Learning the topology of graphs

Convex Group-HKUST

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1 Installation

For installation instructions, please visit https://github.com/dppalomar/spectralGraphTopology

2 Problem Statement

The Laplacian matrix $\boldsymbol{\Theta}$ of a graph contains the information of its topology and weight connections. By definition a Laplacian matrix is positive semi-definite, symmetric, and with sum of rows equal to zero. The Laplacian linear operator $\mathcal{L}\mathbf{w}$ maps a vector of weights $\mathbf{w}$ into a valid Laplacian matrix so that the conditions are satisfied by construction.

The underlying optimization problem of learning a K-component graph may be expressed as follows:

$$\begin{array}{ll} \underset{\mathbf{w},\boldsymbol{\Lambda},\mathbf{U}}{\mathsf{minimize}} & -\log\det(\boldsymbol{\Lambda}) + \mathrm{tr}\left(\mathbf{K}\mathcal{L}\mathbf{w}\right) + \frac{\beta}{2}\left\|\mathcal{L}\mathbf{w} - \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T\right\|_F^2 \\ \mathsf{subject\ to} & \mathbf{w} \geq 0, \boldsymbol{\Lambda} \in \mathcal{S}_{\boldsymbol{\Lambda}},\ \text{and } \mathbf{U}^T\mathbf{U} = \mathbf{I} \end{array}$$

where $\mathcal{S}_{\boldsymbol{\Lambda}}$ further constrains the eigenvalues of Laplacian matrices $\boldsymbol{\Theta} = \mathcal{L}\mathbf{w}$ according to some topology (e.g., a K-component graph has K zero eigenvalues).

In order to solve this problem, we use a block coordinate descent algorithm to iteratively optimize each variable while helding the others fixed.

3 Usage of the package

We illustrate the usage of the package with simulated data, as follows:

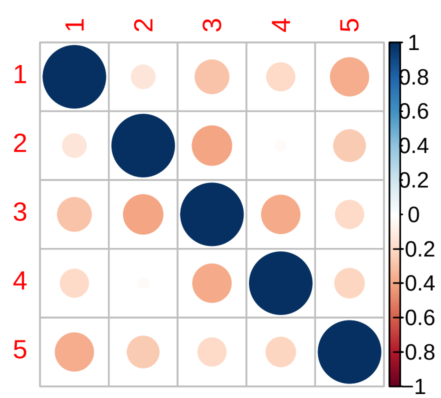
```
library(spectralGraphTopology)
set.seed(123)

# Number of samples
T <- 200
# Vector to generate the Laplacian matrix of the graph
w <- runif(10)
# Laplacian matrix
```

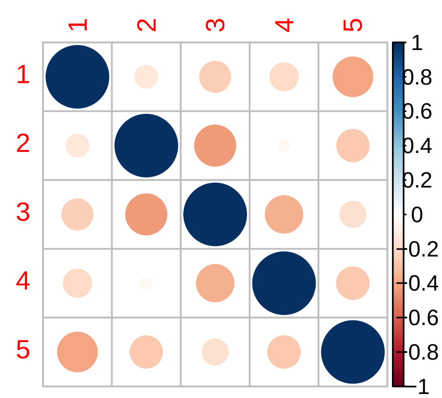
```r
Theta <- L(w)
# Sample data from a Multivariate Gaussian
N <- ncol(Theta)
Y <- MASS::mvrnorm(T, rep(0, N), MASS::ginv(Theta))
# Number of components of the graph
K <- 1
# Learn the Laplacian matrix
res <- learnGraphTopology(Y, K, beta = 10)
```

Let's visually inspect the true Laplacian and the estimated one:

```r
Theta
#>            [,1]       [,2]       [,3]       [,4]       [,5]
#> [1,]  2.3678770 -0.2875775 -0.7883051 -0.4089769 -0.8830174
#> [2,] -0.2875775  1.8017068 -0.9404673 -0.0455565 -0.5281055
#> [3,] -0.7883051 -0.9404673  3.1726265 -0.8924190 -0.5514350
#> [4,] -0.4089769 -0.0455565 -0.8924190  1.8035672 -0.4566147
#> [5,] -0.8830174 -0.5281055 -0.5514350 -0.4566147  2.4191726
res$Theta
#>            [,1]        [,2]       [,3]        [,4]       [,5]
#> [1,]  2.2953931 -0.27079062 -0.6305267 -0.41598450 -0.9780912
#> [2,] -0.2707906  1.95134562 -1.0254774 -0.06127561 -0.5938020
#> [3,] -0.6305267 -1.02547743  2.9706229 -0.83893311 -0.4756856
#> [4,] -0.4159845 -0.06127561 -0.8389331  1.91751385 -0.6013206
#> [5,] -0.9780912 -0.59380196 -0.4756856 -0.60132063  2.6488995
```

```r
library(corrplot)
par(mfrow = c(1, 2))
corrplot(cov2cor(Theta))
corrplot(cov2cor(res$Theta))
```





We evaluate the performance of the learning process in a more objective manner by computing two criterions:

1. relative error
2. percentage improvement in average loss (PRIAL)

```r
relativeError <- function(Xtrue, Xest) {
    return (100 * norm(Xtrue - Xest, type = "F") / norm(Xtrue, type = "F"))
}
```

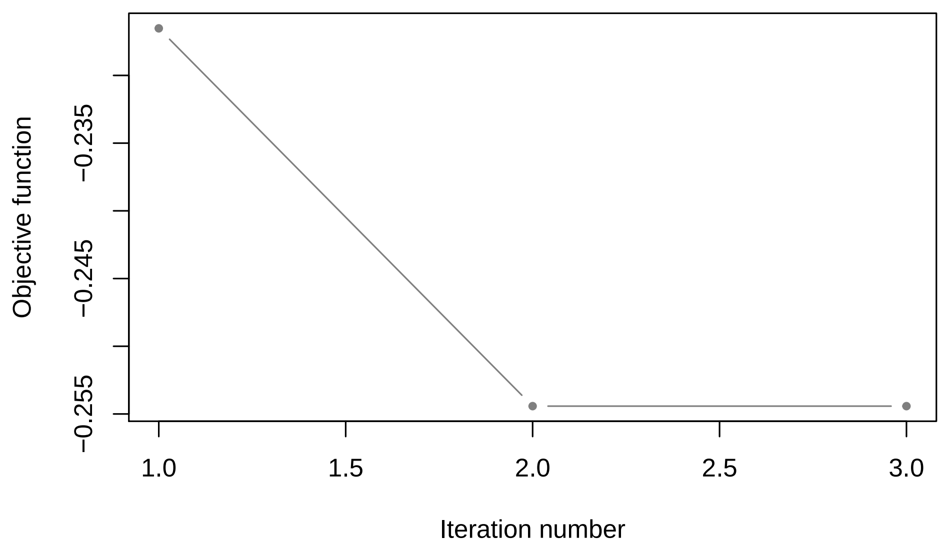
```r
prial <- function(Xtrue, Xest) {
    Xnaive <- MASS::ginv(cov(Xtrue))
    return (100 * (1 - (norm(Xest - Xtrue, type = "F") /
                        norm(Xnaive - Xtrue, type = "F"))^2))
}
```

```r
Theta_naive <- MASS::ginv(cov(Y))
rel_err <- c(proposed = relativeError(Theta, res$Theta),
             naive = relativeError(Theta, Theta_naive))
prial_avg <- c(proposed = prial(Theta, res$Theta),
               naive = prial(Theta, Theta_naive))
rel_err
#> proposed    naive
#> 8.869914 9.224060
prial_avg
#> proposed    naive
#> 98.91276 98.82421
```

In this case, the naive estimation of the Laplacian matrix (i.e., generalized inverse of the sample covariance matrix) performs already quite well since the ratio T/N is large enough 40 for the sample covariance matrix to be accurately estimated.

Let's also look at the convergence of the objective function versus iterations:

```r
N_iter <- length(res$fun)
plot(c(1:N_iter), res$fun, type = "b", pch=19, cex=.6, col = scales::alpha("black", .5),
     xlab = "Iteration number", ylab = "Objective function")
```



For K > 1, we can generate the Laplacian as a block diagonal matrix, as follows

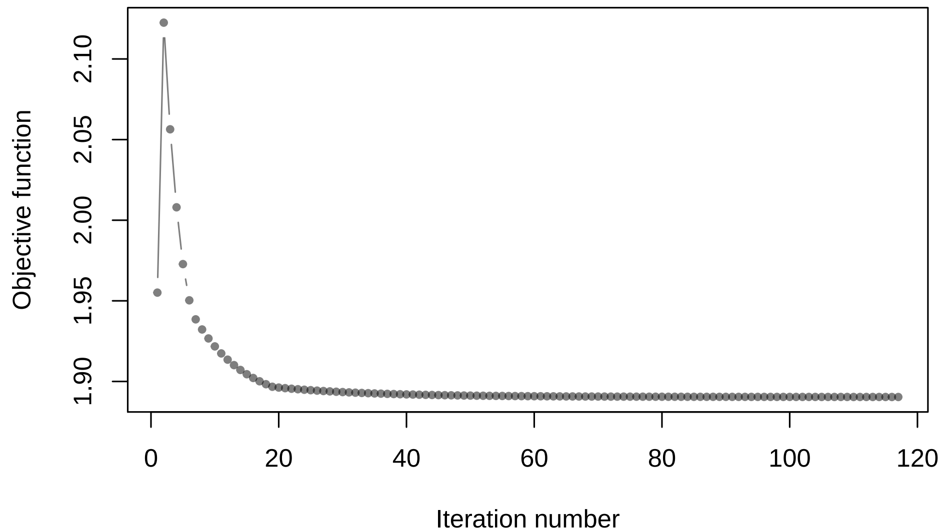
```r
library(spectralGraphTopology)
T <- 50
w1 <- runif(3)
w2 <- runif(3)
Theta1 <- L(w1)
Theta2 <- L(w2)
```

```r
N1 <- ncol(Theta1)
N2 <- ncol(Theta2)
Theta <- rbind(cbind(Theta1, matrix(0, N1, N2)),
               cbind(matrix(0, N2, N1), Theta2))
Y <- MASS::mvrnorm(T, rep(0, N1 + N2), MASS::ginv(Theta))
K <- 2
res <- learnGraphTopology(Y, K, beta = 10)
```

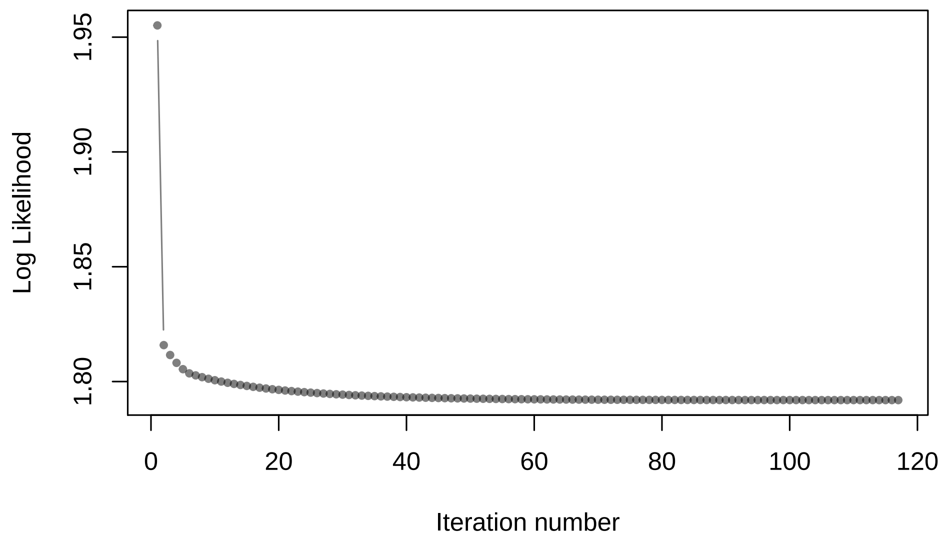
```r
Theta_naive <- MASS::ginv(cov(Y))
rel_err <- c(proposed = relativeError(Theta, res$Theta),
             naive = relativeError(Theta, Theta_naive))
prial_avg <- c(proposed = prial(Theta, res$Theta),
               naive = prial(Theta, Theta_naive))
rel_err
#>  proposed     naive
#>  8.992709 14.027762
prial_avg
#> proposed    naive
#> 99.39504 98.52794
```

```r
Theta
#>            [,1]       [,2]       [,3]       [,4]       [,5]       [,6]
#> [1,]  1.1183094 -0.8509632 -0.2673462  0.0000000  0.0000000  0.0000000
#> [2,] -0.8509632  1.4495635 -0.5986003  0.0000000  0.0000000  0.0000000
#> [3,] -0.2673462 -0.5986003  0.8659465  0.0000000  0.0000000  0.0000000
#> [4,]  0.0000000  0.0000000  0.0000000  1.6007581 -0.6085997 -0.9921584
#> [5,]  0.0000000  0.0000000  0.0000000 -0.6085997  0.7997897 -0.1911900
#> [6,]  0.0000000  0.0000000  0.0000000 -0.9921584 -0.1911900  1.1833484
res$Theta
#>            [,1]       [,2]        [,3]       [,4]        [,5]        [,6]
#> [1,]  1.1839191 -0.8535033 -0.33041578  0.0000000  0.00000000  0.00000000
#> [2,] -0.8535033  1.3384861 -0.48498280  0.0000000  0.00000000  0.00000000
#> [3,] -0.3304158 -0.4849828  0.86057122  0.0000000  0.00000000 -0.04517265
#> [4,]  0.0000000  0.0000000  0.00000000  1.6398148 -0.67676874 -0.96304605
#> [5,]  0.0000000  0.0000000  0.00000000 -0.6767687  0.74520251 -0.06843377
#> [6,]  0.0000000  0.0000000 -0.04517265 -0.9630461 -0.06843377  1.07665247
```

```r
N_iter <- length(res$fun)
plot(c(1:N_iter), res$fun, type = "b", pch=19, cex=.6, col = scales::alpha("black", .5),
     xlab = "Iteration number", ylab = "Objective function")
```




```
plot(c(1:N_iter), res$loglike, type = "b", pch=19, cex=.6, col = scales::alpha("black", .5),
     xlab = "Iteration number", ylab = "Log Likelihood")
```



4 Explanation of the algorithms

In this section we describe in detail the algorithms designed to solve the graph topology learning problem.

4.1 `learnGraphTopology`: Learning the topology of graph

The goal of `learnGraphTopology` is to estimate the Laplacian matrix generated by the weight vector of a graph, $\mathbf{w}$. The algorithm for the function `learnGraphTopology` is stated as follows:

Data: $\mathbf{Y}$ (data matrix), K (#{components}), β (regularization term), $\mathbf{w}^{(0)}$, $\boldsymbol{\lambda}^{(0)}$, $\mathbf{U}^{(0)}$ (initial parameter estimates), α_1, α_2 (lower and upper bound on the eigenvalues of the Laplacian matrix), ρ (how much to increase beta per iteration).
Result: $\boldsymbol{\Theta}$ (Laplacian matrix)
$N \leftarrow$ `ncol`$(\mathbf{Y})$
while *objective function do not converged* ***or*** *max #{iterations} not reached* **do**
  $k \leftarrow 0$
  while *parameters do not converged* ***or*** *max #{iterations} not reached* **do**
    $\mathbf{w}^{(k+1)} \leftarrow \texttt{w\_update}(\mathbf{w}^{(k)}, \mathbf{U}^{(k)}, \boldsymbol{\lambda}^{(k)}, \beta, N, \mathbf{K})$
    $\mathbf{U}^{(k+1)} \leftarrow \texttt{U\_update}(\mathbf{w}^{(k+1)}, N)$
    $\boldsymbol{\lambda}^{(k+1)} \leftarrow \texttt{lambda\_update}(\mathbf{w}^{(k+1)}, \mathbf{U}^{(k+1)}, \alpha_1, \alpha_2, \beta, N, K)$
    $k \leftarrow k + 1$
  end
  $\beta \leftarrow \beta(\rho + 1)$
end
return $\mathcal{L}(\mathbf{w}^{(k+1)})$

Function $\texttt{w\_update}(\mathbf{w}, \mathbf{U}, \boldsymbol{\lambda}, \beta, N, \mathbf{K})$**:**
  $\nabla_{\mathbf{w}} f \leftarrow \mathcal{L}^{\star}\left(\mathcal{L}(\mathbf{w}) - \mathbf{U}\texttt{diag}(\boldsymbol{\lambda})\mathbf{U}^T + \frac{\mathbf{K}}{\beta}\right)$
  return $\texttt{max}\left(0, \mathbf{w} - \frac{\nabla_{\mathbf{w}} f}{2N}\right)$

Function $\texttt{U\_update}(\mathbf{w}, N, K)$**:**
  return `eigenvectors`$(\mathcal{L}(\mathbf{w}))$[K+1:N] # *increasing order w.r.t. eigenvalues*

Function $\texttt{lambda\_update}(\mathbf{w}, \mathbf{U}, \alpha_1, \alpha_2, \beta, N, K)$**:**
  $\mathbf{d} \leftarrow \texttt{diag}\left(\mathbf{U}^T \mathcal{L}(\mathbf{w}) \mathbf{U}\right)$
  $\boldsymbol{\lambda} \leftarrow \frac{1}{2}\left(\mathbf{d} + \sqrt{\mathbf{d} \odot \mathbf{d} + \frac{4}{\beta}}\right)$ # *$\odot$ means element-wise multiplication*
  if $\boldsymbol{\lambda}$ *has its elements in nondecreasing order* ***and*** $\min(\boldsymbol{\lambda}) \geq \alpha_1$ ***and*** $\max(\boldsymbol{\lambda}) \leq \alpha_2$ **then**
    return $\boldsymbol{\lambda}$
  else
    set to α_1 the elements of $\boldsymbol{\lambda}$ whose values are less than α_1
    set to α_2 the elements of $\boldsymbol{\lambda}$ whose values are greater than α_2
  end
  if $\boldsymbol{\lambda}$ *has its elements in nondecreasing order* **then**
    return $\boldsymbol{\lambda}$
  else
    raise `Exception`(*"eigenvalues are not in increasing order"*)
  end

References