MACHINE LEARNING

MEI/1

University of Beira Interior,
Department of Informatics

Hugo Pedro Proença,
hugomcp@di.ubi.pt, 2023/2024

Machine Learning

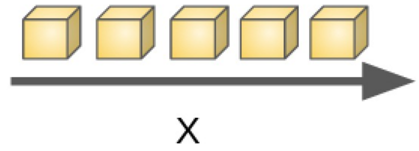
[05]

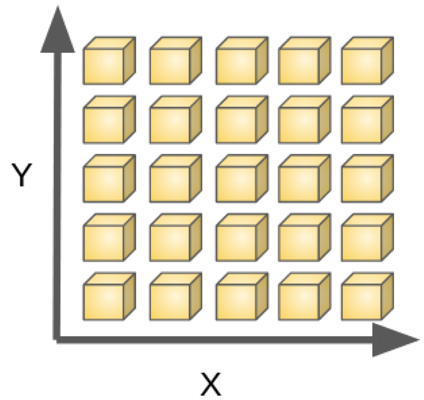
Syllabus

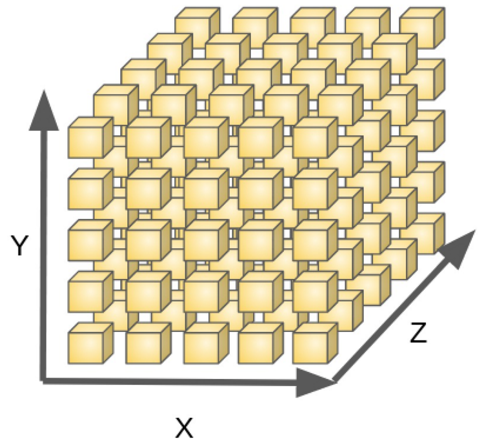
- Feature Representation
- Dimensionality Reduction
- PCA
  - Eigenvectors and Eigenvalues

Dimensionality Reduction

- The **curse of dimensionality** is one of the most classical phenomena in the development of Machine Learning systems.
  - In short, when the dimensionality increases, the volume of the space increases so fast that the data become sparse.
  - Sparsity is problematic for any method that requires statistical significance, i.e., densely populated spaces.
- For example, consider 100 evenly spaced sample points (instances) inside a unit interval.
  - On average, points will be separated around 10^{-2}=0.01
- An equivalent sampling that will yield similar density in a 10-dimensional unit hypercube would require $10^{20}[=(10^2)^{10}]$ sample points

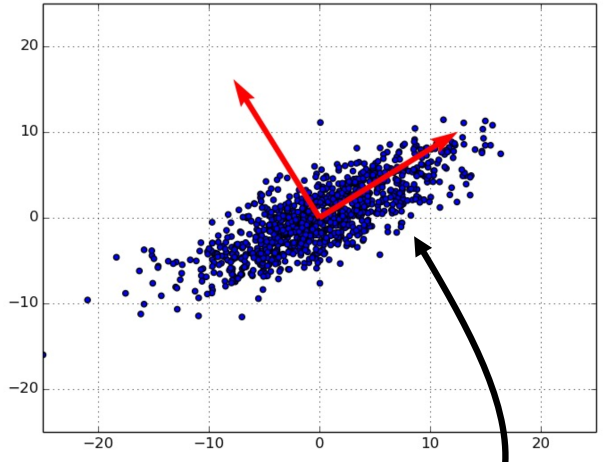






Dimensionality Reduction

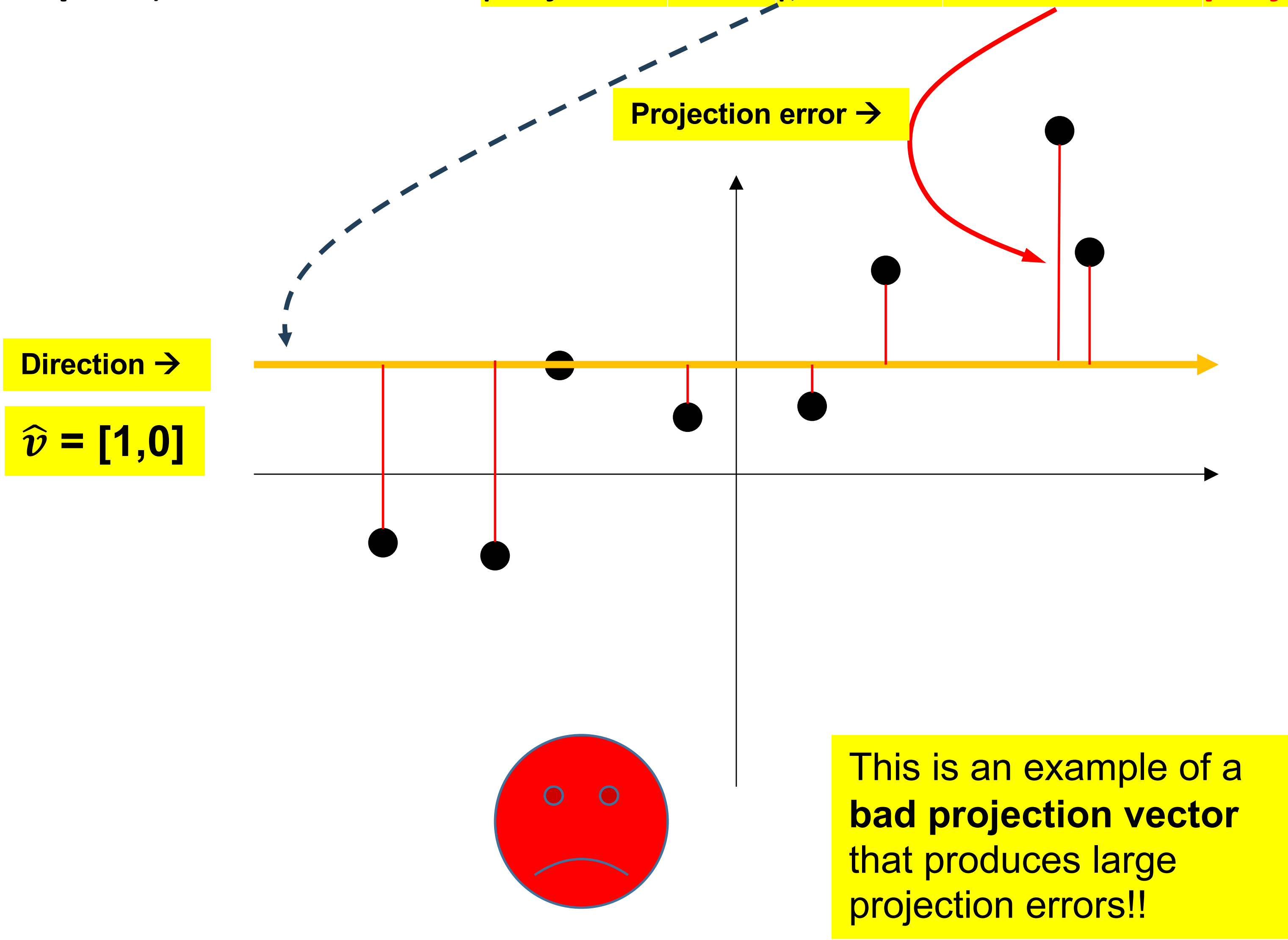
- In statistics, machine learning, and information theory, dimensionality reduction is the process of reducing the number of random variables under consideration by obtaining a set of principal variables.
- In general, there are two families of methods to reduce the dimensionality of a data set:
  - **Feature Selection.** The idea is to find a subset of the original features that better represent the problem, i.e., that minimally decrease the amount of available information, when compared to the original dataset.
    - Most approaches are based in filters (based in information gain), wrappers (based in accuracy) and embedded (features iteratively selected/removed according to prediction errors)
  - **Feature Extraction.** It is often also designated as "**Feature Projection**" and the idea is to transform the original feature space into a space of fewer dimensions, while keeping as much of the original information as we can.
    - **Principal Component Analysis** (**PCA**) is the main technique in this family.



The key idea is to find the direction(s) (vector(s)) onto which data maximally **span**

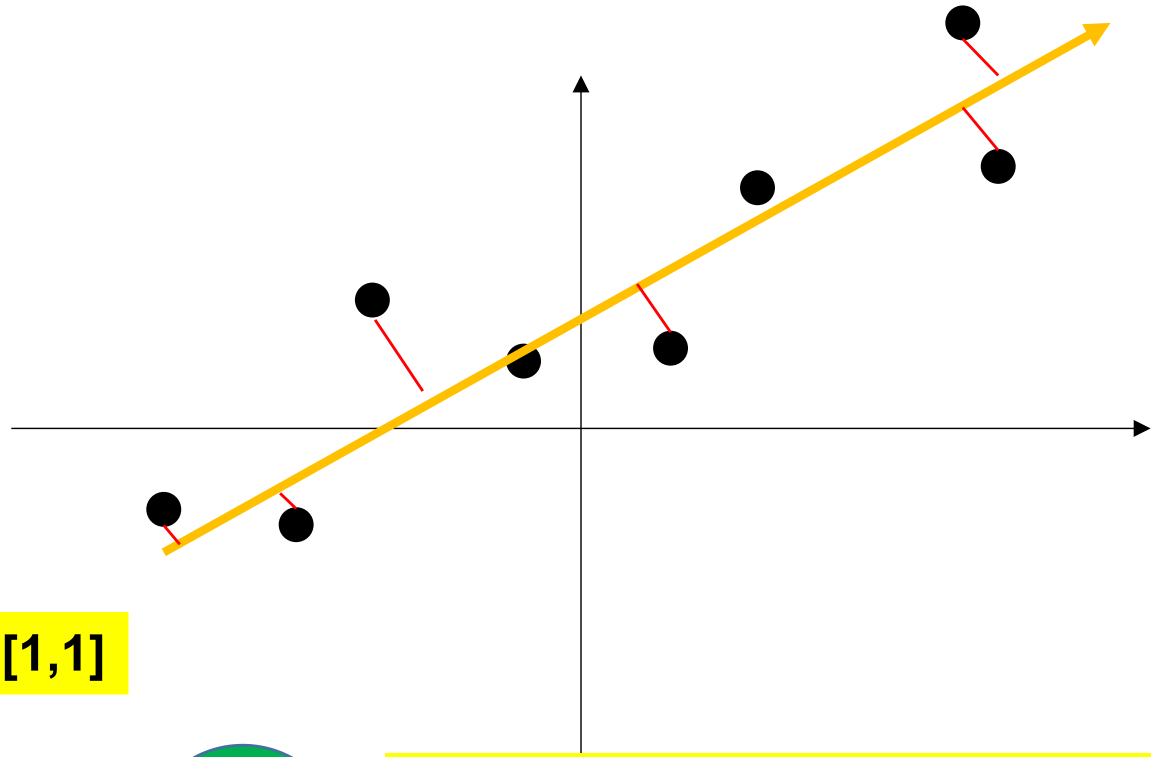
PCA

- Graphically, we are interested in finding the **direction** (**vector in the original space**) onto which the projected data provides the **minimal projection error**:



PCA

- Graphically, we are interested in finding the **direction** (**vector in the original space**) onto which the projected data have **minimal projection error**:

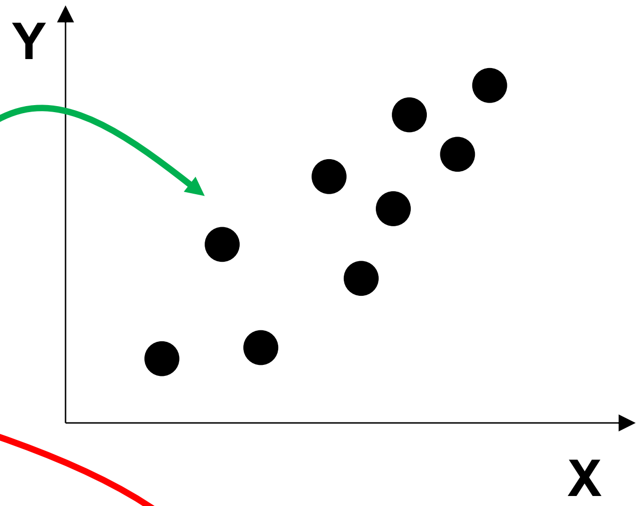


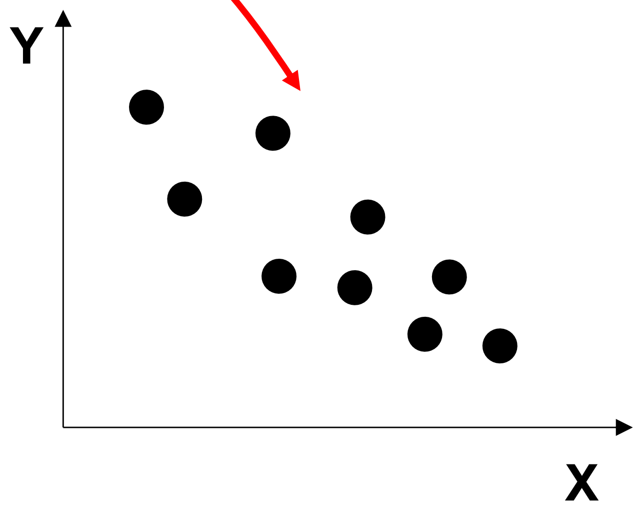
$\hat{v}$ **= [1,1]**

Example of a much better projection vector that produces smaller projection errors

PCA: Covariance

- The **covariance** can be obtained for any two dimensions (features) of a n-dimensional feature space
- It is a measure of the **joint variability** of two features
  - If both variables **vary** in a **direct** way, the covariance is **positive**
  - On the contrary, if both variables **vary inversely**, the variance values will be **negative**.
- The sign of the covariance shows the tendency in the linear relationship between the variables.
- The magnitude of the covariance is not easy to interpret because it is not normalized and hence depends on the magnitudes of the variables.
- The normalized version of the covariance, the correlation coefficient, however, shows by its magnitude the strength of the linear relation.





PCA: Covariance

- The distance between sample points and their mean is multiplied. Then, the result is divided by the number of data points minus 1:

$$cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i \; - X^{\;*})(Yi \; - Y^{\;*})}{n-1}$$

where X_i, Y_i are the ith data points, X^*, Y^* are the sample means and “n” is the number of data points.

- The results is meaningful essentially by analysing it’s sign:
  - Positive: Both dimensions **vary directly**.
  - Negative: Both dimensions **vary inversely.**
  - Zero: Dimensions are **independent**.

PCA: Covariance Matrix

- The **Covariance Matrix C** contains all covariance pair values between every possible dimensions of a feature space :

$$\boldsymbol{C} = [\, cij \mid cij = cov(Xi, Xj)]$$

- For exemple, considering a three dimensional space {X, Y, Z}, the covariance matrix will correspond to:

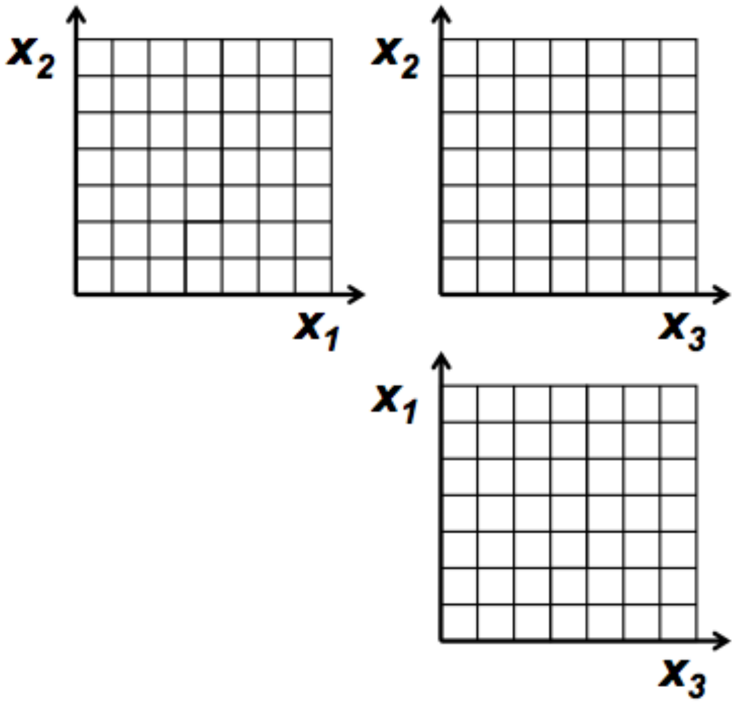
$$\begin{bmatrix} cov(X,X) & cov(X,Y) & cov(X,Z) \\ cov(Y,X) & cov(Y,Y) & cov(Y,Z) \\ cov(Z,X) & cov(Z,Y) & cov(Z,Z) \end{bmatrix}$$

- Values along the main diagonal describe the **variance** of the corresponding dimension.
- Based on its definition, it is obvious that *cov(X,Y)=cov(Y,X),* i.e., the covariance matrix is symetric with respect to its main diagonal.

PCA: Covariance Matrix

- **Exercise**. Obtain the covariance matrix for the given data set:

Obs.	X1	X2	X3
1	2	2	4
2	3	4	6
3	5	4	2
4	6	6	4



	x_1	x_2	x_3	$x_1-\mu_1$	$x_2-\mu_2$	$x_3-\mu_3$	$(x_1-\mu_1)^2$	$(x_2-\mu_2)^2$	$(x_3-\mu_3)^2$	$(x_1-\mu_1)(x_2-\mu_2)$	$(x_1-\mu_1)(x_3-\mu_3)$	$(x_2-\mu_2)(x_3-\mu_3)$
1												
2												
3												
4												

Eigenvectors and eigenvalues

- Consider the multiplication of a **matrix** by a **vector**:

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 11 \\ 5 \end{pmatrix}$$

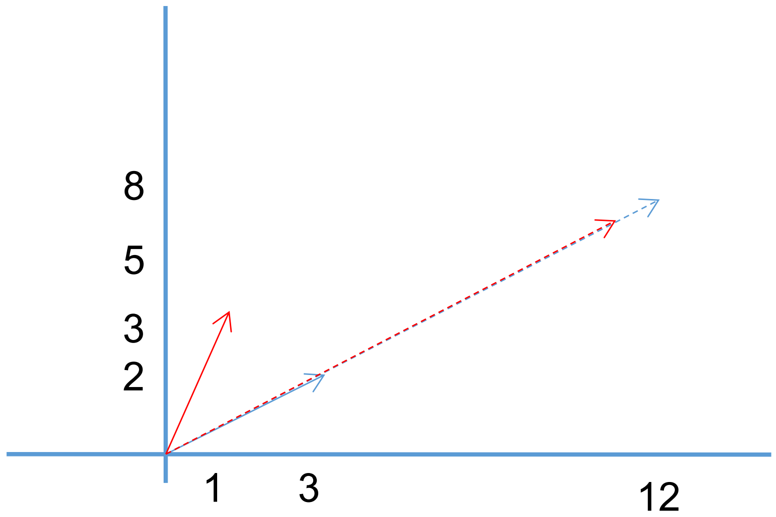
- However, there are some particularly interesting **vectors**:

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \begin{pmatrix} 3 \\ 2 \end{pmatrix}$$

- In the first case, the resulting vector is not a multiple of the original vector.
- Oppositelly, in the second case, the resulting vector (12,8) is a multiple of the multiplier.
- As such, the latter is an **eigenvector**.
  - The correspondong **eigenvalue** is “4”

Eigenvectors and eigenvalues

- By analysing the direction of the original and resultant vectors:



- Considering the matrix as a **transformation**, it can be concluded that in the second case, the direction was not changed. **This is the key insight the notion of eigenvector.**
  - The given matrix does not change the direction of its eigenvectors.

Eigenvectors and eigenvalues

- As we’ve seen, the notion of **eigenvalue** is strongly related to the **eigenvector**.
  - It is the value that should by multiplied by the eigenvector to obtain the original vector.
  - In the above example, 4 was the eigenvalue that corresponds to the given eigenvector.
- As such, eigenvalues and eigenvectors come in pairs and are always inter-related.

Eigenvectors and eigenvalues

- As a summary, the eigenvectors of a matrix correspond to the directions that are not changed by the (transformation) matrix.
- Not all matrices have eigenvectors.
- Matrices have to be square.
- A (n x n) matrix has – at most – "n" eigenvectors.
- The set of eigenvectors of a matrix (image) is widely used to describe the spatial content of that image (feature).
- In MATLAB, this eigenanalysis is made by the "eig()" function:
  - [**V**,**D**] = eig(**A**)
  - Returns the eigenvectors (D) and corresponding eigenvalues (V) of matrix A.
- In Python, this can simply be done by:
  - **V**, **D** = LA.eig(**A**)

Eigenvectors and eigenvalues

- There is an important property to be stressed: **the eigenvectors of a matrix are orthogonal**. This is to say that they form an orthogonal basis of the matrix.
  - We are able to express every point of a data set by linear combinations of its basis-vectors.
  - **This is specially usefull for the analysis of principal components (PCA).**
  - It is usual to determine the eigenvectors/eigenvalues in their normalized version, i.e., with length normalized to 1.
  - As previously seen, the length of a vector does not affect its property of being (or not) an eigenvector.
  - Hence, having an eigenvector (x_1, ..., x_n) it is usual to divide each component by the norm of this vector, in order to obtain length "1":
    - $||(x_1,\ldots, x_n)||$ = sqrt ($x_1^2 + \ldots + x_n^2$)

Eigenvectors and eigenvalues

- **Exercise**
  - Determine, from the following vectors, which are eigenvectors of the matrix given below and, if positive, determine the corresponding eigenvalue.
    - Matrix:

$$\begin{bmatrix} 3 & 0 & 1 \\ -4 & 1 & 2 \\ -6 & 0 & -2 \end{bmatrix}$$

    - Vectors:

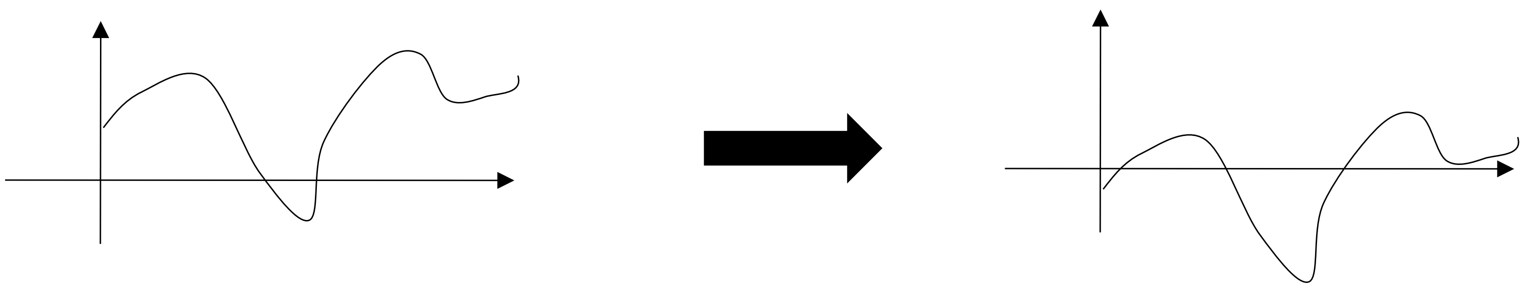
$$\begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix} \quad \begin{bmatrix} -1 \\ 0 \\ 2 \end{bmatrix} \quad \begin{bmatrix} -1 \\ 1 \\ 3 \end{bmatrix} \quad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

PCA: Principal Component Analysis

- **The Principal Component Analysis (PCA)** it’s a well known way to detect patterns on data, by expressing it on a way that enhances similarities or differences.
- Detecting patterns on high dimensional data is a hard task, either for humans or machines.
  - Requires huge amounts of data. An empirical rule says that at the minimum, d^2 instances are required to analyze a d-dimensional data set.
- PCA is typically used to compress data (reduce dimensionality), without loosing substantial information.

PCA: Principal Component Analysis

- **Step 1.** The analysis of principal components requires a data set (with dimension n) and cardinality (k).
- **Step 2.** Removal of energy. For each dimension, the corresponding mean is subtrated to each component. As such, all dimensions of the data set have zero energy.



Principal Component Analysis

- **Step 3.** Calculus of the covariance matrix. Here, the relationships between independent components are detected, together with an assessment of the data dispersion in each dimension (by analysing the main diagonal components).
- **Step 4.** As the covariance matrix is square, it is possible to obtain the set of eigenvectors and correspºonding eigenvalues.
- **Step 4.1.** Eigenvectors normalization. All eigenvectors are normalized to have norm equal to 1.

Principal Component Analysis

- **Step 5.** Selection of components. The set of eigenvectors is sorted by decreasing order, considering the corresponding eigenvalues. From this set, the “k_1” principal components are selected.
  - This is the step that performs the reduction of dimensionality.
- **Step 6.** A transformation matrix is built, by concatenating the eigenvectors selected in the previous step.
  - This matrix will be used to represent all points in the reduced dimensionality feature space. MAT=[vect1, vect2, ... Vectk_1]

Principal Component Analysis

- **Step 7. Data Transformation. As the transformation matrix has “d” lines (corresponding to the dimension of the original feature space and** k_1 columns (corresponding to the dimension of the new feature space), when multipling each original data point by the transformation matrix, we obtain a vector of k_1 components. These are the new representation of the data points, in the principal components space.

$$\mathbf{[1 \times d] \times [d \times k_1] = [1 \times k_1]}$$

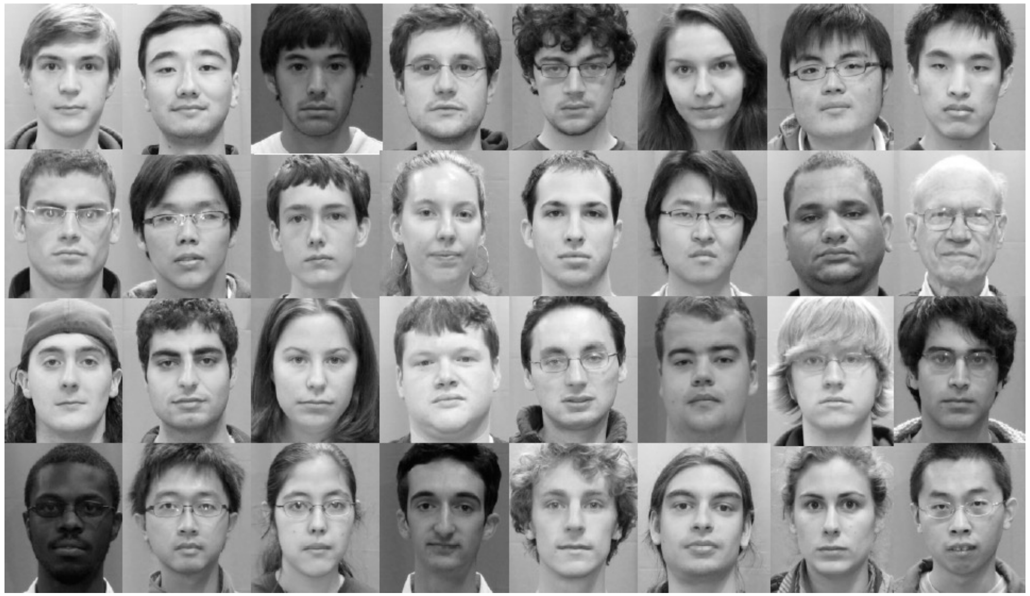
Principal Component Analysis

- **How to choose the value of "k"?**
  - The previously described process does not give any information about a strategy to select the dimensionality of the principal components feature space.
  - There is no formal rule. However, some heuristics about what is generally better exist.
- Usually, the variation in magnitude of consecutive eigenvalues (after sorting) is measured. When changes in magnitude are higher than a threshold, the selection process is stopped.
- But most frequently, the proportion of the data variability that is kept by the selected components is considered as the main criterium.
  - Typically, we are interested in keeping around 90, 95, 99% of the original data variability.
  - The analysis can be done by measuring the proportion of the sum of eigenvalues:

- **Variability**: $\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$, "k": number of selected vectors, and "d": dimensionality

PCA: Example

- Consider a set of 128 face grayscale images (with dimensions 64 x 64).
  - Each image is represented by a 64 x 64 matrix = (4096), where each position represents the intensity at a point (0: black pixel, ... 255: White pixel)
- Each face can be regarded as a point represented in a 4096 dimensional feature space

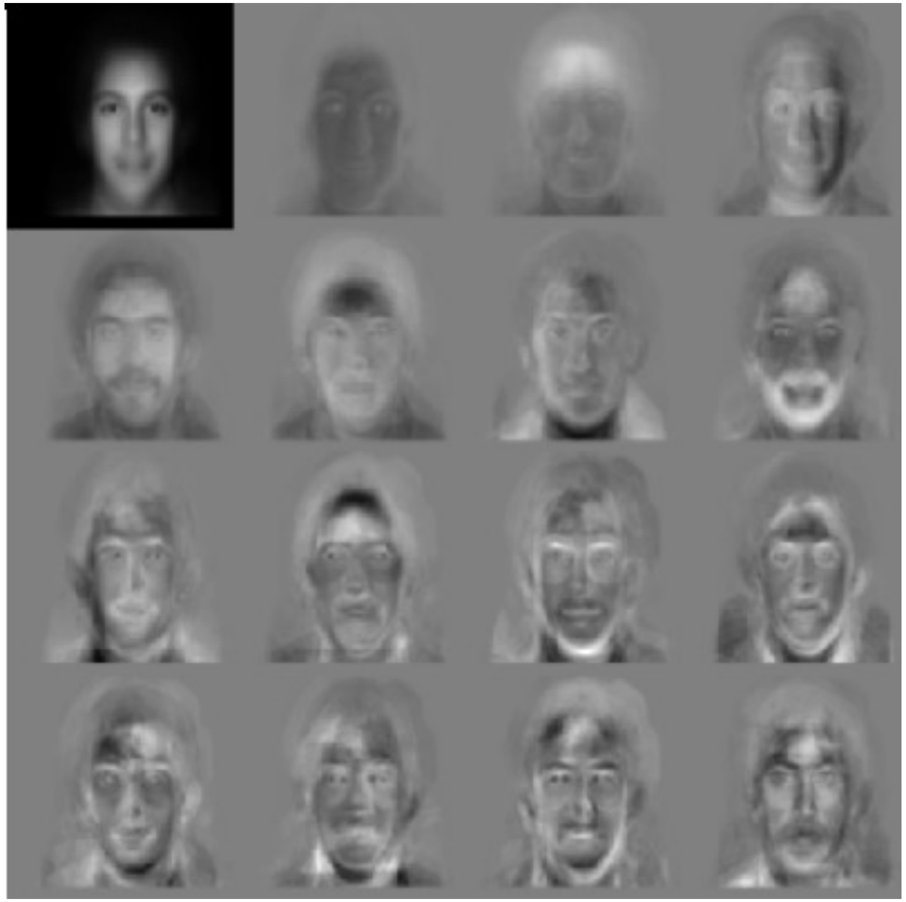


PCA: Example

- We can usethe PCA to select the principal components in this space (i.e., the directions in which the elements mostly span (vary)) .
  - In pratice, the eigenvectors (each one with dimension 4096) with the largest corresponding eigenvalues will be selected.
- Next, each original face can be represented as a weighted combination of the top-k eigenvalues.
  - In such case, each face will actually be represented by weights $\boldsymbol{\alpha}$: $\alpha_1, \dots\ \alpha_k$
  - The PCA can be also regarded as a way to represent a face, with much less information than the originally used, while keeping the most importante information.
- Further, the facial recognition process can be done in the new feature space of (much more) reduced dimension, i.e., typically k << d (original space).

PCA: Example

- Example of the 16 principal components (eigenvectors with the largest eigenvalues) from the above data set:



What do the brightest regions in each vector represent?