Machine Learning

Module 8.2 - Unsupervised Learning: Dimension Reduction

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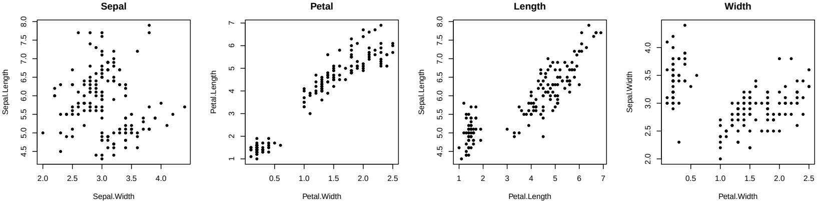
Concept

For unsupervised learning, **data representation and simplification** is an important task. A natural objective is to represent the data on a graph: simplify p features to 2 dimensions and plot on x- and y-axes.

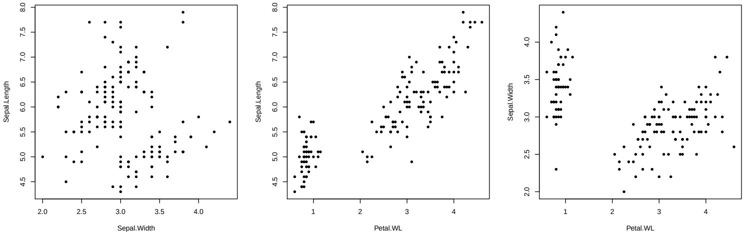
Example: `iris` data has 4 features (species not used). The data cannot be represented on a single graph.



Concept

Observation: `Petal.Length` and `Petal.Width` are highly correlated: if we know one, we can predict the other one.

To simplify the representation, we do not need these two features: replace them by their average `Petal.WL = (Petal.W+Petal.L)/2`:



Same observation for `Petal.WL` and `Sepal.Length`...

Concept

In summary, two correlated features can be replaced by one combination without keeping the information.

The resulting representation shows as much variance as possible: theinformation is kept.

This is the principle of **Principal Component Analysis** (PCA).

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PCA

The PCA is a method that looks for dimensions that are linear combinations of the p features:

$$a_1 x_1 + a_2 x_2 + \cdots + a_p x_p.$$

These linear combinations are called the principal components. There are p principal components.

PCA: the first component

To find the first component (i.e. coefficients a), one should maximize the variance along it. That is, a should be the solution to

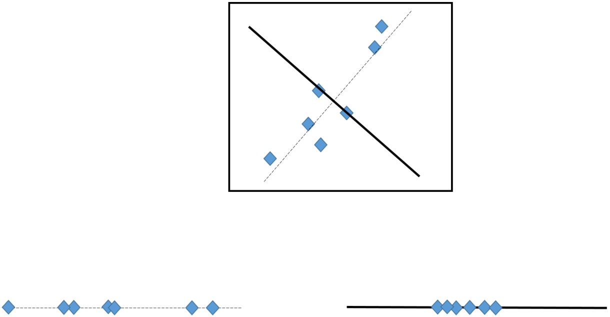
$$\begin{aligned} \max_{a} \quad & Var(a_1 x_1 + \cdots + a_p x_p) \\ s.t. \quad & \sum_j a_j^2 = 1 \end{aligned}$$

where the variance is computed on the data set.

The constraint on a is here because a is only indicating a direction and should therefore be scaled to 1.

PCA: the first component

As an example, let's look at a toy case where we only have 2 features x_1 and x_2 showed below. We want to represent the data in one dimension, that is, along a line (dimension reduction). The dashed line shows more variability of the data and is a better principal component than the solid line.



PCA: the first component

When extended to $p \geq 2$ features, the principle remains the same. For a choice of a with $\sum a_j^2 = 1$,

- $z_i = a_1 x_{i1} + \cdots + a_p x_{ip}$ are computed on the data set $(i = 1, \ldots, n)$,
- the variance of the z_i is computed.

Then this variance is maximized by changing a. The maximum value gives $a^{(1)}$, the first principle component.

PCA: the second component, and third, etc.

The second component $a^{(2)}$ is obtained with the same principle and the extra constraint to be orthogonal to the first one:

$$\sum_{j=1}^{p} a_j^{(1)} a_j^{(2)} = 0.$$

The procedure is repeated until p principal components are found (each one is orthogonal to all the previous ones).

Note: the result can be easily obtained by computing the **spectral decomposition** of the variance matrix of the data.

PCA: scaling

Before computing the PCA, the data can be standardized. Like any standardization, this is a choice of the user, which depends strongly on the application and on the scale (units) of the data.

When the data are first standardized, the **spectral decomposition** is made on the correlation matrix of the data.

PCA: projection

For each PC j, we have the corresponding projections of the data x_i

$$z_i^{(j)} = a_1^{(j)} x_{i1} + \cdots + a_p^{(j)} x_{ip}.$$

We thus have a new data set z whose column are the projection of the features x on the PCA's. These new features $z_1, \ldots, z_p$ can be used

- for data representation (dimension reduction),
- to describe the dependence between the features (factor analysis).

PCA: variance proportion

By construction, the first principal component z_1 has larger variance than z_2 and so on. Also, by construction, the total of the variance is preserved:

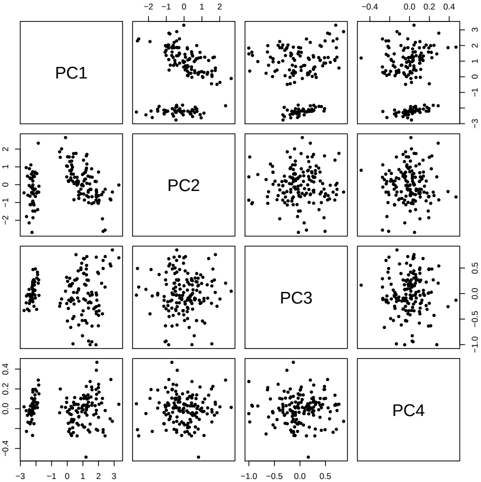
$$\sum_{j=1}^{p} var(x_j) = \sum_{j=1}^{p} var(z_j).$$

The proportion of the total variance explained by the PC z_j is thus

$$var(z_j) / \sum_{j'=1}^{p} var(z_{j'}).$$

It represents how well the data are represented on the component z_j.

PCA: example


PC1
PC2
PC3
PC4
−2 −1 0 1 2
−0.4 0.0 0.2 0.4
3 2 1 0 −1 −3
2 1 0 −1 −2
0.5 0.0 −0.5 −1.0
0.4 0.2 0.0 −0.4
−3 −1 0 1 2 3
−1.0 −0.5 0.0 0.5

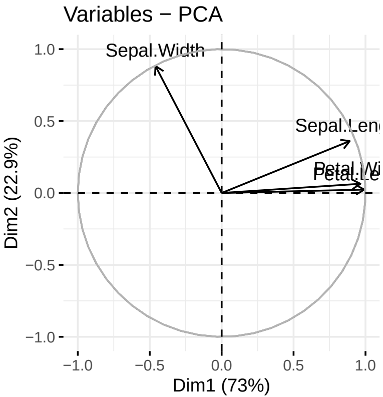
PCA: example

```
> iris.pca <- PCA(iris[,-5], graph=FALSE)
> summary(iris.pca)

Call:
PCA(X = iris[, -5], graph = FALSE)


Eigenvalues
                       Dim.1   Dim.2   Dim.3   Dim.4
Variance               2.918   0.914   0.147   0.021
% of var.             72.962  22.851   3.669   0.518
Cumulative % of var.  72.962  95.813  99.482 100.000
```

Together, PC1 and PC2 explain 95.8% of the variation of the data. The scatter plot matrix shows that it is a good representation of the data with only two dimensions (PC_1, PC_2).

PCA: the circle of correlations

Correlation between the PC and the features x can be computed to see how is PC is correlated to each features.



PCA: the circle of correlations

We see that

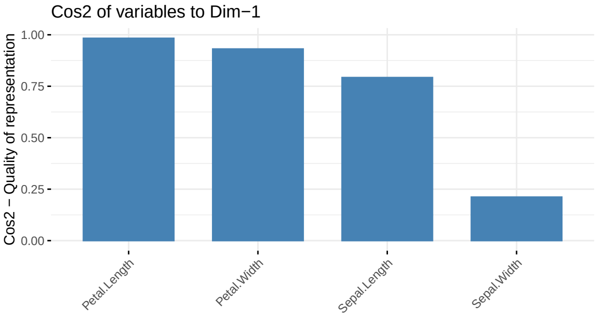
- PC_1 is positively and strongly correlated with petal length, petal width, and sepal length. This component summarizes these 3 features: the larger PC_1, the larger these 3 features.
- PC_2 is (negatively) correlated with sepal width. The larger PC_2 the smaller this feature.
- PC_1 explains 73% of the total data variation. PC_2 explains 23% of it.

With one graph, we know

- which features are correlated/independent
- how to summarize the data into two dimensions.

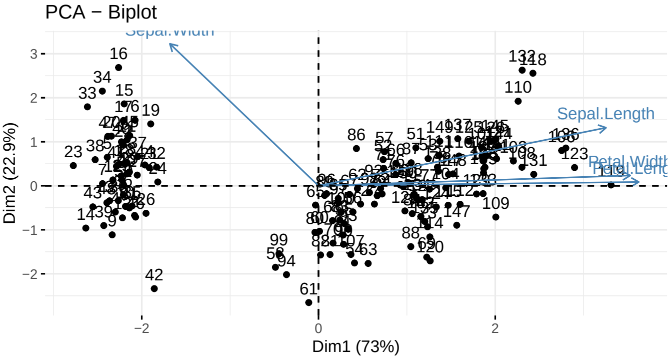
PCA: the cos^2

The circle of correlations relates the dimensions and the features. Another view is the cos^2 graph. It is interpreted as the quality of the representation of the feature by the dimension. Of course this is intimately related to the correlations.



PCA: the biplot

The **biplot** shows a **map of the individuals** in the dimensions and adds the circle of correlations.



PCA: the biplot

For example, we can conclude that

- instance 61 has a sepal width smaller than the average (large PC_2) and an average PC_1 (which indicates an average petal length, width and sepal length).
- instance 119 has an average sepal width but a large PC_1, i.e. petal length and width and sepal length.
- Two clusters can be observed and are well separated by PC_1 (in fact these clusters correspond to species here).

PCA: number of components

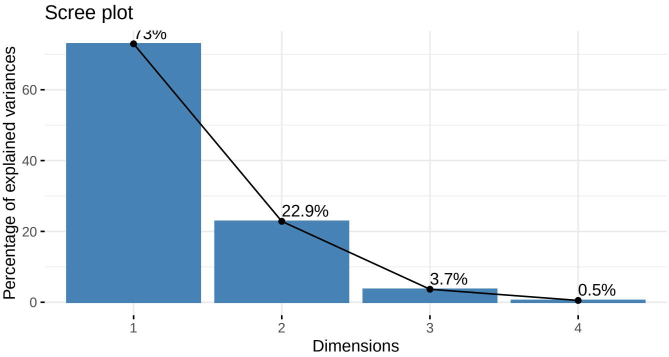
Here, two components explain more than 95% of the data variability. Sometimes, more components are needed.

One way to set the number of components is to target the proportion of explained variance: often between 75% and 95%.

If the features are independent, this number is likely to be large. If the features are correlated, this number will be smaller.

The **screeplot** may help.

PCA: the screeplot



PCA and machine learning

In the context of machine learning, PCA is often used

- To inspect the data, find/explain clusters, find dependence between the features. **PCA** can be used for **EDA**.
- To diminish the number of features when there are too many: dimension reduction $=>$ only keep few first PC.

Categorical data

PCA can only be performed on **numerical features**. When categorical features are also included in the analysis,

- for ordinal data, quick and dirty solution: modalities can be mapped to numbers $(1, 2, \ldots)$ respecting their order,
- for nominal data: there is no correct solution; especially replacing by numbers is **incorrect**.

With only categorical data, **(Multiple) Correspondence Analysis** is a solution. And for mixed data type (categorical and numerical), **Factor Analysis of Mixed Data** (FAMD) is a solution. However, they are not adapted to large data set.

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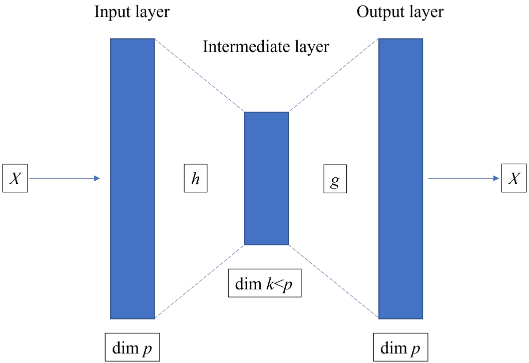
Principle

PCA is a "linear" technique, based on the explanation of the correlation between the features. Auto-encoder are neural network. The idea is to train a model that recovers an instance with an intermediate layer of lower dimension than the number of features.



encoder + decoder = autoencoder

- The input and the output (response) are the same instance (X), of dimension p.
- The intermediate layer (at least one) is of dimension $k < p$.
- The model is trained to recover X ate the end.

If, after traning, the model can recover X from X, then it can recover X from its image in the intermediate layer $h(X)$. Thus, only p dimensions would be needed to recover X.

Thus,

- the left part of the NN **encodes** X in its lower-dimension version $h(X)$
- the right part of the NN **decodes** $h(X)$ in an output $g(h(X))$, hopefully close to the original image X.

The better this final image the better the encoding/decoding:

$$g(h(X)) \overset{?}{\approx} X.$$

Autoencoder vs PCA

In ML, often autoencoder are used to

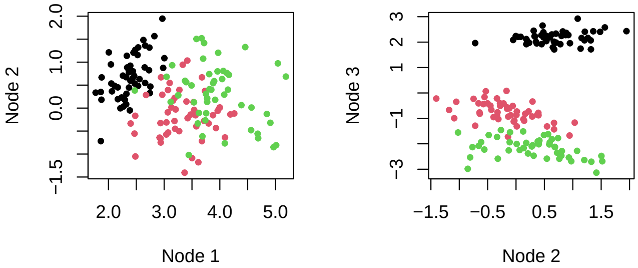
- Reduce the noise in the data (smoothing)
- Reduce the memory needed (compressing)
- Represent the data (dimension reduction)

Unlike PCA, autoencoder do not provide interpretation of the dimensions, which dimension is the most important, etc.

On the other hand, autoencoders can produce better final representation of the data: the recovery of X with k components is better than with PCA.

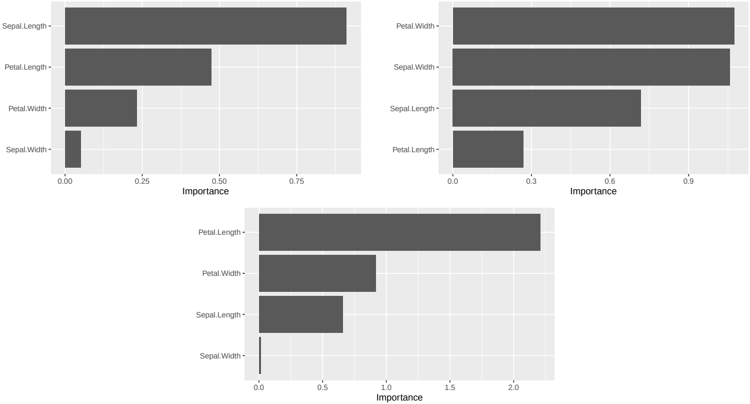
Interpretability

Like PCA make two-dimensional plots to discover pattern. Below, autoencoder (see example file) with 3-node intermediate-layer:



Interpretability

Relate each component of $h(X)$ to each component of X using variable importance (or another technique). Below, Node 1 to 3 (left to right; top to bottom).


Sepal.Length
Petal.Length
Petal.Width
Sepal.Width
Importance
Petal.Width
Sepal.Width
Sepal.Length
Petal.Length
Importance
Petal.Length
Petal.Width
Sepal.Length
Sepal.Width
Importance