Learning the topology of graphs

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Contents

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1 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 <- 10000
# Vector to generate the Laplacian matrix of the graph
w <- runif(10)
# Laplacian matrix
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 as follows::

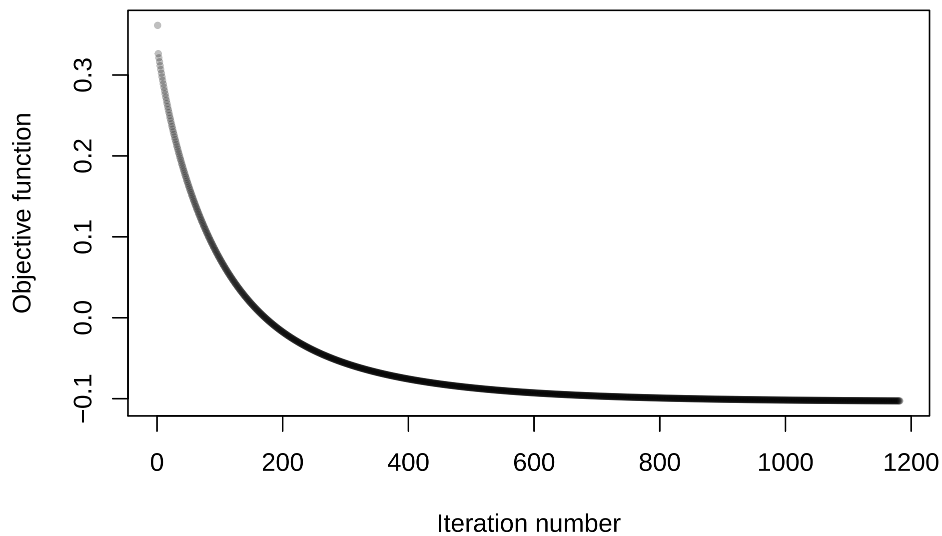
```
Theta
#>            [,1]       [,2]       [,3]       [,4]       [,5]
#> [1,]  2.3678770 -0.2875775 -0.7883051 -0.4089769 -0.8830174
#> [2,] -0.2875775  1.8017068 -0.9404673 -0.0455565 -0.5281055
#> [3,] -0.7883051 -0.9404673  3.1726265 -0.8924190 -0.5514350
#> [4,] -0.4089769 -0.0455565 -0.8924190  1.8035672 -0.4566147
#> [5,] -0.8830174 -0.5281055 -0.5514350 -0.4566147  2.4191726
res$Theta
#>            [,1]        [,2]       [,3]        [,4]       [,5]
#> [1,]  2.3384299 -0.29372890 -0.7864202 -0.38899191 -0.8692889
#> [2,] -0.2937289  1.76412935 -0.9297244 -0.05376403 -0.4869120
#> [3,] -0.7864202 -0.92972444  3.0917157 -0.81448289 -0.5610881
#> [4,] -0.3889919 -0.05376403 -0.8144829  1.74104811 -0.4838093
#> [5,] -0.8692889 -0.48691199 -0.5610881 -0.48380928  2.4010983
```

We can evaluate the performance of the learning process in a more objective manner by computing the relative error between the true Laplacian matrix and the estimated one, which can be done as follows::

```
RE <- norm(Theta - res$Theta, type="F") / max(1., norm(Theta, type="F"))
RE
#> [1] 0.02965113
```

Let's also look at the trend of the objective function per iteration:

```
k <- length(res$fun)
plot(c(1:k), res$fun,  pch=19, cex=.5, col = scales::alpha("black", .25),
     xlab = "Iteration number", ylab = "Objective function")
```



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

```
library(spectralGraphTopology)
w1 <- runif(3)
w2 <- runif(3)
Theta1 <- L(w1)
Theta2 <- L(w2)
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
beta <- 5
res <- learnGraphTopology(Y, K, beta = beta, ftol = 1e-3)
RE <- norm(Theta - res$Theta, type="F") / max(1., norm(Theta, type="F"))
RE
#> [1] 0.8834062
```

```
Theta
#>             [,1]        [,2]       [,3]      [,4]      [,5]      [,6]
#> [1,]  0.96494812 -0.03715792 -0.9277902 0.0000000 0.0000000 0.0000000
#> [2,] -0.03715792  0.48514753 -0.4479896 0.0000000 0.0000000 0.0000000
```

```r
#> [3,] -0.92779020 -0.44798960  1.3757798  0.0000000  0.0000000  0.0000000
#> [4,]  0.00000000  0.00000000  0.0000000  1.2716541 -0.9159023 -0.3557518
#> [5,]  0.00000000  0.00000000  0.0000000 -0.9159023  1.8312150 -0.9153127
#> [6,]  0.00000000  0.00000000  0.0000000 -0.3557518 -0.9153127  1.2710645
res$Theta
#>            [,1]       [,2]       [,3]       [,4] [,5]       [,6]
#> [1,]  1.3891578  0.0000000 -0.3605830 -0.6061550    0 -0.4224198
#> [2,]  0.0000000  0.7412041  0.0000000 -0.3010095    0 -0.4401947
#> [3,] -0.3605830  0.0000000  1.6932700 -0.5816278    0 -0.7510592
#> [4,] -0.6061550 -0.3010095 -0.5816278  1.6025191    0 -0.1137268
#> [5,]  0.0000000  0.0000000  0.0000000  0.0000000    0  0.0000000
#> [6,] -0.4224198 -0.4401947 -0.7510592 -0.1137268    0  1.7274005
```

As we can observe, the matrices' structure do not quite match.

I suspect they might be similar matrices. Let's check some properties:

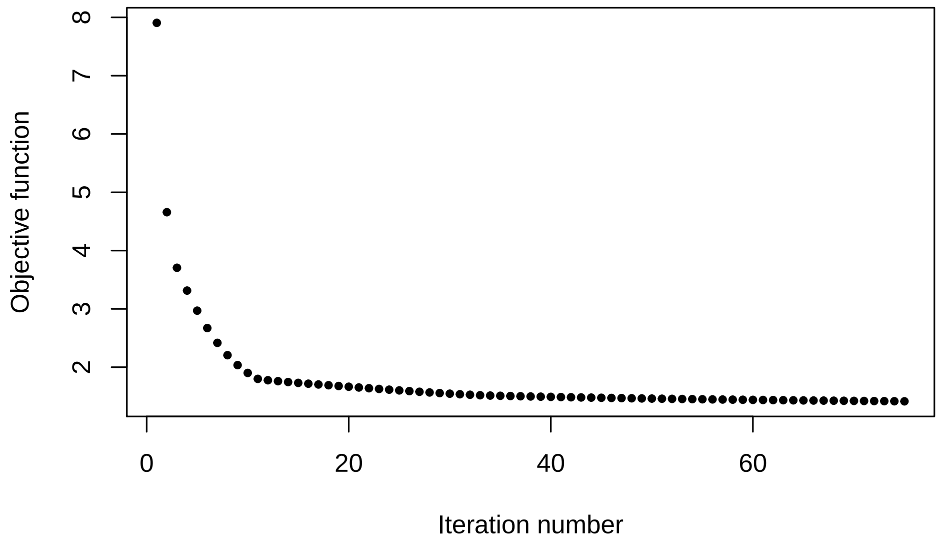
```r
eigen(Theta, only.values = TRUE)
#> $values
#> [1]  2.746823e+00  2.185018e+00  1.627111e+00  6.408571e-01 -3.252607e-18
#> [6] -1.948853e-17
#>
#> $vectors
#> NULL
eigen(res$Theta, only.values = TRUE)
#> $values
#> [1]  2.713545e+00  1.965910e+00  1.661742e+00  8.123542e-01  0.000000e+00
#> [6] -2.220446e-16
#>
#> $vectors
#> NULL
```

```r
sum(diag(Theta))
#> [1] 7.199809
sum(diag(res$Theta))
#> [1] 7.153552
```

```r
det(Theta)
#> [1] 0
det(res$Theta)
#> [1] 0
```

```r
N <- N1 + N2
objFunction(Theta, res$U, res$lambda, res$Km, beta, N, K)
objFunction(res$Theta, res$U, res$lambda, res$Km, beta, N, K)
```

```r
k <- length(res$fun)
plot(c(1:k), res$fun, pch=19, cex=.6, xlab = "Iteration number",
     ylab = "Objective function")
```



2 Explanation of the algorithms

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

2.1 `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**

    $\mathbf{w}^{(k+1)} \leftarrow$ `w_update`$(\mathbf{w}^{(k)}, \mathbf{U}^{(k)}, \boldsymbol{\lambda}^{(k)}, \beta, N, \mathbf{K})$

    $\mathbf{U}^{(k+1)} \leftarrow$ `U_update`$(\mathbf{w}^{(k+1)}, N)$

    $\boldsymbol{\lambda}^{(k+1)} \leftarrow$ `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 `w_update`$(\mathbf{w}, \mathbf{U}, \boldsymbol{\lambda}, \beta, N, \mathbf{K})$**:**

  $\nabla_{\mathbf{w}} f \leftarrow \mathcal{L}^{\star}\left(\mathcal{L}\left(\mathbf{w}\right) - \mathbf{U}\texttt{diag}(\boldsymbol{\lambda})\mathbf{U}^T + \dfrac{\mathbf{K}}{\beta}\right)$

  return $\texttt{max}\left(0, \mathbf{w} - \dfrac{\nabla_{\mathbf{w}} f}{2N}\right)$

Function `U_update`$(\mathbf{w}, N)$**:**

  return `eigen`$(\mathcal{L}(\mathbf{w}))$`$vectors`$[, N:1]$

Function `lambda_update`$(\mathbf{w}, \mathbf{U}, \alpha_1, \alpha_2, \beta, N, K)$**:**

  $\mathbf{d} \leftarrow \texttt{diag}\left(\mathbf{U}^T\mathcal{L}(\mathbf{w})\mathbf{U}\right)$

  $\boldsymbol{\lambda} \leftarrow \frac{1}{2}\left(\mathbf{d} + \sqrt{\mathbf{d} \odot \mathbf{d} + \frac{4}{\beta}}\right)$

  if $\boldsymbol{\lambda}$ *has its elements in increasing order* **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 increasing order* **then**

    return $\boldsymbol{\lambda}$

  else

    raise `Exception`(*"eigenvalues are not in increasing order"*)

  end

References