Algorithm Foundations of Data Science and Engineering

Lecture 5: SVD and PCA

MING GAO

DaSE @ ECNU
(for course related communications)
mgao@dase.ecnu.edu.cn

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Outline

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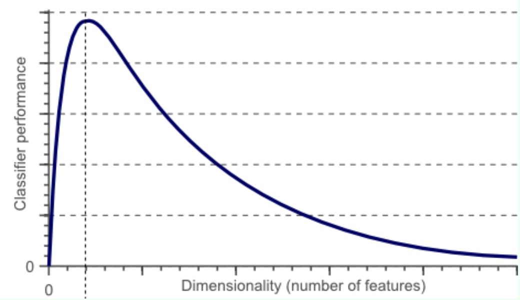
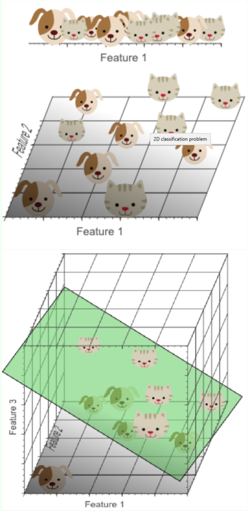
- However, these three color-describing numbers, called features, will obviously not suffice to obtain a perfect classification.
- Maybe we can obtain a perfect classification by carefully defining a few hundred of these features?

Classifier performance



As the dimensionality increases, the classifier's performance increases until the optimal number of features is reached. Further increasing the dimensionality without increasing the number of training samples results in a decrease in classifier performance.

Adding features



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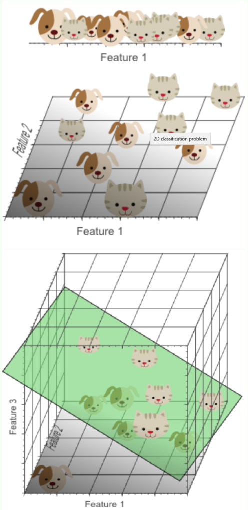

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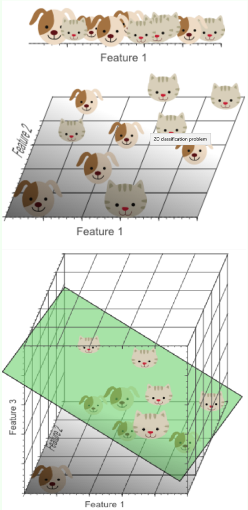

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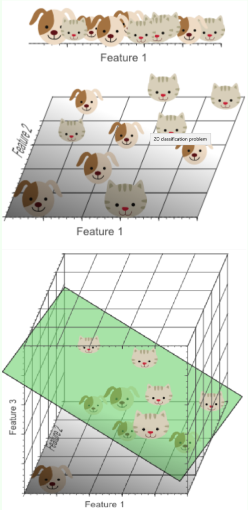

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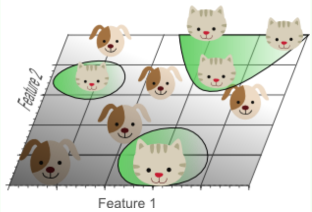
- Adding a second feature still does not result in a linearly separable classification problem: No single line can separate all cats from all dogs in this example.
- The more features we use, the higher the likelihood that we can successfully separate the classes perfectly.

Non-separable classification in low-dimensional space



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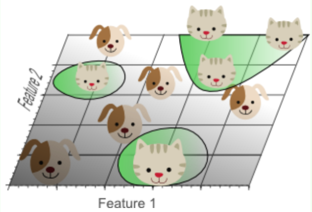

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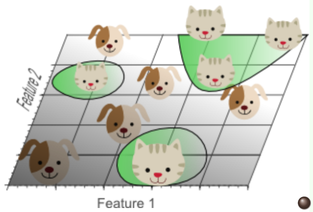

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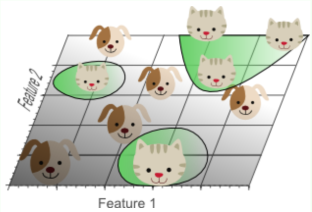

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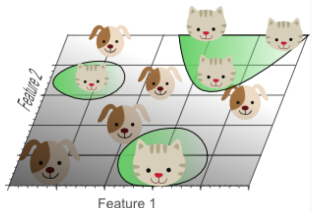

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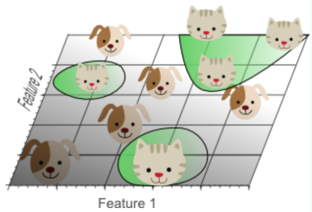

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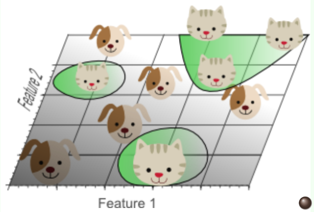

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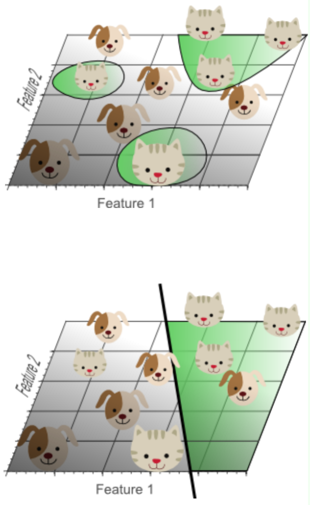

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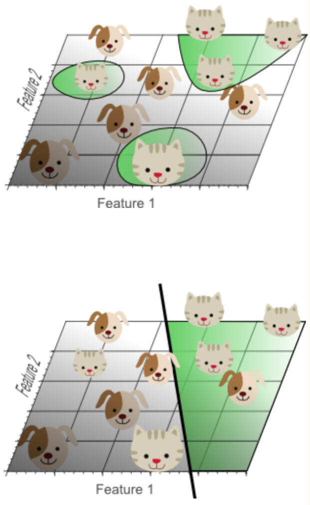

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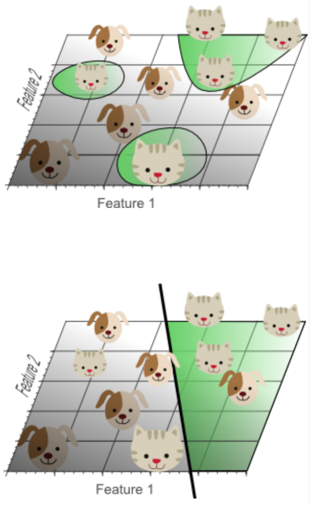

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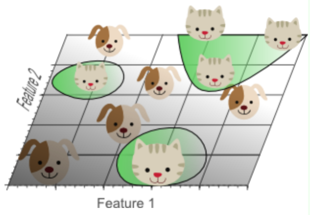

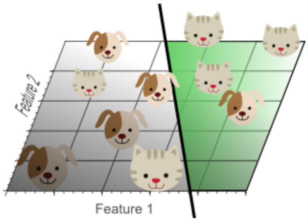

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- This concept is called overfitting and is a direct result of the curse of dimensionality.

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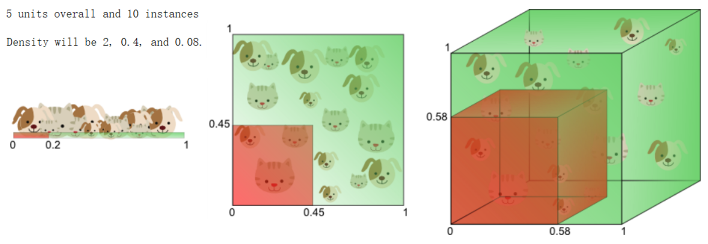

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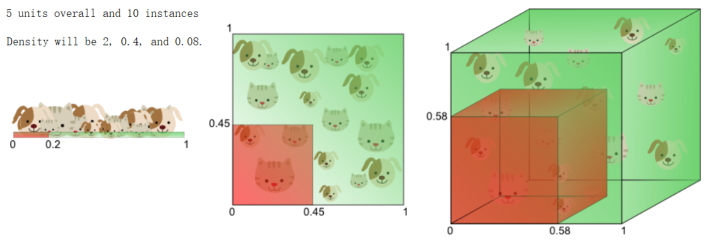

- For 2D feature space, to cover 20% of the 2D feature range, we now need to obtain 45% of the complete population ($0.45^2 = 0.2$). In the 3D case this gets even worse, the proportion will be 58% ($0.58^3 = 0.2$).

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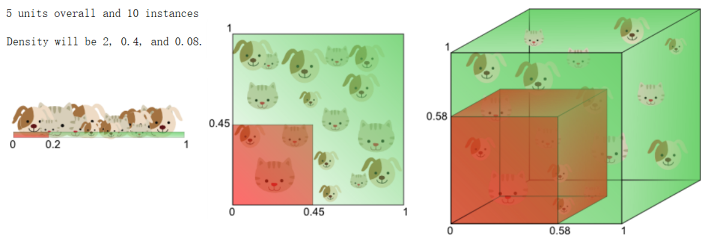

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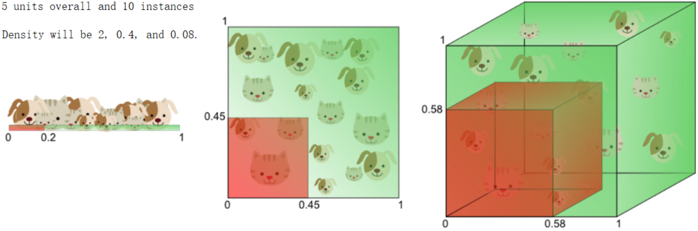
5 units overall and 10 instances

Density will be 2, 0.4, and 0.08.



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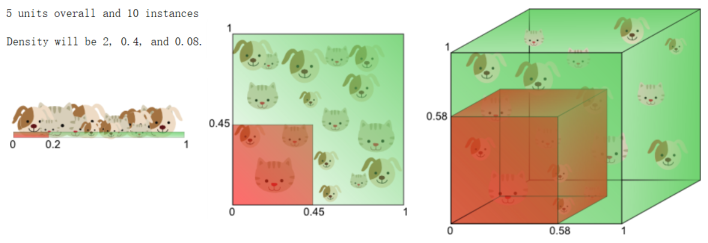

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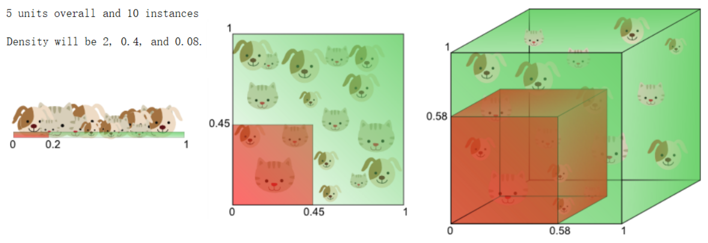

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- The other approach, **Dimensionality reduction**, would be to replace the set of N features by a set of M features, each of which is a combination of the original feature values.

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  - Matrix decomposition, such as SVD, PCA, MF, PMF, etc

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- If we think of the squared matrix A as a transformation matrix, then multiply it with the eigenvector do not change its direction.

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  - Why useful? If A is diagonalizable, then $A^k = PD^kP^{-1}$ for $k > 0$.
  - How to find diagonal matrix? If $v_1, \cdots, v_n$ are linearly independent eigenvectors of A and λ_i are their corresponding eignevalues, then $A = PDP^{-1}$, where $P = [v_1 \ \cdots \ v_n]$ and $D = Diag(\lambda_1, \cdots, \lambda_n)$.

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- Hence, the matrix is not diagonalizable.

Diagonalization of of symmetric matrix

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Geometric explanation of diagonalization

Example

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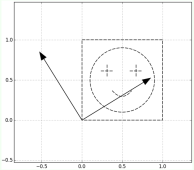

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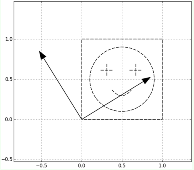

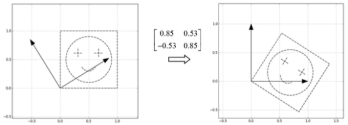

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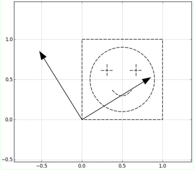

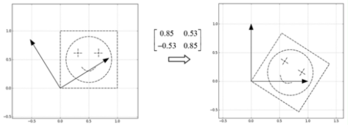

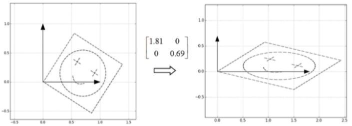

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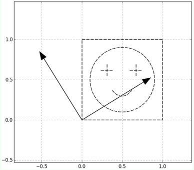

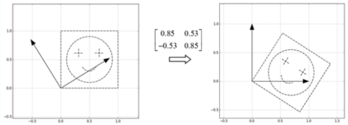

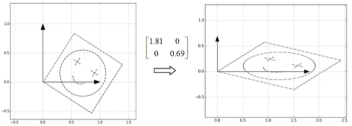

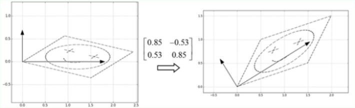

Outline

1. The Curse of Dimensionality
2. Singular Value Decomposition
   - Diagonalization
   - Singular Value Decomposition
3. Principal Component Analysis

Singular value decomposition: SVD

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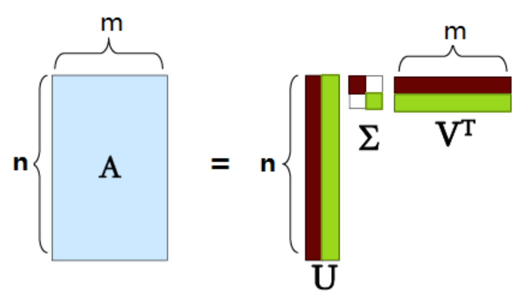

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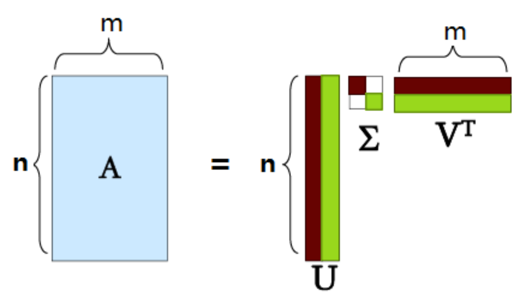

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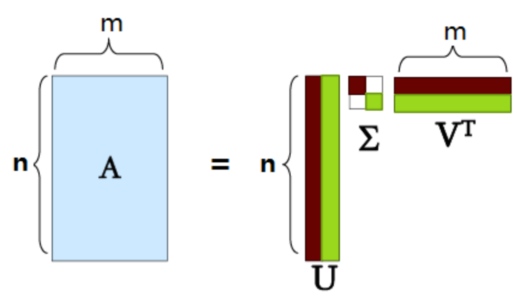

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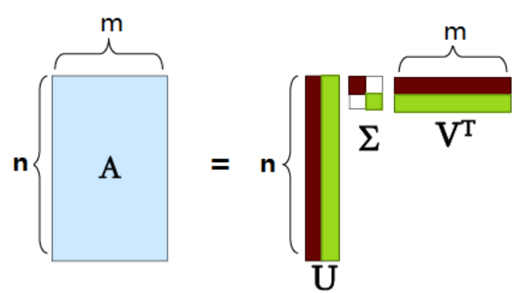

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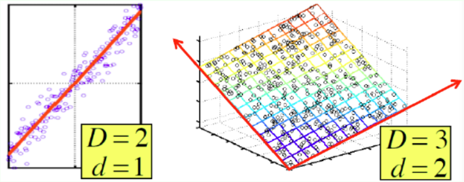

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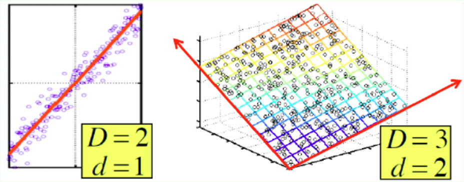

Assumptions

- Data lies on or near a low $d-$dimensional subspace.
- Axes of this subspace are effective representation of the data.

Methodology of decomposition

Diagonalization

- $$AA^T = UDV^TVDU^T = UD^2U^T,$$

  where $D = diag(\sigma_1^2, \sigma_2^2, \cdots, \sigma_k^2)$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_k$.

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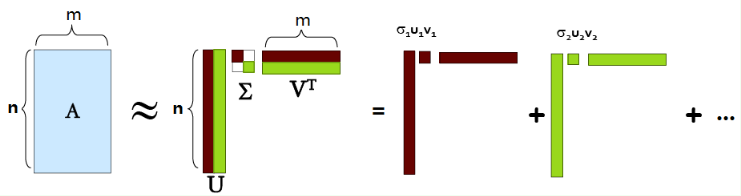

Methodology of dimensionality reduction

$$A = \left[\begin{array}{ccc|ccc} u_1 & \cdots & u_k & u_{k+1} & \cdots & u_m \end{array}\right] \left[\begin{array}{ccc|c} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_k & \\ \hline & 0 & & 0 \end{array}\right] \left[\begin{array}{c} v_1^T \\ \vdots \\ v_k^T \\ \hline v_{k+1}^T \\ \vdots \\ v_n^T \end{array}\right]$$

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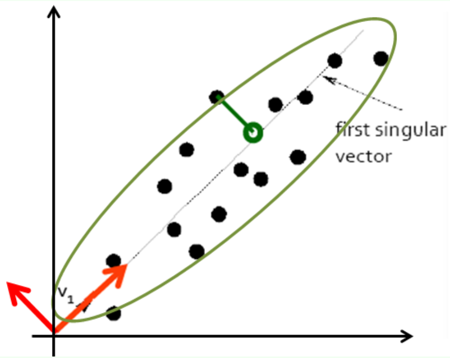
- For example

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \approx \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

SVD interpretation



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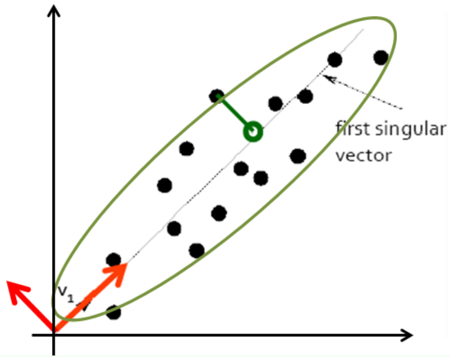

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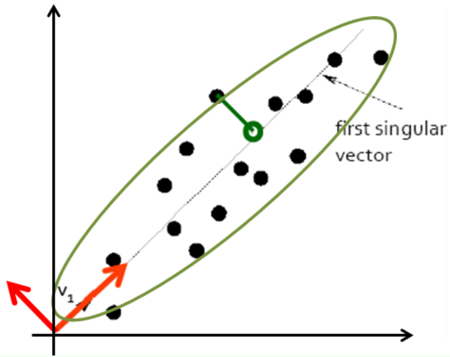

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- SVD can be helpful to similarity query or join.

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  - If A is a nonsingular matrix, then its inverse is given by $A^{-1} = V^T D^{-1} U$.
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- Consider linear system $Ax = b$, where $A \in \mathbb{R}^{n \times m}$. If $A^T A$ is ill-conditioned (small changes in b can lead to relatively large changes in the solution x) or singular, $x \approx VD_0^{-1}U^T b$.
- SVD can be helpful to similarity query or join.
- Data compression and anomaly detection.

PCA: an important application of SVD

Motivation

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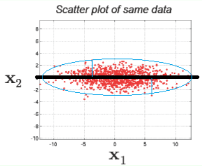

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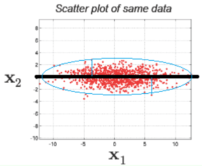

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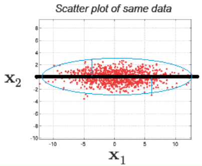

Goals

- Find a good representation for features (what?)
- Reduce redundancy in the data (how?)

PCA Cont'd

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- Minimize relation of the different dimensions.

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- It also gives best axis to project data, where "best" means to minimize sum of squares of projection errors.

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- It also gives the minimum reconstruction errors.
- It can be determined by the "best" eigenvectors of the covariance matrix of x (i.e., the eigenvectors corresponding to the "largest" eigenvalues, also called "principal components").

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5. Keep only the terms corresponding to the k largest eigenvalues: $\widehat{\mathbf{x}} - \bar{\mathbf{x}} \approx \sum_{i=1}^{k} b_i \mathbf{u}_i$, i.e., the representation of $\widehat{\mathbf{x}} - \bar{\mathbf{x}}$ into the basis $\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_k$.

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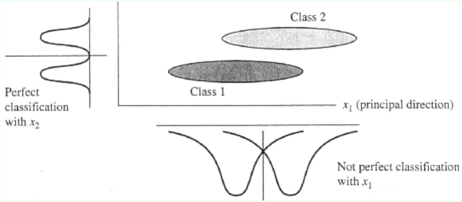
- It can be shown that the error is equal to $e = \sqrt{\sum_{i=k+1}^{d} \lambda_i}$.
- PCA is not always an optimal dimensionality-reduction procedure, e.g., classification problem.



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- We need an approach that can simply ignore missing values and reduce the complexity.

Take-home messages

- The Curse of Dimensionality
- Singular Value Decomposition
  - Diagonalization
  - Singular Value Decomposition
- Principal Component Analysis