Package ‘apComplex’

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Title Estimate protein complex membership using AP-MS protein data
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Description Functions to estimate a bipartite graph of protein complex membership using AP-MS data.
Depends R (>= 2.10), graph, RBGL
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Suggests
Maintainer Denise Scholtens <dscholtens@northwestern.edu>
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NeedsCompilation no

R topics documented:

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AP-MS complexes

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Both sets of estimates are reported as lists of length three, corresponding to MBME, SBMH, and UnRBB complex estimate types (see Scholtens et al., 2005). Each of the three elements contains a list of character vectors of estimated complex members.

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**Description**

A matrix and corresponding graph of AP-MS purifications from a small hypothetical experiment.

**Usage**

```r
data(apEX)
data(apEXG)
```

**Details**

`apEX` is a matrix of hypothetical AP-MS data. The 4 rows correspond to bait proteins and the 8 columns correspond to proteins found as hits in the hypothetical experiment and are named accordingly. The first 4 column names are the same as the 4 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in `apEX`. An entry of "1" in the ith row and jth column of `apEX` indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of 9 "1" entries in the matrix, corresponding to 9 comemberships detected in the experiment.

`apEXG` is a `graphNEL` object in which 8 nodes represent proteins and 9 directed edges represent comemberships detected in the purification. Each directed edge originates at the bait and ends at the hit. Each edge in `apEXG` corresponds to an entry of "1" in the `apEX` matrix.

These data are used in the `apComplex` vignette.

**Examples**

```r
data(apEX)
apEX
data(apEXG)
adj(apEXG,"P1")
```

---

**bhmaxSubgraph**

*Find maximal BH-complete subgraph*

**Description**

Given an adjacency matrix of bait-hit AP-MS protein data, this function finds the maximal BH-complete subgraphs and reports them as an affiliation matrix.

**Usage**

```r
bhmaxSubgraph(adjMat, VBs=NULL, VPs=NULL, unrecip=1)
```
bhmaxSubgraph

Arguments

adjMat  adjMat is an N by (N+M) adjacency matrix with N equal to the number of bait proteins and M equal to the number of hit-only proteins. adjMat should have row and column names corresponding to the proteins in the experiment. An entry of "1" in the ith row and jth column of adjMat corresponds to bait protein i finding protein j as a hit. All other entries should be 0.

VBs  VBs is an optional vector of viable baits.

VPs  VPs is an optional vector of viable prey.

unrecip  By default set to 1 so that unreciprocated bait-bait edges are treated as present. If set to 0, unreciprocated bait-bait edges will be treated as absent.

Details

A BH-complete subgraph with n bait nodes and m hit-only nodes for AP-MS data is defined as a subgraph for which all n*(n-1)+nm directed edges exist. A maximal BH-complete subgraph is a BH-complete subgraph which is not contained in any other BH-complete subgraph.

If VBs and/or VPs are not specified, then by default VBs will be assigned the set of baits that detect at least one prey and VPs the set of prey that are detected by at least one bait. By default, unreciprocated bait-bait observations will be treated as present. If unrecip is set to 0, they will be treated as absent. If the sensitivity of the AP-MS technology is believed to be less than the specificity, then it is suggested that unrecip=1.

This function calls maxCliques from the RBGL package.

Value

A list of length one named 'maxCliques' which is itself a list of character vectors containing the names of the elements in the cliques.

Author(s)

Denise Scholtens

References


See Also

mergeComplexes, findComplexes

Examples

data(apEX)
PCMG0 <- bhmaxSubgraph(apEX)
PCMG1 <- mergeComplexes(PCMG0, apEX, sensitivity=.7, specificity=.75)
**findComplexes**

Estimate a Protein Complex Membership Graph (PCMG) using protein complex comembership data from AP-MS technology

**Description**

Performs all steps in the local modeling algorithm described by Scholtens and Gentleman (2004) and Scholtens, Vidal, and Gentleman (submitted), beginning with an adjacency matrix recording bait-hit AP-MS data.

**Usage**

```r
findComplexes(adjMat, V Bs=NULL, V Ps=NULL, simMat=NULL, sensitivity=.75, specificity=.995, Beta=0, commonFrac=2/3, wsVal = 2e7)
```

**Arguments**

- `adjMat`: Adjacency matrix of bait-hit data from an AP-MS experiment. Rows correspond to baits and columns to hits.
- `VBs`: VBs is an optional vector of viable baits.
- `VPs`: VPs is an optional vector of viable prey.
- `simMat`: An optional square matrix with entries between 0 and 1. Rows and columns correspond to the proteins in the experiment, and should be reported in the same order as the columns of `adjMat`. Higher values in this matrix are interpreted to mean higher similarity for protein pairs.
- `sensitivity`: Believed sensitivity of AP-MS technology.
- `specificity`: Believed specificity of AP-MS technology.
- `Beta`: Optional additional parameter for the weight to give data in `simMat` in the logistic regression model.
- `commonFrac`: This is the fraction of baits that need to be overlapping for a complex combination to be considered.
- `wsVal`: A numeric. This is the value assigned as the work-space in the call to fisher.test

**Details**

`findComplexes` performs all steps in the complex estimation algorithm using the apComplex package functions `bhmaxSubgraph`, `LCdelta`, and `mergeComplexes`. These steps can also be performed separately by the user.

If `VBs` and/or `VPs` are not specified, then by default `VBs` will be assigned the set of baits that detect at least one prey and `VPs` the set of prey that are detected by at least one bait.

By default `commonFrac` is set relatively high at 2/3. This means that some potentially reasonable complex combinations could be missed. For smaller data sets, users may consider decreasing the fraction. For larger data sets, this may cause a large increase in computation time.

**Value**

A list of character vectors containing the names of the proteins in the estimated complexes.
Author(s)

Denise Scholtens

References


See Also

bhmaxSubgraph,mergeComplexes

Examples

data(apEX)
PCMG2 <- findComplexes(apEX,sensitivity=.7,specificity=.75)

---

gavinBP2006  Tandem Affinity Purification (TAP) Data from Gavin et al. (2006)

Description


Usage

data(gavinBP2006)

Details

gavinBP2006 is a matrix of the TAP data published by Gavin, et al. (2006). The 1752 rows correspond to bait proteins and the 2551 columns correspond to proteins found as hits in the TAP experiment and are named accordingly. The first 1752 column names are the same as the 1752 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in gavinBP2006. An entry of "1" in the ith row and jth column of gavinBP2006 indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of 19105 "1" entries in the matrix, corresponding to the 19105 comemberships detected in the experiment. These data are available in the IntAct repository under Gavin et al - 2006.

Source


See Also

yTAP,MBMEcTAP,SBMHCcTAP,UnRBBcTAP,HMSPCI
**Examples**

```r
data(gavinBP2006)
which(gavinBP2006[1,]==1)
```

**Description**

HMS-PCI data published by Ho, et al. (2002).

**Usage**

```r
data(HMSPCI)
data(HMSPCIgraph)
```

**Details**

HMSPCI is a matrix of the HMS-PCI data published by Ho, et al. (2002). The 493 rows correspond to bait proteins and the 1578 columns correspond to proteins found as hits in the HMSPCI experiment and are named accordingly. The first 493 column names are the same as the 493 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in HMSPCI. An entry of "1" in the ith row and jth column of HMSPCI indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of 3687 "1" entries in the matrix, corresponding to the 3687 comemberships detected in the experiment.

HMSPCIgraph is a graphNEL object in which 1578 nodes represent proteins and 3687 directed edges represent comemberships detected in the purification. Each directed edge originates at the bait and ends at the hit. Each edge in HMSPCIgraph corresponds to an entry of "1" in the HMSPCI matrix.

These data are available at http://www.mdsp.com/yeast.

**Source**


**References**


**See Also**

MBMEcHMSPCI, SBMHcHMSPCI, UnRBBcHMSPCI, TAP
Examples

```r
data(HMSPCI)
which(HMSPCI["YAL015C",]==1)

data(HMSPCIgraph)
adj(HMSPCIgraph,"YAL015C")
```

### Description

Affiliation matrices with rows corresponding to proteins and columns corresponding to complexes.

### Usage

```r
data(MBMEcHMSPCI)
data(SBMHcHMSPCI)
data(UnRBBcHMSPCI)
```

### Details

These are the results from an analysis of the HMS-PCI data (Ho et al., 2002) described by Scholtens and Gentleman (2004) and Scholtens, Vidal, and Gentleman (submitted). These estimates were constructed using `findComplexes` with a sensitivity parameter of .75, specificity of .99, and Beta=-0.2 for externally derived similarity measure based on Gene Ontology cellular component annotation (see Scholtens and Gentleman (2004)).

- **MBMEcHMSPCI** contains 242 multi-bait-multi-edge complex estimates.
- **SBMHcHMSPCI** contains 437 single-bait-multi-hit complex estimates.
- **UnRBBcHMSPCI** contains 329 unreciprocated bait-bait complex estimates. These data are also available at http://www.bioconductor.org/Docs/Papers/2003/apComplex.

### Source


### References


### See Also

`HMSPCI`, `HMSPCIgraph`, `findComplexes`
Krogan

Examples

```r
data(MBMEcHMSPCI)
MBMEcHMSPCI[1:4,1:4]
which(MBMEcHMSPCI[,"MBME1"] == 1)
```

---

### Description

AP-MS data published by Krogan et al. (2004)

### Usage

```r
data(Krogan)
```

### Details

**Krogan** is a matrix of the AP-MS data published by Krogan et al (2004). The 153 rows correspond to bait proteins and the 485 columns correspond to proteins found as hits in the AP-MS experiment and are named accordingly. The first 153 column names are the same as the 153 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in **Krogan**. An entry of "1" in the ith row and jth column of **Krogan** indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of 1132 "1" entries in the matrix, corresponding to the 1132 comemberships detected in the experiment.

These data are available at [http://www.molecule.org/cgi/content/full/13/2/225/DC1/](http://www.molecule.org/cgi/content/full/13/2/225/DC1/).

### Source


### References


### See Also

- **MBMEcKrogan**

### Examples

```r
data(Krogan)
```
Krogan complexes

Description
Affiliation matrices with rows corresponding to proteins and columns corresponding to complexes.

Usage
data(MBMEcKrogan)

Details
These are the results from an analysis of the AP-MS data (Krogan et al., 2004). These estimates were constructed using findComplexes with a sensitivity parameter of .75, specificity of .99, and Beta=-0.2 for externally derived similarity measure based on Gene Ontology cellular component annotation (see Scholtens and Gentleman (2004)).

MBMEchMSPCI contains 82 multi-bait-multi-edge complex estimates.

Source

References
High-Definition Macromolecular Composition of Yeast RNA-Processing Complexes; Molecular Cell, Vol 13, 225-239, 30 January 2004

Examples
data(MBMEcKrogan)
MBMEcKrogan[1:4,1:4]

Tandem Affinity Purification (TAP) Data from Krogan et al. (2006)

Description

Usage
data(kroganBPMat2006)
**Details**

kroganBPMat2006 is a matrix of the TAP data published by Krogan, et al. (2006). The 2264 rows correspond to bait proteins and the 5361 columns correspond to proteins found as hits in the TAP experiment and are named accordingly. The first 2264 column names are the same as the 2264 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in kroganBPMat2006. An entry of "1" in the ith row and jth column of kroganBPMat2006 indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of "1" entries in the matrix, corresponding to the 63360 comemberships detected in the experiment.

These data were obtained from the Primary Source -

**Source**


**See Also**
yTAP, MBMEcTAP, SBMHcTAP, UnRBBcTAP, HMSPCI

**Examples**

data(kroganBPMat2006)
which(kroganBPMat2006[,1]==1)

---

**LCjoin**

*Computes change in LxC measure*

**Description**

Computes the change in the P=LxC measure for AP-MS protein data when two protein complex estimates are combined into one complex.

**Details**

These functions are used to evaluate changes in the penalized likelihood when two complexes are combined. They are not meant to be directly used.

**Value**

The numeric value of the change in P=LxC when two complexes are combined.

**Author(s)**

Denise Scholtens

**References**


mergeComplexes

**See Also**

bhmaxSubgraph, mergeComplexes, findComplexes

**Examples**

```r
data(apEX)
PCMG0 <- bhmaxSubgraph(apEX)
PCMG1 <- mergeComplexes(PCMG0, apEX, sensitivity=.7, specificity=.75)
```

---

**mergeComplexes**

*Iteratively combine columns in initial PCMG estimate*

**Description**

Repeatedly applies the function `LCdelta` to make combinations of columns in the affiliation matrix representing the protein complex membership graph (PCMG) for AP-MS data.

**Usage**

```r
mergeComplexes(bhmax, adjMat, VBs=NULL, VPs=NULL, simMat=NULL, sensitivity=.75, specificity=.995, Beta=0, commonFrac=2/3, wsVal = 2e7)
```

**Arguments**

- `bhmax`: Initial complex estimates coming from `bhmaxSubgraph`
- `adjMat`: Adjacency matrix of bait-hit data from an AP-MS experiment. Rows correspond to baits and columns to hits.
- `VBs`: VBs is an optional vector of viable baits.
- `VPs`: VPs is an optional vector of viable prey.
- `simMat`: An optional square matrix with entries between 0 and 1. Rows and columns correspond to the proteins in the experiment, and should be reported in the same order as the columns of `adjMat`. Higher values in this matrix are interpreted to mean higher similarity for protein pairs.
- `sensitivity`: Believed sensitivity of AP-MS technology.
- `specificity`: Believed specificity of AP-MS technology.
- `Beta`: Optional additional parameter for the weight to give data in `simMat` in the logistic regression model.
- `commonFrac`: This is the fraction of baits that need to be overlapping for a complex combination to be considered.
- `wsVal`: A numeric. This is the value assigned to the work-space in the call to `fisher.test`. 
Details
The local modeling algorithm for AP-MS data described by Scholtens and Gentleman (2004) and Scholtens, Vidal, and Gentleman (2005) uses a two-component measure of protein complex estimate quality, namely $P=L\times C$. Columns in $cMat$ represent individual complex estimates. The algorithm works by starting with a maximal BH-complete subgraph estimate of $cMat$, and then improves the estimate by combining complexes such that $P=L\times C$ increases.

By default commonFrac is set relatively high at 2/3. This means that some potentially reasonable complex combinations could be missed. For smaller data sets, users may consider decreasing the fraction. For larger data sets, this may cause a large increase in computation time.

Value
A list of character vectors containing the names of the proteins in the estimated complexes.

Author(s)
Denise Scholtens

References

See Also
bhmaxSubgraph, findComplexes

Examples

```r
data(apEX)
PCMG0 <- bhmaxSubgraph(apEX)
PCMG1 <- mergeComplexes(PCMG0, apEX, sensitivity=.7, specificity=.75)
```

Description
plotComplex renders complex estimates from the apComplex algorithm using Rgraphviz.

Usage

```r
plotComplex(complexMembers, g, VBs, VPs, geneName=FALSE, baitColor="yellow", preyColor="white", recipLineColor="red", unrecipBBLineColor="blue", unrecipBPLineColor="gray", y="neato")
```
Arguments

complexMembers  A character vector of proteins composing a complex estimate.
g  An object of class graph, the full bait-prey graph of AP-MS data used in analysis. complexMembers must be a subset of the node names of g.
VBs  A vector of viable baits used in the AP-MS experiment.
VPs  A vector of viable prey used in the AP-MS experiment.
geneName  A logical indicating whether or not nodes should be plotted with common gene names as labels rather than systematic names.
baitColor  Color of bait nodes.
preyColor  Color of prey nodes.
recipLineColor  Color of edges connecting baits which both detected each other as prey.
unrecipBBLineColor  Color of edges connecting baits in which one bait finds the other as prey but not vice versa.
unrecipBPLineColor  Color of edges extending from baits to proteins that were only used as prey, hence reciprocity is not possible.
y  Layout of plot

Details

This is a simple function for plotting complex estimates resulting from the apComplex algorithm. Giving the upcoming changes in Rgraphviz, it will likely be changed substantially.

Value

A plotted graph of the complex estimate subgraph.

Author(s)

Denise Scholtens

References


See Also

findComplexes

Examples

data(apEX)
data(apEXG)
PCMG2 <- findComplexes(apEX,sensitivity=.7,specificity=.75)
PCMG2sorted <- sortComplexes(PCMG2,apEX)
sortComplexes

VBs <- rownames(apEX)
VPs <- setdiff(colnames(apEX), VBs)

plotComplex(PCMG2sorted$MBME[[1]], g=apEXG, VBs=VBs, VPs=VPs)

sortComplexes
Sort complex estimates

Description
Sorts complexes recorded in PCMG list into three separate lists containing MBME, SBMH, and UnRBB complexes.

Usage
sortComplexes(PCMG, adjMat)

Arguments
PCMG
Current PCMG estimate
adjMat
Adjacency matrix of bait-hit data from an AP-MS experiment. Rows correspond to baits and columns to hits.

Details
MBME complexes contain multiple bait proteins and multiple edges. SBMH complexes contain one bait and a collection of hit-only proteins. UnRBB complexes contain only two baits (no hit-only proteins) that are connected by an unreciprocated edge.

Value
A list of lists representing the MBME, SBMH, and UnRBB complex estimates.

Author(s)
Denise Scholtens

References

See Also
findComplexes
Examples

```r
data(apEX)
PCMG2 <- findComplexes(apEX,sensitivity=.7,specificity=.75)
sortComplexes(PCMG2,apEX)
```

---

**TAP**  
**Tandem Affinity Purification (TAP) Data from Gavin et al. (2002)**

**Description**


**Usage**

```r
data(TAP)
data(TAPgraph)
```

**Details**

TAP is a matrix of the TAP data published by Gavin, et al. (2002). The 455 rows correspond to bait proteins and the 1364 columns correspond to proteins found as hits in the TAP experiment and are named accordingly. The first 455 column names are the same as the 455 row names; bait proteins can also be found as hits by other baits, hence their inclusion as columns in TAP. An entry of "1" in the ith row and jth column of TAP indicates that bait protein i found protein j as a hit. All other entries are "0". There are a total of 3420 "1" entries in the matrix, corresponding to the 3420 comemberships detected in the experiment.

TAPgraph is a graphNEL object in which 1364 nodes represent proteins and 3420 directed edges represent comemberships detected in the purification. Each directed edge originates at the bait and ends at the hit. Each edge in TAPgraph corresponds to an entry of "1" in the TAP matrix.

These data are available in Supplementary Table S1 of Gavin et al. at http://www.nature.com.

**Source**


**References**


**See Also**

yTAP, MBMEcTAP, SBMHcTAP, UnRBBcTAP, HMSPCI
Examples

```r
data(TAP)
which(TAP["Abd1",]==1)

data(TAPgraph)
adj(TAPgraph,"Abd1")
```

Description

Affiliation matrices with rows corresponding to proteins and columns corresponding to complexes.

Usage

```r
data(MBMEcTAP)
data(SBMHcTAP)
data(UnRBBcTAP)
```

Details

These are the results from an analysis of the TAP data (Gavin et al., 2002) by Scholtens and Gentleman (2004) and Scholtens, Vidal, and Gentleman (submitted). These estimates were constructed using findComplexes with a sensitivity parameter of .75, specificity of .995, and Beta=-0.2 for externally derived similarity measure based on Gene Ontology cellular component annotation (see Scholtens and Gentleman (2004)).


Source


References


See Also

*TAP, TAPgraph, yTAP, findComplexes*
**Examples**

```r
data(MBMEcTAP)
MBMEcTAP[1:10,1:3]
which(MBMEcTAP[,"MBME1"]==1)
```

**Description**

Affiliation matrices with rows corresponding to proteins and columns corresponding to complexes.

**Usage**

```r
data(yNameTAP)
```

**Details**

These are the results from an analysis of the TAP data (Gavin et al., 2002) by Scholtens and Gentleman (2004) and Scholtens, Vidal, and Gentleman (submitted). These estimates were constructed using `findComplexes` with a sensitivity parameter of .75, specificity of .995, and Beta=-0.2 for externally derived similarity measure based on Gene Ontology cellular component annotation (see Scholtens and Gentleman (2004)).

`yNameTAP` contains 260 multi-bait-multi-edge complex estimates.

**Source**


**References**


**See Also**

`TAP`, `TAPgraph`, `yTAP`, `findComplexes`

**Examples**

```r
data(yNameTAP)
yNameTAP[1:10,1:3]
```
Description

Usage
data(yTAP)

Details
Each element of the yTAP list contains a vector of the proteins reported as part of the complex, as well as the functional annotation category published by Gavin, et al. (2002).
These data are available in Supplementary Table S3 of Gavin, et al. (2002) at http://www.nature.com and at http://yeast.cellzome.com.

Source

See Also
TAP, TAPgraph, MBMEcTAP, SBMHcTAP, UnRBBcTAP, HMSPC1

Examples
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