Linear Dimensionality Reduction

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CS5350/6350: Machine Learning

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High-Dimensional Datasets Abound..

face images

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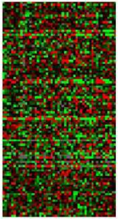
documents



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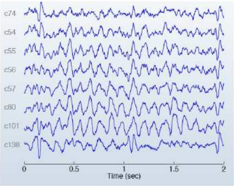

MEG readings

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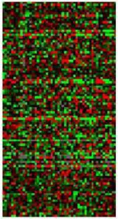

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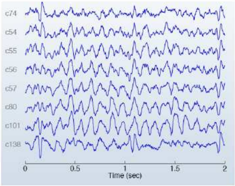

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Goal: Find a low-dimensional, yet useful representation of the data

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  - .. although the goals are kind of the same
- Dimensionality reduction is more like "Feature Extraction"
  - Constructing a small set of new features from the original features

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$$\mathbf{z} = \mathbf{U}^\top \mathbf{x}$$

- $\mathbf{z} \in \mathbb{R}^K$ is the projection
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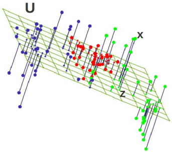

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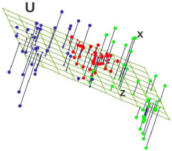
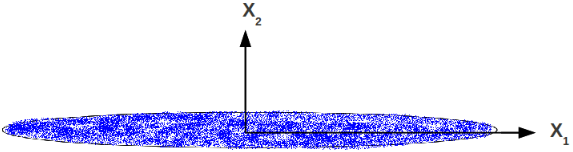


- Different methods differ in how $\mathbf{U}$ is defined/learned
- The differences depend on what properties of data we want to capture

Dimensionality Reduction: A Simple Illustration



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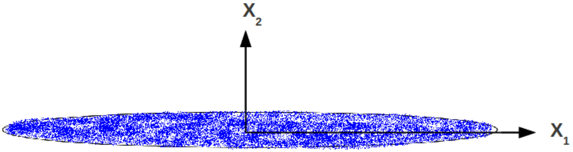

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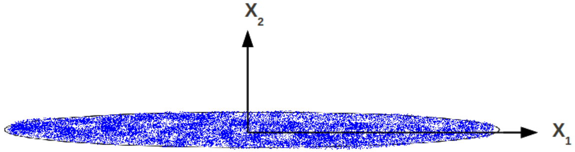

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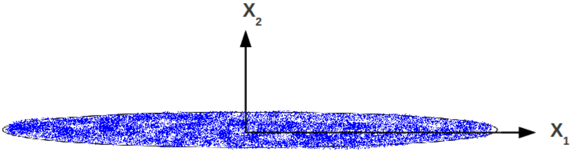

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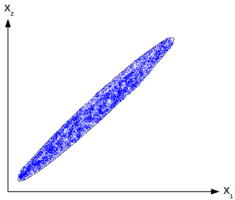

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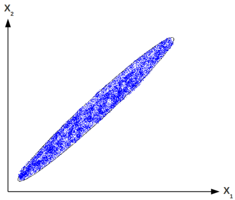

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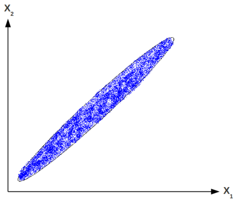

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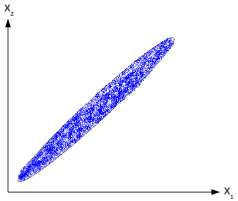

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- Yes. The data has substantial variance along both features (i.e., both axes)

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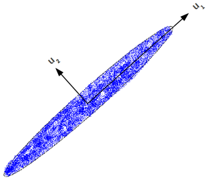

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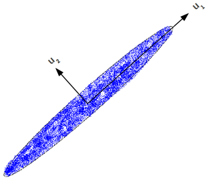

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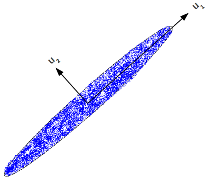

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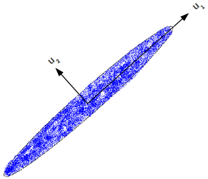

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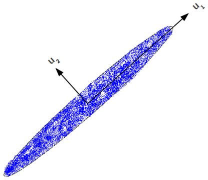

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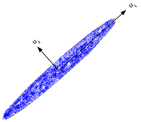

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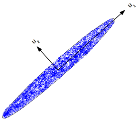

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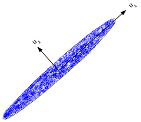

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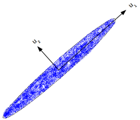

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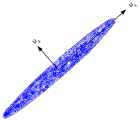

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- PCA: Take top K PC's and project the data along those

PCA: Finding the Principal Components

- Given: N examples $\mathbf{x}_1, \ldots, \mathbf{x}_N$, each example $\mathbf{x}_n \in \mathbb{R}^D$
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- We want only the first K principal components

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- Variance of the projected data (along projection direction $\mathbf{u}_1$):

$$\frac{1}{N}\sum_{n=1}^{N}\left\{\mathbf{u}_1^\top \mathbf{x}_n - \mathbf{u}_1^\top \bar{\mathbf{x}}\right\}^2 = \mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1$$

where $\mathbf{S}$ is the data covariance matrix defined as

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- Want to have $\mathbf{u}_1$ that maximizes the projected data variance $\mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1$
  - Subject to the constraint: $\mathbf{u}_1^\top \mathbf{u}_1 = 1$
  - We will introduce a Lagrange multiplier λ_1 for this constraint

PCA: Finding the Principal Components

- Objective function: $\mathbf{u}_1^\top \mathbf{S}\mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^\top \mathbf{u}_1)$
- Taking derivative w.r.t. $\mathbf{u}_1$ and setting it to zero gives:

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  - Thus λ_1 should be the largest eigenvalue
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- Subsequent PC's are given by the subsequent eigenvectors of $\mathbf{S}$

PCA: The Algorithm

- Compute the mean of the data

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n$$

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- Call these $\mathbf{u}_1, \ldots, \mathbf{u}_K$ (s.t. $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_{K-1} \geq \lambda_K$)
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PCA: The Algorithm

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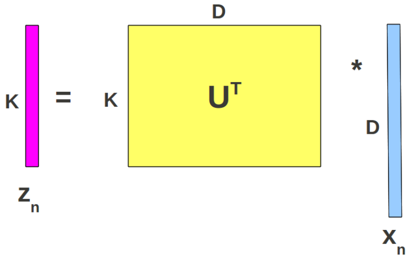
- Projection of each example $\mathbf{x}_n$ is computed as $\mathbf{z}_n = \mathbf{U}^\top \mathbf{x}_n$
  - $\mathbf{z}_n$ is a $K \times 1$ vector (also called the embedding of $\mathbf{x}_n$)

PCA: Pictorially

- For a single example $\mathbf{x}_n$:



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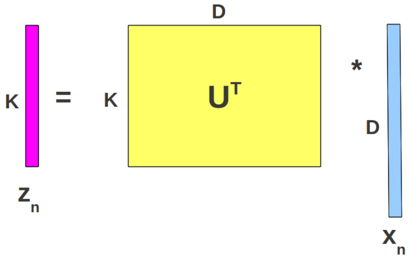
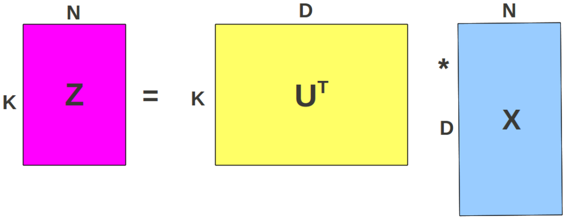
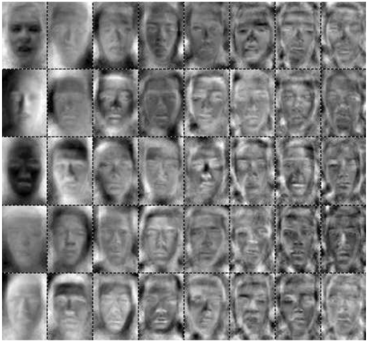


- For a set of N examples:



PCA Example: Eigenfaces

- Principal Components learned using a face image dataset



PCA: Approximate Reconstruction

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- The eigenvectors aren't exactly the same (but still related)
- The relationship is $\mathbf{u}_i = \frac{1}{(N\lambda_i)^2}\mathbf{X}\mathbf{v}_i$
- $\{\lambda_i, \mathbf{v}_i\}$ is an eigenvalue-eigenvector pair of the $N \times N$ matrix $\frac{1}{N}\mathbf{X}^\top\mathbf{X}$, and $\mathbf{u}_i$ is the corresponding eigenvector of $\mathbf{S} = \frac{1}{N}\mathbf{X}\mathbf{X}^\top$ (that we want)

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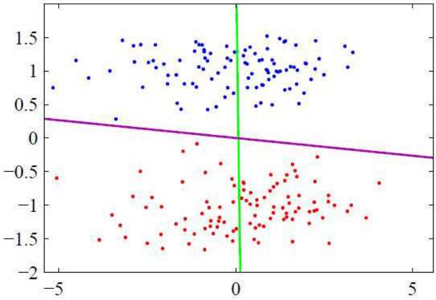
PCA vs FDA/LDA

- PCA: magenta line, FDA: green line



- PCA based projection makes the classes overlap (which is bad)
- LDA/FDA is often better if the final goal is classification