# fbpca Documentation 

Release 1.0

## Facebook Inc

Functions for principal component analysis (PCA) and accuracy checks

This module contains eight functions:
pca principal component analysis (singular value decomposition)
eigens eigendecomposition of a self-adjoint matrix
eigenn eigendecomposition of a nonnegative-definite self-adjoint matrix
diffsnorm spectral-norm accuracy of a singular value decomposition
diffsnormc spectral-norm accuracy of a centered singular value decomposition
diffsnorms spectral-norm accuracy of a Schur decomposition
mult default matrix multiplication
set_matrix_mult re-definition of the matrix multiplication function "mult"

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fbpca.diffsnorm ( $A, U, s$, Va, n_iter=20)
2-norm accuracy of an approx to a matrix.
Computes an estimate snorm of the spectral norm (the operator norm induced by the Euclidean vector norm) of $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$, using n_iter iterations of the power method started with a random vector; $\mathrm{n} \_i t e r$ must be a positive integer.
Increasing $n \_i t e r$ improves the accuracy of the estimate snorm of the spectral norm of $A-U \operatorname{diag}(s) V a$.
Parameters A: array_like
first matrix in A-U diag(s) Va whose spectral norm is being estimated
$\mathbf{U}$ : array_like
second matrix in A - U diag(s) Va whose spectral norm is being estimated
s: array_like
vector in $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s})$ Va whose spectral norm is being estimated
Va : array_like
fourth matrix in A - U diag(s) Va whose spectral norm is being estimated
n_iter : int, optional
number of iterations of the power method to conduct; $n$ _iter must be a positive integer, and defaults to 20

Returns float
an estimate of the spectral norm of $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$ (the estimate fails to be accurate with exponentially low prob. as n_iter increases; see references DM1, DM2, and DM3 below)

## See also:

diffsnormc, pca

## Notes

To obtain repeatable results, reset the seed for the pseudorandom number generator.

## References

[DM1], [DM2], [DM3]

## Examples

```
>>> from fbpca import diffsnorm, pca
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> A = uniform(low=-1.0, high=1.0, size=(100, 2))
>>> A = A.dot(uniform(low=-1.0, high=1.0, size=(2, 100)))
>>> (U, s, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>> (U, S, Va) = pca(A, 2, True)
```

```
>>> err = diffsnorm(A, U, S, Va)
```

>>> print (err)

This example produces a rank-2 approximation $U \operatorname{diag}(\mathrm{~s})$ Va to A such that the columns of U are orthonormal, as are the rows of Va , and the entries of s are all nonnegative and are nonincreasing. diffsnorm $(\mathrm{A}, \mathrm{U}, \mathrm{s}, \mathrm{Va})$ outputs an estimate of the spectral norm of $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$, which should be close to the machine precision.
fbpca.diffsnorme ( $A, U, s$, Va, $n \_$iter $=20$ )
2-norm approx error to a matrix upon centering.
Computes an estimate snorm of the spectral norm (the operator norm induced by the Euclidean vector norm) of $\mathrm{C}(\mathrm{A})-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$, using n_iter iterations of the power method started with a random vector, where $\mathrm{C}(\mathrm{A})$ refers to A from the input, after centering its columns; $\mathrm{n}_{\mathrm{i}}$ iter must be a positive integer.

Increasing $n \_i t e r$ improves the accuracy of the estimate snorm of the spectral norm of $C(A)-U \operatorname{diag}(s) V a$, where $\mathrm{C}(\mathrm{A})$ refers to A after centering its columns.

Parameters A: array_like
first matrix in the column-centered A - U diag(s) Va whose spectral norm is being estimated
$\mathbf{U}$ : array_like
second matrix in the column-centered A - U diag(s) Va whose spectral norm is being estimated
s: array_like
vector in the column-centered A - U diag(s) Va whose spectral norm is being estimated
Va : array_like
fourth matrix in the column-centered A - U diag(s) Va whose spectral norm is being estimated
n_iter : int, optional
number of iterations of the power method to conduct; $n$ _iter must be a positive integer, and defaults to 20

## Returns float

an estimate of the spectral norm of the column-centered $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$ (the estimate fails to be accurate with exponentially low probability as n_iter increases; see references DC1, DC2, and DC3 below)

## See also:

diffsnorm, pca

## Notes

To obtain repeatable results, reset the seed for the pseudorandom number generator.

## References

[DC1], [DC2], [DC3]

## Examples

```
>>> from fbpca import diffsnormc, pca
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> A = uniform(low=-1.0, high=1.0, size=(100, 2))
>>> A = A.dot(uniform(low=-1.0, high=1.0, size=(2, 100)))
>>> (U, s, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>> (U, s, Va) = pca(A, 2, False)
>>> err = diffsnormc(A, U, s, Va)
>>> print(err)
```

This example produces a rank-2 approximation U diag(s) Va to the column-centered A such that the columns of U are orthonormal, as are the rows of Va, and the entries of s are nonnegative and nonincreasing. diffsnormc(A, $\mathrm{U}, \mathrm{s}, \mathrm{Va}$ ) outputs an estimate of the spectral norm of the column-centered A-U diag(s) Va, which should be close to the machine precision.

## fbpca.diffsnorms ( $\left.A, S, V, n \_i t e r=20\right)$

2-norm accuracy of a Schur decomp. of a matrix.
Computes an estimate snorm of the spectral norm (the operator norm induced by the Euclidean vector norm) of A-VSV', using n_iter iterations of the power method started with a random vector; $n \_i t e r$ must be a positive integer.
Increasing $n \_i t e r$ improves the accuracy of the estimate snorm of the spectral norm of A-VSV'.
Parameters A: array_like
first matrix in A-VSV' whose spectral norm is being estimated
S : array_like
third matrix in A-VSV' whose spectral norm is being estimated
V : array_like
second matrix in A-VSV' whose spectral norm is being estimated
n_iter : int, optional
number of iterations of the power method to conduct; $n \_i t e r$ must be a positive integer, and defaults to 20

## Returns float

an estimate of the spectral norm of A-VSV' (the estimate fails to be accurate with exponentially low probability as n_iter increases; see references DS1, DS2, and DS3 below)

## See also:

```
eigenn,eigens
```


## Notes

To obtain repeatable results, reset the seed for the pseudorandom number generator.

## References

[DS1], [DS2], [DS3]

## Examples

>>> from fbpca import diffsnorms, eigenn
>>> from numpy import diag
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> $A=$ uniform(low=-1.0, high=1.0, size=(2, 100))
$\ggg \mathrm{A}=\mathrm{A} \cdot \mathrm{T} \cdot \operatorname{dot}(\mathrm{A})$
>>> (U, s, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>> ( $\mathrm{d}, \mathrm{V}$ ) $=$ eigenn $(\mathrm{A}, 2)$
>>> err = diffsnorms(A, diag(d), V)
>>> print(err)
This example produces a rank-2 approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}$ ' to A such that the columns of V are orthonormal and the entries of d are nonnegative and are nonincreasing. diffsnorms $(\mathrm{A}, \operatorname{diag}(\mathrm{d}), \mathrm{V})$ outputs an estimate of the spectral norm of A - V diag(d) $\mathrm{V}^{\prime}$, which should be close to the machine precision.

## fbpca.eigenn ( $A, k=6, n \_$iter $=4, l=$ None $)$

Eigendecomposition of a NONNEGATIVE-DEFINITE matrix.
Constructs a nearly optimal rank-k approximation V diag(d) V ' to a NONNEGATIVE-DEFINITE matrix A, using n_iter normalized power iterations, with block size 1 , started with an $n \times 1$ random matrix, when A is n x n ; the reference EGN below explains "nearly optimal." k must be a positive integer $<=$ the dimension n of A , n _iter must be a nonnegative integer, and 1 must be a positive integer $>=\mathrm{k}$.
The rank-k approximation V diag(d) $\mathrm{V}^{\prime}$ comes in the form of an eigendecomposition - the columns of V are orthonormal and d is a real vector such that its entries are nonnegative and nonincreasing. V is nx k and len(d) $=\mathrm{k}$, when A is nx n .

Increasing $n \_i t e r$ or 1 improves the accuracy of the approximation $V \operatorname{diag}(d) V^{\prime}$; the reference EGN below describes how the accuracy depends on $n_{-}$iter and 1 . Please note that even $n_{-} i t e r=1$ guarantees superb accuracy, whether or not there is any gap in the singular values of the matrix A being approximated, at least when measuring accuracy as the spectral norm II A - V diag(d) V' II of the matrix A - V diag(d) V' (relative to the spectral norm IIAll of A).

Parameters A: array_like, shape (n, n)
matrix being approximated
$\mathbf{k}$ : int, optional
rank of the approximation being constructed; k must be a positive integer $<=$ the dimension of A , and defaults to 6
n_iter : int, optional
number of normalized power iterations to conduct; $\mathrm{n}_{\text {_ }}$ iter must be a nonnegative integer, and defaults to 4
$\mathbf{l}$ : int, optional
block size of the normalized power iterations; 1 must be a positive integer $>=k$, and defaults to $\mathrm{k}+2$

Returns d: ndarray, shape (k,)
vector of length $k$ in the rank- k approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ to A , such that its entries are nonnegative and nonincreasing
$\mathbf{V}$ : ndarray, shape ( $\mathrm{n}, \mathrm{k}$ )
$\mathrm{n} x \mathrm{k}$ matrix in the rank-k approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ to A , where A is $\mathrm{n} x \mathrm{n}$

## See also:

diffsnorms, eigens, pca

## Notes

## THE MATRIX A MUST BE SELF-ADJOINT AND NONNEGATIVE DEFINITE.

To obtain repeatable results, reset the seed for the pseudorandom number generator.
The user may ascertain the accuracy of the approximation $V \operatorname{diag}(\mathrm{~d}) \mathrm{V}$ ' to A by invoking diffsnorms(A, numpy.diag(d), V).

## References

[EGN]

## Examples

```
>>> from fbpca import diffsnorms, eigenn
>>> from numpy import diag
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> A = uniform(low=-1.0, high=1.0, size=(2, 100))
>>> A = A.T.dot(A)
>>>(U, S, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>> (d, V) = eigenn(A, 2)
>>> err = diffsnorms(A, diag(d), V)
>>> print(err)
```

This example produces a rank-2 approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}$ ' to A such that the columns of V are orthonormal and the entries of $d$ are nonnegative and nonincreasing. diffsnorms $(\mathrm{A}, \operatorname{diag}(\mathrm{d}), \mathrm{V})$ outputs an estimate of the spectral norm of A - V diag(d) $\mathrm{V}^{\prime}$, which should be close to the machine precision.

## fbpca. eigens ( $A, k=6, n \_$iter $=4, l=$ None $)$

Eigendecomposition of a SELF-ADJOINT matrix.
Constructs a nearly optimal rank-k approximation V diag(d) V' to a SELF-ADJOINT matrix A, using n_iter normalized power iterations, with block size 1 , started with an $n x l$ random matrix, when $A$ is $n x n$; the reference EGS below explains "nearly optimal." k must be a positive integer $<=$ the dimension n of A , $\mathrm{n} \_$iter must be a nonnegative integer, and 1 must be a positive integer $>=k$.

The rank-k approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ comes in the form of an eigendecomposition - the columns of V are orthonormal and d is a vector whose entries are real-valued and their absolute values are nonincreasing. V is n xk and $\operatorname{len}(\mathrm{d})=\mathrm{k}$, when A is n xn .

Increasing n_iter or 1 improves the accuracy of the approximation $V \operatorname{diag}(\mathrm{~d}) \mathrm{V}$ '; the reference EGS below describes how the accuracy depends on n_iter and 1 . Please note that even n_iter=1 guarantees superb accuracy, whether or not there is any gap in the singular values of the matrix A being approximated, at least when measuring accuracy as the spectral norm II $\mathrm{A}-\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime} \| l$ of the matrix $\mathrm{A}-\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ (relative to the spectral norm IIAll of A).

Parameters A : array_like, shape (n, n)
matrix being approximated
k: int, optional
rank of the approximation being constructed; $k$ must be a positive integer $<=$ the dimen-
sion of $A$, and defaults to 6
n_iter : int, optional
number of normalized power iterations to conduct; $n \_i t e r$ must be a nonnegative integer, and defaults to 4
l : int, optional
block size of the normalized power iterations; 1 must be a positive integer $>=\mathrm{k}$, and defaults to $\mathrm{k}+2$

Returns d: ndarray, shape (k,)
vector of length $k$ in the rank-k approximation $V \operatorname{diag}(d) V^{\prime}$ to $A$, such that its entries are real-valued and their absolute values are nonincreasing
$\mathbf{V}$ : ndarray, shape ( $\mathrm{n}, \mathrm{k}$ )
$\mathrm{n} x \mathrm{k}$ matrix in the rank-k approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ to A , where A is $\mathrm{n} \mathrm{x} n$

## See also:

diffsnorms, eigenn, pca

## Notes

## THE MATRIX A MUST BE SELF-ADJOINT.

To obtain repeatable results, reset the seed for the pseudorandom number generator.
The user may ascertain the accuracy of the approximation $V \operatorname{diag}(\mathrm{~d}) \mathrm{V}$ ' to A by invoking diffsnorms(A, numpy.diag(d), V).

## References

[EGS]

## Examples

```
>>> from fbpca import diffsnorms, eigens
```

>>> from numpy import diag
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> $A=$ uniform(low=-1.0, high=1.0, size=(2, 100))

```
>> A = A.T.dot(A)
>>> (U, s, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>> (d, V) = eigens(A, 2)
>>> err = diffsnorms(A, diag(d), V)
>>> print(err)
```

This example produces a rank-2 approximation $\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$ to A such that the columns of V are orthonormal, and the entries of d are real-valued and their absolute values are nonincreasing. diffsnorms(A, diag(d), V) outputs an estimate of the spectral norm of $\mathrm{A}-\mathrm{V} \operatorname{diag}(\mathrm{d}) \mathrm{V}^{\prime}$, which should be close to the machine precision.

```
fbpca.mult (A,B)
    default matrix multiplication.
```

Multiplies A and B together via the "dot" method.
Parameters A : array_like
first matrix in the product $\mathrm{A} * \mathrm{~B}$ being calculated
B : array_like
second matrix in the product $\mathrm{A} * \mathrm{~B}$ being calculated
Returns array_like
product of the inputs A and B

## Examples

>>> from fbpca import mult
>>> from numpy import array
>>> from numpy.linalg import norm
>>>
>>> A $=\operatorname{array}([[1 ., 2],.[3 ., 4]]$.
>>> $B=\operatorname{array}([[5 ., 6],.[7 ., 8]]$.
>>> norm(mult(A, B) - A.dot(B))
This example multiplies two matrices two ways - once with mult, and once with the usual "dot" method - and then calculates the (Frobenius) norm of the difference (which should be near 0).
fbpca.pca ( $A, k=6$, raw $=$ False, $n$ _iter $=2, l=$ None )
Principal component analysis.
Constructs a nearly optimal rank-k approximation $U \operatorname{diag}(s)$ Va to $A$, centering the columns of A first when raw is False, using n_iter normalized power iterations, with block size 1 , started with a $\min (m, n) \times 1$ random matrix, when A is mx n ; the reference PCA below explains "nearly optimal." k must be a positive integer $<=$ the smaller dimension of $\mathrm{A}, \mathrm{n} \_$iter must be a nonnegative integer, and 1 must be a positive integer $>=\mathrm{k}$.

The rank-k approximation $\mathrm{U} \operatorname{diag}(\mathrm{s})$ Va comes in the form of a singular value decomposition (SVD) - the columns of U are orthonormal, as are the rows of Va , and the entries of s are all nonnegative and nonincreasing. U is $\mathrm{mxk}, V$ is kxn , and len $(\mathrm{s})=\mathrm{k}$, when A is mxn .

Increasing $n \_i t e r$ or 1 improves the accuracy of the approximation $U \operatorname{diag}(s) \mathrm{Va}$; the reference PCA below describes how the accuracy depends on n_iter and 1 . Please note that even n_iter=1 guarantees superb accuracy, whether or not there is any gap in the singular values of the matrix A being approximated, at least when measuring accuracy as the spectral norm II A - U diag(s) Va II of the matrix A - U diag(s) Va (relative to the spectral norm IIAll of A, and accounting for centering when raw is False).

Parameters A: array_like, shape (m, n)
matrix being approximated
$\mathbf{k}$ : int, optional
rank of the approximation being constructed; k must be a positive integer $<=$ the smaller dimension of $A$, and defaults to 6
raw : bool, optional
centers A when raw is False but does not when raw is True; raw must be a Boolean and defaults to False
n_iter : int, optional
number of normalized power iterations to conduct; $n \_i t e r$ must be a nonnegative integer, and defaults to 2

I : int, optional
block size of the normalized power iterations; 1 must be a positive integer $>=\mathrm{k}$, and defaults to $\mathrm{k}+2$

Returns U : ndarray, shape (m, k)
$m x k$ matrix in the rank-k approximation $U \operatorname{diag}(s)$ Va to $A$ or $C(A)$, where $A$ is $m x n$, and $\mathrm{C}(\mathrm{A})$ refers to A after centering its columns; the columns of U are orthonormal
$\mathbf{s}$ : ndarray, shape (k,)
vector of length $k$ in the rank-k approximation $U \operatorname{diag}(s)$ Va to $A$ or $C(A)$, where $A$ is $m$ $\mathrm{x} n$, and $\mathrm{C}(\mathrm{A})$ refers to A after centering its columns; the entries of s are all nonnegative and nonincreasing
Va : ndarray, shape (k, n)
kx n matrix in the rank-k approximation $U \operatorname{diag}(\mathrm{~s})$ Va to A or $\mathrm{C}(\mathrm{A})$, where A is $\mathrm{m} \mathrm{x} n$, and $\mathrm{C}(\mathrm{A})$ refers to A after centering its columns; the rows of Va are orthonormal

## See also:

diffsnorm, diffsnormc, eigens, eigenn

## Notes

To obtain repeatable results, reset the seed for the pseudorandom number generator.
The user may ascertain the accuracy of the approximation $U \operatorname{diag}(s)$ Va to $A$ by invoking diffsnorm $(A, U, s, V a)$, when raw is True. The user may ascertain the accuracy of the approximation $U \operatorname{diag}(s)$ Va to $C(A)$, where $C(A)$ refers to A after centering its columns, by invoking diffsnormc(A, U, s, Va), when raw is False.

## References

[PCA]

## Examples

```
>>> from fbpca import diffsnorm, pca
>>> from numpy.random import uniform
>>> from scipy.linalg import svd
>>>
>>> A = uniform(low=-1.0, high=1.0, size=(100, 2))
>>> A = A.dot(uniform(low=-1.0, high=1.0, size=(2, 100)))
>>> (U, s, Va) = svd(A, full_matrices=False)
>>> A = A / s[0]
>>>
>>>(U, s, Va) = pca(A, 2, True)
>>> err = diffsnorm(A, U, S, Va)
>>> print(err)
```

This example produces a rank-2 approximation $U \operatorname{diag}(s) V a$ to A such that the columns of $U$ are orthonormal, as are the rows of Va , and the entries of s are all nonnegative and are nonincreasing. diffsnorm $(\mathrm{A}, \mathrm{U}, \mathrm{s}, \mathrm{Va})$ outputs an estimate of the spectral norm of $\mathrm{A}-\mathrm{U} \operatorname{diag}(\mathrm{s}) \mathrm{Va}$, which should be close to the machine precision.
fbpca.set_matrix_mult (newmult)
re-definition of the matrix multiplication function "mult".
Sets the matrix multiplication function "mult" used in fbpca to be the input "newmult" - which must return the product $\mathrm{A} * \mathrm{~B}$ of its two inputs A and B , i.e., newmult $(\mathrm{A}, \mathrm{B})$ must be the product of A and B .

## Parameters newmult : callable

matrix multiplication replacing mult in fbpca; newmult must return the product of its two array_like inputs

## Returns None

## Examples

```
>>> from fbpca import set_matrix_mult
>>>
>>> def newmult(A, B):
... return A*B
...
>>> set_matrix_mult(newmult)
```

This example redefines the matrix multiplication used in fbpca to be the entrywise product.
[DM1] Jacek Kuczynski and Henryk Wozniakowski, Estimating the largest eigenvalues by the power and Lanczos methods with a random start, SIAM Journal on Matrix Analysis and Applications, 13 (4): 1094-1122, 1992.
[DM2] Edo Liberty, Franco Woolfe, Per-Gunnar Martinsson, Vladimir Rokhlin, and Mark Tygert, Randomized algorithms for the low-rank approximation of matrices, Proceedings of the National Academy of Sciences (USA), 104 (51): 20167-20172, 2007. (See the appendix.)
[DM3] Franco Woolfe, Edo Liberty, Vladimir Rokhlin, and Mark Tygert, A fast randomized algorithm for the approximation of matrices, Applied and Computational Harmonic Analysis, 25 (3): 335-366, 2008. (See Section 3.4.)
[DC1] Jacek Kuczynski and Henryk Wozniakowski, Estimating the largest eigenvalues by the power and Lanczos methods with a random start, SIAM Journal on Matrix Analysis and Applications, 13 (4): 1094-1122, 1992.
[DC2] Edo Liberty, Franco Woolfe, Per-Gunnar Martinsson, Vladimir Rokhlin, and Mark Tygert, Randomized algorithms for the low-rank approximation of matrices, Proceedings of the National Academy of Sciences (USA), 104 (51): 20167-20172, 2007. (See the appendix.)
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[DS2] Edo Liberty, Franco Woolfe, Per-Gunnar Martinsson, Vladimir Rokhlin, and Mark Tygert, Randomized algorithms for the low-rank approximation of matrices, Proceedings of the National Academy of Sciences (USA), 104 (51): 20167-20172, 2007. (See the appendix.)
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