Machine Learning
Lab 8

Principal Component Analysis

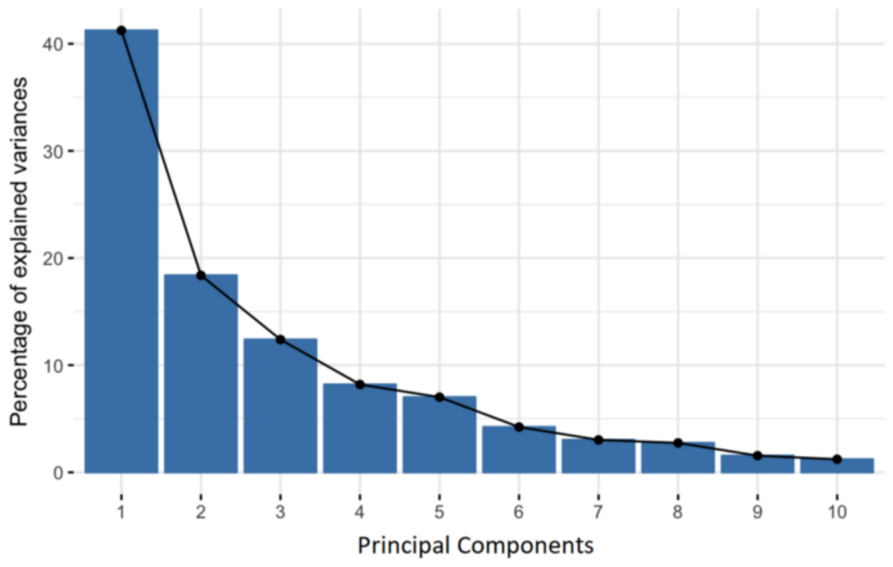
Principal component analysis, or PCA, is a dimensionality-reduction method that is often used to reduce the dimensionality of large data sets, by transforming a large set of variables into a smaller one that still contains most of the information in the large set.

Reducing the number of variables of a data set naturally comes at the expense of accuracy, but the trick in dimensionality reduction is to trade a little accuracy for simplicity. Because smaller data sets are easier to explore and visualize and make analysing data much easier and faster for machine learning algorithms without extraneous variables to process.

So, to sum up, the idea of PCA is simple — **reduce the number of variables of a data set, while preserving as much information as possible.**

Principal components

Principal components are new variables that are constructed as linear combinations or mixtures of the initial variables. These combinations are done in such a way that the new variables (i.e., principal components) are uncorrelated and most of the information within the initial variables is squeezed or compressed into the first components. So, the idea is 10-dimensional data gives you 10 principal components, but PCA tries to put maximum possible information in the first component, then maximum remaining information in the second and so on, until having something like shown in the scree plot below.



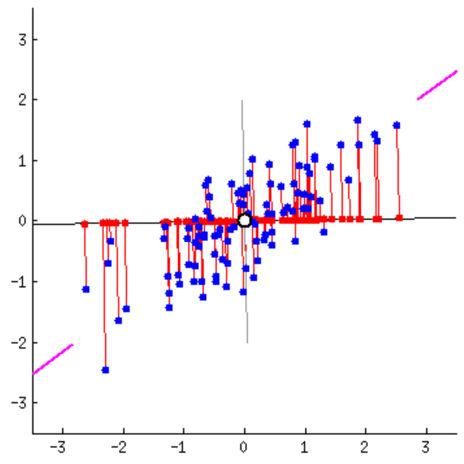
Organizing information in principal components this way, will allow you to reduce dimensionality without losing much information, and this by discarding the components with low information and considering the remaining components as your new variables.

An important thing to realize here is that the principal components are less interpretable and don't have any real meaning since they are constructed as linear combinations of the initial variables.

Geometrically speaking, principal components represent the directions of the data that explain a **maximal amount of variance**, that is to say, the lines that capture most information of the data. The relationship between variance and information here, is that, the larger the variance carried by a line, the larger the dispersion of the data points along it, and the larger the dispersion along a line, the more information it has. To put all this simply, just think of principal components as new axes that provide the best angle to see and evaluate the data, so that the differences between the observations are better visible.

How PCA Constructs the Principal Components

As there are as many principal components as there are variables in the data, principal components are constructed in such a manner that the first principal component accounts for the **largest possible variance** in the data set. For example, let's assume that the scatter plot of our data set is as shown below, can we guess the first principal component ? Yes, it's approximately the line that matches the purple marks because it goes through the origin and it's the line in which the projection of the points (red dots) is the most spread out. Or mathematically speaking, it's the line that maximizes the variance (the average of the squared distances from the projected points (red dots) to the origin).



The second principal component is calculated in the same way, with the condition that it is uncorrelated with (i.e., perpendicular to) the first principal component and that it accounts for the next highest variance.

This continues until a total of p principal components have been calculated, equal to the original number of variables.

HOW DO YOU DO A PRINCIPAL COMPONENT ANALYSIS?

1. Standardize the range of continuous initial variables.
2. Compute the covariance matrix to identify correlations.
3. Compute the eigenvectors and eigenvalues of the covariance matrix to identify the principal components.
4. Create a feature vector to decide which principal components to keep.
5. Recast the data along the principal components axes.

Python Implementation

PCA is a dimensionality reduction technique; it lets you distil multi-dimensional data down to fewer dimensions, selecting new dimensions that preserve variance in the data as best it can.

We're not talking about Star Trek stuff here; let's make it real - a black & white image for example, contains three dimensions of data: X position, Y position, and brightness at each point. Distilling that down to two dimensions can be useful for things like image compression and facial recognition, because it distils out the information that contributes most to the variance in the data set.

Let's do this with a simpler example: the Iris data set that comes with scikit-learn. It's just a small collection of data that has four dimensions of data for three different kinds of Iris flowers: The length and width of both the petals and sepals of many individual flowers from each species. Let's load it up and have a look:

```
from sklearn.datasets import load_iris
from sklearn.decomposition import PCA
import pylab as pl
from itertools import cycle

iris = load_iris()

numSamples, numFeatures = iris.data.shape
print(numSamples)
print(numFeatures)
print(list(iris.target_names))
```

So, this tells us our data set has 150 samples (individual flowers) in it. It has 4 dimensions - called features here, and three distinct Iris species that each flower is classified into.

While we can visualize 2 or even 3 dimensions of data pretty easily, visualizing 4D data isn't something our brains can do. So let's distil this down to 2 dimensions, and see how well it works:

```
X = iris.data
pca = PCA(n_components=2, whiten=True).fit(X)
X_pca = pca.transform(X)
```

What we have done is distil our 4D data set down to 2D, by projecting it down to two orthogonal 4D vectors that make up the basis of our new 2D projection. We can see what those 4D vectors are, although it's not something you can really wrap your head around:

```
print(pca.components_)
```

Let's see how much information we've managed to preserve:

```
print(pca.explained_variance_ratio_)
print(sum(pca.explained_variance_ratio_))
```

That's pretty cool. Although we have thrown away two of our four dimensions, PCA has chosen the remaining two dimensions well enough that we've captured 92% of the variance in our data in a single dimension alone! The second dimension just gives us an additional 5%; altogether we've only really lost less than 3% of the variance in our data by projecting it down to two dimensions.

As promised, now that we have a 2D representation of our data, we can plot it:

```
%matplotlib inline
from pylab import *

colors = cycle('rgb')
target_ids = range(len(iris.target_names))
pl.figure()
for i, c, label in zip(target_ids, colors, iris.target_names):
    pl.scatter(X_pca[iris.target == i, 0], X_pca[iris.target == i, 1],
        c=c, label=label)
pl.legend()
pl.show()
```

You can see the three different types of Irises are still clustered pretty well. If you think about it, this probably works well because the overall size of an individual flower probably makes both the petal and sepal sizes increase by a similar amount. Although the actual numbers on this graph have no intuitive meaning, what we're probably seeing is measure of the ratio of width to height for petals and sepals - and PCA distilled our data down to that on its own.

Activity

- Our results suggest we could distil this data down to a single dimension and still preserve most of its variance. Try it! Do a PCA down to one component and measure the results.

- Think of whether PCA can be applied to the previous regression and classification problems.