sklearn.decomposition.PCA

» *class* `sklearn.decomposition.`**`PCA`**(*n_components=None*, *copy=True*, *whiten=False*, *svd_solver='auto'*, *tol=0.0*, *iterated_power='auto'*, *random_state=None*) ¶ [source]

Principal component analysis (PCA)

Linear dimensionality reduction using Singular Value Decomposition of the data to project it to a lower dimensional space.

It uses the LAPACK implementation of the full SVD or a randomized truncated SVD by the method of Halko et al. 2009, depending on the shape of the input data and the number of components to extract.

It can also use the scipy.sparse.linalg ARPACK implementation of the truncated SVD.

Notice that this class does not support sparse input. See `TruncatedSVD` for an alternative with sparse data.

Read more in the User Guide.

Parameters: **n_components** : int, float, None or string

Number of components to keep. if n_components is not set all components are kept:

```
n_components == min(n_samples, n_features)
```

if n_components == 'mle' and svd_solver == 'full', Minka's MLE is used to guess the dimension if `0 < n_components < 1` and svd_solver == 'full', select the number of components such that the amount of variance that needs to be explained is greater than the percentage specified by n_components n_components cannot be equal to n_features for svd_solver == 'arpack'.

copy : bool (default True)

If False, data passed to fit are overwritten and running fit(X).transform(X) will not yield the expected results, use fit_transform(X) instead.

whiten : bool, optional (default False)

When True (False by default) the *components_* vectors are multiplied by the square root of n_samples and then divided by the singular values to ensure uncorrelated outputs with unit component-wise variances.

Whitening will remove some information from the transformed signal (the relative variance scales of the components) but can sometime improve the predictive accuracy of the downstream estimators by making their data respect some hard-wired assumptions.

svd_solver : string {'auto', 'full', 'arpack', 'randomized'} auto :

the solver is selected by a default policy based on *X.shape* and *n_components*: if the input data is larger than 500x500 and the number of components to extract is lower than 80% of the smallest dimension of the data, then the more efficient 'randomized' method is enabled. Otherwise the exact full SVD is computed and optionally truncated afterwards.

full :

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run exact full SVD calling the standard LAPACK solver via *scipy.linalg.svd* and select the components by postprocessing

arpack :

run SVD truncated to n_components calling ARPACK solver via *scipy.sparse.linalg.svds*. It requires strictly 0 < n_components < X.shape[1]

randomized :

run randomized SVD by the method of Halko et al.

New in version 0.18.0.

tol : float >= 0, optional (default .0)

Tolerance for singular values computed by svd_solver == 'arpack'.

New in version 0.18.0.

iterated_power : int >= 0, or 'auto', (default 'auto')

Number of iterations for the power method computed by svd_solver == 'randomized'.

New in version 0.18.0.

random_state : int or RandomState instance or None (default None)

Pseudo Random Number generator seed control. If None, use the numpy.random singleton. Used by svd_solver == 'arpack' or 'randomized'.

New in version 0.18.0.

Attributes: **components_** : array, [n_components, n_features]

Principal axes in feature space, representing the directions of maximum variance in the data. The components are sorted by `explained_variance_`.

explained_variance_ : array, [n_components]

The amount of variance explained by each of the selected components.

New in version 0.18.

explained_variance_ratio_ : array, [n_components]

Percentage of variance explained by each of the selected components.

If `n_components` is not set then all components are stored and the sum of explained variances is equal to 1.0.

mean_ : array, [n_features]

Per-feature empirical mean, estimated from the training set.

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Equal to *X.mean(axis=1)*.

n_components_ : int

The estimated number of components. When n_components is set to ‘mle’ or a number between 0 and 1 (with svd_solver == ‘full’) this number is estimated from input data. Otherwise it equals the parameter n_components, or n_features if n_components is None.

noise_variance_ : float

The estimated noise covariance following the Probabilistic PCA model from Tipping and Bishop 1999. See “Pattern Recognition and Machine Learning” by C. Bishop, 12.2.1 p. 574 or http://www.miketipping.com/papers/met-mppca.pdf. It is required to computed the estimated data covariance and score samples.

See also: `KernelPCA`, `SparsePCA`, `TruncatedSVD`, `IncrementalPCA`

References

For n_components == ‘mle’, this class uses the method of *Thomas P. Minka: Automatic Choice of Dimensionality for PCA. NIPS 2000: 598-604*

Implements the probabilistic PCA model from: M. Tipping and C. Bishop, Probabilistic Principal Component Analysis, Journal of the Royal Statistical Society, Series B, 61, Part 3, pp. 611-622 via the score and score_samples methods. See http://www.miketipping.com/papers/met-mppca.pdf

For svd_solver == ‘arpack’, refer to *scipy.sparse.linalg.svds*.

For svd_solver == ‘randomized’, see: *Finding structure with randomness: Stochastic algorithms for constructing approximate matrix decompositions Halko, et al., 2009 (arXiv:909) A randomized algorithm for the decomposition of matrices Per-Gunnar Martinsson, Vladimir Rokhlin and Mark Tygert*

Examples

```
>>> import numpy as np
>>> from sklearn.decomposition import PCA
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> pca = PCA(n_components=2)
>>> pca.fit(X)
PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
>>> print(pca.explained_variance_ratio_)
[ 0.99244...  0.00755...]
```

```
>>> pca = PCA(n_components=2, svd_solver='full')
>>> pca.fit(X)
```

```
PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
  svd_solver='full', tol=0.0, whiten=False)
>>> print(pca.explained_variance_ratio_)
[ 0.99244...  0.00755...]
```

```
>>> pca = PCA(n_components=1, svd_solver='arpack')
>>> pca.fit(X)
PCA(copy=True, iterated_power='auto', n_components=1, random_state=None,
  svd_solver='arpack', tol=0.0, whiten=False)
>>> print(pca.explained_variance_ratio_)
[ 0.99244...]
```

Methods

`fit`(X[, y])	Fit the model with X.
`fit_transform`(X[, y])	Fit the model with X and apply the dimensionality reduction on X.
`get_covariance`()	Compute data covariance with the generative model.
`get_params`([deep])	Get parameters for this estimator.
`get_precision`()	Compute data precision matrix with the generative model.
`inverse_transform`(X[, y])	Transform data back to its original space.
`score`(X[, y])	Return the average log-likelihood of all samples.
`score_samples`(X)	Return the log-likelihood of each sample.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X[, y])	Apply dimensionality reduction to X.

`__init__`(*n_components=None*, *copy=True*, *whiten=False*, *svd_solver='auto'*, *tol=0.0*, *iterated_power='auto'*, *random_state=None*) [source]

`fit`(*X*, *y=None*) [source]

Fit the model with X.

Parameters: **X: array-like, shape (n_samples, n_features)** :

Training data, where n_samples in the number of samples and n_features is the number of features.

Returns: **self** : object

Returns the instance itself.

`fit_transform`(*X*, *y=None*) [source]

Fit the model with X and apply the dimensionality reduction on X.

Parameters: **X** : array-like, shape (n_samples, n_features)

Training data, where n_samples is the number of samples and n_features is the number of features.

Returns: **X_new** : array-like, shape (n_samples, n_components) `get_covariance()` [source]

Compute data covariance with the generative model.

`cov = components_.T * S**2 * components_ + sigma2 * eye(n_features)` where S**2 contains the explained variances, and sigma2 contains the noise variances.

Returns: **cov** : array, shape=(n_features, n_features)

Estimated covariance of data.

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`get_params(deep=True)` [source]

Get parameters for this estimator.

Parameters: **deep** : boolean, optional

If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns: **params** : mapping of string to any

Parameter names mapped to their values.

`get_precision()` [source]

Compute data precision matrix with the generative model.

Equals the inverse of the covariance but computed with the matrix inversion lemma for efficiency.

Returns: **precision** : array, shape=(n_features, n_features)

Estimated precision of data.

`inverse_transform(X, y=None)` [source]

Transform data back to its original space.

In other words, return an input X_original whose transform would be X.

Parameters: **X** : array-like, shape (n_samples, n_components)

New data, where n_samples is the number of samples and n_components is the number of components.

Returns: **X_original array-like, shape (n_samples, n_features)** :

Notes

If whitening is enabled, inverse_transform will compute the exact inverse operation, which includes reversing whitening.

`score`(*X*, *y=None*) [source]

Return the average log-likelihood of all samples.

See. “Pattern Recognition and Machine Learning” by C. Bishop, 12.2.1 p. 574 or http://www.miketipping.com/papers/met-mppca.pdf

Parameters:	**X: array, shape(n_samples, n_features)** : The data.
Returns:	**ll: float** : Average log-likelihood of the samples under the current model

`score_samples`(*X*) [source]

Return the log-likelihood of each sample.

See. “Pattern Recognition and Machine Learning” by C. Bishop, 12.2.1 p. 574 or http://www.miketipping.com/papers/met-mppca.pdf

Parameters:	**X: array, shape(n_samples, n_features)** : The data.
Returns:	**ll: array, shape (n_samples,)** : Log-likelihood of each sample under the current model

`set_params`(***params*) [source]

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it’s possible to update each component of a nested object.

Returns:	**self** :

`transform`(*X*, *y=None*) [source]

Apply dimensionality reduction to X.

X is projected on the first principal components previously extracted from a training set.

Parameters:	**X** : array-like, shape (n_samples, n_features)

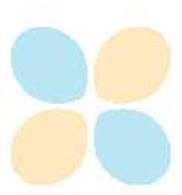
New data, where n_samples is the number of samples and n_features is the number of features.

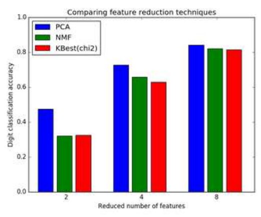
Returns: **X_new** : array-like, shape (n_samples, n_components)

Examples

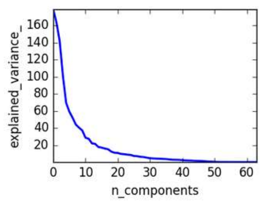
```
>>> import numpy as np
>>> from sklearn.decomposition import IncrementalPCA
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> ipca = IncrementalPCA(n_components=2, batch_size=3)
>>> ipca.fit(X)
IncrementalPCA(batch_size=3, copy=True, n_components=2, whiten=False)
>>> ipca.transform(X)
```

Examples using `sklearn.decomposition.PCA`

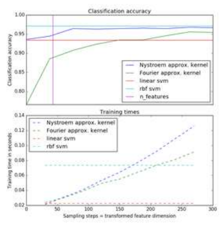

Concatenating multiple feature extraction methods



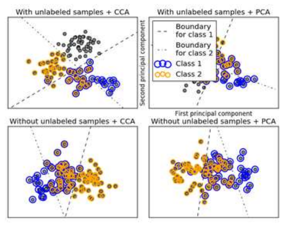
Selecting dimensionality reduction with Pipeline and GridSearchCV



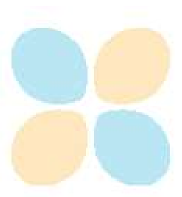
Pipelining: chaining a PCA and a logistic regression

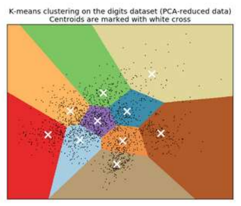


Explicit feature map approximation for RBF kernels

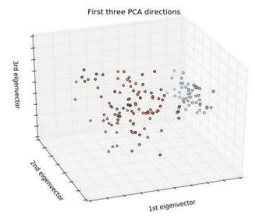


Multilabel classification

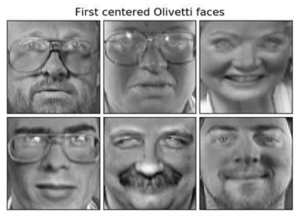

Faces recognition example using eigenfaces and SVMs



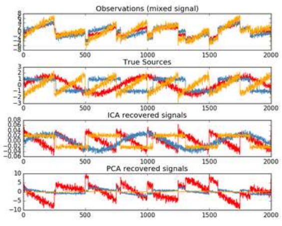
A demo of K-Means clustering on the handwritten digits data

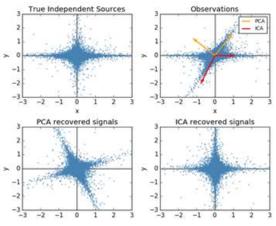


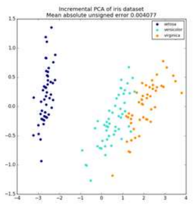
The Iris Dataset



Faces dataset decompositions


Blind source separation using FastICA


FastICA on 2D point clouds


Incremental PCA

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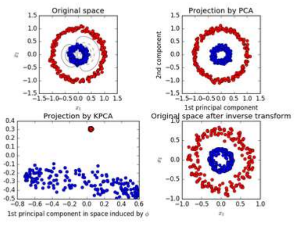
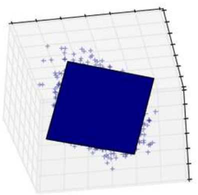
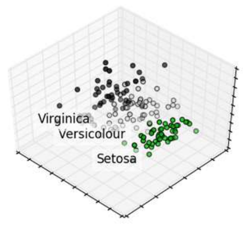
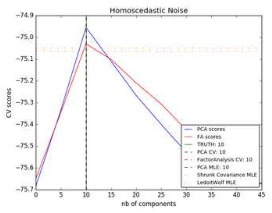
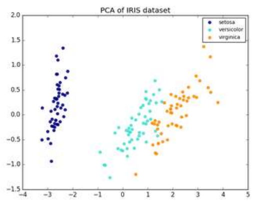
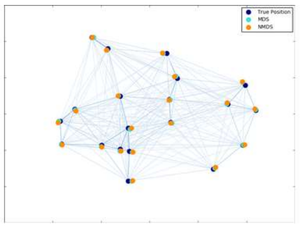

Kernel PCA

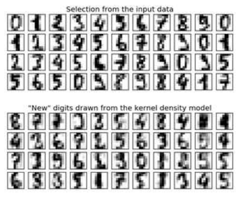

Principal components analysis (PCA)

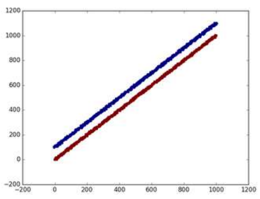

PCA example with Iris Data-set


Model selection with Probabilistic PCA and Factor Analysis (FA)


Comparison of LDA and PCA 2D projection of Iris dataset


Multi-dimensional scaling


Kernel Density Estimation


Using FunctionTransformer to select columns