sklearn.decomposition.PCA

class `sklearn.decomposition.`**`PCA`**(*n_components=None*, ***, *copy=True*, *whiten=False*, *svd_solver='auto'*, *tol=0.0*, *iterated_power='auto'*, *n_oversamples=10*, *power_iteration_normalizer='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. The input data is centered but not scaled for each feature before applying the SVD.

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.

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Parameters:

n_components : *int, float or 'mle', default=None*

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. Use of `n_components == 'mle'` will interpret `svd_solver == 'auto'` as `svd_solver == 'full'`.

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.

If `svd_solver == 'arpack'`, the number of components must be strictly less than the minimum of n_features and n_samples.

Hence, the None case results in:

```
n_components == min(n_samples, n_features) - 1
```

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, 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 : *{'auto', 'full', 'arpack', 'randomized'}, default='auto'*

If 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.

If full :

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

If arpack :

run SVD truncated to n_components calling ARPACK solver via `scipy.sparse.linalg.svds`. It requires strictly 0 < n_components < min(X.shape)

If randomized :

run randomized SVD by the method of Halko et al.

New in version 0.18.0.

tol : *float, default=0.0*

Tolerance for singular values computed by svd_solver == 'arpack'. Must be of range [0.0, infinity).

New in version 0.18.0.

iterated_power : *int or 'auto', default='auto'*

Number of iterations for the power method computed by svd_solver == 'randomized'. Must be of range [0, infinity).

New in version 0.18.0.

n_oversamples : *int, default=10*

This parameter is only relevant when `svd_solver="randomized"`. It corresponds to the additional number of random vectors to sample the range of `X` so as to ensure proper conditioning. See [`randomized_svd`] for more details.

New in version 1.1.

power_iteration_normalizer : *{'auto', 'QR', 'LU', 'none'}, default='auto'*

Power iteration normalizer for randomized SVD solver. Not used by ARPACK. See [`randomized_svd`] for more details.

New in version 1.1.

random_state : *int, RandomState instance or None, default=None*

n the 'arpack' or 'randomized' solvers are used. Pass an int for reproducible results across multiple function calls. See Glossary.

New in version 0.18.0.

Attributes:

components_ : *ndarray of shape (n_components, n_features)*

Principal axes in feature space, representing the directions of maximum variance in the data. Equivalently, the right singular vectors of the centered input data, parallel to its eigenvectors. The components are sorted by decreasing `explained_variance_`.

explained_variance_ : *ndarray of shape (n_components,)*

The amount of variance explained by each of the selected components. The variance estimation uses `n_samples - 1` degrees of freedom.

Equal to n_components largest eigenvalues of the covariance matrix of X.

New in version 0.18.

explained_variance_ratio_ : *ndarray of shape (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 the ratios is equal to 1.0.

singular_values_ : *ndarray of shape (n_components,)*

The singular values corresponding to each of the selected components. The singular values are equal to the 2-norms of the `n_components` variables in the lower-dimensional space.

New in version 0.19.

mean_ : *ndarray of shape (n_features,)*

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

Equal to `X.mean(axis=0)`.

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 the lesser value of n_features and n_samples if n_components is None.

n_features_ : *int*

Number of features in the training data.

n_samples_ : *int*

Number of samples in the training data.

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 compute the estimated data covariance and score samples.

Equal to the average of (min(n_features, n_samples) - n_components) smallest eigenvalues of the covariance matrix of X.

n_features_in_ : *int*

Number of features seen during fit.

New in version 0.24.

feature_names_in_ : *ndarray of shape (`n_features_in_`,)*

Names of features seen during fit. Defined only when `X` has feature names that are all strings.

New in version 1.0.

See also:

`KernelPCA`

Kernel Principal Component Analysis.

`SparsePCA`

Sparse Principal Component Analysis.

`TruncatedSVD`

D ality reduction using truncated SVD.

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`IncrementalPCA`
Incremental Principal Component Analysis.

References

For n_components == 'mle', this class uses the method from: Minka, T. P.. "Automatic choice of dimensionality for PCA". In NIPS, pp. 598-604

Implements the probabilistic PCA model from: Tipping, M. E., and Bishop, C. M. (1999). "Probabilistic principal component analysis". Journal of the Royal Statistical Society: Series B (Statistical Methodology), 61(3), 611-622. via the score and score_samples methods.

For svd_solver == 'arpack', refer to `scipy.sparse.linalg.svds`.

For svd_solver == 'randomized', see: Halko, N., Martinsson, P. G., and Tropp, J. A. (2011). "Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions". SIAM review, 53(2), 217-288. and also Martinsson, P. G., Rokhlin, V., and Tygert, M. (2011). "A randomized algorithm for the decomposition of matrices". Applied and Computational Harmonic Analysis, 30(1), 47-68.

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(n_components=2)
>>> print(pca.explained_variance_ratio_)
[0.9924... 0.0075...]
>>> print(pca.singular_values_)
[6.30061... 0.54980...]
```

```
>>> pca = PCA(n_components=2, svd_solver='full')
>>> pca.fit(X)
PCA(n_components=2, svd_solver='full')
>>> print(pca.explained_variance_ratio_)
[0.9924... 0.00755...]
>>> print(pca.singular_values_)
[6.30061... 0.54980...]
```

```
>>> pca = PCA(n_components=1, svd_solver='arpack')
>>> pca.fit(X)
PCA(n_components=1, svd_solver='arpack')
>>> print(pca.explained_variance_ratio_)
[0.99244...]
>>> print(pca.singular_values_)
[6.30061...]
```

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_feature_names_out`([input_features])	Get output feature names for transformation.
`get_metadata_routing`()	Get metadata routing of this object.
`get_params`([deep])	Get parameters for this estimator.
`get_precision`()	Compute data precision matrix with the generative model.
`inverse_transform`(X)	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_output`(*[, transform])	Set output container.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X)	Apply dimensionality reduction to X.

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

Fit the model with X.

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Parameters:

X : *array-like of shape (n_samples, n_features)*
Training data, where `n_samples` is the number of samples and `n_features` is the number of features.

y : *Ignored*
Ignored.

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 of shape (n_samples, n_features)*
Training data, where `n_samples` is the number of samples and `n_features` is the number of features.

y : *Ignored*
Ignored.

Returns:

X_new : *ndarray of shape (n_samples, n_components)*
Transformed values.

Notes

This method returns a Fortran-ordered array. To convert it to a C-ordered array, use 'np.ascontiguousarray'.

`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 of shape=(n_features, n_features)*
Estimated covariance of data.

`get_feature_names_out`(*input_features=None*) [source]

Get output feature names for transformation.

The feature names out will prefixed by the lowercased class name. For example, if the transformer outputs 3 features, then the feature names out are: `["class_name0", "class_name1", "class_name2"]`.

Parameters:

input_features : *array-like of str or None, default=None*
Only used to validate feature names with the names seen in `fit`.

Returns:

feature_names_out : *ndarray of str objects*
Transformed feature names.

`get_metadata_routing`() [source]

Get metadata routing of this object.

Please check User Guide on how the routing mechanism works.

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Returns:

routing : *MetadataRequest*
A `MetadataRequest` encapsulating routing information.

`get_params`(*deep=True*) [source]

Get parameters for this estimator.

Parameters:

deep : *bool, default=True*
If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns:

params : *dict*
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*) [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 of 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 of shape (n_samples, n_features)
Original data, where `n_samples` is the number of samples and `n_features` is the number of 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-like of shape (n_samples, n_features)*
The data.

y : *Ignored*
Ignored.

Returns:

ll : *float*
Average log-likelihood of the samples under the current model.

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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-like of shape (n_samples, n_features)*
The data.

Returns:

ll : *ndarray of shape (n_samples,)*
Log-likelihood of each sample under the current model.

set_output(*, *transform=None*) [source]

Set output container.

See Introducing the set_output API for an example on how to use the API.

Parameters:

transform : *{“default”, “pandas”}, default=None*
Configure output of `transform` and `fit_transform`.

- `"default"`: Default output format of a transformer
- `"pandas"`: DataFrame output
- `None`: Transform configuration is unchanged

Returns:

self : *estimator instance*
Estimator instance.

set_params(***params*) [source]

Set the parameters of this estimator.

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

Parameters:

****params : *dict***
Estimator parameters.

Returns:

self : *estimator instance*
Estimator instance.

transform(*X*) [source]

Apply dimensionality reduction to X.

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

Parameters:

X : *array-like of 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 of shape (n_samples, n_components)*
Projection of X in the first principal components, where `n_samples` is the number of samples and `n_components` is the number of the components.

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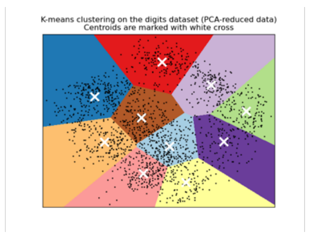
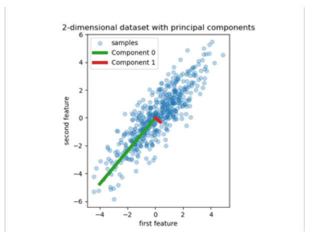
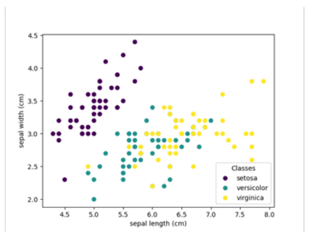
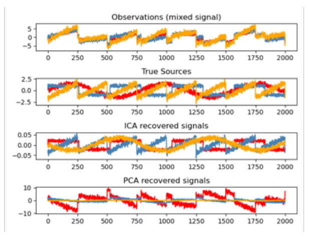
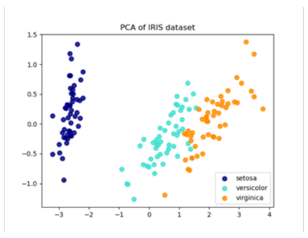
Examples using `sklearn.decomposition.PCA`

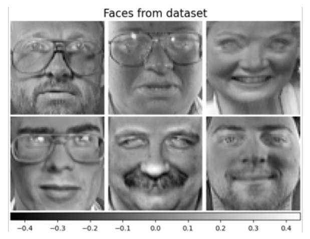

A demo of K-Means clustering on the handwritten digits data

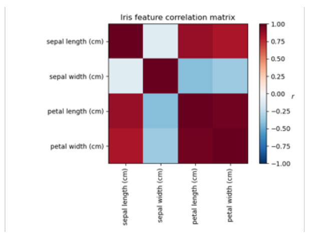

Principal Component Regression vs Partial Least Squares Regression

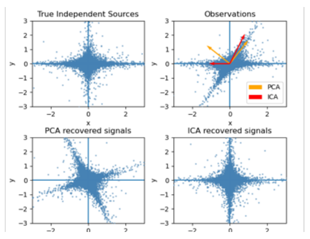

The Iris Dataset

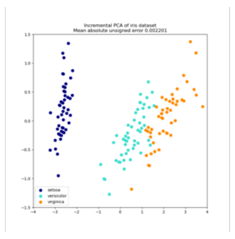

Blind source separation using FastICA

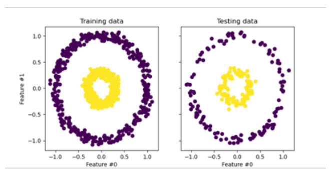

Comparison of LDA and PCA 2D projection of Iris dataset

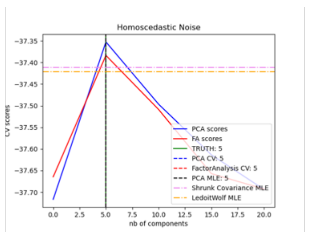

Faces dataset decompositions

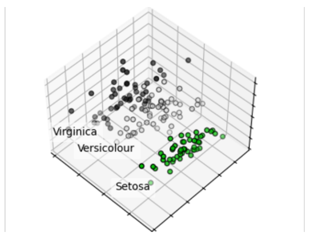

Factor Analysis (with rotation) to visualize patterns

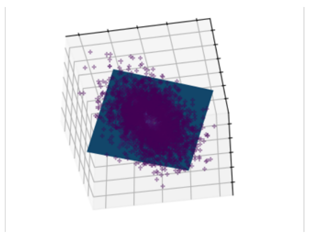

FastICA on 2D point clouds


Incremental PCA


Kernel PCA


Model selection with Probabilistic PCA and Factor Analysis (FA)


PCA example with Iris Data-set


Principal components analysis (PCA)

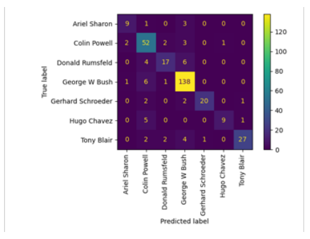
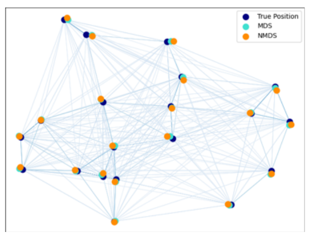
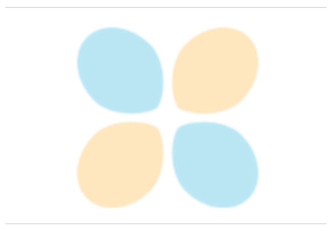
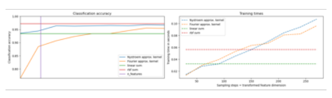
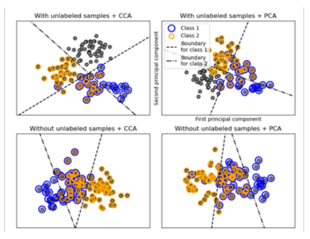

Faces recognition example using eigenfaces and SVMs

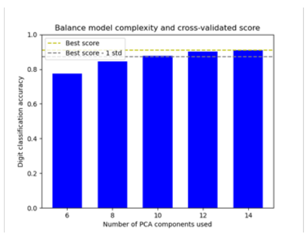
Image denoising using kernel PCA

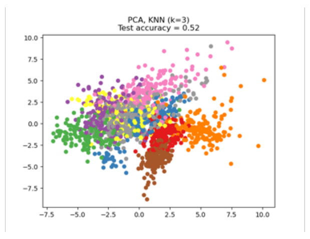

Multi-dimensional scaling


Displaying Pipelines

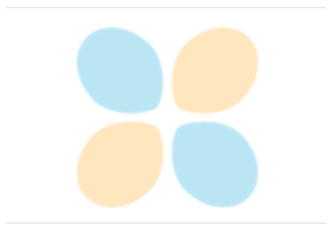

Explicit feature map approximation for RBF kernels

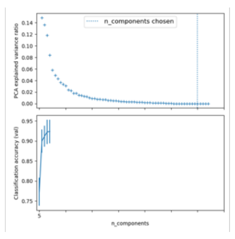

Multilabel classification

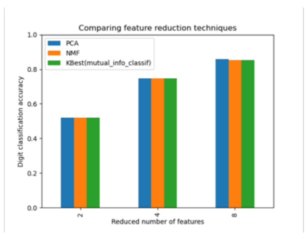

Balance model complexity and cross-validated score


Dimensionality Reduction with Neighborhood Components Analysis

Kernel Density Estimation


Concatenating multiple feature extraction methods


Pipelining: chaining a PCA and a logistic regression


Selecting dimensionality reduction with Pipeline and GridSearchCV

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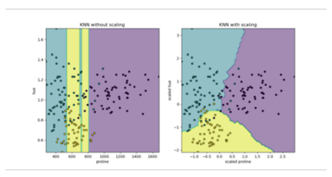

Importance of Feature Scaling

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