CS559 Lecture 17

Dimension Reduction and Feature Selection - PCA

Reading: Chapter 12.1, Bishop book

The curse of dimensionality

The curse of dimensionality

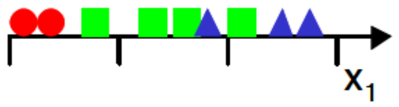
– A term coined by Bellman in 1961

– Refers to the problems associated with multivariate data analysis as the dimensionality increases

Consider a 3-class pattern recognition problem

– A simple approach would be to
  - Divide the feature space into uniform bins
  - Compute the ratio of examples for each class at each bin and,
  - For a new example, choose the predominant class in its bin

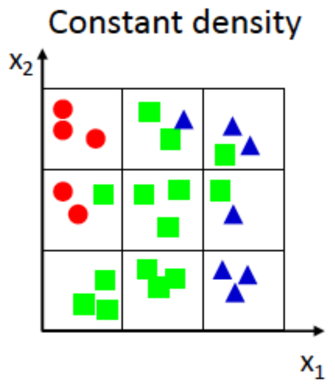
– In our toy problem we decide to start with one single feature and divide the real line into 3 segments

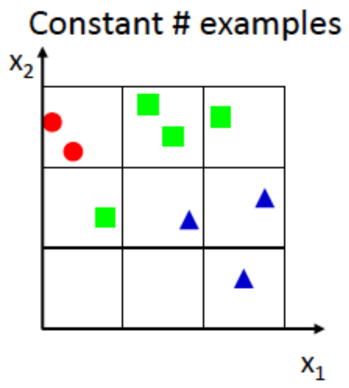


– After doing this, we notice that there exists too much overlap among the classes, so we decide to incorporate a second feature to try and improve separability

We decide to preserve the granularity of each axis, which raises the number of bins from 3 (in 1D) to $3^2 = 9$ (in 2D)

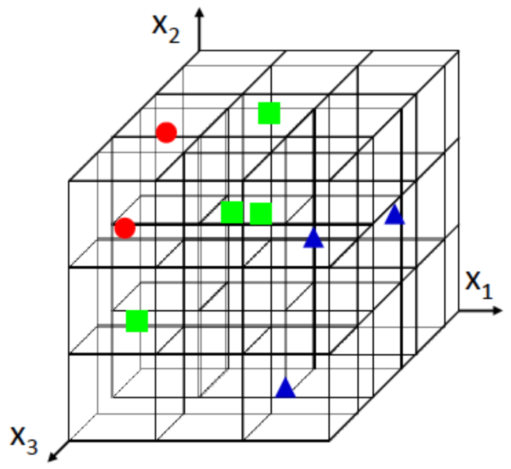
- At this point we need to make a decision: do we maintain the density of examples per bin or do we keep the number of examples had for the one-dimensional case?
- Choosing to maintain the density increases the number of examples from 9 (in 1D) to 27 (in 2D)
- Choosing to maintain the number of examples results in a 2D scatter plot that is very sparse





Moving to three features makes the problem worse

- The number of bins grows to $3^3 = 27$
- For the same density of examples the number of needed examples becomes 81
- For the same number of examples, the 3D scatter plot is almost empty



Obviously, our approach to divide the sample space into equally spaced bins was quite inefficient

- There are other approaches that are much less susceptible to the curse of dimensionality, **but the problem still exists**

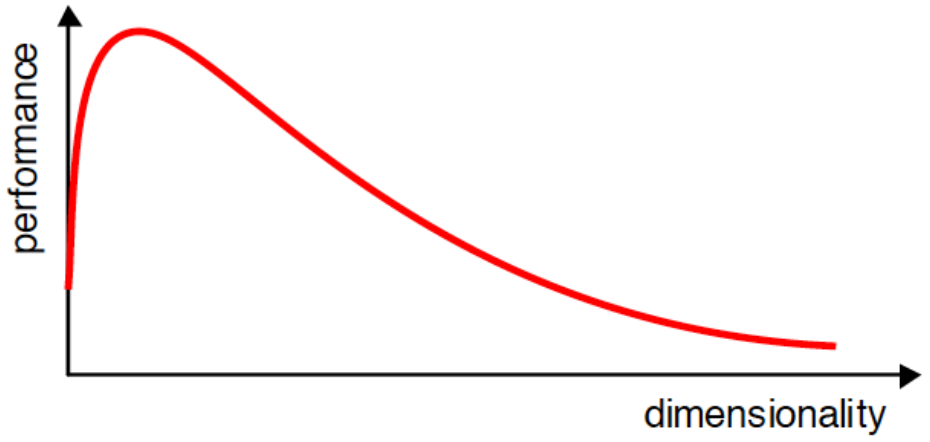
How do we beat the curse of dimensionality?

- By incorporating prior knowledge
- By providing increasing smoothness of the target function
- By reducing the dimensionality

What does the curse of dimensionality mean, in practice?

– For a given sample size, there is a maximum number of features above which the performance of our classifier will degrade rather than improve

– In most cases, the additional information that is lost by discarding some features is (more than) compensated by a more accurate mapping in the lower-dimensional space



Additional implications

- Exponential growth in the #examples required to maintain a given sampling density
  - For a density of N examples/bin and D dimensions, the total number of examples is N^D
- Exponential growth in the complexity of the target function (a density estimate) with increasing dimensionality
  - *"A function defined in high-dimensional space is likely to be much more complex than a function defined in a lower-dimensional space, and those complications are harder to discern"* –J. Friedman
  - This means that, in order to learn it well, a more complex target function requires denser sample points!
- What to do if it ain't Gaussian?
  - For 1D a large number of density functions can be found in textbooks, but for high-dimensions only the multivariate Gaussian density is available.
  - Moreover, for large D the Gaussian can only be handled in a simplified form!
- Humans have an extraordinary capacity to discern patterns and clusters in 1D, 2D and 3D, but these capabilities break down for $D \geq 4$

Dimensionality reduction

Two approaches are available to reduce dimensionality

- **Feature extraction**: creating a subset of new features by combinations of the existing features
- **Feature selection**: choosing a subset of all the features

$$\begin{bmatrix} x_1 \\ x_2 \\ \\ x_N \end{bmatrix} \rightarrow \begin{bmatrix} x_{i_1} \\ x_{i_2} \\ \\ x_{i_M} \end{bmatrix} \qquad \begin{bmatrix} x_1 \\ x_2 \\ \\ x_N \end{bmatrix} \rightarrow \begin{bmatrix} y_1 \\ y_2 \\ \\ y_M \end{bmatrix} = f\left(\begin{bmatrix} x_1 \\ x_2 \\ \\ x_N \end{bmatrix}\right)$$

The problem of feature extraction can be stated as

- Given a feature space $x_i \in \Re^N$ find a mapping $y = f(x): R^N \rightarrow R^M$ with $M < N$ such that the transformed feature vector $y \in R^M$ preserves (most of) the information or structure in R^N
- An optimal mapping $y = f(x)$ is one that does not increase $P[error]$
- This is, a Bayes decision rule applied to the initial space R^N and to the reduced space R^M yield the same classification rate

Linear dimensionality reduction

- In general, the optimal mapping $y = f(x)$ will be a non-linear function
  - However, there is no systematic way to generate non-linear transforms
  - The selection of a particular subset of transforms is problem dependent
- For these reasons, feature extraction is commonly based on linear transforms, of the form $y = Wx$

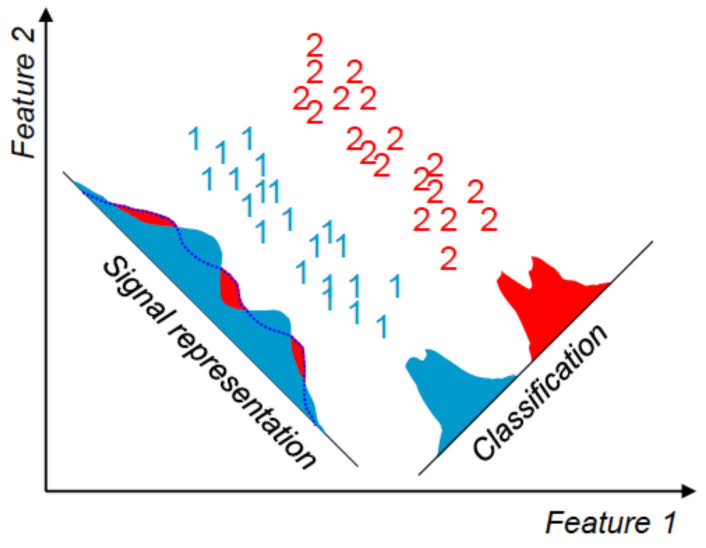
$$\begin{bmatrix} x_1 \\ x_2 \\ \\ \\ x_N \end{bmatrix} \rightarrow \begin{bmatrix} y_1 \\ y_2 \\ \\ y_M \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & & w_{1N} \\ & & & \\ w_{M1} & & & w_{MN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \\ \\ x_N \end{bmatrix}$$

  - NOTE: When the mapping is a non-linear function, the reduced space is called a manifold
- We will focus on linear feature extraction for now, and revisit non-linear techniques when we cover multi-layer perceptrons, manifold learning, and kernel methods

Signal representation versus classification

Finding the mapping $y = f(x)$ is guided by an objective function that we seek to maximize (or minimize)

- Depending on the criteria used by the objective function, feature extraction techniques are grouped into two categories:
  - **Signal representation**: The goal of the feature extraction mapping is to represent the samples accurately in a lower-dimensional space
  - **Classification**: The goal of the feature extraction mapping is to enhance the class-discriminatory information in the lower-dimensional space
- Within the realm of linear feature extraction, two techniques are commonly used
  - Principal components analysis (**PCA**): uses a signal representation criterion
  - Linear discriminant analysis (**LDA**): uses a signal classification criterion



Principal Components Analysis, PCA (1)

- **The objective of PCA is to perform dimensionality reduction while preserving as much of the randomness in the high-dimensional space as possible**
  - Let x be an N-dimensional random vector, represented as a linear combination of orthonormal basis vectors $[\varphi_1 | \varphi_2 | \ldots | \varphi_N]$ as

$$x = \sum_{i=1}^{N} y_i \varphi_i \quad \text{where} \quad \varphi_i | \varphi_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

  - Suppose we choose to represent x with only M (M<N) of the basis vectors. We can do this by replacing the components $[y_{M+1}, \ldots, y_N]^T$ with some pre-selected constants

$$\hat{x}(M) = \sum_{i=1}^{M} y_i \varphi_i + \sum_{i=M+1}^{N} b_i \varphi_i$$

  - The representation error is then

$$\Delta x(M) = x - \hat{x}(M) = \sum_{i=1}^{N} y_i \varphi_i - \left(\sum_{i=1}^{M} y_i \varphi_i - \sum_{i=M+1}^{N} b_i \varphi_i \right) = \sum_{i=M+1}^{M} (y_i - b_i) \varphi_i$$

  - We choose to measure this representation error by the mean-squared magnitude of Δx

$$\bar{\varepsilon}^2(M) = E\left[|\Delta x(M)|^2 \right] = E\left[\sum_{i=M+1}^{N} \sum_{j=M+1}^{N} (y_i - b_i)(y_j - b_j) \varphi_i^T \varphi_j \right] = \sum_{i=M+1}^{N} E\left[(y_i - b_i)^2 \right]$$

  - Among all the basis vectors ϕi and constants bi we choose the ones that minimize this mean-square error

Principal Components Analysis, PCA (2)

- The optimal values of b_i are found by computing the partial derivative of the objective function and equating to zero

$$\frac{\partial}{\partial b_i} E\left[(y_i - b_i)^2\right] = -2\left(E[y_i] - b_i\right) = 0 \Rightarrow b_i = E[y_i]$$

  - So we will replace the discarded y_i's by their expected value (an intuitive solution)

- The mean-square error can be written as

$$\bar{\varepsilon}^2(M) = \sum_{i=M+1}^{N} E\left[(y_i - E[y_i])^2\right] = \sum_{i=M+1}^{N} E\left[(x\varphi_i - E[x\varphi_i])^T (x\varphi_i - E[x\varphi_i])\right]$$

$$= \sum_{i=M+1}^{N} \varphi_i^T E\left[(x - E[x])(x - E[x])^T\right]\varphi_i = \sum_{i=M+1}^{N} \varphi_i^T \Sigma_x \varphi_i$$

- We seek to find the solution that minimizes this expression subject to the orthonormality constraint, which we incorporate into the expression using a set of Lagrange multipliers λ_i

$$\bar{\varepsilon}^2(M) = \sum_{i=M+1}^{N} \varphi_i^T \Sigma_x \varphi_i + \sum_{i=M+1}^{N} \lambda_i (1 - \varphi_i^T \varphi_i)$$

- Computing the partial derivative with respect to the basis vectors

$$\frac{\partial}{\partial \varphi_i} \bar{\varepsilon}^2(M) = \frac{\partial}{\partial \varphi_i}\left[\sum_{i=M+1}^{N} \varphi_i^T \Sigma_x \varphi_i + \sum_{i=M+1}^{N} \lambda_i (1 - \varphi_i^T \varphi_i)\right] = 2\left(\Sigma_x \varphi_i - \lambda_i \varphi_i\right) = 0 \Rightarrow \Sigma_x \varphi_i = \lambda_i \varphi_i$$

$$\text{NOTE: } \frac{d}{dx}\left(x^T A x\right) = \left(A + A^T\right)x \overset{\substack{\text{if A is} \\ \text{symmmetric}}}{=} 2Ax$$

  - So φ_i and λ_i are the eigenvectors and eigenvalues of the covariance matrix Σ_x

Principal Components Analysis, PCA (3)

- We can express the sum-square error as

$$\bar{\varepsilon}^2(M) = \sum_{i=M+1}^{N} \varphi_i^T \Sigma_x \varphi_i = \sum_{i=M+1}^{N} \varphi_i^T \lambda_i \varphi_i = \sum_{i=M+1}^{N} \lambda_i$$

- In order to minimize this measure, λ_i will have to be smallest eigenvalues
  - Therefore, to represent x with minimum sum-square error, we will choose the eigenvectors φ_i corresponding to the largest eigenvalues λ_i

PCA dimensionality reduction

The optimal* approximation of a random vector $x \in \Re^N$ by a linear combination of M (M<N) independent vectors is obtained by projecting the random vector x onto the eigenvectors φ_i corresponding to the largest eigenvalues λ_i of the covariance matrix Σ_x

*optimality is defined as the minimum of the sum-square magnitude of the approximation error

Principal Components Analysis, PCA (4)

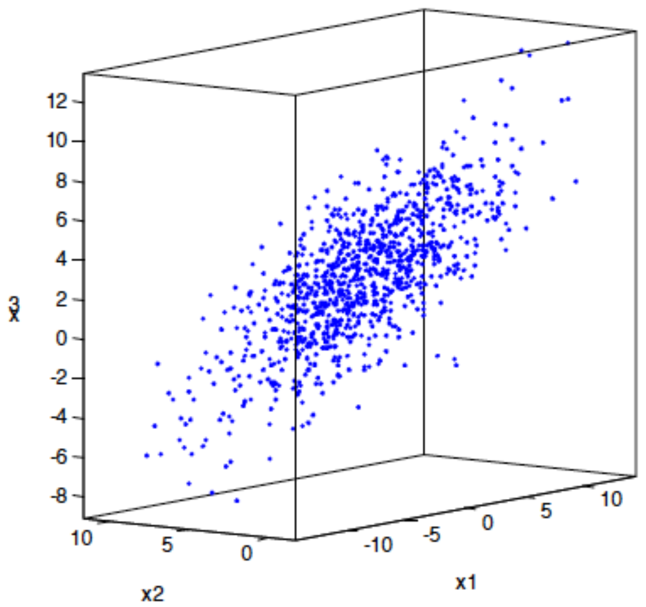
- **NOTES**
  - Since PCA uses the eigenvectors of the covariance matrix Σ_x, it is able to find the independent axes of the data under the unimodal Gaussian assumption
    - For non-Gaussian or multi-modal Gaussian data, PCA simply de-correlates the axes
  - The main limitation of PCA is that it does not consider class separability since it does not take into account the class label of the feature vector
    - PCA simply performs a coordinate rotation that aligns the transformed axes with the directions of maximum variance
    - <u>**There is no guarantee that the directions of maximum variance will contain good features for discrimination!!!**</u>
- **Historical remarks**
  - Principal Components Analysis is the oldest technique in multivariate analysis
  - PCA is also known as the Karhunen-Loève transform (communication theory)
  - PCA was first introduced by Pearson in 1901, and it experienced several modifications until it was generalized by Loève in 1963

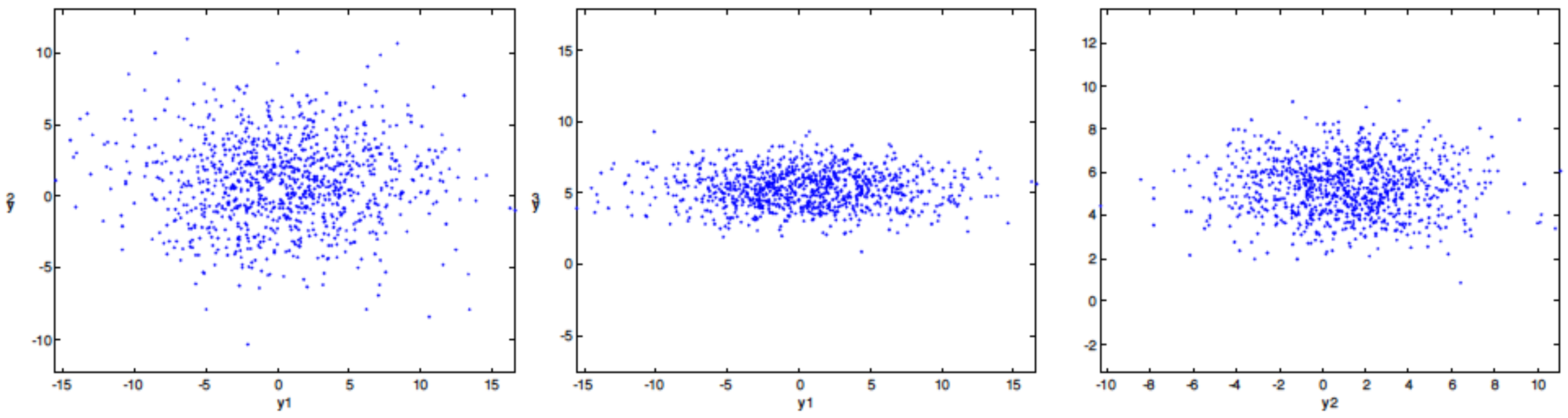
PCA examples (1)

- **In this example we have a three-dimensional Gaussian distribution with the following parameters**

$$\mu = [0\ 5\ 2]^T \text{ and } \Sigma = \begin{bmatrix} 25 & -1 & 7 \\ -1 & 4 & -4 \\ 7 & -4 & 10 \end{bmatrix}$$

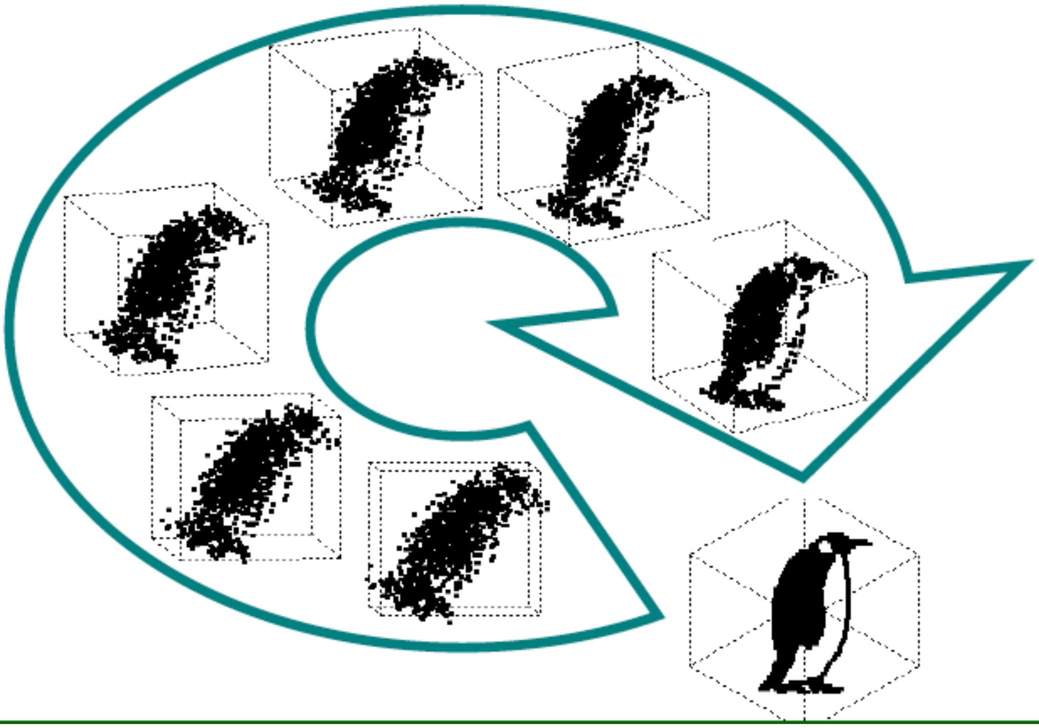
- **The three pairs of principal component projections are shown below**
  - Notice that the first projection has the largest variance, followed by the second projection
  - Also notice that the PCA projections de-correlate the axis (we knew this since Lecture 2)

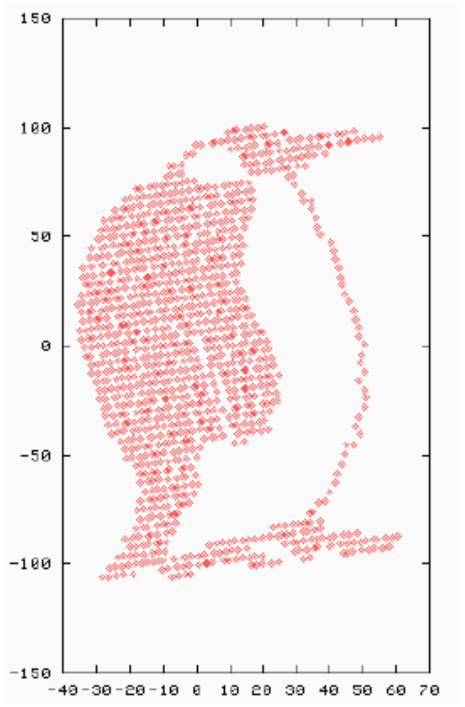




PCA examples (2)

- **This example shows a projection of a three-dimensional data set into two dimensions**
  - Initially, except for the elongation of the cloud, there is no apparent structure in the set of points
  - Choosing an appropriate rotation allows us to unveil the underlying structure. (You can think of this rotation as "walking around" the three-dimensional set, looking for the best viewpoint)
- **PCA can help find such underlying structure. It selects a rotation such that most of the variability within the data set is represented in the first few dimensions of the rotated data**
  - In our three-dimensional case, this may seem of little use
  - However, when the data is highly multidimensional (10's of dimensions), the analysis is quite powerful





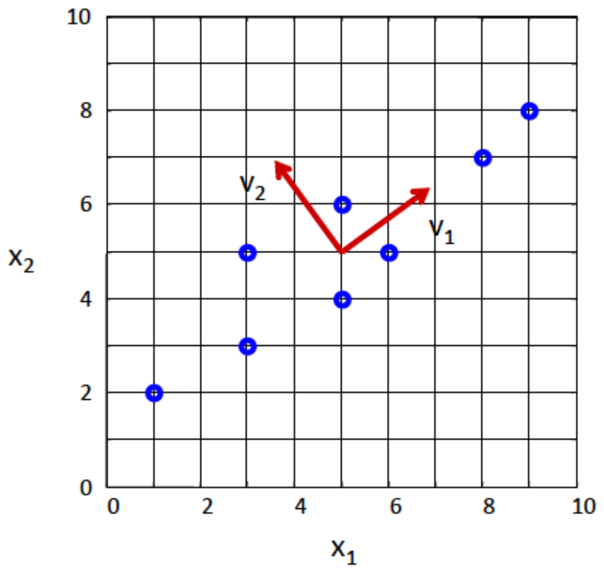
Example III

Problem statement

- Compute the PCA for dataset

$X = \{(1,2),(3,3),(3,5),(5,4),(5,6),(6,5),(8,7),(9,8)\}$

- Let's first plot the data to get an idea of which solution we should expect



Solution

- The sample covariance is

$$\Sigma_x = \begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix}$$

- The eigenvalues are the zeros of the characteristic equation

$$\Sigma_x v = \lambda v \Rightarrow |\Sigma_x - \lambda I| = 0$$
$$\Rightarrow \begin{vmatrix} 6.25-\lambda & 4.25 \\ 4.25 & 3.5-\lambda \end{vmatrix} = 0$$
$$\Rightarrow \boldsymbol{\lambda_1 = 9.34; \lambda_2 = 0.41}$$

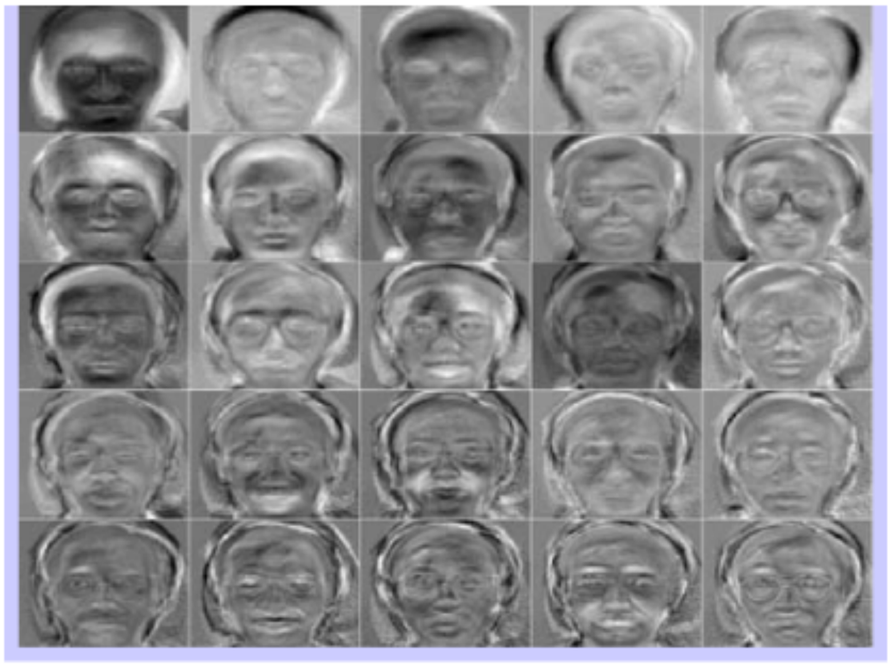
– The eigenvectors are the solutions of the system

$$\begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix} \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} = \begin{bmatrix} \lambda_1 v_{11} \\ \lambda_1 v_{12} \end{bmatrix} \Rightarrow \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} = \begin{bmatrix} 0.81 \\ 0.59 \end{bmatrix}$$

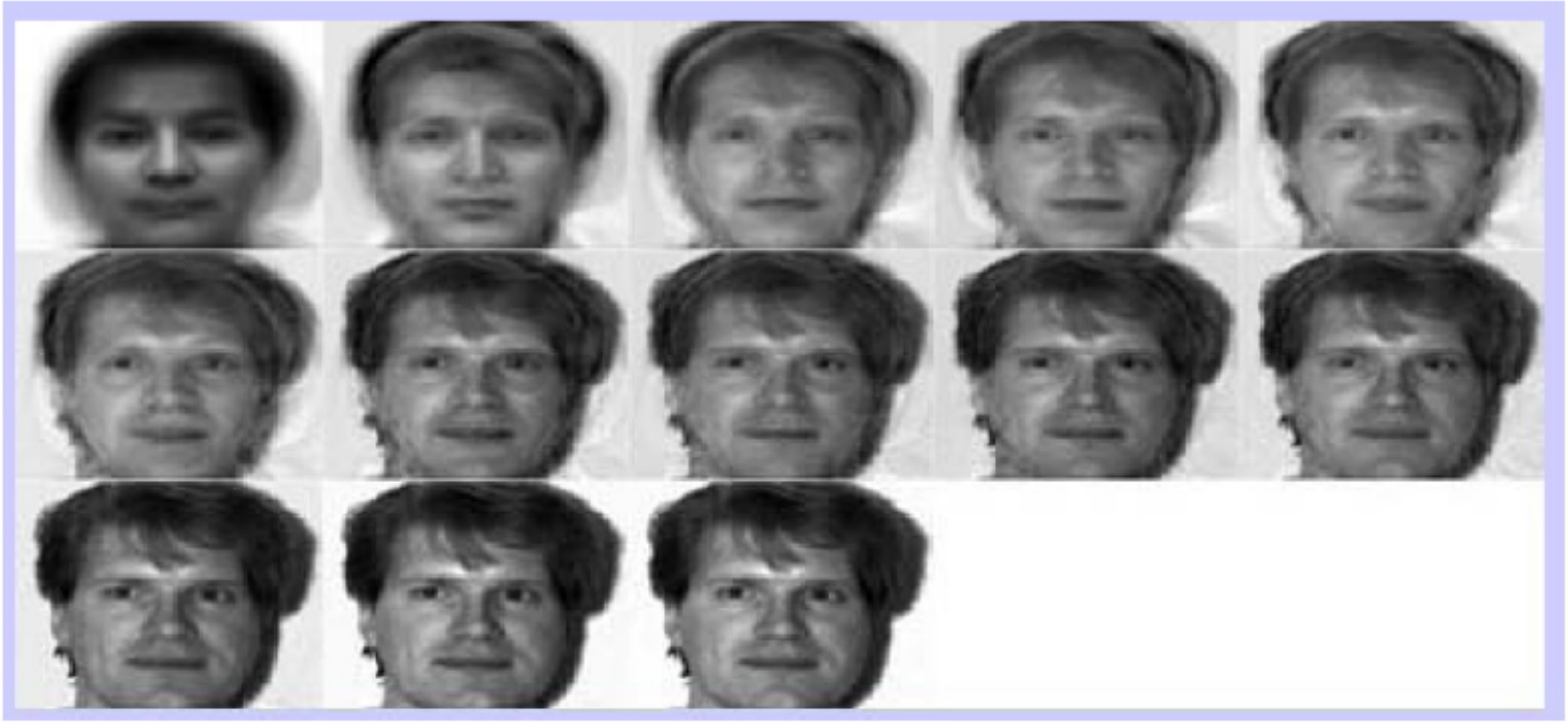
$$\begin{bmatrix} 6.25 & 4.25 \\ 4.25 & 3.5 \end{bmatrix} \begin{bmatrix} v_{21} \\ v_{22} \end{bmatrix} = \begin{bmatrix} \lambda_2 v_{21} \\ \lambda_2 v_{22} \end{bmatrix} \Rightarrow \begin{bmatrix} v_{21} \\ v_{22} \end{bmatrix} = \begin{bmatrix} -0.59 \\ 0.81 \end{bmatrix}$$

– HINT: To solve each system manually, first assume that one of the variables is equal to one (i.e. $v_{i1} = 1$), then find the other one and finally normalize the vector to make it unit-length

Principal Component Analysis: Example



Principal Component Analysis: Example



Reconstruction with increments of 8 eigenvectors