Package 'MCODER'

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Title MCODER, an R Implementation Of MCODE Network Clustering Algorithm

Type Package

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<pre>URL https://sourceforge.net/projects/mcoder, https: //github.com/ginokwon-yuhs/MCODER</pre>	
Description Molecular Complex Detection (MCODE) network analysis and visualization based on Bader et al. 2003, "An automated method for finding molecular complexes in large protein interaction networks". The algorithm detects densely interconnected clusters (complex, subgraph). MCODER is an R-implementations of MCODE with additional functions, comprising: a) node annotation, b) visualize of multiple edges and c) visualize of directed graph	
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add.annotation Adding annotation information to vertices

Description

Adding annotation information to vertices

Usage

```
add.annotation(x, vertices.par, edges.par, annotation.table)
```

Arguments

x A List of adjacency matrix

vertices.par A matrix of graphical parameters for vertices that is created by the function

graph.par.vertex

edges.par A matrix of graphical parameters for edges that is created by the function graph.par.edge

annotation.table

A table for annotation. It must be consist of two columns including vertex label and description

Details

A table for annotation that must include vertex names in its first column and description of vertex in its second column. Return adjacency matrixes of subgraph, tables of graphical parameter for vertices and nodes including annotation information.

Value

A list consists of three matrixes: adjacency matrix for subgraph cluster, matrix of graphical parameters for vertexes, and matrix of graphical parameters for edges

See Also

```
cluster.adj.matrix, graph.par.vertex, graph.par.edge
```

```
# vertex value table (label,K-core,node density, node score)
vertex_table <- calc.vertex.value(x=adj_mat,loop=F)
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)
# make table
int_tb <- as.data.frame(c('Gene2','Gene210','Gene6'),stringsAsFactors=F )
colnames(int_tb) <- 'label'
int_tb$desc <- c('Drug_A','Drug_D','Drug_E')
int_tb <- as.matrix(int_tb)
# add annotation
rst <- add.annotation(x=clusters_edges,vertices.par=graph_par_vertex,edges.par=graph_par_edge,annotation.taclusters_edges <- rst[[1]]
graph_par_vertex <- rst[[2]]
graph_par_edge <- rst[[3]]</pre>
```

adjacency.matrix 3

adjacency.matrix	Transforming a table of connection information into an adjacency matrix

Description

To transform a table of connections (two vertices connected by edge, i.e. PPI) consist of at least two columns into adjacency matrix

Usage

```
adjacency.matrix(input_tb, v1 = NULL, v2 = NULL, sampling = NULL,
  remove.loop = T, directed = F, multiple.edge = F)
```

Arguments

input_tb	A matrix contains connections between two vertices	
v1	For directed graph, the column name of out-degree vertex in the table x (table of connections). If NULL, it takes first column.	
v2	v1 For directed graph, the column name of in-degree vertex in the table x (table of connections). If NULL, it takes second column.	
sampling	A vector of characters for extracting specific nodes. By default NULL, it ignores the sampling step and transform the all connections.	
remove.loop	If FALSE, adjacency matrix will include loop edges. By default, it removes loop edges.	
directed	If TRUE, adjacency matrix will be built from v1 (out-degree) to v2 (in-degree) otherwise, it returns a symmetric.	
x	A list of adjacency matrix that is created by the function cluster.adj.matrix	
multitple.edges		
	If TRUE, element of adjacency matrix will be bigger than 1 where it has multiple connections between nodes. Otherwise, default value is the result matrix that contains either 1 or 0.	

Details

An adjacency matrix of an undirected graph is a symmetric matrix and it contains boolean values. A case for directed network, adjacency matrix contains the directions from vertex (i.e. A) to vertex (i.e. B) such as vertices on the row of adjacency matrix (i.e. A) to vertices of the column of adjacency matrix (i.e. B). For instance, the directional connection from A to B can be defined by 'matrix [A, B]'. However, the MCODE algorithm is an undirected graph algorithm. Therefore, the following result of network clustering in this r package is based on undirected graph.

```
#' # ideal undirected graph for MCODE
adj_mat <- adjacency.matrix(raw_table1,v1='X',v2='Y')
# directed graph with multple edges
adj_mat_directed <- adjacency.matrix(raw_table2,v1='outdegree_node',v2='indegree_node',direct=T,multiple.edge)</pre>
```

4 calc.node.scores

calc.local.density Calculating density value of a node

Description

To calculate vertex density and used for function fluff

Usage

```
calc.local.density(x, vertex)
```

Arguments

x A vector of character that is the label of vertex

vertex An adjacency matrix

Value

A numeric vector of the vertex density

See Also

```
post.fluff
```

calc.node.scores

Calculating density, score and k-core of the single vertex

Description

Calculate density, score and k-core of the single vertex. The function for calculating k-core of vertex is imported from package 'sna' kcores

Usage

```
calc.node.scores(x, adj.mat, minimum.edges = 2, loop = F)
```

Arguments

x A vector of character that is the name of vertex

adj.mat An adjacency matrix and it is created by function adjacency.matrix

minimum.edges The minimum numbers of connected edges to a vertex (degree). By default,

vertex should have more than two edges

loop By default, loop edges would remove loops. The method of the maximum num-

ber of edges depends on loop inclusion

calc.vertex.value 5

Details

The k-core value is calculated by the function that is imported from the package, sna. k-core measures cliquishness of a network. The principle of MCODE algorithm is to detect densely interconnected clusters. This idea goes from local density within neighborhoods. Node density is calculated by the number of edges, D = |E|/|E| max in Graph = (V,E). |E| = number of edges to a vertex. |E| max = maximum number of possible connection to a vertex. If graph includes loops, |E| max = |V| (|V| + 1) / 2 and graph excludes loops, |E| max = |V| (|V| - 1) / 2. |V| is the number of connected vertexes to seed vertex.

Value

A list includes the density, score and k-core of vetex

References

Butts CT, Social Network Analysis with sna, 2008, Journal of Statistical Software, 24 (6), Bader GD et al. BMC Bioinformatics 2003, 4, 2. PMID 12525261

See Also

```
calc.vertex.value, adjacency.matrix
```

calc.vertex.value	Calculating the density, score and k-core of the all vertices in a net-
	work

Description

Calculating the density, score and k-core of the all vertices in a network

Usage

```
calc.vertex.value(x, loop = F, minimum.edges = 2)
```

Arguments

x An adjacency matrix

loop By default, loop edges would remove loops. The method of the maximum num-

ber of edges depends on loop inclusion

minimum.edges The minimum numbers of connected edges to a vertex (degree). By default,

vertex should have more than two edges

Value

A table including k-core, density and scores of the all vertices in a network

```
adj_mat <- adjacency.matrix(raw_table1,v1='X',v2='Y')
#vertex value table (label,K-core,node density, node score)
vertex_table <- calc.vertex.value(x=adj_mat,loop=F)</pre>
```

6 find.cluster

cluster.adj.matrix Extracting adjacency matrixes of subgraphs

Description

Extracting adjacency matrixes of subgraphs

Usage

```
cluster.adj.matrix(x, adj.mat)
```

Arguments

x List of clusters is created by the function find.cluster adj.mat An adjacency matrix

Value

A list consists of adjacency matrixes that are separated by individual sub clusters

See Also

```
find.cluster
```

Examples

```
adj_mat <- adjacency.matrix(raw_table1,v1='X',v2='Y')
vertex_table <- calc.vertex.value(x=adj_mat,loop=F)
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)
# edge matrix order by cluster number
clusters_edges <- cluster.adj.matrix(x=clusters,adj_mat)</pre>
```

find.cluster

Detecting subgraphs (clusters) in a network

Description

Detecting subgraphs (clusters) in a network. The derived score is used in clustering

Usage

```
find.cluster(vertex.score, adj.mat, node.score.cutoff = 0.2, min.k.core = 2,
   max.depth = 100)
```

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Arguments

vertex.score A table of score is created by the function calc.vertex.value

adj.mat An adjacency matrix

node.score.cutoff

The cutoff for derived score. Otherwise, default value is 0.2

min.k.core The minimum K-core for clustering. Default value is 2

max.depth The maximum depth is the number of path along the longest path from seed

node to destination. By default, maximum depth is 100.

Details

MCODE algorithm finds the densely connected vertices that are started from a seed vertex and use several parametric variables such as cutoff score, the maximum depth, and k-core. First, connected vertices its scores have to be bigger than a derived score, vertex score = vertex density * k-core, derived score = seed score * score cutoff. Second, destination node should be in a range of maximum depth from a seed node. Third, k-core value should be bigger than or equal to the minimum k-core value. The cutoff must be in a range between from 0 to 1. The minimum K-core value is bigger than or equal to 2 and it represents complexity.

Value

A list of clusters

Examples

```
adj_mat <- adjacency.matrix(raw_table1,v1='X',v2='Y') # import raw data
vertex_table <- calc.vertex.value(x=adj_mat,loop=F) # adjacency matrix transfoming
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)</pre>
```

graph.par.edge

Making matrix of graphical parameters for edges

Description

Making matrix of graphical parameters for edges

Usage

```
graph.par.edge(x, directed = F, multiple.edge = F)
```

Arguments

x A list of adjacency matrixes for each cluster (subgraph)

directed If TRUE, x (input adjacency matrix) must be directed graph. By defualt, result

table generates connections on an upper triangular matrix.

should not be on result table.

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Details

Default colour of edge is 'blue', width of edge is 1

Value

A matrix contains graphical variables for edges including vertex x (from), vertex y (to), number (cluster number), colour (edge colour), and width (edge width)

graph.par.vertex

Making matrix of graphical parameters for vertices

Description

Making matrix of graphical parameters for vertices

Usage

```
graph.par.vertex(x)
```

Arguments

Х

A list of clusters (subgraph) created by the function find.cluster

Details

The only possible shape of vertex is 'rectangle' and 'circle'. Default vertex frame colour is 'white', vertex size is 27, vertex label size is 1, vertex shape is 'circle' and vertex border colour is 'black'.

Value

A matrix contains graphical variables for vertices including x (vertex name), number (cluster number), colour (vertex frame colour), size (vertex size), font (vertex label size), shape (vertex shape), lab_col (vertex label colour), and border (vertex border colour)

network.format

Transforms an adjacency matrix of clusters into the format of network for igraph

Description

Transforms an adjacency matrix of clusters into the format of network for igraph

Usage

```
network.format(x, vertices.par = NULL, edges.par = NULL, direct = F)
```

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Arguments

x An adjacency matrix

vertices.par A matrix of graphical parameters for vertices that is created by the function

graph.par.vertex

edges.par A matrix of graphical parameters for edges that is created by the function graph.par.edge

directed If TRUE, x must be a directed adjacency matrix. By default, it returns an undi-

rected graph.

Value

A list of network format for igraph

References

Csardi G, Nepusz T: The igraph software package for complex network research, InterJournal, Complex Systems 1695. 2006.

Examples

```
adj_mat <- adjacency.matrix(input_tb,v1='X',v2='Y',remove.loop=T,directed=F,multiple.edge=T)
vertex_table <- calc.vertex.value(x=adj_mat,loop=F) # tansforming to matrix
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)
# subgraphs adjancecy matrixes
clusters_edges <- cluster.adj.matrix(x=clusters,adj_mat)
#prepare for essential plotting input
graph_par_vertex <- graph.par.vertex(x=clusters)
graph_par_edge <- graph.par.edge(x=clusters_edges) #option here for multiple edge, direction
# adjacency matrix to graph format, includes graphical parameters
IG <- network.format(x=clusters_edges,vertices.par=graph_par_vertex,edges.par=graph_par_edge,direct=F)</pre>
```

plot.network

Plotting function of networks

Description

Plotting function of networks

Usage

```
## S3 method for class 'network'
plot(input, network.layout = "layout.fruchterman.reingold",
    arrow.size = 0.5)
```

Arguments

input A list of network format

network.layout The drawing algorithm for plotting. Default drawing algorithm is 'Frucherman

Reingold'. It is also possible to apply other drawing algorithms, which are supported on R package, 'igraph'. Other layouts are in layout.reingold.tilford

arrow. size size of arrow. Default size is 0.5

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Examples

```
### draw an whole network (directed), Example 1
adj_mat_directed <- adjacency.matrix(raw_table2,v1='outdegree_node',v2='indegree_node',direct=T,multiple.ec
# vertex value table (label,K-core,node density, node score)
clusters <- list()</pre>
clusters[[1]] <- rownames(adj_mat_directed)</pre>
clusters_edges <- list()</pre>
clusters_edges[[1]] <- adj_mat_directed</pre>
##prepare for essential plotting input
graph_par_vertex <- graph.par.vertex(x=clusters)</pre>
graph_par_edge <- graph.par.edge(x=clusters_edges)</pre>
# transform to network
IG <- \ network.format(x=clusters\_edges, vertices.par=graph\_par\_vertex, edges.par=graph\_par\_edge, direct=T)
# plotting
plot(plot.network(IG[1])
### draw clusters with multiple edges, example 2
adj_mat_directed <- adjacency.matrix(raw_table2,v1='outdegree_node',v2='indegree_node',direct=F,multiple.ec
vertex_table <- calc.vertex.value(x=adj_mat_directed,loop=F)</pre>
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat_directed,node.score.cutoff=0.2)</pre>
clusters <- post.fluff(x=clusters,adj_mat_directed,vertex_table)</pre>
clusters <- post.fluff.bind(x=clusters)</pre>
# haircut
clusters <- post.haircut(clusters,adj_mat_directed)</pre>
# edge matrix order by cluster number
clusters_edges <- cluster.adj.matrix(x=clusters,adj_mat_directed)</pre>
#prepare for essential plotting input
graph_par_vertex <- graph.par.vertex(x=clusters)</pre>
graph_par_edge <- graph.par.edge(x=clusters_edges)</pre>
# network format
IG <- \ network.format(x=clusters\_edges, vertices.par=graph\_par\_vertex, edges.par=graph\_par\_edge, direct=T)
# plotting
for(i in 1:length(IG)) { plot.network(IG[i]) }
```

post.fluff

Performing post processing, Fluff

Description

Performing post processing, Fluff, after detecting cluster complex

Usage

```
post.fluff(x, adj.mat, vertex.score.table, density.cutoff = 0.6)
```

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Arguments

```
x A list of clusters

adj.mat An adjacency matrix

vertex.score.table

A matrix of the score of the vertices that is created by the function calc.vertex.value

density.cutoff A cutoff value of the node density
```

Details

The fluff step is the post process after clustering. In this step, cluster expands to neighbourhoods. It is decided by derived density, derived density = seed density * cutoff. Density of candidate vertices has to be bigger than the derived density of the seed node. If a neighbour vertex has satisfied enough density, it belongs to the expanded cluster. If procedure contains either fluff and haircut, fluff has to be performed before haircut.

Value

A list of clusters

Examples

```
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)
# Fluff
clusters <- post.fluff(x=clusters,adj_mat,vertex_table)
clusters <- post.fluff.bind(x=clusters)</pre>
```

post.fluff.bind

Combining overlapping clusters (subgraphs)

Description

Combining overlapping clusters (subgraphs), after it performed post-process step post.fluff

Usage

```
post.fluff.bind(x)
```

Arguments

x A list of clusters that is generated after the post processing function post.fluff

Value

A list of clusters

See Also

```
post.fluff
```

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post.haircut

Performing post processing, Haircut

Description

Performing post processing, Haircut, after detecting cluster complex

Usage

```
post.haircut(x, adj.mat)
```

Arguments

x A list of clusters (subgraph) that is created by the function find.cluster

adj.mat An adjacency matrix

Details

The haircut removes singly connected vertices within a cluster. Post process have to performed after clustering. This haircut process comes after fluff when fluff is needed.

Value

A list of clusters

```
# finding clusters
clusters <- find.cluster(vertex_table,adj_mat,node.score.cutoff=0.2)
# Haircut, post process
clusters <- post.haircut(clusters,adj_mat)</pre>
```

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