Package 'sparsepca'

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Type Package

Title Sparse Principal Component Analysis (SPCA)

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Description Sparse principal component analysis (SPCA) attempts to find sparse weight vectors (loadings), i.e., a weight vector with only a few 'active' (nonzero) values. This approach provides better interpretability for the principal components in high-dimensional data settings. This is, because the principal components are formed as a linear combination of only a few of the original variables. This package provides efficient routines to compute SPCA. Specifically, a variable projection solver is used to compute the sparse solution. In addition, a fast randomized accelerated SPCA routine and a robust SPCA routine is provided. Robust SPCA allows to capture grossly corrupted entries in the data. The methods are discussed in detail by N. Benjamin Erichson et al. (2018) <arXiv:1804.00341>.

License GPL (>= 3)

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LazyData true

URL https://github.com/erichson/spca

BugReports https://github.com/erichson/spca/issues Imports rsvd RoxygenNote 6.0.1 NeedsCompilation no Repository CRAN Date/Publication 2018-04-11 08:17:42 UTC

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robspca

Description

Implementation of robust SPCA, using variable projection as an optimization strategy.

Usage

```
robspca(X, k = NULL, alpha = 1e-04, beta = 1e-04, gamma = 100,
center = TRUE, scale = FALSE, max_iter = 1000, tol = 1e-05,
verbose = TRUE)
```

Arguments

| Х | array_like; a real (n, p) input matrix (or data frame) to be decomposed. |
|----------|---|
| k | integer; specifies the target rank, i.e., the number of components to be computed. |
| alpha | float; Sparsity controlling parameter. Higher values lead to sparser components. |
| beta | float; Amount of ridge shrinkage to apply in order to improve conditioning. |
| gamma | float; Sparsity controlling parameter for the error matrix S. Smaller values lead to a larger amount of noise removeal. |
| center | bool; logical value which indicates whether the variables should be shifted to be zero centered (TRUE by default). |
| scale | bool; logical value which indicates whether the variables should be scaled to have unit variance (FALSE by default). |
| max_iter | integer; maximum number of iterations to perform before exiting. |
| tol | float; stopping tolerance for the convergence criterion. |
| verbose | bool; logical value which indicates whether progress is printed. |

Details

Sparse principal component analysis is a modern variant of PCA. Specifically, SPCA attempts to find sparse weight vectors (loadings), i.e., a weight vector with only a few 'active' (nonzero) values. This approach leads to an improved interpretability of the model, because the principal components

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are formed as a linear combination of only a few of the original variables. Further, SPCA avoids overfitting in a high-dimensional data setting where the number of variables p is greater than the number of observations n.

Such a parsimonious model is obtained by introducing prior information like sparsity promoting regularizers. More concreatly, given an (n, p) data matrix X, robust SPCA attemps to minimize the following objective function:

$$f(A,B) = \frac{1}{2} \|X - XBA^{\top} - S\|_F^2 + \psi(B) + \gamma \|S\|_1$$

where B is the sparse weight matrix (loadings) and A is an orthonormal matrix. ψ denotes a sparsity inducing regularizer such as the LASSO (ℓ_1 norm) or the elastic net (a combination of the ℓ_1 and ℓ_2 norm). The matrix S captures grossly corrupted outliers in the data.

The principal components Z are formed as

$$Z = XB$$

and the data can be approximately rotated back as

$$\tilde{X} = ZA^{\top}$$

The print and summary method can be used to present the results in a nice format.

Value

spca returns a list containing the following three components:

| loadings | array_like; sparse loadings (weight) vector; (p, k) dimensional array. |
|---------------|---|
| transform | array_like; the approximated inverse transform; (p, k) dimensional array. |
| scores | array_like; the principal component scores; (n, k) dimensional array. |
| sparse | array_like; sparse matrix capturing outliers in the data; (n, p) dimensional array. |
| eigenvalues | array_like; the approximated eigenvalues; (k) dimensional array. |
| center, scale | array_like; the centering and scaling used. |

Author(s)

N. Benjamin Erichson, Peng Zheng, and Sasha Aravkin

References

 [1] N. B. Erichson, P. Zheng, K. Manohar, S. Brunton, J. N. Kutz, A. Y. Aravkin. "Sparse Principal Component Analysis via Variable Projection." Submitted to IEEE Journal of Selected Topics on Signal Processing (2018). (available at 'arXiv https://arxiv.org/abs/ 1804.00341).

See Also

rspca, spca

Examples

```
# Create artifical data
m <- 10000
V1 <- rnorm(m, 0, 290)
V2 <- rnorm(m, 0, 300)
V3 <- -0.1*V1 + 0.1*V2 + rnorm(m,0,100)
X <- cbind(V1,V1,V1,V1, V2,V2,V2,V2, V3,V3)
X <- X + matrix(rnorm(length(X),0,1), ncol = ncol(X), nrow = nrow(X))
# Compute SPCA
out <- robspca(X, k=3, alpha=1e-3, beta=1e-5, gamma=5, center = TRUE, scale = FALSE, verbose=0)
print(out)
summary(out)</pre>
```

rspca

Randomized Sparse Principal Component Analysis (rspca).

Description

Randomized accelerated implementation of SPCA, using variable projection as an optimization strategy.

Usage

```
rspca(X, k = NULL, alpha = 1e-04, beta = 1e-04, center = TRUE,
    scale = FALSE, max_iter = 1000, tol = 1e-05, o = 20, q = 2,
    verbose = TRUE)
```

Arguments

| Х | array_like; a real (n, p) input matrix (or data frame) to be decomposed. |
|---|--|
| k | integer; specifies the target rank, i.e., the number of components to be computed. |

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| alpha | float; Sparsity controlling parameter. Higher values lead to sparser components. |
|----------|--|
| beta | float; Amount of ridge shrinkage to apply in order to improve conditioning. |
| center | bool; logical value which indicates whether the variables should be shifted to be zero centered (TRUE by default). |
| scale | bool; logical value which indicates whether the variables should be scaled to have unit variance (FALSE by default). |
| max_iter | integer; maximum number of iterations to perform before exiting. |
| tol | float; stopping tolerance for the convergence criterion. |
| 0 | integer; oversampling parameter (default $o = 20$). |
| q | integer; number of additional power iterations (default $q = 2$). |
| verbose | bool; logical value which indicates whether progress is printed. |

Details

Sparse principal component analysis is a modern variant of PCA. Specifically, SPCA attempts to find sparse weight vectors (loadings), i.e., a weight vector with only a few 'active' (nonzero) values. This approach leads to an improved interpretability of the model, because the principal components are formed as a linear combination of only a few of the original variables. Further, SPCA avoids overfitting in a high-dimensional data setting where the number of variables p is greater than the number of observations n.

Such a parsimonious model is obtained by introducing prior information like sparsity promoting regularizers. More concreatly, given an (n, p) data matrix X, SPCA attemps to minimize the following objective function:

$$f(A,B) = \frac{1}{2} \|X - XBA^{\top}\|_{F}^{2} + \psi(B)$$

where B is the sparse weight (loadings) matrix and A is an orthonormal matrix. ψ denotes a sparsity inducing regularizer such as the LASSO (ℓ_1 norm) or the elastic net (a combination of the ℓ_1 and ℓ_2 norm). The principal components Z are formed as

$$Z = XB$$

and the data can be approximately rotated back as

$$\tilde{X} = ZA^{\top}$$

The print and summary method can be used to present the results in a nice format.

Value

spca returns a list containing the following three components:

| loadings | array_like; sparse loadings (weight) vector; (p, k) dimensional array. |
|---------------|---|
| transform | array_like; the approximated inverse transform; (p, k) dimensional array. |
| scores | array_like; the principal component scores; (n, k) dimensional array. |
| eigenvalues | array_like; the approximated eigenvalues; (k) dimensional array. |
| center, scale | array_like; the centering and scaling used. |

Note

This implementation uses randomized methods for linear algebra to speedup the computations. o is an oversampling parameter to improve the approximation. A value of at least 10 is recommended, and o = 20 is set by default.

The parameter q specifies the number of power (subspace) iterations to reduce the approximation error. The power scheme is recommended, if the singular values decay slowly. In practice, 2 or 3 iterations achieve good results, however, computing power iterations increases the computational costs. The power scheme is set to q = 2 by default.

If k > (min(n, p)/4), a the deterministic spca algorithm might be faster.

Author(s)

N. Benjamin Erichson, Peng Zheng, and Sasha Aravkin

References

- [1] N. B. Erichson, P. Zheng, K. Manohar, S. Brunton, J. N. Kutz, A. Y. Aravkin. "Sparse Principal Component Analysis via Variable Projection." Submitted to IEEE Journal of Selected Topics on Signal Processing (2018). (available at 'arXiv https://arxiv.org/abs/ 1804.00341).
- [1] N. B. Erichson, S. Voronin, S. Brunton, J. N. Kutz. "Randomized matrix decompositions using R." Submitted to Journal of Statistical Software (2016). (available at 'arXiv http://arxiv.org/abs/1608.02148).

See Also

spca, robspca

spca

Examples

```
# Create artifical data
m <- 10000
V1 <- rnorm(m, 0, 290)
V2 <- rnorm(m, 0, 300)
V3 <- -0.1*V1 + 0.1*V2 + rnorm(m,0,100)
X <- cbind(V1,V1,V1,V1, V2,V2,V2,V2, V3,V3)
X <- X + matrix(rnorm(length(X),0,1), ncol = ncol(X), nrow = nrow(X))
# Compute SPCA
out <- rspca(X, k=3, alpha=1e-3, beta=1e-3, center = TRUE, scale = FALSE, verbose=0)
print(out)
summary(out)
```

```
spca
```

Sparse Principal Component Analysis (spca).

Description

Implementation of SPCA, using variable projection as an optimization strategy.

Usage

spca(X, k = NULL, alpha = 1e-04, beta = 1e-04, center = TRUE, scale = FALSE, max_iter = 1000, tol = 1e-05, verbose = TRUE)

Arguments

| Х | array_like; a real (n, p) input matrix (or data frame) to be decomposed. |
|--------|--|
| k | integer; specifies the target rank, i.e., the number of components to be computed. |
| alpha | float; Sparsity controlling parameter. Higher values lead to sparser components. |
| beta | float; Amount of ridge shrinkage to apply in order to improve conditioning. |
| center | bool; logical value which indicates whether the variables should be shifted to be zero centered (TRUE by default). |
| scale | bool; logical value which indicates whether the variables should be scaled to have unit variance (FALSE by default). |

| <pre>max_iter</pre> | integer; maximum number of iterations to perform before exiting. |
|---------------------|---|
| tol | float; stopping tolerance for the convergence criterion. |
| verbose | bool; logical value which indicates whether progress is printed. |

Details

Sparse principal component analysis is a modern variant of PCA. Specifically, SPCA attempts to find sparse weight vectors (loadings), i.e., a weight vector with only a few 'active' (nonzero) values. This approach leads to an improved interpretability of the model, because the principal components are formed as a linear combination of only a few of the original variables. Further, SPCA avoids overfitting in a high-dimensional data setting where the number of variables p is greater than the number of observations n.

Such a parsimonious model is obtained by introducing prior information like sparsity promoting regularizers. More concreatly, given an (n, p) data matrix X, SPCA attemps to minimize the following objective function:

$$f(A,B) = \frac{1}{2} \|X - XBA^{\top}\|_{F}^{2} + \psi(B)$$

where B is the sparse weight (loadings) matrix and A is an orthonormal matrix. ψ denotes a sparsity inducing regularizer such as the LASSO (ℓ_1 norm) or the elastic net (a combination of the ℓ_1 and ℓ_2 norm). The principal components Z are formed as

$$Z = XB$$

and the data can be approximately rotated back as

$$\tilde{X} = ZA^{\mathsf{T}}$$

The print and summary method can be used to present the results in a nice format.

Value

spca returns a list containing the following three components:

| loadings | array_like; sparse loadings (weight) vector; (p, k) dimensional array. |
|---------------|---|
| transform | array_like; the approximated inverse transform; (p,k) dimensional array. |
| scores | array_like; the principal component scores; (n, k) dimensional array. |
| eigenvalues | array_like; the approximated eigenvalues; (k) dimensional array. |
| center, scale | array_like; the centering and scaling used. |

spca

Author(s)

N. Benjamin Erichson, Peng Zheng, and Sasha Aravkin

References

 [1] N. B. Erichson, P. Zheng, K. Manohar, S. Brunton, J. N. Kutz, A. Y. Aravkin. "Sparse Principal Component Analysis via Variable Projection." Submitted to IEEE Journal of Selected Topics on Signal Processing (2018). (available at 'arXiv https://arxiv.org/abs/ 1804.00341).

See Also

rspca, robspca

Examples

```
# Create artifical data
m <- 10000
V1 <- rnorm(m, 0, 290)
V2 <- rnorm(m, 0, 300)
V3 <- -0.1*V1 + 0.1*V2 + rnorm(m,0,100)
X <- cbind(V1,V1,V1,V1, V2,V2,V2,V2, V3,V3)
X <- X + matrix(rnorm(length(X),0,1), ncol = ncol(X), nrow = nrow(X))
# Compute SPCA
out <- spca(X, k=3, alpha=1e-3, beta=1e-3, center = TRUE, scale = FALSE, verbose=0)
print(out)
summary(out)
```

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