Principal Component Analysis

Principal Component Analysis (PCA) is a linear dimensionality reduction technique that can be utilized for extracting information from a high-dimensional space by projecting it into a lower-dimensional sub-space. It tries to preserve the essential parts that have more variation of the data and remove the non-essential parts with fewer variation.

Dimensions are nothing but features that represent the data. For example, A 28 X 28 image has 784 picture elements (pixels) that are the dimensions or features which together represent that image.

One important thing to note about PCA is that it is an Unsupervised dimensionality reduction technique, you can cluster the similar data points based on the feature correlation between them without any supervision (or labels), and you will learn how to achieve this practically using Python in later sections of this tutorial!

One important thing to note about PCA is that it is an Unsupervised dimensionality reduction technique, you can cluster the similar data points based on the feature correlation between them without any supervision (or labels). PCA is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables (entities each of which takes on various numerical values) into a set of values of linearly uncorrelated variables called principal components. Features, Dimensions, and Variables are all referring to the same thing in this notebook.

Main usage of PCA

Data Visualization

When working on any data related problem, extensive data exploration like finding out how the variables are correlated or understanding the distribution of a few variables is crucial. Considering that there are a large number of variables or dimensions along which the data is distributed, visualization can be a challenge and almost impossible. Using dimensionality reduction, data can be projected into a lower dimension, thereby allowing you to visualize the data in a 2D or 3D space.

Speeding Machine Learning Algorithm

Since PCA's main idea is dimensionality reduction, you can leverage that to speed up your machine learning algorithm's training and testing time considering your data has a lot of features, and the ML algorithm's learning is too slow.

Principal Component

Principal components are the key to PCA; they represent what's underneath the hood of your data. In a layman term, when the data is projected into a lower dimension (assume three dimensions) from a higher space, the three dimensions are nothing but the three

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Principal Components that captures (or holds) most of the variance (information) of your data.

Principal components have both direction and magnitude. The direction represents across which principal axes the data is mostly spread out or has most variance and the magnitude signifies the amount of variance that Principal Component captures of the data when projected onto that axis. The principal components are a straight line, and the first principal component holds the most variance in the data. Each subsequent principal component is orthogonal to the last and has a lesser variance. In this way, given a set of x correlated variables over y samples you achieve a set of u uncorrelated principal components over the same y samples.

The reason you achieve uncorrelated principal components from the original features is that the correlated features contribute to the same principal component, thereby reducing the original data features into uncorrelated principal components; each representing a different set of correlated features with different amounts of variation.

Each principal component represents a percentage of total variation captured from the data.

PCA on iris dataset

In this section we will decompose with PCA very simple 4-dimensional data set. This is ono eg the best known pattern recognition dataset. The data set contains 3 classes of 50 instances each, where each class refers to a type of iris plant. One class is linearly separable from the other 2; the latter are NOT linearly separable from each other.

```
In [1]: import pandas as pd
        import numpy as np
        import matplotlib.pyplot as plt
        import seaborn as sns
        from sklearn.decomposition import PCA
        from sklearn.preprocessing import StandardScaler
        # from sklearn.datasets import load boston
        #from sklearn.model selection import train test split
        from sklearn.linear_model import LinearRegression
        from sklearn.feature_selection import RFE
        #from sklearn.linear model import RidgeCV, LassoCV, Ridge, Lasso
        %matplotlib inline
In [2]: %%javascript
        IPython.OutputArea.prototype._should_scroll = function(lines) {
            return false;
In [3]: | iris_url = "https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.dat
In [4]: # Loading dataset into Pandas DataFrame
        df_iris = pd.read_csv(iris_url ,names=['sepal length','sepal width','petal length'
In [5]: df iris.head(15)
```

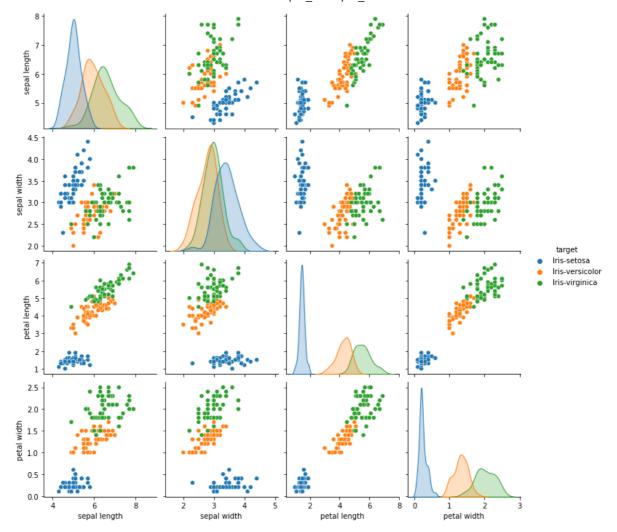
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	sepal length	sepal width	petal length	petal width	target
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa
5	5.4	3.9	1.7	0.4	Iris-setosa
6	4.6	3.4	1.4	0.3	Iris-setosa
7	5.0	3.4	1.5	0.2	Iris-setosa
8	4.4	2.9	1.4	0.2	Iris-setosa
9	4.9	3.1	1.5	0.1	Iris-setosa
10	5.4	3.7	1.5	0.2	Iris-setosa
11	4.8	3.4	1.6	0.2	Iris-setosa
12	4.8	3.0	1.4	0.1	Iris-setosa
13	4.3	3.0	1.1	0.1	Iris-setosa
14	5.8	4.0	1.2	0.2	Iris-setosa

In the case that the dimensionality of the data allows it, it is good practice to see how each pair of features correlate with each other. In the followinglink you will find more methods for visualizing multidimensional data using matplotlib and seaborn libraries https://towardsdatascience.com/the-art-of-effective-visualization-of-multi-dimensional-data-6c7202990c57

```
In [6]: sns.pairplot(df_iris, hue='target')
```

Out[6]: <seaborn.axisgrid.PairGrid at 0x2796b411730>



You can immediately see that the features petal length and petal width are strongly correlated

Standardize the Data

Since PCA yields a feature subspace that maximizes the variance along the axes, it makes sense to standardize the data, especially, if it was measured on different scales. Although, all features in the Iris dataset were measured in centimeters, let us continue with the transformation of the data onto unit scale (mean=0 and variance=1), which is a requirement for the optimal performance of many machine learning algorithms.

```
In [7]: features_iris = ['sepal length', 'sepal width', 'petal length', 'petal width']
    x_iris = df_iris.loc[:, features_iris].values

In [8]: y_iris = df_iris.loc[:,['target']].values

In [9]: x_iris = StandardScaler().fit_transform(x_iris)

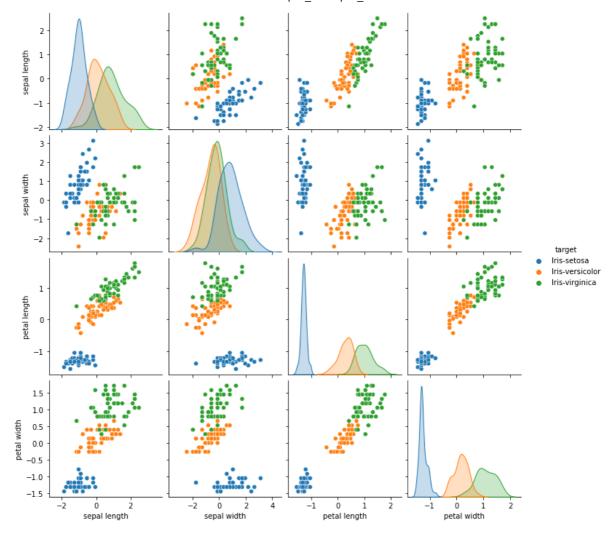
In [10]: df_iris_standarize = pd.DataFrame(data = x_iris, columns = features_iris)
    df_iris_standarize['target'] = df_iris['target']
    df_iris_standarize.head(15)
```

Out[10]:

	sepal length	sepal width	petal length	petal width	target
0	-0.900681	1.032057	-1.341272	-1.312977	Iris-setosa
1	-1.143017	-0.124958	-1.341272	-1.312977	Iris-setosa
2	-1.385353	0.337848	-1.398138	-1.312977	Iris-setosa
3	-1.506521	0.106445	-1.284407	-1.312977	Iris-setosa
4	-1.021849	1.263460	-1.341272	-1.312977	Iris-setosa
5	-0.537178	1.957669	-1.170675	-1.050031	Iris-setosa
6	-1.506521	0.800654	-1.341272	-1.181504	Iris-setosa
7	-1.021849	0.800654	-1.284407	-1.312977	Iris-setosa
8	-1.748856	-0.356361	-1.341272	-1.312977	Iris-setosa
9	-1.143017	0.106445	-1.284407	-1.444450	Iris-setosa
10	-0.537178	1.494863	-1.284407	-1.312977	Iris-setosa
11	-1.264185	0.800654	-1.227541	-1.312977	Iris-setosa
12	-1.264185	-0.124958	-1.341272	-1.444450	Iris-setosa
13	-1.870024	-0.124958	-1.511870	-1.444450	Iris-setosa
14	-0.052506	2.189072	-1.455004	-1.312977	Iris-setosa

In [11]: sns.pairplot(df_iris_standarize, hue='target')

Out[11]: <seaborn.axisgrid.PairGrid at 0x2794fadd850>



We can see that the distributions are now standardized

PCA Projection to 2D

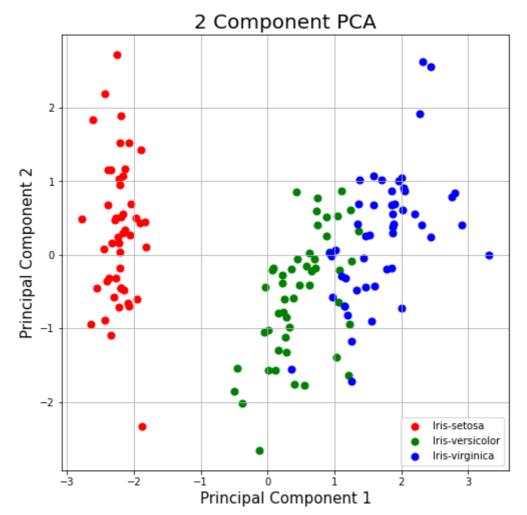
```
In [12]: pca_iris = PCA(n_components=2)
In [13]: principalComponents_iris = pca_iris.fit_transform(x_iris)
In [14]: principalDf_iris = pd.DataFrame(data = principalComponents_iris ,columns = ['princ:
In [15]: finalDf_iris = pd.concat([principalDf_iris, df_iris[['target']]], axis = 1)
    finalDf_iris.head(15)
```

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Out[15]: principal component 1 principal component 2 target -2.264542 0.505704 Iris-setosa -2.086426 1 -0.655405 Iris-setosa 2 -2.367950 -0.318477 Iris-setosa 3 -2.304197 -0.575368 Iris-setosa 4 -2.388777 0.674767 Iris-setosa 5 -2.070537 1.518549 Iris-setosa 6 -2.445711 0.074563 Iris-setosa 7 -2.233842 0.247614 Iris-setosa 8 -2.341958 -1.095146 Iris-setosa 9 -2.188676 -0.448629 Iris-setosa 10 -2.163487 1.070596 Iris-setosa 11 -2.327378 0.158587 Iris-setosa 12 -2.224083 -0.709118 Iris-setosa 13 -2.639716 -0.938282 Iris-setosa 14 -2.192292 1.889979 Iris-setosa

Visualize 2D Projection

Use a PCA projection to 2d to visualize the entire data set. You should plot different classes using different colors or shapes.



iris-setosa is linearry separablo from others class

Explained Variance

The explained variance tells us how much information (variance) can be attributed to each of the principal components.

```
In [17]: pca_iris.explained_variance_ratio_
```

Out[17]: array([0.72770452, 0.23030523])

Together, the first two principal components contain 95.80% of the information. The first principal component contains 72.77% of the variance and the second principal component contains 23.03% of the variance. The third and fourth principal component contained the rest of the variance of the dataset.

limitations of PCA

- PCA is not scale invariant. check: we need to scale our data first.
- The directions with largest variance are assumed to be of the most interest
- Only considers orthogonal transformations (rotations) of the original variables

- PCA is only based on the mean vector and covariance matrix. Some distributions (multivariate normal) are characterized by this, but some are not.
- If the variables are correlated, PCA can achieve dimension reduction. If not, PCA just orders them according to their variances.

Exercises - Perform PCA for breast cancer dataset

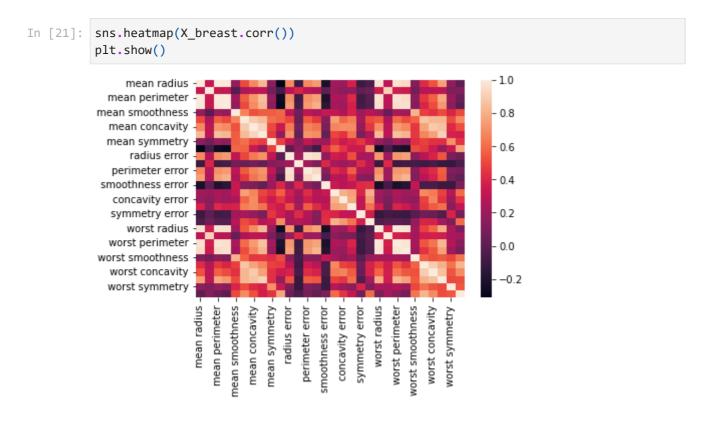
• You can find this dataset it in the scikit learn library, import it and convert to pandas dataframe, original label are '0' and '1' for better readability change these names to: 'benign' and 'malignant'

```
In [18]: from sklearn.datasets import load_breast_cancer
from sklearn.svm import SVR

In [19]: data = load_breast_cancer(as_frame=True)
    X_breast = data.data
    y_breast = data.target
    y_01 = data.target

In [20]: y_breast = np.array(['benign' if i == 0 else 'malignant' for i in y_breast])
```

• Visualizes correlations between pairs of features (due to the greater number of features use pandas corr () function instead of pairplot instead of seaborn heatmap ())

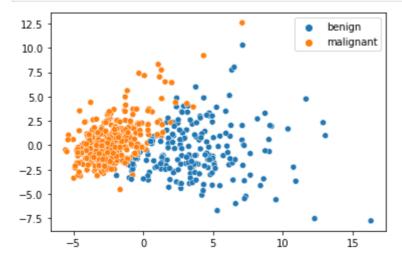


Perform PCA and visualize the data

```
In [22]: X_breast_scaled = StandardScaler().fit_transform(X_breast)
In [23]: pca_breast = PCA()
```

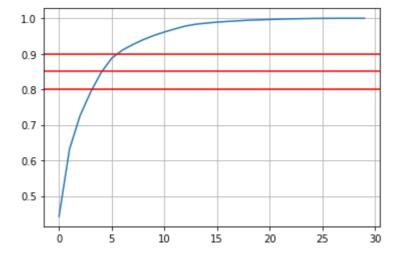
```
X_breast_pcaed = pca_breast.fit_transform(X_breast_scaled)
```

```
In [24]: sns.scatterplot(x=X_breast_pcaed[:, 0], y=X_breast_pcaed[:, 1], hue=y_breast)
plt.show()
```



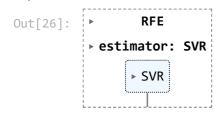
 Examine explained variance, draw a plot showing relation between total explained variance and number of principal components used

```
In [25]: plt.plot(np.cumsum(pca_breast.explained_variance_ratio_))
    plt.axhline(y=0.85, c='r')
    plt.axhline(y=0.8, c='r')
    plt.axhline(y=0.9, c='r')
    plt.grid()
    plt.show()
```

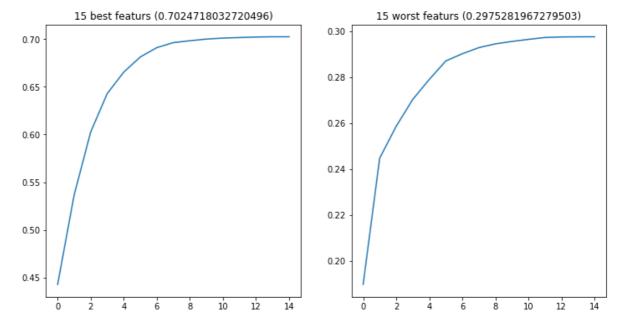


• Use recursive feature elimination (available in scikit-learn module) or another feature ranking algorithm to split 30 features to on 15 "more important" and "less important" features. Then repeat the last step from the full data set - draw a plot showing relation between total explained variance and number of principal components used for all 3 cases. Explain the result briefly.

```
In [26]: feature_selector = RFE(estimator=SVR(kernel='linear'), n_features_to_select=15)
    feature_selector.fit(X_breast_scaled, y_01)
```



```
In [27]: features_breast = X_breast.columns
         best = []
         worst = []
         for idx, cl in enumerate(feature selector.ranking ):
             if cl == 1:
                 best.append(idx)
             else:
                 worst.append(idx)
         print(best)
         print(worst)
         print(features breast)
         print(feature_selector.ranking_)
         [0, 2, 3, 5, 6, 7, 10, 13, 16, 17, 20, 23, 24, 25, 29]
         [1, 4, 8, 9, 11, 12, 14, 15, 18, 19, 21, 22, 26, 27, 28]
         Index(['mean radius', 'mean texture', 'mean perimeter', 'mean area',
                'mean smoothness', 'mean compactness', 'mean concavity',
                'mean concave points', 'mean symmetry', 'mean fractal dimension',
                'radius error', 'texture error', 'perimeter error', 'area error',
                'smoothness error', 'compactness error', 'concavity error',
                'concave points error', 'symmetry error', 'fractal dimension error',
                'worst radius', 'worst texture', 'worst perimeter', 'worst area',
                'worst smoothness', 'worst compactness', 'worst concavity',
                'worst concave points', 'worst symmetry', 'worst fractal dimension'],
               dtype='object')
         [ 1 5 1 1 13 1 1 1 15 9 1 10 3 1 6 14 1 1 2 8 1 11 4 1
           1 1 12 16 7 1]
In [28]: plt.figure(figsize=(12, 6))
         plt.subplot(1,2,1)
         plt.title(f'15 best featurs ({sum(pca_breast.explained_variance_ratio_[best])})')
         plt.plot(np.cumsum(pca breast.explained variance ratio [best]))
         plt.subplot(1,2,2)
         plt.title(f'15 worst featurs ({sum(pca_breast.explained_variance_ratio_[worst])})'
         plt.plot(np.cumsum(pca breast.explained variance ratio [worst]))
         plt.show()
```



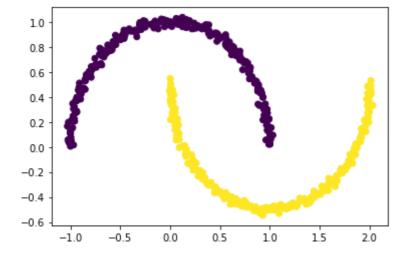
Kernel PCA

PCA is a linear method. That is it can only be applied to datasets which are linearly separable. It does an excellent job for datasets, which are linearly separable. But, if we use it to non-linear datasets, we might get a result which may not be the optimal dimensionality reduction. Kernel PCA uses a kernel function to project dataset into a higher dimensional feature space, where it is linearly separable. It is similar to the idea of Support Vector Machines.

```
import matplotlib.pyplot as plt
from sklearn.datasets import make_moons

X, y = make_moons(n_samples = 500, noise = 0.02, random_state = 417)

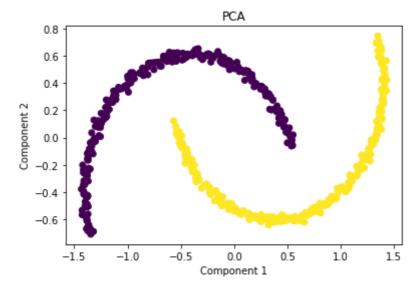
plt.scatter(X[:, 0], X[:, 1], c = y)
plt.show()
```



Let's apply PCA on this dataset

```
In [30]: pca = PCA(n_components = 2)
X_pca = pca.fit_transform(X)
```

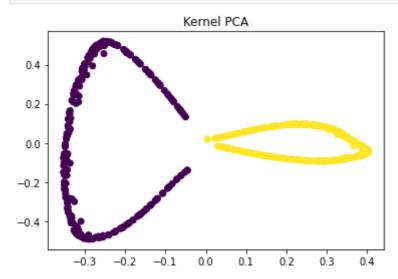
```
plt.title("PCA")
plt.scatter(X_pca[:, 0], X_pca[:, 1], c = y)
plt.xlabel("Component 1")
plt.ylabel("Component 2")
plt.show()
```



PCA failed to distinguish the two classes

```
In [31]: from sklearn.decomposition import KernelPCA
    kpca = KernelPCA(kernel = 'rbf', gamma = 15)
    X_kpca = kpca.fit_transform(X)

plt.title("Kernel PCA")
    plt.scatter(X_kpca[:, 0], X_kpca[:, 1], c = y)
    plt.show()
```

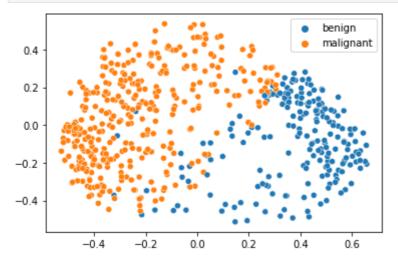


Applying kernel PCA on this dataset with RBF kernel with a gamma value of 15

KernelPCA exercises

 Visualize in 2d datasets used in this labs, experiment with the parameters of the KernelPCA method change kernel and gamma params. Docs: https://scikitlearn.org/stable/modules/generated/sklearn.decomposition.KernelPCA.html

```
In [32]: breast_kpca = KernelPCA(kernel ='rbf', gamma=0.04)
X_breast_kpcaed = breast_kpca.fit_transform(X_breast_scaled)
sns.scatterplot(x=X_breast_kpcaed[:, 0], y=X_breast_kpcaed[:, 1], hue = y_breast)
plt.show()
```



Homework

- Download the MNIST data set (there is a function to load this set in libraries such as scikit-learn, keras). It is a collection of black and white photos of handwritten digits with a resolution of 28x28 pixels. which together gives 784 dimensions.
- Try to visualize this dataset using PCA and KernelPCA, don't expect full separation of the data
- Similar to the exercises, examine explained variance. draw explained variance vs number of principal Components plot.
- Find number of principal components for 99%, 95%, 90%, and 85% of explained variance.
- Draw some sample MNIST digits and from PCA of its images transform data back to its
 original space (https://scikitlearn.org/stable/modules/generated/sklearn.decomposition.PCA.html#sklearn.decompositic
 Make an inverse transformation for number of components coresponding with
 explained variance shown above and draw the reconstructed images. The idea of this
 exercise is to see visually how depending on the number of components some
 information is lost.
- Perform the same reconstruction using KernelPCA (make comparisons for the same components number)

https://scikit-

learn.org/stable/modules/generated/sklearn.decomposition.KernelPCA.html#sklearn.decomposi

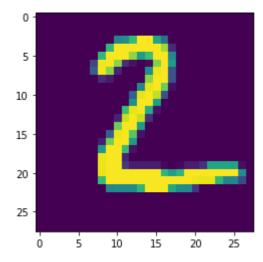


Useful links

https://scikit-learn.org https://towardsdatascience.com/introduction-to-principal-component-analysis-pca-with-python-code-69d3fcf19b57 https://towardsdatascience.com/kernel-pca-vs-pca-vs-ica-in-tensorflow-sklearn-60e17eb15a64

```
In [46]: mnist_df = pd.read_csv('https://pjreddie.com/media/files/mnist_test.csv')
In [100... mnist_data = mnist_df.values[:, 1:] mnist_target = mnist_df.values[:,0] mnist_data = mnist_data/255
In [101... plt.imshow(mnist_data[0].reshape(28, -1))
```

Out[101]: <matplotlib.image.AxesImage at 0x27907ac4400>

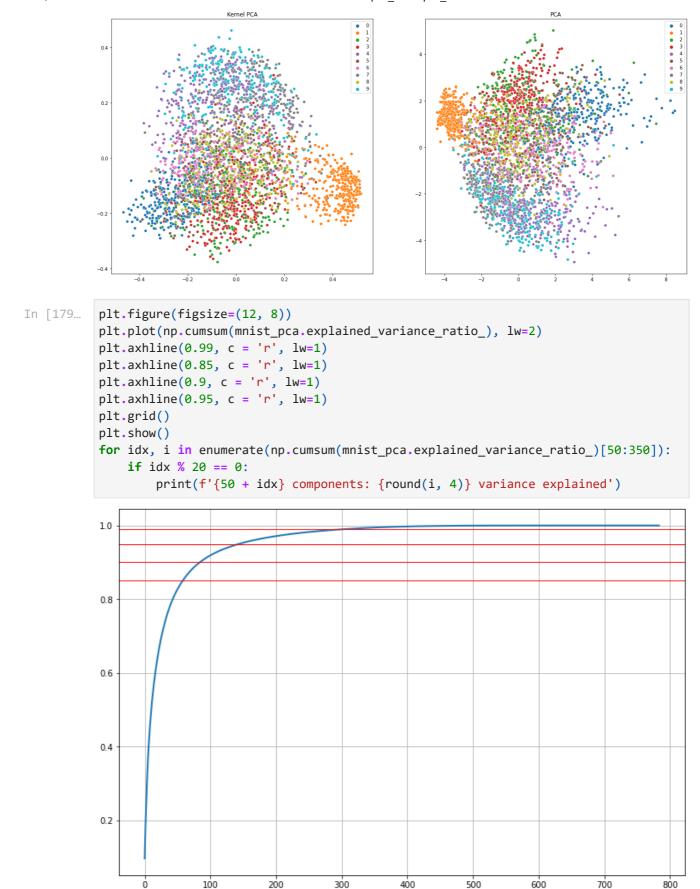


```
In [177... mnist_kpca = KernelPCA(kernel='rbf', gamma=0.01, fit_inverse_transform=True)
mnist_pca = PCA()

n = 3000

mnist_kpcaed = mnist_kpca.fit_transform(mnist_data[:n,:])
mnist_pcaed = mnist_pca.fit_transform(mnist_data[:n,:])
In [178... plt.figure(figsize=(22, 10))
nlt.subplot(1.2.1)
```

```
In [178... plt.figure(figsize=(22, 10))
    plt.subplot(1,2,1)
    plt.title('Kernel PCA')
    sns.scatterplot(x=mnist_kpcaed[:, 0], y=mnist_kpcaed[:,1], hue=mnist_target[:n], paplt.subplot(1,2,2)
    plt.title('PCA')
    sns.scatterplot(x=mnist_pcaed[:, 0], y=mnist_pcaed[:,1], hue=mnist_target[:n], pale plt.show()
```



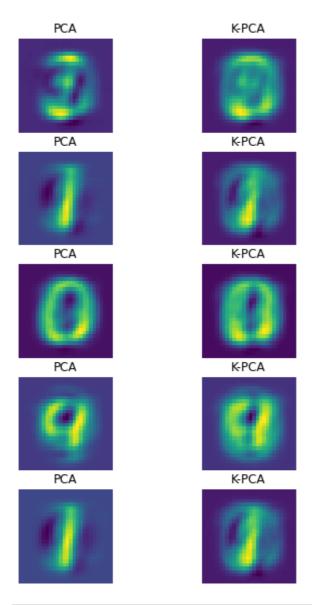
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```
50 components: 0.8273 variance explained
70 components: 0.975 variance explained
90 components: 0.908 variance explained
110 components: 0.9281 variance explained
130 components: 0.9424 variance explained
150 components: 0.9533 variance explained
170 components: 0.9617 variance explained
170 components: 0.9684 variance explained
170 components: 0.9739 variance explained
170 components: 0.9785 variance explained
170 components: 0.9823 variance explained
170 components: 0.9824 variance explained
170 components: 0.9884 variance explained
170 components: 0.9884 variance explained
170 components: 0.9884 variance explained
170 components: 0.98907 variance explained
170 components: 0.9907 variance explained
170 components: 0.9927 variance explained
```

Jestem z tych funkcji poniżej BAAARDZO dumny

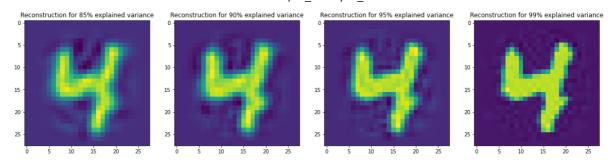
```
In [220...
         def inverse_transform_pca(model, data, n_components: int):
              # transform data
              tmp = (data - model.mean_) @ model.components_[:n_components].T
              # inverse transform
              return tmp @ model.components_[:n_components] + model.mean_
          def inverse_transform_kpca(model, data, n_components: int):
              # transform data
              K = model._centerer.transform(model._get_kernel(data, model.X_fit_))
              non zeros = np.flatnonzero(model.eigenvalues [:n components])
              scaled_alphas = np.zeros_like(model.eigenvectors_[:, :n_components])
              scaled_alphas[:, non_zeros] = model.eigenvectors_[:, non_zeros] / np.sqrt(model
              tmp = K @ scaled_alphas
              # inverse transform
              K = model._get_kernel(tmp, model.X_transformed_fit_[:, :n_components])
              return K @ model.dual_coef_
In [225...
          n comp = 3
          inv_pca = inverse_transform_pca(mnist_pca, mnist_data[:5], n_comp)
          inv kpca = inverse transform kpca(mnist kpca, mnist data[:5], n comp)
          plt.figure(figsize=(6, 10))
          plt.suptitle(f"PCA vs KPCA for {n_comp} components")
          for i in range(10):
              plt.subplot(5,2,i+1)
              plt.axis('off')
              if i % 2 == 0:
                  plt.title("PCA")
                  plt.imshow(inv_pca[i//2].reshape(28, 28))
              else:
                  plt.title("K-PCA")
                  plt.imshow(inv_kpca[i//2].reshape(28, 28))
```

PCA vs KPCA for 3 components



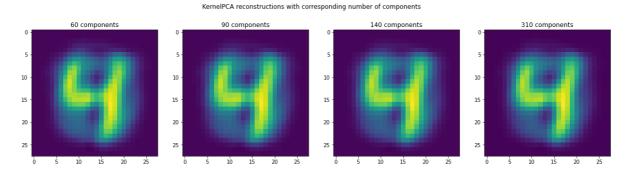
```
In [243... k = 84
    plt.figure(figsize=(20, 5))
    plt.subplot(1, 4, 1)
    plt.title('Reconstruction for 85% explained variance')
    plt.imshow(inverse_transform_pca(mnist_pca, mnist_data[k], 60).reshape(28, 28))
    plt.subplot(1, 4, 2)
    plt.title('Reconstruction for 90% explained variance')
    plt.imshow(inverse_transform_pca(mnist_pca, mnist_data[k], 90).reshape(28, 28))
    plt.subplot(1, 4, 3)
    plt.title('Reconstruction for 95% explained variance')
    plt.imshow(inverse_transform_pca(mnist_pca, mnist_data[k], 140).reshape(28, 28))
    plt.subplot(1, 4, 4)
    plt.title('Reconstruction for 99% explained variance')
    plt.imshow(inverse_transform_pca(mnist_pca, mnist_data[k], 310).reshape(28, 28))
```

Out[243]: <matplotlib.image.AxesImage at 0x279071b2fa0>



```
plt.figure(figsize=(20, 5))
  plt.suptitle('KernelPCA reconstructions with corresponding number of components')
  plt.subplot(1, 4, 1)
  plt.title('60 components')
  plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 60).res
  plt.subplot(1, 4, 2)
  plt.title('90 components')
  plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 90).res
  plt.subplot(1, 4, 3)
  plt.title('140 components')
  plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 140).res
  plt.subplot(1, 4, 4)
  plt.title('310 components')
  plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 310).res
  plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 310).res
```

Out[254]: <matplotlib.image.AxesImage at 0x27909008160>



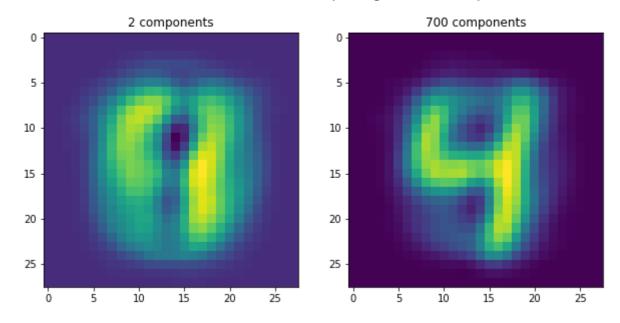
Niby wyglądają wszystkie tak samo ale poniżej widać dla innych komponentów, że działa to poprawnie

```
In [256... plt.figure(figsize=(10, 5))
    plt.suptitle('KernelPCA reconstructions with corresponding number of components')
    plt.subplot(1, 2, 1)
    plt.title('2 components')
    plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 2).resh
    plt.subplot(1, 2, 2)
    plt.title('700 components')
    plt.imshow(inverse_transform_kpca(mnist_kpca, mnist_data[k].reshape(1, -1), 700).reshape(1, -1), 700).reshape(1, -1)
```

Out[256]: <matplotlib.image.AxesImage at 0x27906dd4130>

18.03.2023, 11:21 pca_kernelpca_lab

KernelPCA reconstructions with corresponding number of components



In []: