Computing sparse eigenvectors

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This vignette illustrates the computation of sparse eigenvectors or sparse PCA with the package `sparseEigen` (with a comparison with other packages) and gives a description of the algorithms used.

1 Comparison with other packages

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2 Usage of the package

2.1 Computation of sparse eigenvectors of a given matrix

We start by loading the package and generating synthetic data with sparse eigenvectors:

```
library(sparseEigen)
set.seed(42)

# parameters
m <- 500  # dimension
n <- 100  # number of samples
q <- 3  # number of sparse eigenvectors to be estimated
sp_card <- 0.2*m  # cardinality of each sparse eigenvector
rho <- 0.6  # sparsity level

# generate non-overlapping sparse eigenvectors
V <- matrix(rnorm(m^2), ncol = m)
tmp <- matrix(0, m, q)
for (i in 1:max(q, 2)) {
  ind1 <- (i - 1)*sp_card + 1
  ind2 <- i*sp_card
  tmp[ind1:ind2, i] = 1/sqrt(sp_card)
  V[, i] <- tmp[, i]
```

```
}
V <- qr.Q(qr(V))  # keep first q eigenvectors the same (already orthogonal) and orthogonalize the rest

# generate eigenvalues
lmd <- rep(1, m)
lmd[1:q] <- 100*seq(from = q, to = 1)

# generate covariance matrix from sparse eigenvectors and eigenvalues
R <- V %*% diag(lmd) %*% t(V)

# generate data matrix from a zero-mean multivariate Gaussian distribution with the constructed covaria
X <- MASS::mvrnorm(n, rep(0, m), R)  # random data with underlying sparse structure
X <- scale(X, center = TRUE, scale = FALSE)  # center the data
```

Then we estimate the covariance matrix with `cov(X)` and compute its sparse eigenvectors:

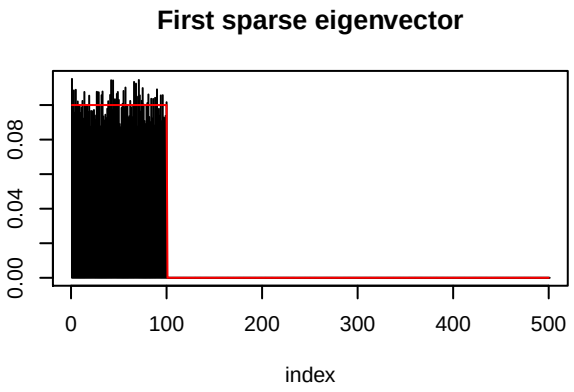
```
# computation of sparse eigenvectors
res_standard <- eigen(cov(X))
res_sparse1 <- spEigen(cov(X), q, rho)
res_sparse2 <- spEigen(X, q, rho, data = TRUE)
```

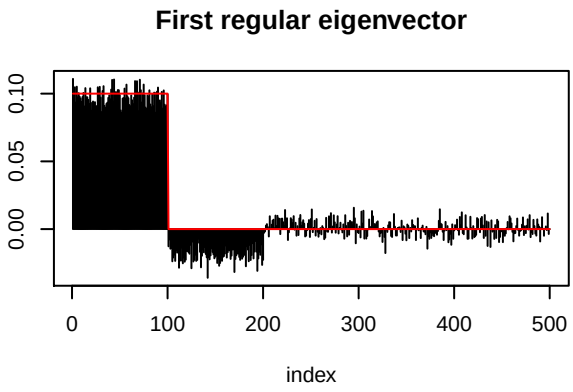
We can assess how good the estimated eigenvectors are by computing the inner product with the original eigenvectors (the closer to 1 the better):

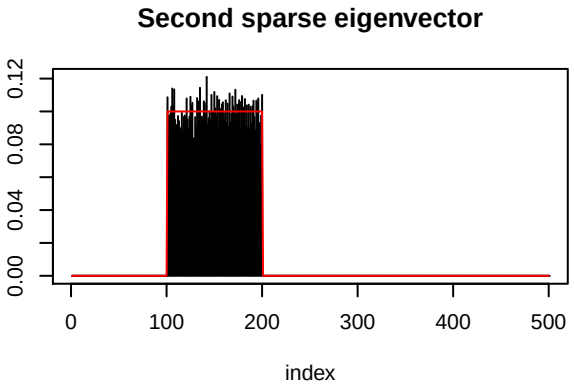
```
# show inner product between estimated eigenvectors and originals
abs(diag(t(res_standard$vectors) %*% V[, 1:q]))   #for standard estimated eigenvectors
#> [1] 0.9726306 0.9488030 0.9623054
abs(diag(t(res_sparse1$vectors) %*% V[, 1:q]))    #for sparse estimated eigenvectors
#> [1] 0.9975791 0.9968073 0.9956102
abs(diag(t(res_sparse2$vectors) %*% V[, 1:q]))    #for sparse estimated eigenvectors
#> [1] 0.9975774 0.9968051 0.9956073
```

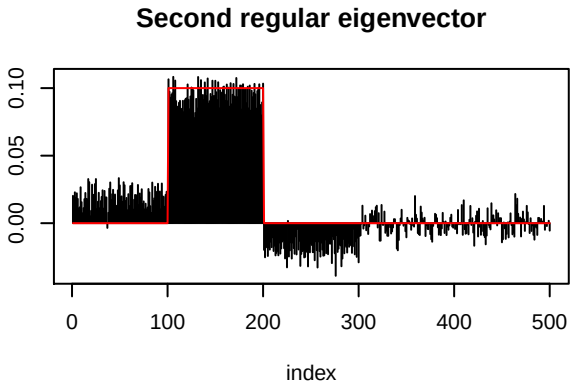
Finally, the following plot shows the sparsity pattern of the eigenvectors (sparse computation vs. classical computation):

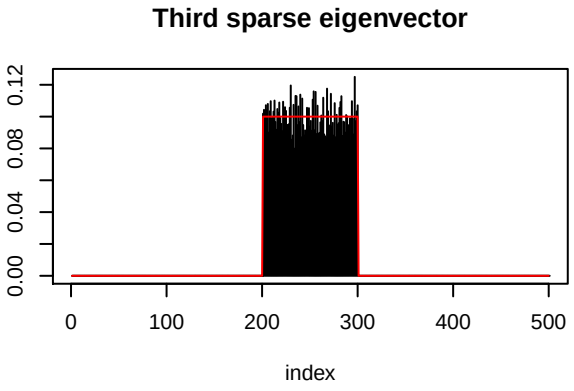
```
par(mfcol = c(3, 2))
plot(res_sparse1$vectors[, 1]*sign(res_sparse1$vectors[1, 1]),
     main = "First sparse eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 1]*sign(V[1, 1]), col = "red")
plot(res_sparse1$vectors[, 2]*sign(res_sparse1$vectors[sp_card+1, 2]),
     main = "Second sparse eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 2]*sign(V[sp_card+1, 2]), col = "red")
plot(res_sparse1$vectors[, 3]*sign(res_sparse1$vectors[2*sp_card+1, 3]),
     main = "Third sparse eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 3]*sign(V[2*sp_card+1, 3]), col = "red")

plot(res_standard$vectors[, 1]*sign(res_standard$vectors[1, 1]),
     main = "First regular eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 1]*sign(V[1, 1]), col = "red")
plot(res_standard$vectors[, 2]*sign(res_standard$vectors[sp_card+1, 2]),
     main = "Second regular eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 2]*sign(V[sp_card+1, 2]), col = "red")
plot(res_standard$vectors[, 3]*sign(res_standard$vectors[2*sp_card+1, 3]),
     main = "Third regular eigenvector", xlab = "index", ylab = "", type = "h")
lines(V[, 3]*sign(V[2*sp_card+1, 3]), col = "red")
```

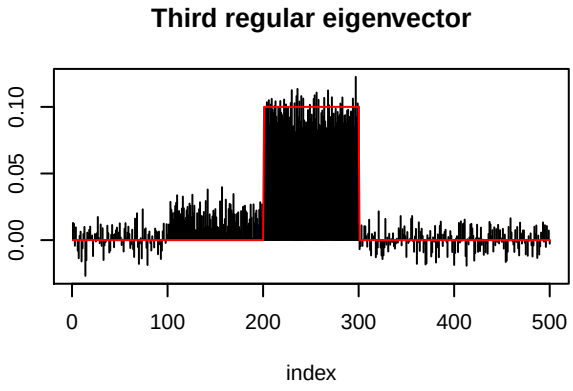












2.2 Covariance matrix estimation with sparse eigenvectors

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3 Explanation of the algorithms

3.1 `spEigen()`: Sparse eigenvectors from a given covariance matrix

The goal of `spEigen()` is the estimation of the q leading sparse eigenvectors (with $q \leq \text{rank}(\mathbf{S})$) from an $m \times m$ covariance matrix $\mathbf{S}$ (typically the sample covariance matrix obtained from n samples) based on [1].

The underlying optimization problem that is solved is

$$\begin{aligned} \underset{\mathbf{U}}{\text{maximize}} \quad & \operatorname{Tr}\left(\mathbf{U}^\top \mathbf{S}\mathbf{U}\operatorname{Diag}(\mathbf{d})\right) - \sum_{i=1}^{q} \rho_i \|\mathbf{u}_i\|_0 \\ \text{subject to} \quad & \mathbf{U}^\top \mathbf{U} = \mathbf{I}_q, \end{aligned}$$

where $\mathbf{U} \in \mathbb{R}^{m\times q}$ is a matrix containing the q leading eigenvectors, $\mathbf{d}$ is a vector of weights to ensure that $\mathbf{U}$ contains the leading eigenvectors without an arbitrary rotation, and the ρ_i's are the regularization parameters to control how much sparsity is desired. This problem is the typical PCA formulation with an extra penalty term in the objective that penalizes the cardinality of the eigenvectors, controled by the regularization parameters ρ_i's.

The ℓ_0-"norm" is approximated by the continuous and differentiable function

$$g_p^\epsilon(x) = \begin{cases} \frac{x^2}{2\epsilon(p+\epsilon)\log(1+1/p)}, & |x| \le \epsilon, \\ \frac{\log\left(\frac{p+|x|}{p+\epsilon}\right) + \frac{\epsilon}{2(p+\epsilon)}}{\log(1+1/p)}, & |x| > \epsilon, \end{cases}$$

where $p > 0$ and $0 < \epsilon \ll 1$ are parameters that control the approximation. This leads to the following approximate problem:

$$\begin{aligned} \underset{\mathbf{U}}{\text{maximize}} \quad & \operatorname{Tr}\left(\mathbf{U}^\top \mathbf{S}\mathbf{U}\operatorname{Diag}(\mathbf{d})\right) - \sum_{j=1}^{q} \rho_j \sum_{i=1}^{m} g_p^\epsilon(u_{ij}) \\ \text{subject to} \quad & \mathbf{U}^\top \mathbf{U} = \mathbf{I}_q. \end{aligned}$$

This problem can be solved via Majorization-Minimization (MM) [2] with an iterative closed-form update algorithm. For this, at each iteration (denoted by k) two key quantities are needed:

$$\mathbf{G}^{(k)} = \mathbf{S}\mathbf{U}^{(k)}\operatorname{Diag}(\mathbf{d})$$

$$\mathbf{H}^{(k)} = \left[\operatorname{diag}\left(\mathbf{w}^{(k)} - \mathbf{w}_{\max}^{(k)} \otimes \mathbf{1}_m\right)\tilde{\mathbf{u}}^{(k)}\right]_{m\times q},$$

where

$$w_i^{(k)} = \begin{cases} \frac{\rho_i}{2\epsilon(p+\epsilon)\log(1+1/p)}, & |\tilde{u}_i^{(k)}| \le \epsilon, \\ \frac{\rho_i}{2\log(1+1/p)|\tilde{u}_i^{(k)}|\left(|\tilde{u}_i^{(k)}|+p\right)}, & |\tilde{u}_i^{(k)}| > \epsilon, \end{cases}$$

with $\mathbf{w} \in \mathbb{R}_+^{mq}$, $\tilde{\mathbf{u}}^{(k)} = \operatorname{vec}(\mathbf{U}^{(k)}) \in \mathbb{R}_+^{mq}$, $\mathbf{w}_{\max} \in \mathbb{R}_+^q$, with $w_{\max,i}$ being the maximum weight that corresponds to the i-th eigenvector $\mathbf{u}_i^{(k)}$.

The iterative closed-form update algorithm is:

1. Set $k = 0$ and choose an initial point $\mathbf{U}^{(0)}$
2. Compute $\mathbf{G}^{(k)}$ and $\mathbf{H}^{(k)}$
3. Compute $\mathbf{V}_\mathrm{L}$, $\mathbf{V}_\mathrm{R}$ as the left and right singular vectors of $\left(\mathbf{G}^{(k)} - \mathbf{H}^{(k)}\right)$
4. $\mathbf{U}^{(k+1)} \leftarrow \mathbf{V}_\mathrm{L}\mathbf{V}_\mathrm{R}^\top$
5. $k \leftarrow k + 1$
6. Repeat steps 2-5 until convergence

7. Return $\mathbf{U}^{(k)}$

The initial point of the algorithm $\mathbf{U}^{(0)}$ is set by default to the q leading standard eigenvectors, unless the user specifies otherwise. Internally, all the computations of $\mathbf{G}^{(k)}$ and $\mathbf{H}^{(k)}$ are done through the eigenvalue decomposition (EVD) of $\mathbf{S}$. Since we can also retrieve the eigenvectors and eigenvalues of $\mathbf{S}$ through the singular value decomposition (SVD) of the data matrix $\mathbf{X}$, with $\mathbf{S} = \frac{1}{n-1}\mathbf{X}^\top\mathbf{X}$, it becomes possible to use as an input to 'spEigen()' either the covariance matrix $\mathbf{S}$ or directly the data matrix $\mathbf{X}$.

Although $\mathbf{H}^{(k)}$ does not depend directly on $\mathbf{S}$, the parameters ρ_j are set based on its eigenvalues. In particular, each ρ_j takes a value in an interval $[0, \rho_j^{\max}]$ based on the input variable $\rho \in [0, 1]$ that the user selects, i.e., $\rho_j = \rho\rho_j^{\max}$. The uppperbound $\rho_j^{\max}$ depends, among others, on the eigenvalues of $\mathbf{S}$. Note that the theoretical upperbound is derived based on the initial problem and not the approximate. Therefore, although a suggested range for ρ is the interval $[0, 1]$, any nonnegative value is accepted by the algorithm.

3.2 `spEigenCov()`: Covariance matrix estimation with sparse eigenvectors

References

[1] K. Benidis, Y. Feng, and D. P. Palomar, "Sparse portfolios for high-dimensional financial index tracking," *IEEE Transactions on Signal Processing*, vol. 66, no. 1, pp. 155–170, jan. 2018.

[2] Y. Sun, P. Babu, and D. P. Palomar, "Majorization-minimization algorithms in signal processing, communications, and machine learning," *IEEE Transactions on Signal Processing*, vol. 65, no. 3, pp. 794–816, feb. 2011.