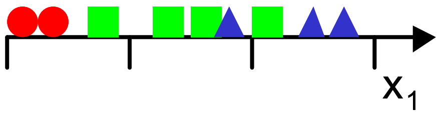
LECTURE 9: Principal Components Analysis

- The curse of dimensionality
- Dimensionality reduction
- Feature selection vs. feature extraction
- Signal representation vs. signal classification
- Principal Components Analysis

The curse of dimensionality (1)

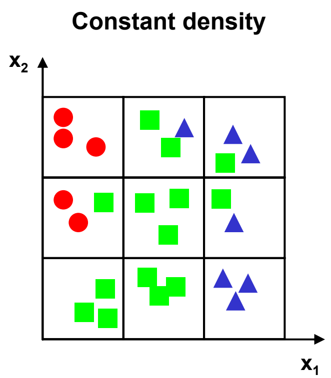
- **The <u>curse of dimensionality</u>**
  - A term coined by Bellman in 1961
  - Refers to the problems associated with multivariate data analysis as the dimensionality increases
  - We will illustrate these problems with a simple example
- **Consider a 3-class pattern recognition problem**
  - A simple 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, find its bin and choose the predominant class in that bin
  - In our toy problem we decide to start with one single feature and divide the real line into 3 segments

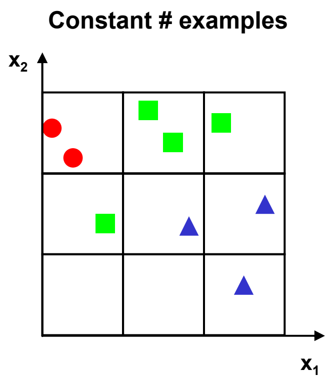


  - After doing this, we notice that there exists too much overlap among the classes, so we decide to incorporate a second feature to try and improve separability

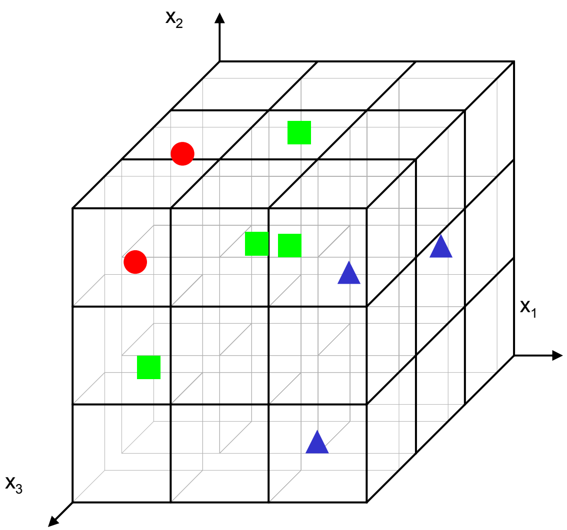
The curse of dimensionality (2)

- **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



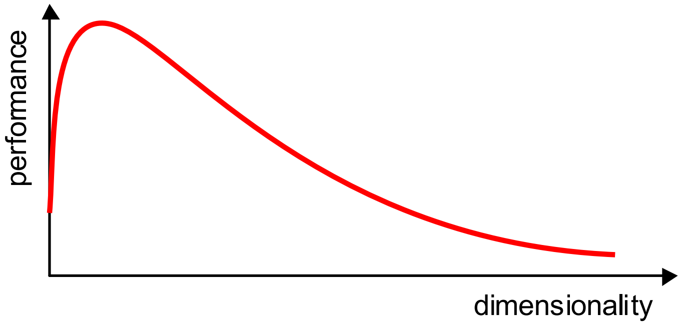


- **Moving to three features makes the problem worse:**
  - The number of bins grows to 3^3=27
  - For the same density of examples the number of needed examples becomes 81
  - For the same number of examples, well, the 3D scatter plot is almost empty



The curse of dimensionality (3)

- **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
- **In practice, the curse of dimensionality means that, 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



The curse of dimensionality (4)

- **There are many implications of the curse of dimensionality**
  - Exponential growth in the number of 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*" –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 one dimension a large number of density functions can be found in textbooks, but for high-dimensions only the multivariate Gaussian density is available. Moreover, for larger values of D the Gaussian density can only be handled in a simplified form!
  - Humans have an extraordinary capacity to discern patterns and clusters in 1, 2 and 3-dimensions, but these capabilities degrade drastically for 4 or higher dimensions

Dimensionality reduction (1)

- **Two approaches are available to perform dimensionality reduction**
  - **Feature extraction**: creating a subset of new features by combinations of the existing features
  - **Feature selection**: choosing a subset of all the features (the ones more informative)

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_N \end{bmatrix} \xrightarrow{\text{feature selection}} \begin{bmatrix} x_{i_1} \\ x_{i_2} \\ \\ x_{i_M} \end{bmatrix} \qquad \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_N \end{bmatrix} \xrightarrow{\text{feature extraction}} \begin{bmatrix} y_1 \\ y_2 \\ \\ y_M \end{bmatrix} = f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \\ x_N \end{bmatrix}\right)$$

- **The problem of feature extraction can be stated as**
  - Given a feature space $\mathbf{x_i} \in \mathbf{R^N}$ find a mapping $\mathbf{y=f(x):R^N \rightarrow R^M}$ with $\mathbf{M<N}$ such that the transformed feature vector $y_i \in R^M$ preserves (most of) the information or structure in R^N.
  - An **optimal** mapping **y=f(x)** will be one that results in **no increase in the minimum probability of 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

Dimensionality reduction (2)

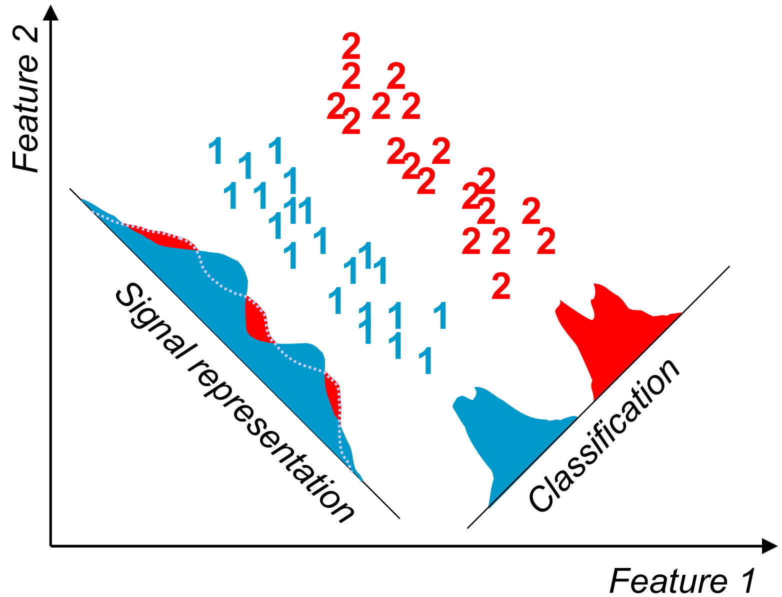
- **In general, the optimal mapping y=f(x) will be a non-linear function**
  - However, there is no systematic way to generate non-linear transforms
    - The selection of a particular subset of transforms is problem dependent
  - For this reason, feature extraction is commonly limited to linear transforms: ***y=Wx***
    - This is, *y* is a linear projection of *x*
    - NOTE: When the mapping is a non-linear function, the reduced space is called a **manifold**

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} \xrightarrow{\text{linear feature extraction}} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1N} \\ w_{21} & w_{22} & \cdots & w_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ w_{M1} & w_{M2} & & w_{MN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

- **We will focus on linear feature extraction for now, and revisit non-linear techniques when we cover multi-layer perceptrons**

Signal representation versus classification

- **The selection of the feature extraction 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 (variance) 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 b_i

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

  - 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 can measure this representation error by the mean-squared magnitude of Δx
  - Our goal is to find the basis vectors φ_i and constants b_i that minimize this mean-square error

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

Principal Components Analysis, PCA (2)

- As we have done earlier in the course, the optimal values of b_i can be found by computing the partial derivative of the objective function and equating it to zero

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

  - Therefore, we will replace the discarded dimensions y_i's by their expected value (an intuitive solution)
- The mean-square error can then be written as

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

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

  - where Σ_x is the covariance matrix of x
- 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 then 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

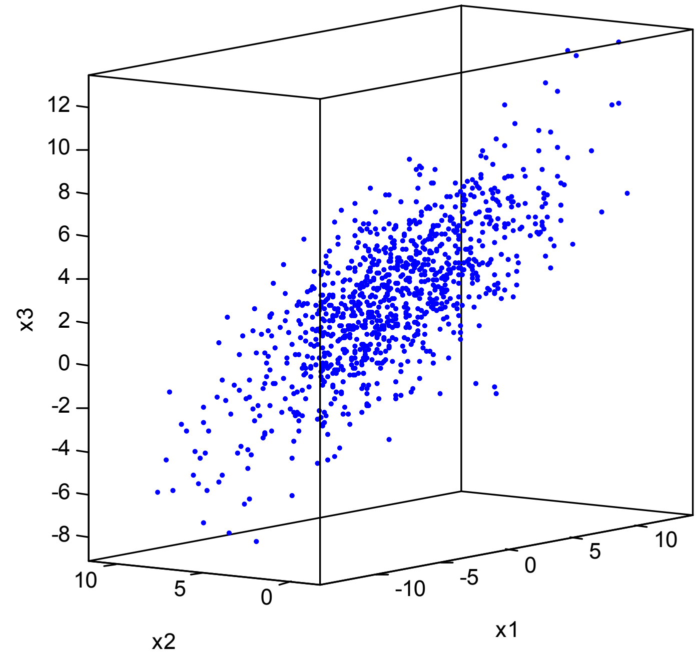
Principal Components Analysis, PCA (4)

- **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
    - **There is no guarantee that the directions of maximum variance will contain good features for discrimination**
- **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

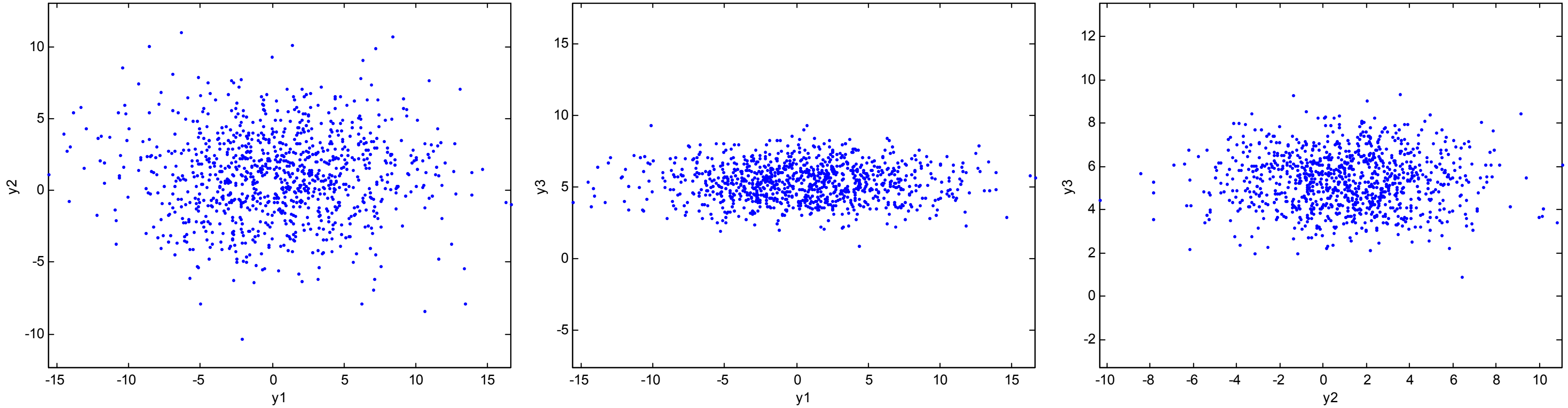
PCA example (1)

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

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

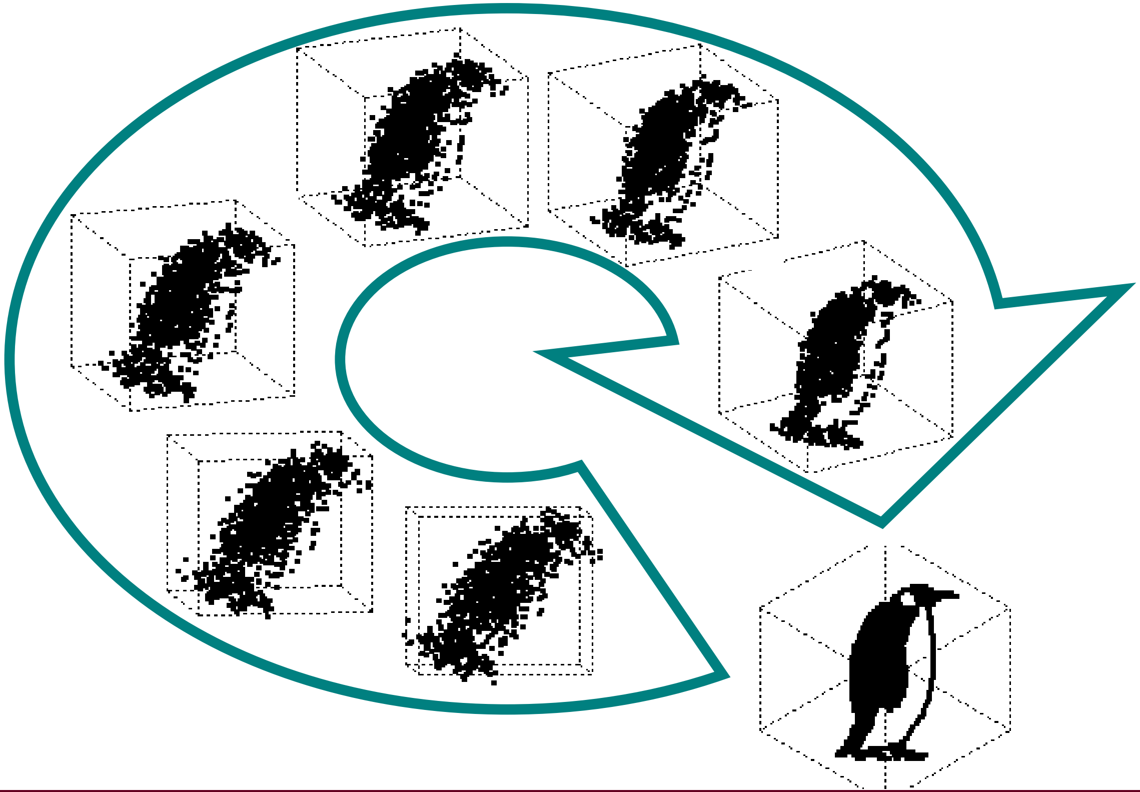


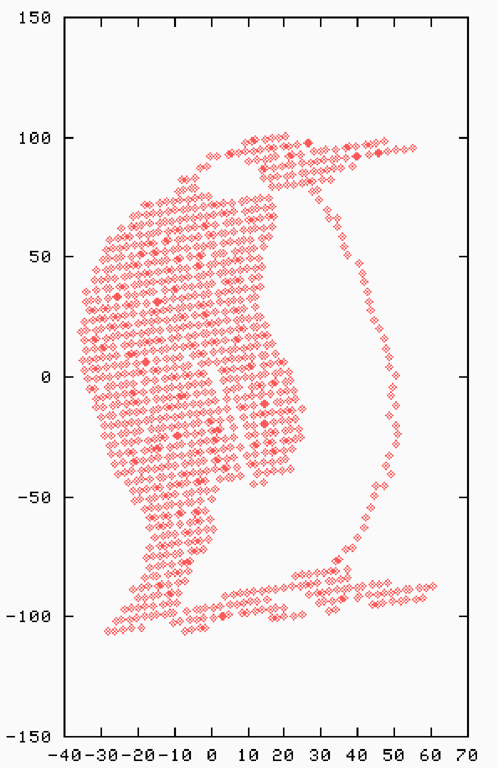
- **The three pairs of principal component projections are shown below**
  - Notice that the first projection has the largest variance, followed by the second projection
  - Also notice that the PCA projections de-correlates the axis (we knew this since Lecture 3, though)



PCA example (2)

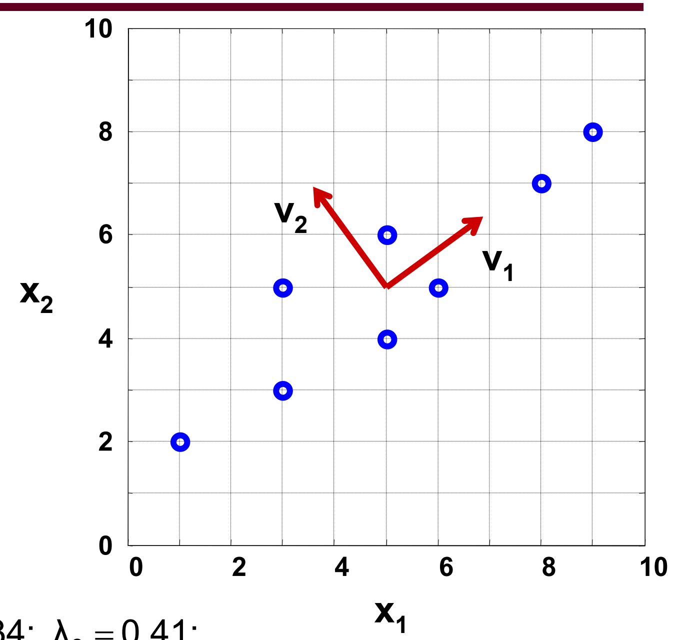
- **This example shows a projection of a three-dimensional data set into two dimensions**
  - Initially, except for the elongation of the cloud, there is no apparent structure in the set of points
  - Choosing an appropriate rotation allows us to unveil the underlying structure. (You can think of this 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), this analysis is quite powerful





PCA example (3)

- **Compute the principal components for the following two-dimensional dataset**
  - $X=(x_1,x_2)=\{(1,2),(3,3),(3,5),(5,4),(5,6),(6,5),(8,7),(9,8)\}$
    - Let's first plot the data to get an idea of which solution we should expect



- **SOLUTION (by hand)**
  - The (biased) covariance estimate of the data is:

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

  - The eigenvalues are the zeros of the characteristic equation

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

  - 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