to zero and sparsify.

Set the diagonal entries of a matrix to zero and convert it to sparse form.

Parameters some_mat (*matrix*) – A square matrix.

Returns sparse_mat – A sparse-form copy of *some_mat* with its diagonal entries set to zero.

Return type sparse matrix

```
\verb|_random_sparse_matrix| (m, n, p, sample_weight_type='constant', w=1)
```

Build a random sparse matrix.

Build a sparse matrix of size m * n with non-zero probability p. Edge weights can be unweighted, constant-weighted or Poisson-weighted.

Parameters

- \mathbf{m} , \mathbf{n} (*int*) Dimension of matrix to build is (m, n).
- **p** (*float*) Probability that each entry is non-zero (before weighting).

- **sample_weight_type** (*str*) Type of weighting scheme.
- w (*float*) Weight parameter.

Returns A random sparse matrix.

Return type sparse matrix

```
get_largest_component (adj_mat)
```

Get largest connected component.

Get the indices of the vertices in the largest connected component of a graph from its adjacency matrix.

Parameters adj_mat (*matrix*) – An adjacency matrix of a graph.

Returns verts_to_keep – A list of indices corresponding to the vertices in the largest connected component.

Return type list

Examples

```
>>> adj_mat = np.array([0, 1, 0, 0, 0, 0, 0, 0]).reshape((3, 3))
>>> get_largest_component(adj_mat)
```

get_motif_names()

Get common motif names.

Get the names of some common motifs as strings.

Returns motif_names – A list of names (strings) of common motifs.

Return type list

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