Package: spectralGraphTopology (via r-universe)

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Title Learning Graphs from Data via Spectral Constraints

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Description In the era of big data and hyperconnectivity, learning high-dimensional structures such as graphs from data has become a prominent task in machine learning and has found applications in many fields such as finance, health care, and networks. 'spectralGraphTopology' is an open source, documented, and well-tested R package for learning graphs from data. It provides implementations of state of the art algorithms such as Combinatorial Graph Laplacian Learning (CGL), Spectral Graph Learning (SGL), Graph Estimation based on Majorization-Minimization (GLE-MM), and Graph Estimation based on Alternating Direction Method of Multipliers (GLE-ADMM). In addition, graph learning has been widely employed for clustering, where specific algorithms are available in the literature. To this end, we provide an implementation of the Constrained Laplacian Rank (CLR) algorithm.

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URL https://github.com/dppalomar/spectralGraphTopology, https://mirca.github.io/spectralGraphTopology/, https://www.danielppalomar.com

BugReports https://github.com/dppalomar/spectralGraphTopology/issues

License GPL-3

Encoding UTF-8

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Imports Rcpp (>= 0.11.0), MASS, Matrix, progress, rlist

RoxygenNote 7.1.1

Suggests CVXR, bookdown, knitr, prettydoc, rmarkdown, R.rsp, testthat, patrick, corrplot, igraph, kernlab, pals, clusterSim, viridis, quadprog, matrixcalc

VignetteBuilder CVXR, knitr, rmarkdown, R.rsp

NeedsCompilation yes

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Package spectralGraphTopology

Description

This package provides estimators to learn k-component, bipartite, and k-component bipartite graphs from data by imposing spectral constraints on the eigenvalues and eigenvectors of the Laplacian and adjacency matrices. Those estimators leverages spectral properties of the graphical models as a prior information, which turn out to play key roles in unsupervised machine learning tasks such as community detection.

Functions

`learn_k_component_graph` `learn_bipartite_graph` `learn_bipartite_k_component_graph` `cluster_k_component_g`
`learn_laplacian_gle_mm` `learn_laplacian_gle_admm` `L` `A`

Help

For a quick help see the README file: GitHub-README.

Author(s)

Ze Vinicius and Daniel P. Palomar

References

S. Kumar, J. Ying, J. V. de Miranda Cardoso, and D. P. Palomar (2019). <https://arxiv.org/abs/1904.09792>

N., Feiping, W., Xiaoqian, J., Michael I., and H., Heng. (2016). The Constrained Laplacian Rank Algorithm for Graph-based Clustering, AAAI'16. <http://dl.acm.org/citation.cfm?id=3016100.3016174>

Licheng Zhao, Yiwei Wang, Sandeep Kumar, and Daniel P. Palomar. Optimization Algorithms for Graph Laplacian Estimation via ADMM and MM IEEE Trans. on Signal Processing, vol. 67, no. 16, pp. 4231-4244, Aug. 2019

A
Computes the Adjacency linear operator which maps a vector of weights into a valid Adjacency matrix.

Description

Computes the Adjacency linear operator which maps a vector of weights into a valid Adjacency matrix.

Usage

```
A(w)
```

Arguments

`w`	weight vector of the graph

Value

Aw the Adjacency matrix

Examples

```
library(spectralGraphTopology)
Aw <- A(c(1, 0, 1))
Aw
```

`accuracy` *Computes the accuracy between two matrices*

Description

Computes the accuracy between two matrices

Usage

```
accuracy(Wtrue, West, eps = 1e-04)
```

Arguments

`Wtrue`	true matrix
`West`	estimated matrix
`eps`	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
accuracy(X, X)
```

`Astar` *Computes the Astar operator.*

Description

Computes the Astar operator.

Usage

```
Astar(M)
```

Arguments

M	matrix

Value

w vector

`block_diag` *Constructs a block diagonal matrix from a list of square matrices*

Description

Constructs a block diagonal matrix from a list of square matrices

Usage

```
block_diag(...)
```

Arguments

...	list of matrices or individual matrices

Value

block diagonal matrix

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
Y <- L(c(1, 0, 1, 0, 0, 1))
B <- block_diag(X, Y)
B
```

`cluster_k_component_graph`

Cluster a k-component graph from data using the Constrained Laplacian Rank algorithm Cluster a k-component graph on the basis of an observed data matrix. Check out https://mirca.github.io/spectralGraphTopology for code examples.

Description

Cluster a k-component graph from data using the Constrained Laplacian Rank algorithm

Cluster a k-component graph on the basis of an observed data matrix. Check out https://mirca.github.io/spectralGraphTopolog for code examples.

Usage

```
cluster_k_component_graph(
  Y,
  k = 1,
  m = 5,
  lmd = 1,
  eigtol = 1e-09,
  edgetol = 1e-06,
  maxiter = 1000
)
```

Arguments

`Y`	a pxn data matrix, where p is the number of nodes and n is the number of features (or data points per node)
`k`	the number of components of the graph
`m`	the maximum number of possible connections for a given node used to build an affinity matrix
`lmd`	L2-norm regularization hyperparameter
`eigtol`	value below which eigenvalues are considered to be zero
`edgetol`	value below which edge weights are considered to be zero
`maxiter`	the maximum number of iterations

Value

A list containing the following elements:

`laplacian`	the estimated Laplacian Matrix
`adjacency`	the estimated Adjacency Matrix
`eigvals`	the eigenvalues of the Laplacian Matrix

`lmd_seq`	sequence of lmd values at every iteration
`elapsed_time`	elapsed time at every iteration

Author(s)

Ze Vinicius and Daniel Palomar

References

Nie, Feiping and Wang, Xiaoqian and Jordan, Michael I. and Huang, Heng. The Constrained Laplacian Rank Algorithm for Graph-based Clustering, 2016, AAAI'16. http://dl.acm.org/citation.cfm?id=3016100.3016174

Examples

```
library(clusterSim)
library(spectralGraphTopology)
library(igraph)
set.seed(1)
# number of nodes per cluster
N <- 30
# generate datapoints
twomoon <- shapes.two.moon(N)
# estimate underlying graph
graph <- cluster_k_component_graph(twomoon$data, k = 2)
# build network
net <- graph_from_adjacency_matrix(graph$adjacency, mode = "undirected", weighted = TRUE)
# colorify nodes and edges
colors <- c("#706FD3", "#FF5252", "#33D9B2")
V(net)$cluster <- twomoon$clusters
E(net)$color <- apply(as.data.frame(get.edgelist(net)), 1,
                      function(x) ifelse(V(net)$cluster[x[1]] == V(net)$cluster[x[2]],
                                         colors[V(net)$cluster[x[1]]], '#000000'))
V(net)$color <- c(colors[1], colors[2])[twomoon$clusters]
# plot network
plot(net, layout = twomoon$data, vertex.label = NA, vertex.size = 3)
```

D — *Computes the degree operator from the vector of edge weights.*

Description

Computes the degree operator from the vector of edge weights.

Usage

```
D(w)
```

Arguments

`w`	vector

Value

Dw vector

`Dstar` *Computes the Dstar operator, i.e., the adjoint of the D operator.*

Description

Computes the Dstar operator, i.e., the adjoint of the D operator.

Usage

```
Dstar(w)
```

Arguments

`w`	vector

Value

Dstar(w) vector

`fdr` *Computes the false discovery rate between two matrices*

Description

Computes the false discovery rate between two matrices

Usage

```
fdr(Wtrue, West, eps = 1e-04)
```

Arguments

`Wtrue`	true matrix
`West`	estimated matrix
`eps`	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
fdr(X, X)
```

`fscore` *Computes the fscore between two matrices*

Description

Computes the fscore between two matrices

Usage

```
fscore(Wtrue, West, eps = 1e-04)
```

Arguments

`Wtrue`	true matrix
`West`	estimated matrix
`eps`	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
fscore(X, X)
```

`L` *Computes the Laplacian linear operator which maps a vector of weights into a valid Laplacian matrix.*

Description

Computes the Laplacian linear operator which maps a vector of weights into a valid Laplacian matrix.

Usage

```
L(w)
```

Arguments

`w`	weight vector of the graph

Value

Lw the Laplacian matrix

Examples

```
library(spectralGraphTopology)
Lw <- L(c(1, 0, 1))
Lw
```

---

learn_bipartite_graph *Learn a bipartite graph Learns a bipartite graph on the basis of an observed data matrix*

Description

Learn a bipartite graph

Learns a bipartite graph on the basis of an observed data matrix

Usage

```
learn_bipartite_graph(
  S,
  is_data_matrix = FALSE,
  z = 0,
  nu = 10000,
  alpha = 0,
  w0 = "naive",
  m = 7,
  maxiter = 10000,
  abstol = 1e-06,
  reltol = 1e-04,
  record_weights = FALSE,
  verbose = TRUE
)
```

Arguments

S	either a pxp sample covariance/correlation matrix, or a pxn data matrix, where p is the number of nodes and n is the number of features (or data points per node)
is_data_matrix	whether the matrix S should be treated as data matrix or sample covariance matrix
z	the number of zero eigenvalues for the Adjancecy matrix
nu	regularization hyperparameter for the term ||A(w) - V Psi V'||^2_F
alpha	L1 regularization hyperparameter
w0	initial estimate for the weight vector the graph or a string selecting an appropriate method. Available methods are: "qp": finds w0 that minimizes ||ginv(S) - L(w0)||_F, w0 >= 0; "naive": takes w0 as the negative of the off-diagonal elements of the pseudo inverse, setting to 0 any elements s.t. w0 < 0

`m`	in case is_data_matrix = TRUE, then we build an affinity matrix based on Nie et. al. 2017, where m is the maximum number of possible connections for a given node
`maxiter`	the maximum number of iterations
`abstol`	absolute tolerance on the weight vector w
`reltol`	relative tolerance on the weight vector w
`record_weights`	whether to record the edge values at each iteration
`verbose`	whether to output a progress bar showing the evolution of the iterations

Value

A list containing possibly the following elements:

`laplacian`	the estimated Laplacian Matrix
`adjacency`	the estimated Adjacency Matrix
`w`	the estimated weight vector
`psi`	optimization variable accounting for the eigenvalues of the Adjacency matrix
`V`	eigenvectors of the estimated Adjacency matrix
`elapsed_time`	elapsed time recorded at every iteration
`convergence`	boolean flag to indicate whether or not the optimization converged
`obj_fun`	values of the objective function at every iteration in case record_objective = TRUE
`negloglike`	values of the negative loglikelihood at every iteration in case record_objective = TRUE
`w_seq`	sequence of weight vectors at every iteration in case record_weights = TRUE

Author(s)

Ze Vinicius and Daniel Palomar

References

S. Kumar, J. Ying, J. V. M. Cardoso, D. P. Palomar. A unified framework for structured graph learning via spectral constraints. Journal of Machine Learning Research, 2020. http://jmlr.org/papers/v21/19-276.html

Examples

```
library(spectralGraphTopology)
library(igraph)
library(viridis)
library(corrplot)
set.seed(42)
n1 <- 10
n2 <- 6
n <- n1 + n2
```

```
pc <- .9
bipartite <- sample_bipartite(n1, n2, type="Gnp", p = pc, directed=FALSE)
# randomly assign edge weights to connected nodes
E(bipartite)$weight <- runif(gsize(bipartite), min = 0, max = 1)
# get true Laplacian and Adjacency
Ltrue <- as.matrix(laplacian_matrix(bipartite))
Atrue <- diag(diag(Ltrue)) - Ltrue
# get samples
Y <- MASS::mvrnorm(100 * n, rep(0, n), Sigma = MASS::ginv(Ltrue))
# compute sample covariance matrix
S <- cov(Y)
# estimate Adjacency matrix
graph <- learn_bipartite_graph(S, z = 4, verbose = FALSE)
graph$adjacency[graph$adjacency < 1e-3] <- 0
# Plot Adjacency matrices: true, noisy, and estimated
corrplot(Atrue / max(Atrue), is.corr = FALSE, method = "square",
         addgrid.col = NA, tl.pos = "n", cl.cex = 1.25)
corrplot(graph$adjacency / max(graph$adjacency), is.corr = FALSE,
         method = "square", addgrid.col = NA, tl.pos = "n", cl.cex = 1.25)
# build networks
estimated_bipartite <- graph_from_adjacency_matrix(graph$adjacency,
                                                   mode = "undirected",
                                                   weighted = TRUE)
V(estimated_bipartite)$type <- c(rep(0, 10), rep(1, 6))
la = layout_as_bipartite(estimated_bipartite)
colors <- viridis(20, begin = 0, end = 1, direction = -1)
c_scale <- colorRamp(colors)
E(estimated_bipartite)$color = apply(
  c_scale(E(estimated_bipartite)$weight / max(E(estimated_bipartite)$weight)), 1,
                          function(x) rgb(x[1]/255, x[2]/255, x[3]/255))
E(bipartite)$color = apply(c_scale(E(bipartite)$weight / max(E(bipartite)$weight)), 1,
                      function(x) rgb(x[1]/255, x[2]/255, x[3]/255))
la = la[, c(2, 1)]
# Plot networks: true and estimated
plot(bipartite, layout = la, vertex.color=c("red","black")[V(bipartite)$type + 1],
     vertex.shape = c("square", "circle")[V(bipartite)$type + 1],
     vertex.label = NA, vertex.size = 5)
plot(estimated_bipartite, layout = la,
     vertex.color=c("red","black")[V(estimated_bipartite)$type + 1],
     vertex.shape = c("square", "circle")[V(estimated_bipartite)$type + 1],
     vertex.label = NA, vertex.size = 5)
```

`learn_bipartite_k_component_graph` *Learns a bipartite k-component graph Jointly learns the Laplacian and Adjacency matrices of a graph on the basis of an observed data matrix*

Description

Learns a bipartite k-component graph

Jointly learns the Laplacian and Adjacency matrices of a graph on the basis of an observed data matrix

Usage

```
learn_bipartite_k_component_graph(
  S,
  is_data_matrix = FALSE,
  z = 0,
  k = 1,
  w0 = "naive",
  m = 7,
  alpha = 0,
  beta = 10000,
  rho = 0.01,
  fix_beta = TRUE,
  beta_max = 1e+06,
  nu = 10000,
  lb = 0,
  ub = 10000,
  maxiter = 10000,
  abstol = 1e-06,
  reltol = 1e-04,
  eigtol = 1e-09,
  record_weights = FALSE,
  record_objective = FALSE,
  verbose = TRUE
)
```

Arguments

`S`	either a pxp sample covariance/correlation matrix, or a pxn data matrix, where p is the number of nodes and n is the number of features (or data points per node)
`is_data_matrix`	whether the matrix S should be treated as data matrix or sample covariance matrix
`z`	the number of zero eigenvalues for the Adjancecy matrix
`k`	the number of components of the graph
`w0`	initial estimate for the weight vector the graph or a string selecting an appropriate method. Available methods are: "qp": finds w0 that minimizes ||ginv(S) - L(w0)||_F, w0 >= 0; "naive": takes w0 as the negative of the off-diagonal elements of the pseudo inverse, setting to 0 any elements s.t. w0 < 0
`m`	in case is_data_matrix = TRUE, then we build an affinity matrix based on Nie et. al. 2017, where m is the maximum number of possible connections for a given node
`alpha`	L1 regularization hyperparameter
`beta`	regularization hyperparameter for the term ||L(w) - U Lambda U'||^2_F
`rho`	how much to increase (decrease) beta in case fix_beta = FALSE

`fix_beta`	whether or not to fix the value of beta. In case this parameter is set to false, then beta will increase (decrease) depending whether the number of zero eigenvalues is lesser (greater) than k
`beta_max`	maximum allowed value for beta
`nu`	regularization hyperparameter for the term ||A(w) - V Psi V'||^2_F
`lb`	lower bound for the eigenvalues of the Laplacian matrix
`ub`	upper bound for the eigenvalues of the Laplacian matrix
`maxiter`	the maximum number of iterations
`abstol`	absolute tolerance on the weight vector w
`reltol`	relative tolerance on the weight vector w
`eigtol`	value below which eigenvalues are considered to be zero
`record_weights`	whether to record the edge values at each iteration
`record_objective`	whether to record the objective function values at each iteration
`verbose`	whether to output a progress bar showing the evolution of the iterations

Value

A list containing possibly the following elements:

`laplacian`	the estimated Laplacian Matrix
`adjacency`	the estimated Adjacency Matrix
`w`	the estimated weight vector
`psi`	optimization variable accounting for the eigenvalues of the Adjacency matrix
`lambda`	optimization variable accounting for the eigenvalues of the Laplacian matrix
`V`	eigenvectors of the estimated Adjacency matrix
`U`	eigenvectors of the estimated Laplacian matrix
`elapsed_time`	elapsed time recorded at every iteration
`beta_seq`	sequence of values taken by beta in case fix_beta = FALSE
`convergence`	boolean flag to indicate whether or not the optimization converged
`obj_fun`	values of the objective function at every iteration in case record_objective = TRUE
`negloglike`	values of the negative loglikelihood at every iteration in case record_objective = TRUE
`w_seq`	sequence of weight vectors at every iteration in case record_weights = TRUE

Author(s)

Ze Vinicius and Daniel Palomar

References

S. Kumar, J. Ying, J. V. M. Cardoso, D. P. Palomar. A unified framework for structured graph learning via spectral constraints. Journal of Machine Learning Research, 2020. http://jmlr.org/papers/v21/19-276.html

Examples

```
library(spectralGraphTopology)
library(igraph)
library(viridis)
library(corrplot)
set.seed(42)
w <- c(1, 0, 0, 1, 0, 1) * runif(6)
Laplacian <- block_diag(L(w), L(w))
Atrue <- diag(diag(Laplacian)) - Laplacian
bipartite <- graph_from_adjacency_matrix(Atrue, mode = "undirected", weighted = TRUE)
n <- ncol(Laplacian)
Y <- MASS::mvrnorm(40 * n, rep(0, n), MASS::ginv(Laplacian))
graph <- learn_bipartite_k_component_graph(cov(Y), k = 2, beta = 1e2, nu = 1e2, verbose = FALSE)
graph$adjacency[graph$adjacency < 1e-2] <- 0
# Plot Adjacency matrices: true, noisy, and estimated
corrplot(Atrue / max(Atrue), is.corr = FALSE, method = "square", addgrid.col = NA, tl.pos = "n",
         cl.cex = 1.25)
corrplot(graph$adjacency / max(graph$adjacency), is.corr = FALSE, method = "square",
         addgrid.col = NA, tl.pos = "n", cl.cex = 1.25)
# Plot networks
estimated_bipartite <- graph_from_adjacency_matrix(graph$adjacency, mode = "undirected",
                                                   weighted = TRUE)
V(bipartite)$type <- rep(c(TRUE, FALSE), 4)
V(estimated_bipartite)$type <- rep(c(TRUE, FALSE), 4)
la = layout_as_bipartite(estimated_bipartite)
colors <- viridis(20, begin = 0, end = 1, direction = -1)
c_scale <- colorRamp(colors)
E(estimated_bipartite)$color = apply(
          c_scale(E(estimated_bipartite)$weight / max(E(estimated_bipartite)$weight)), 1,
                                      function(x) rgb(x[1]/255, x[2]/255, x[3]/255))
E(bipartite)$color = apply(c_scale(E(bipartite)$weight / max(E(bipartite)$weight)), 1,
                           function(x) rgb(x[1]/255, x[2]/255, x[3]/255))
la = la[, c(2, 1)]
# Plot networks: true and estimated
plot(bipartite, layout = la,
     vertex.color = c("red","black")[V(bipartite)$type + 1],
     vertex.shape = c("square", "circle")[V(bipartite)$type + 1],
     vertex.label = NA, vertex.size = 5)
plot(estimated_bipartite, layout = la,
     vertex.color = c("red","black")[V(estimated_bipartite)$type + 1],
     vertex.shape = c("square", "circle")[V(estimated_bipartite)$type + 1],
     vertex.label = NA, vertex.size = 5)
```

learn_combinatorial_graph_laplacian

Learn the Combinatorial Graph Laplacian from data Learns a graph Laplacian matrix using the Combinatorial Graph Laplacian (CGL) algorithm proposed by Egilmez et. al. (2017)

Description

Learn the Combinatorial Graph Laplacian from data

Learns a graph Laplacian matrix using the Combinatorial Graph Laplacian (CGL) algorithm proposed by Egilmez et. al. (2017)

Usage

```
learn_combinatorial_graph_laplacian(
  S,
  A_mask = NULL,
  alpha = 0,
  reltol = 1e-05,
  max_cycle = 10000,
  regtype = 1,
  record_objective = FALSE,
  verbose = TRUE
)
```

Arguments

S	sample covariance matrix
A_mask	binary adjacency matrix of the graph
alpha	L1-norm regularization hyperparameter
reltol	minimum relative error considered for the stopping criteri
max_cycle	maximum number of cycles
regtype	type of L1-norm regularization. If reg_type == 1, then all elements of the Laplacian matrix will be regularized. If reg_type == 2, only the off-diagonal elements will be regularized
record_objective	whether or not to record the objective function value at every iteration. Default is FALSE
verbose	if TRUE, then a progress bar will be displayed in the console. Default is TRUE

Value

A list containing possibly the following elements

laplacian	estimated Laplacian Matrix

`elapsed_time`	elapsed time recorded at every iteration
`frod_norm`	relative Frobenius norm between consecutive estimates of the Laplacian matrix
`convergence`	whether or not the algorithm has converged within the tolerance and max number of iterations
`obj_fun`	objective function value at every iteration, in case record_objective = TRUE

References

H. E. Egilmez, E. Pavez and A. Ortega, "Graph Learning From Data Under Laplacian and Structural Constraints", in IEEE Journal of Selected Topics in Signal Processing, vol. 11, no. 6, pp. 825-841, Sept. 2017. Original MATLAB source code is available at: https://github.com/STAC-USC/Graph_Learning

---

`learn_graph_sigrep` *Learn graphs from a smooth signal representation approach This function learns a graph from a observed data matrix using the method proposed by Dong (2016).*

Description

Learn graphs from a smooth signal representation approach

This function learns a graph from a observed data matrix using the method proposed by Dong (2016).

Usage

```
learn_graph_sigrep(
  X,
  alpha = 0.001,
  beta = 0.5,
  maxiter = 1000,
  ftol = 1e-04,
  verbose = TRUE
)
```

Arguments

`X`	a p-by-n data matrix, where p is the number of nodes and n is the number of observations
`alpha`	hyperparameter that controls the importance of the Dirichlet energy penalty
`beta`	hyperparameter that controls the importance of the L2-norm regularization
`maxiter`	maximum number of iterations
`ftol`	relative error on the objective function to be used as the stopping criteria
`verbose`	if TRUE, then a progress bar will be displayed in the console. Default is TRUE

Value

A list containing the following items

`laplacian`	estimated Laplacian Matrix
`Y`	a smoothed approximation of the data matrix X
`convergence`	whether or not the algorithm has converged within the tolerance and max number of iterations
`obj_fun`	objective function value at every iteration, in case record_objective = TRUE

References

X. Dong, D. Thanou, P. Frossard and P. Vandergheynst, "Learning Laplacian Matrix in Smooth Graph Signal Representations," in IEEE Transactions on Signal Processing, vol. 64, no. 23, pp. 6160-6173, Dec.1, 2016.

`learn_k_component_graph`

Learn the Laplacian matrix of a k-component graph Learns a k-component graph on the basis of an observed data matrix. Check out https://mirca.github.io/spectralGraphTopology for code examples.

Description

Learn the Laplacian matrix of a k-component graph

Learns a k-component graph on the basis of an observed data matrix. Check out https://mirca.github.io/spectralGraphTopolog
for code examples.

Usage

```
learn_k_component_graph(
  S,
  is_data_matrix = FALSE,
  k = 1,
  w0 = "naive",
  lb = 0,
  ub = 10000,
  alpha = 0,
  beta = 10000,
  beta_max = 1e+06,
  fix_beta = TRUE,
  rho = 0.01,
  m = 7,
  eps = 1e-04,
  maxiter = 10000,
  abstol = 1e-06,
  reltol = 1e-04,
```

```
  eigtol = 1e-09,
  record_objective = FALSE,
  record_weights = FALSE,
  verbose = TRUE
)
```

Arguments

S	either a pxp sample covariance/correlation matrix, or a pxn data matrix, where p is the number of nodes and n is the number of features (or data points per node)
is_data_matrix	whether the matrix S should be treated as data matrix or sample covariance matrix
k	the number of components of the graph
w0	initial estimate for the weight vector the graph or a string selecting an appropriate method. Available methods are: "qp": finds w0 that minimizes ||ginv(S) - L(w0)||_F, w0 >= 0; "naive": takes w0 as the negative of the off-diagonal elements of the pseudo inverse, setting to 0 any elements s.t. w0 < 0
lb	lower bound for the eigenvalues of the Laplacian matrix
ub	upper bound for the eigenvalues of the Laplacian matrix
alpha	reweighted l1-norm regularization hyperparameter
beta	regularization hyperparameter for the term ||L(w) - U Lambda U'||^2_F
beta_max	maximum allowed value for beta
fix_beta	whether or not to fix the value of beta. In case this parameter is set to false, then beta will increase (decrease) depending whether the number of zero eigenvalues is lesser (greater) than k
rho	how much to increase (decrease) beta in case fix_beta = FALSE
m	in case is_data_matrix = TRUE, then we build an affinity matrix based on Nie et. al. 2017, where m is the maximum number of possible connections for a given node
eps	small positive constant
maxiter	the maximum number of iterations
abstol	absolute tolerance on the weight vector w
reltol	relative tolerance on the weight vector w
eigtol	value below which eigenvalues are considered to be zero
record_objective	whether to record the objective function values at each iteration
record_weights	whether to record the edge values at each iteration
verbose	whether to output a progress bar showing the evolution of the iterations

Value

A list containing possibly the following elements:

`laplacian`	the estimated Laplacian Matrix
`adjacency`	the estimated Adjacency Matrix
`w`	the estimated weight vector
`lambda`	optimization variable accounting for the eigenvalues of the Laplacian matrix
`U`	eigenvectors of the estimated Laplacian matrix
`elapsed_time`	elapsed time recorded at every iteration
`beta_seq`	sequence of values taken by beta in case fix_beta = FALSE
`convergence`	boolean flag to indicate whether or not the optimization converged
`obj_fun`	values of the objective function at every iteration in case record_objective = TRUE
`negloglike`	values of the negative loglikelihood at every iteration in case record_objective = TRUE
`w_seq`	sequence of weight vectors at every iteration in case record_weights = TRUE

Author(s)

Ze Vinicius and Daniel Palomar

References

S. Kumar, J. Ying, J. V. M. Cardoso, D. P. Palomar. A unified framework for structured graph learning via spectral constraints. Journal of Machine Learning Research, 2020. http://jmlr.org/papers/v21/19-276.html

Examples

```
# design true Laplacian
Laplacian <- rbind(c(1, -1, 0, 0),
                   c(-1, 1, 0, 0),
                   c(0, 0, 1, -1),
                   c(0, 0, -1, 1))
n <- ncol(Laplacian)
# sample data from multivariate Gaussian
Y <- MASS::mvrnorm(n * 500, rep(0, n), MASS::ginv(Laplacian))
# estimate graph on the basis of sampled data
graph <- learn_k_component_graph(cov(Y), k = 2, beta = 10)
graph$laplacian
```

---

learn_laplacian_gle_admm
Learn the weighted Laplacian matrix of a graph using the ADMM method

---

Description

Learn the weighted Laplacian matrix of a graph using the ADMM method

Usage

```
learn_laplacian_gle_admm(
  S,
  A_mask = NULL,
  alpha = 0,
  rho = 1,
  maxiter = 10000,
  reltol = 1e-05,
  record_objective = FALSE,
  verbose = TRUE
)
```

Arguments

`S`	a pxp sample covariance/correlation matrix
`A_mask`	the binary adjacency matrix of the graph
`alpha`	L1 regularization hyperparameter
`rho`	ADMM convergence rate hyperparameter
`maxiter`	the maximum number of iterations
`reltol`	relative tolerance on the Laplacian matrix estimation
`record_objective`	whether or not to record the objective function. Default is FALSE
`verbose`	if TRUE, then a progress bar will be displayed in the console. Default is TRUE

Value

A list containing possibly the following elements:

`Laplacian`	the estimated Laplacian Matrix
`Adjacency`	the estimated Adjacency Matrix
`convergence`	boolean flag to indicate whether or not the optimization converged
`obj_fun`	values of the objective function at every iteration in case record_objective = TRUE

Author(s)

Ze Vinicius, Jiaxi Ying, and Daniel Palomar

References

Licheng Zhao, Yiwei Wang, Sandeep Kumar, and Daniel P. Palomar. Optimization Algorithms for Graph Laplacian Estimation via ADMM and MM. IEEE Trans. on Signal Processing, vol. 67, no. 16, pp. 4231-4244, Aug. 2019

---

learn_laplacian_gle_mm

Learn the weighted Laplacian matrix of a graph using the MM method

---

Description

Learn the weighted Laplacian matrix of a graph using the MM method

Usage

```
learn_laplacian_gle_mm(
  S,
  A_mask = NULL,
  alpha = 0,
  maxiter = 10000,
  reltol = 1e-05,
  record_objective = FALSE,
  verbose = TRUE
)
```

Arguments

S	a pxp sample covariance/correlation matrix
A_mask	the binary adjacency matrix of the graph
alpha	L1 regularization hyperparameter
maxiter	the maximum number of iterations
reltol	relative tolerance on the weight vector w
record_objective	whether or not to record the objective function. Default is FALSE
verbose	if TRUE, then a progress bar will be displayed in the console. Default is TRUE

Value

A list containing possibly the following elements:

`laplacian`	the estimated Laplacian Matrix
`Adjacency`	the estimated Adjacency Matrix
`convergence`	boolean flag to indicate whether or not the optimization converged
`obj_fun`	values of the objective function at every iteration in case record_objective = TRUE

Author(s)

Ze Vinicius, Jiaxi Ying, and Daniel Palomar

References

Licheng Zhao, Yiwei Wang, Sandeep Kumar, and Daniel P. Palomar. Optimization Algorithms for Graph Laplacian Estimation via ADMM and MM. IEEE Trans. on Signal Processing, vol. 67, no. 16, pp. 4231-4244, Aug. 2019

`learn_smooth_approx_graph`

Learns a smooth approximated graph from an observed data matrix. Check out https://mirca.github.io/spectralGraphTopology for code examples.

Description

Learns a smooth approximated graph from an observed data matrix. Check out https://mirca.github.io/spectralGraphTopology for code examples.

Usage

```
learn_smooth_approx_graph(Y, m)
```

Arguments

`Y`	a p-by-n data matrix, where p is the number of nodes and n is the number of features (or data points per node)
`m`	the maximum number of possible connections for a given node used to build an affinity matrix

Value

A list containing the following elements:

`laplacian`	the estimated Laplacian Matrix

Author(s)

Ze Vinicius and Daniel Palomar

References

Nie, Feiping and Wang, Xiaoqian and Jordan, Michael I. and Huang, Heng. The Constrained Laplacian Rank Algorithm for Graph-based Clustering, 2016, AAAI'16. http://dl.acm.org/citation.cfm?id=3016100.3016174

`learn_smooth_graph` *Learn a graph from smooth signals This function learns a connected graph given an observed signal matrix using the method proposed by Kalofilias (2016).*

Description

Learn a graph from smooth signals

This function learns a connected graph given an observed signal matrix using the method proposed by Kalofilias (2016).

Usage

```
learn_smooth_graph(
  X,
  alpha = 0.01,
  beta = 1e-04,
  step_size = 0.01,
  maxiter = 1000,
  tol = 1e-04
)
```

Arguments

`X`	a p-by-n data matrix, where p is the number of nodes and n is the number of observations
`alpha`	hyperparameter that controls the importance of the Dirichlet energy penalty
`beta`	hyperparameter that controls the importance of the L2-norm regularization
`step_size`	learning rate
`maxiter`	maximum number of iterations
`tol`	relative tolerance used as stopping criteria

References

V. Kalofolias, "How to learn a graph from smooth signals", in Proc. Int. Conf. Artif. Intell. Statist., 2016, pp. 920–929.

Lstar — *Computes the Lstar operator.*

Description

Computes the Lstar operator.

Usage

```
Lstar(M)
```

Arguments

M	matrix

Value

w vector

npv — *Computes the negative predictive value between two matrices*

Description

Computes the negative predictive value between two matrices

Usage

```
npv(Wtrue, West, eps = 1e-04)
```

Arguments

Wtrue	true matrix
West	estimated matrix
eps	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
npv(X, X)
```

recall — *Computes the recall between two matrices*

Description

Computes the recall between two matrices

Usage

```
recall(Wtrue, West, eps = 1e-04)
```

Arguments

Wtrue	true matrix
West	estimated matrix
eps	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
recall(X, X)
```

relative_error — *Computes the relative error between the true and estimated matrices*

Description

Computes the relative error between the true and estimated matrices

Usage

```
relative_error(West, Wtrue)
```

Arguments

West	estimated matrix
Wtrue	true matrix

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
relative_error(X, X)
```

`specificity` *Computes the specificity between two matrices*

Description

Computes the specificity between two matrices

Usage

```
specificity(Wtrue, West, eps = 1e-04)
```

Arguments

`Wtrue`	true matrix
`West`	estimated matrix
`eps`	real number such that edges whose values are smaller than eps are not considered in the computation of the fscore

Examples

```
library(spectralGraphTopology)
X <- L(c(1, 0, 1))
specificity(X, X)
```

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