Principle Component Analysis

Announcement:

Recap on K-means

Given any K disjoint groups $C_1, C_2, \ldots, C_K$, and any K centroids $\mu_1, \ldots, \mu_K$, define

$$\ell(\{C_i\}, \{\mu_i\}) = \sum_{i=1}^{K} \left[\sum_{x \in C_i} \|x - \mu_i\|_2^2 \right]$$

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K-means Algorithm:

Initialize $\mu_1, \ldots, \mu_K$

Repeat until convergence:

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Outline for today:

1. Intro of PCA

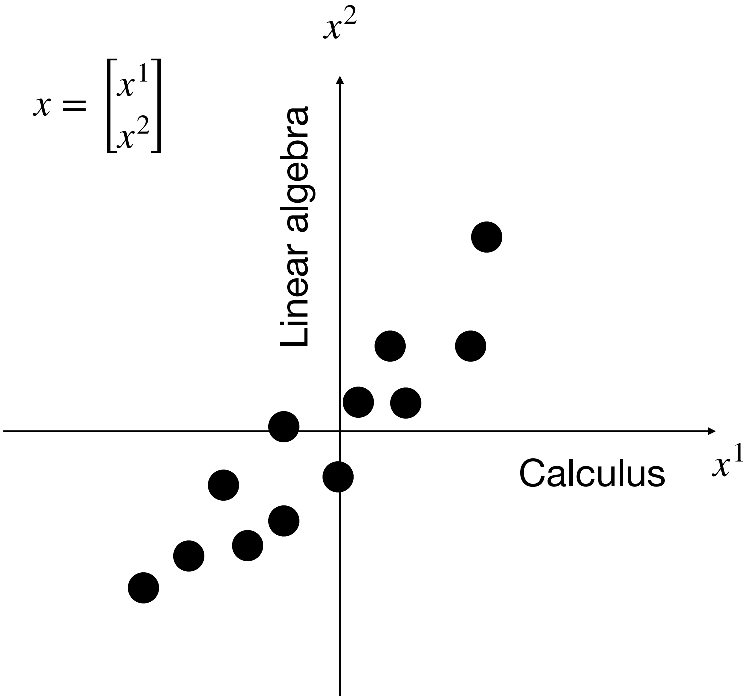
2. PCA via eigendecomposition

3. Example of PCA: eigenfaces

Data compression

Goal: reduce high dimensional data to low dimensional

$$x = \begin{bmatrix} x^1 \\ x^2 \end{bmatrix}$$



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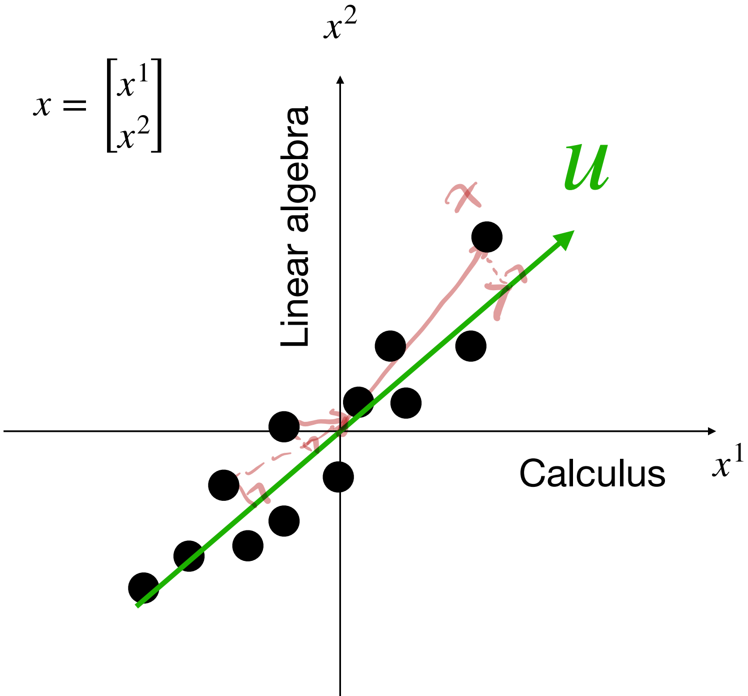

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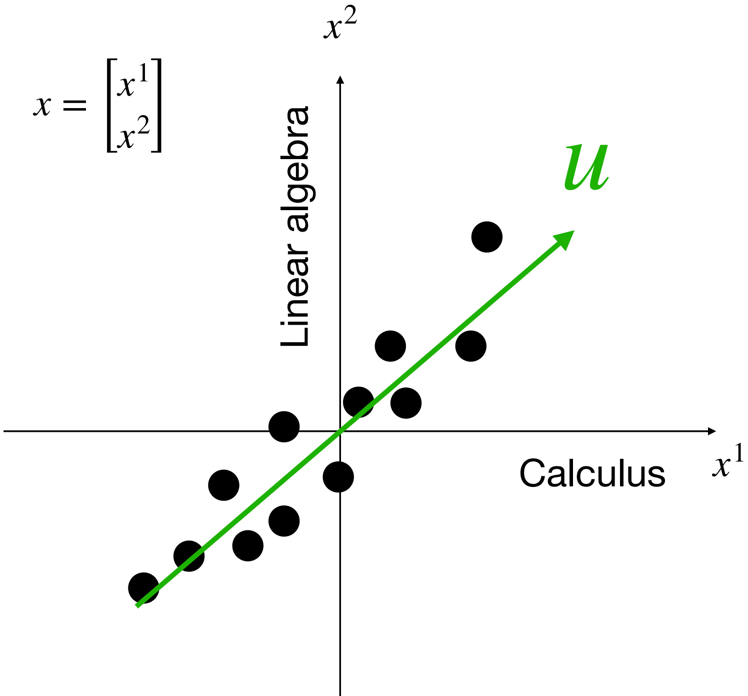

Normalize u s.t. $\|u\|_2 = 1$

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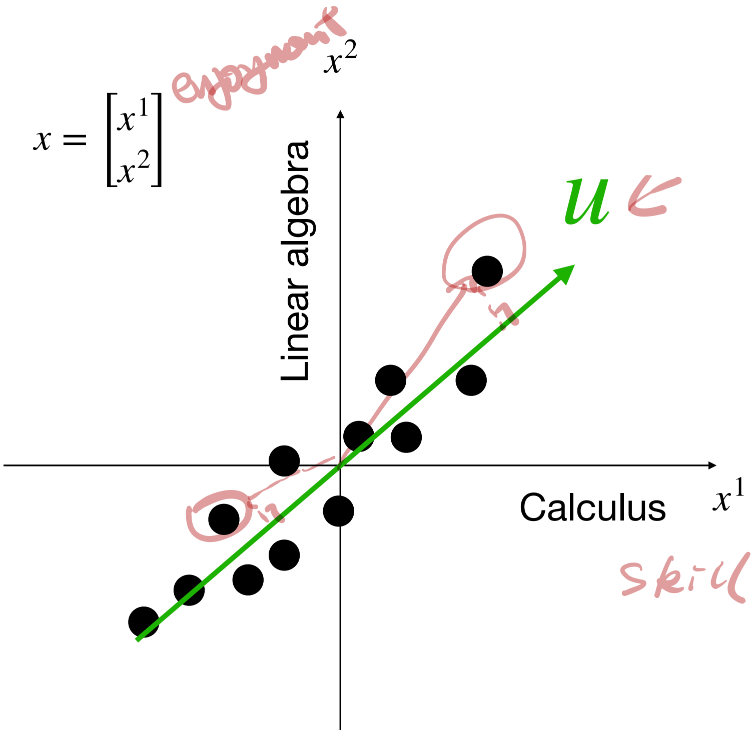

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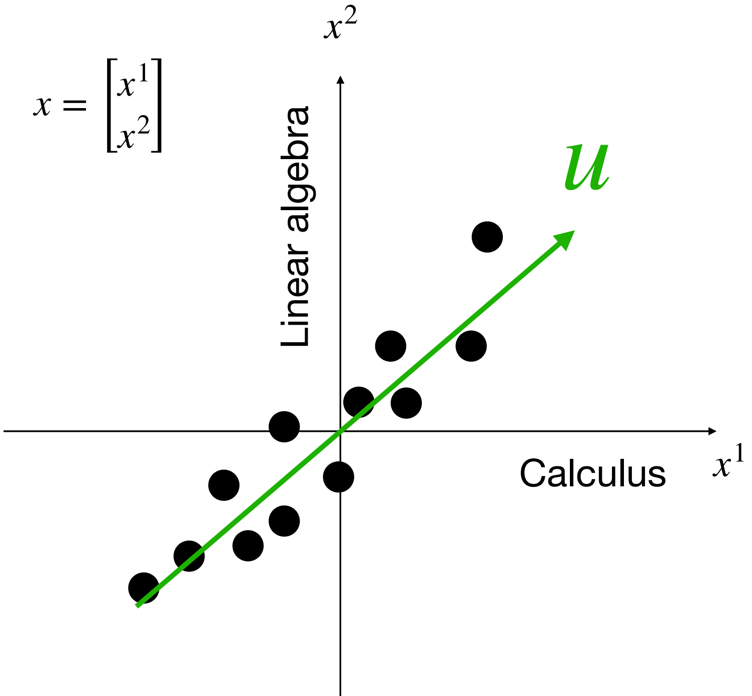

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Given $\mathcal{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^2$

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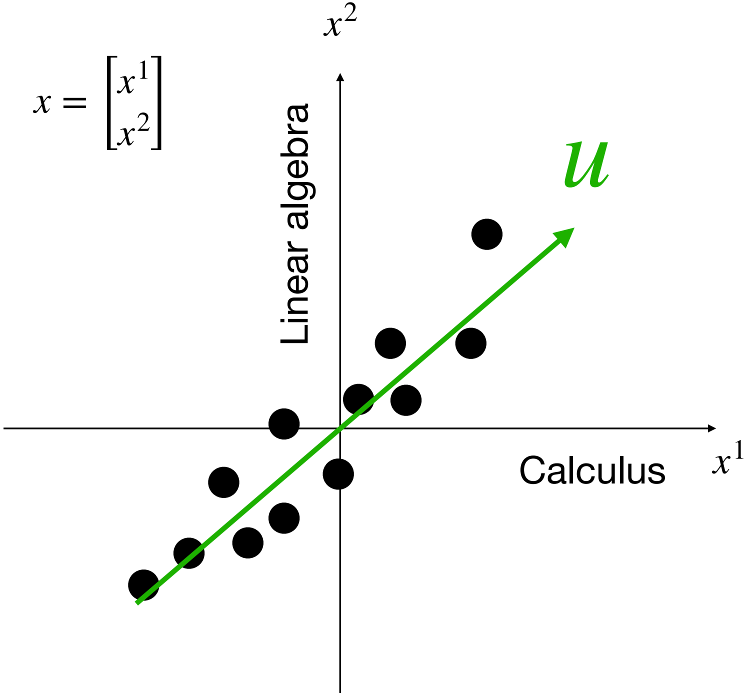

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Dim-reduction:

Given $\mathcal{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^2$

We get a 1-d dataset

$\mathcal{Z} = \{z_1, \ldots, z_n\}$, where $z_i = u^\top x_i$

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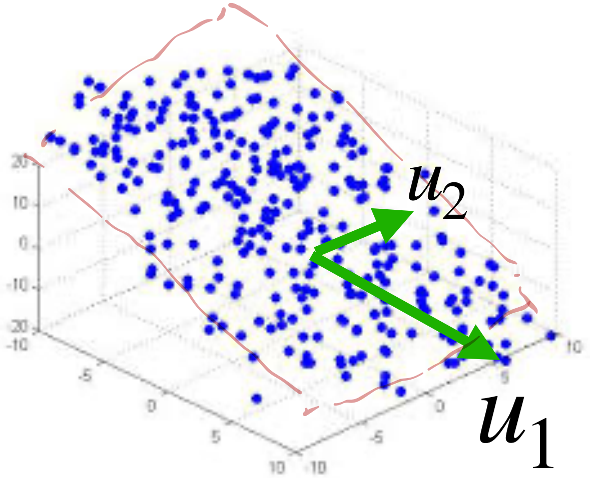

Reduce data from 3-d to 2-d:

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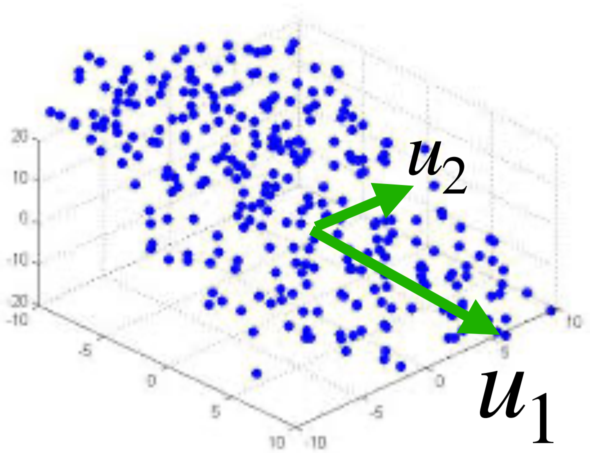

Reduce data from 3-d to 2-d:

$$u_1 \in \mathbb{R}^3, u_2 \in \mathbb{R}^3$$

$$\mathscr{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^3$$

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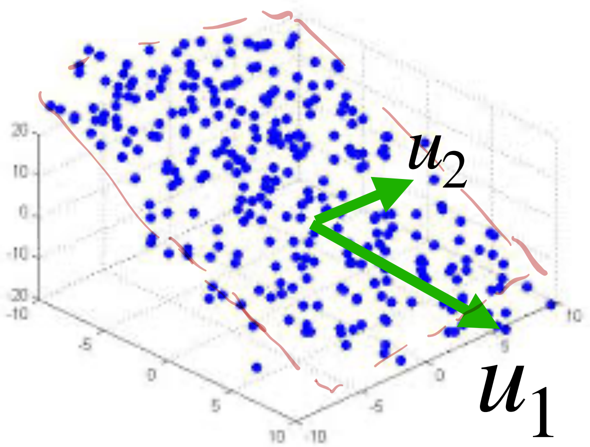

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$$\mathcal{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^3$$

$$\Downarrow$$

$$\mathcal{Z} = \{z_1, \ldots, z_n\}, z_i \in \mathbb{R}^3, z_i = [u_1^\top x_i, u_2^\top x_i]^\top$$

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1. Intro of PCA

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3. Example of PCA: eigenfaces

Compute the Principle Component

Setup

Input: dataset $\mathscr{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^d$ $X = [x_1, x_2, \ldots, x_n] \in \mathbb{R}^{d \times n}$

$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix}$

Compute the Principle Component

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Assume data is centered, i.e.,

$$\sum_{i=1}^{n} x_i / n = 0$$

(Otherwise, compute the mean and shift every data point)

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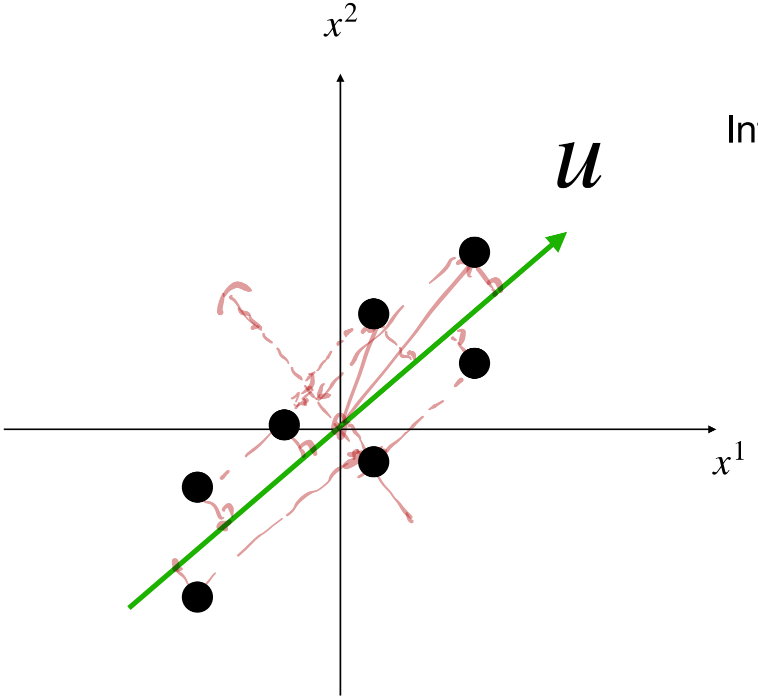
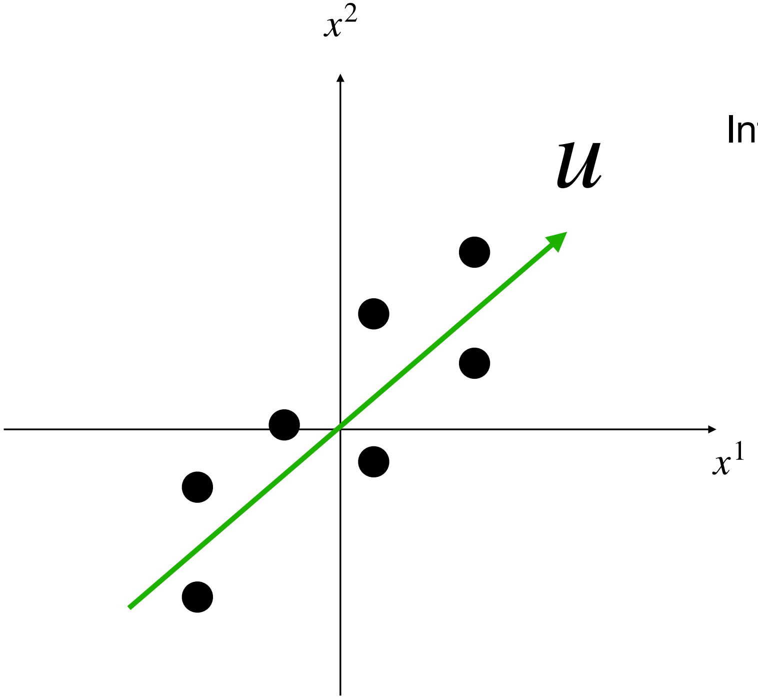
Output: K principle components $u_1, \ldots, u_K$ (they are orthonormal)

Compute the Principle Component



Intuition: find a direction such that the projected points are spread out

Compute the Principle Component



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Mathematically, maximizes the variance of projected points

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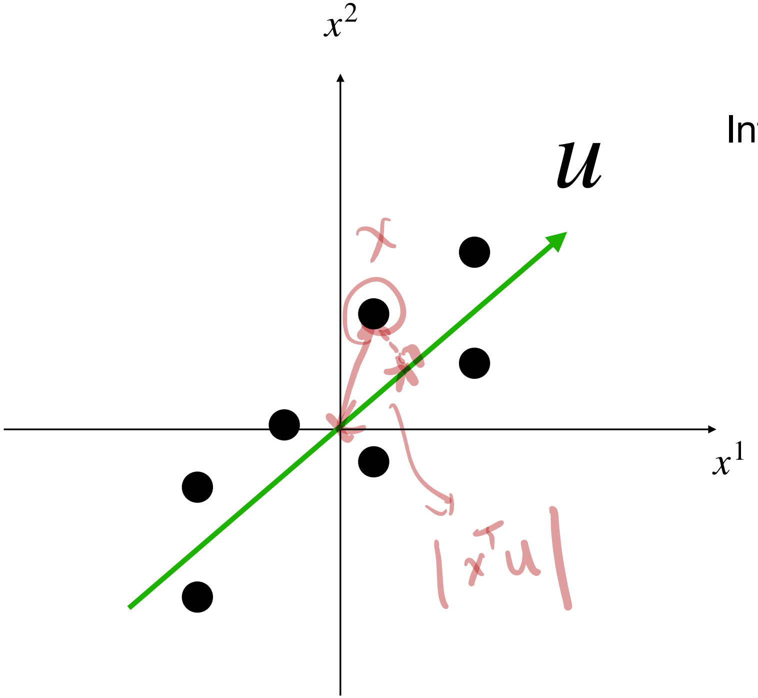
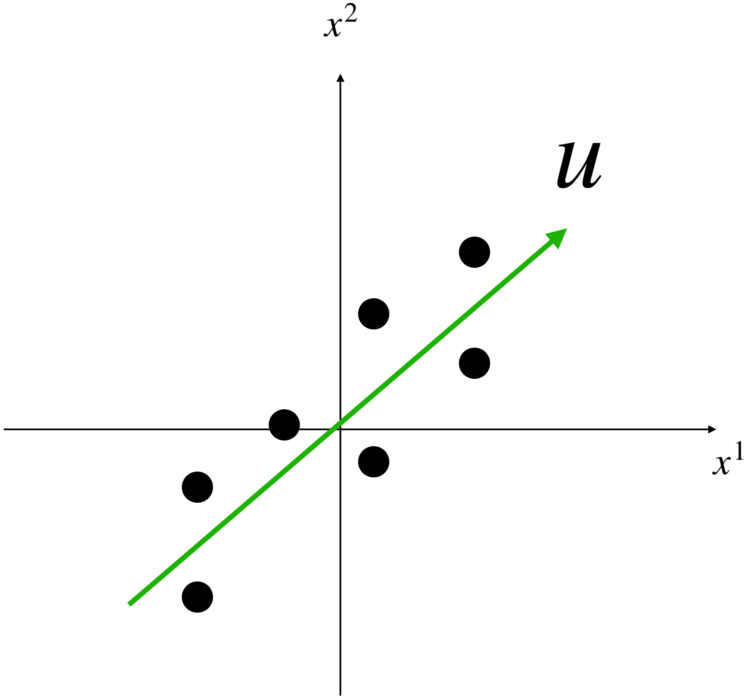


Intuition: find a direction such that the projected points are spread out

Mathematically, maximizes the variance of projected points

$$\max_{u:\|u\|_2=1} \sum_{i=1}^{n} (x_i^\top u)^2$$

Compute the Principle Component



$$(x_i^\top u)^2 = (u^\top x_i x_i^\top u)$$

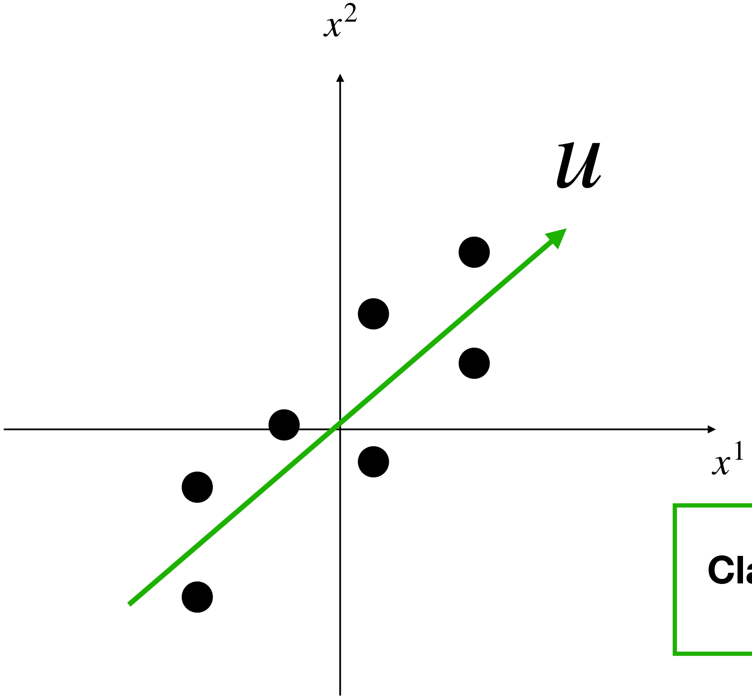
$$\arg\max_{u:\|u\|_2=1} \sum_{i=1}^{n} (x_i^\top u)^2$$

$$= \arg\max_{u:\|u\|_2=1} u^\top \underbrace{\left[\sum_{i=1}^{n} x_i x_i^\top\right]}_{XX^\top} u$$

$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \dots & x_n \\ | & | & & | \end{bmatrix}$$

$$\sum_{i=1}^{n} x_i x_i^\top = XX^\top$$

Compute the Principle Component



$$\arg\max_{u:\|u\|_2=1} \sum_{i=1}^{n} (x_i^\top u)^2$$

$$= \arg\max_{u:\|u\|_2=1} u^\top \underbrace{\left[\sum_{i=1}^{n} x_i x_i^\top\right]}_{XX^\top} u$$

Claim: the maximizer is the first eigenvector of $XX^\top$

Compute the Principle Component

Definition of Eigenvalue/Eigenvectors

(λ, u) is a pair of eigenvalue / eigenvector if:

$$(XX^\top)u = \lambda u$$

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$$XX^\top = \sum_{i=1}^{n} x_i x_i^\top \in \mathbb{R}^{d\times d}$$

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Eigendecomposition:

$$XX^\top = U\Lambda U^\top$$

$$= \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_d \\ | & | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_d \end{bmatrix} \begin{bmatrix} - & u_1^\top & - \\ - & u_2^\top & - \\ & \vdots & \\ - & u_d^\top & - \end{bmatrix}$$

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \lambda_d \geq 0$$

$$\arg\max_{u:\|u\|_2=1} \sum_{i=1}^{n} (x_i^\top u)^2$$

$$= \arg\max_{u:\|u\|_2=1} u^\top \underbrace{\left[\sum_{i=1}^{n} x_i x_i^\top\right]}_{XX^\top} u$$

$$u_1^\top (XX^\top) u_1 = \lambda_1$$

↑ largest eigenvalue

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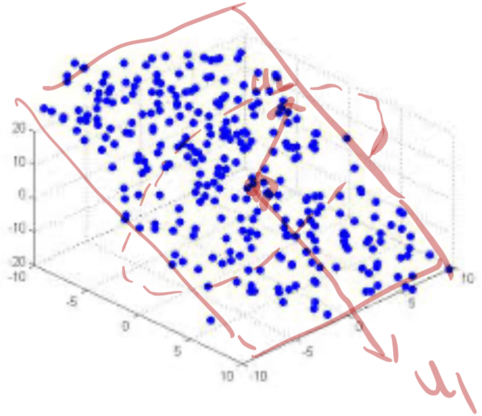
Solution:

The arg max returns the first eigenvector of $XX^\top$

What about computing the second principle component?

First Principle component $u_1 = \arg\max_{u:\|u\|_2=1} \sum_{i=1}^{n} (x_i^\top u)^2$



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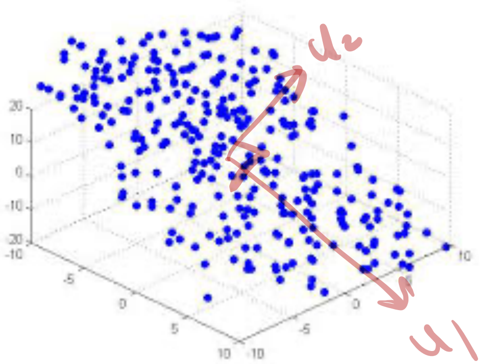

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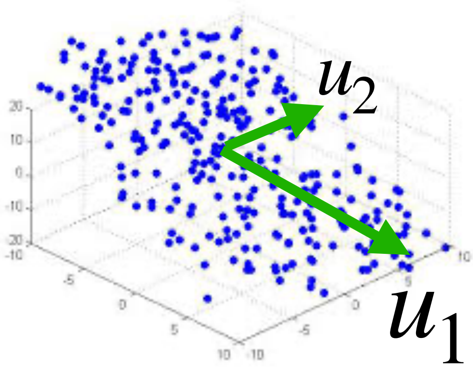

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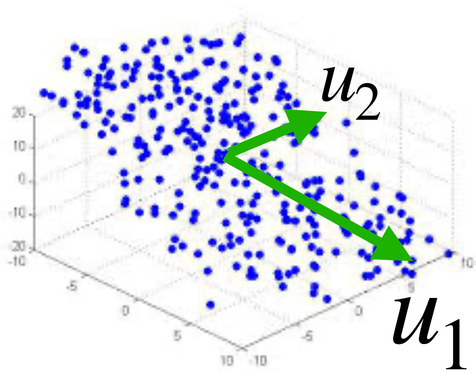

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Force constraints: $\|u_2\|_2 = 1,\ u_2^\top u_1 = 0$

$$u_2 = \arg \max_{u:\|u\|_2=1, u^\top u_1 = 0} \sum_{i=1}^{n} (x_i^\top u)^2$$

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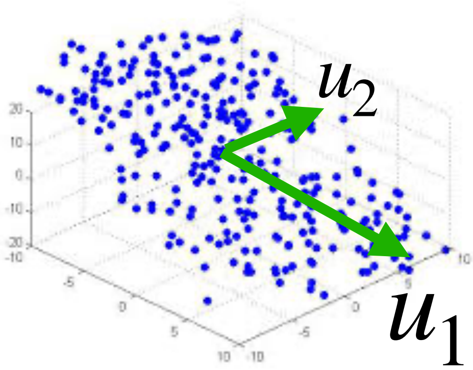

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u_2

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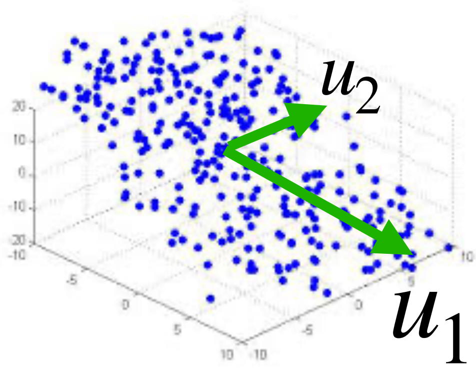

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Solution: u_2 will be the second eigenvector

Algorithm: PCA

Input: given the centered dateset $\mathscr{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^d$, and parameter $K < d$

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Algorithm: PCA

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λ

1. Compute **Eigendecomposition** of $XX^\top := U\Sigma U^\top$

2. Return the **top K eigenvectors** (corresponding to the top k largest eigenvalues)

$$U = [\quad \underbrace{u_1, u_2, \ldots, u_k,}_{\text{top k eigenvectors}} \quad u_{k+1} \ldots, u_d], u_i \in \mathbb{R}^d$$

Algorithm for data compression via PCA

$x_i \in \mathbb{R}^d$

Input: the centered dateset $\mathscr{D} = \{x_1, \ldots, x_n\}$, parameter K

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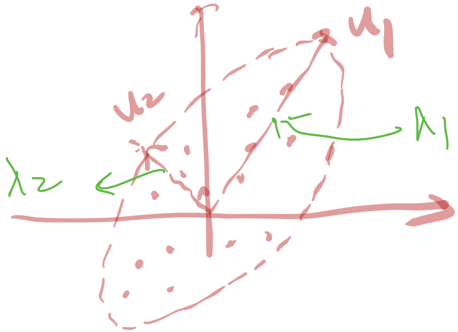
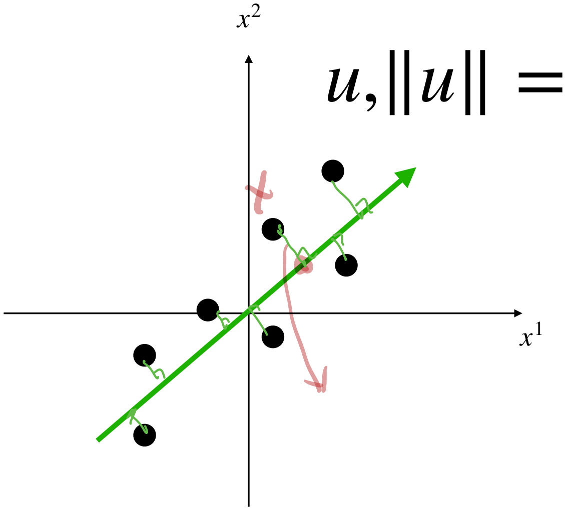
$\det(xx^\top)$

2. $\forall x \in \mathscr{D}$, compute $z = [u_1^\top x, u_2^\top x, \ldots, u_K^\top x]^\top \in \mathbb{R}^K$

Output: K-dim dataset $\mathscr{Z} = \{z_1, \ldots, z_n\}, z_i \in \mathbb{R}^K$



Think about PCA from a data re-construction perspective



$$u, \|u\| = 1$$

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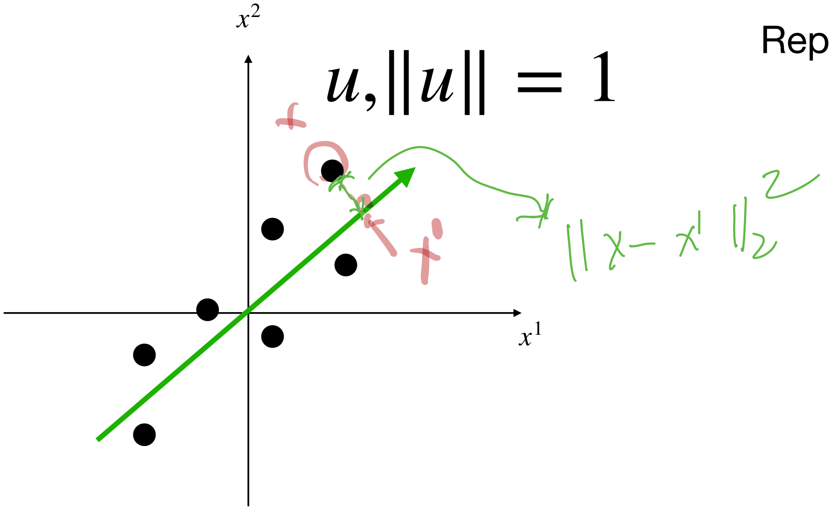

Represent x using u: $x \rightarrow (x^\top u)u$
(i.e., project x on u)

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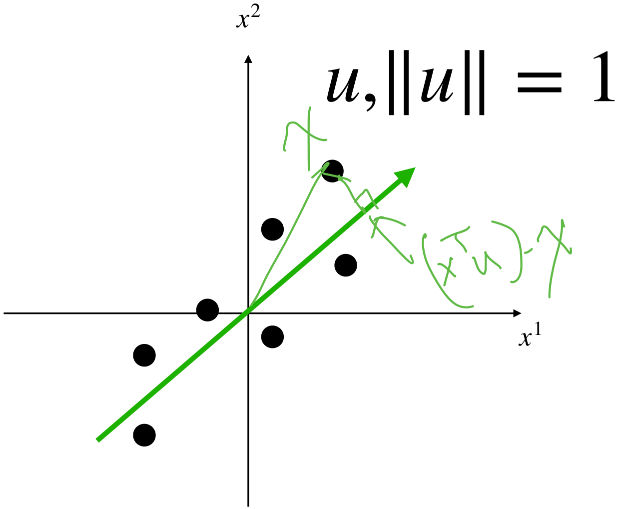

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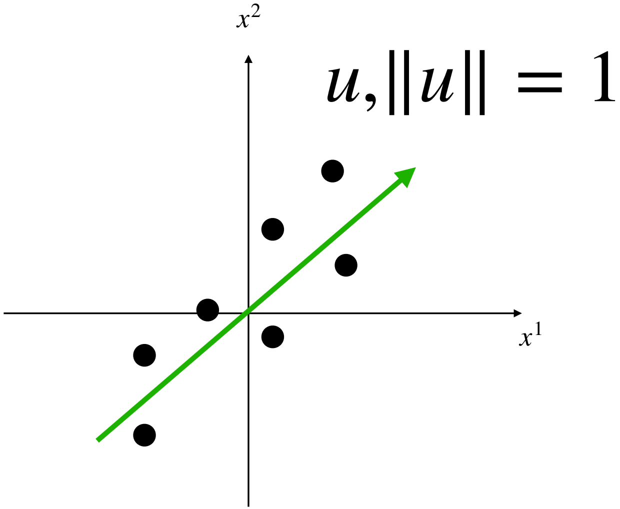

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PCA first principle component procedure : find u that minimizes the total reconstruction error

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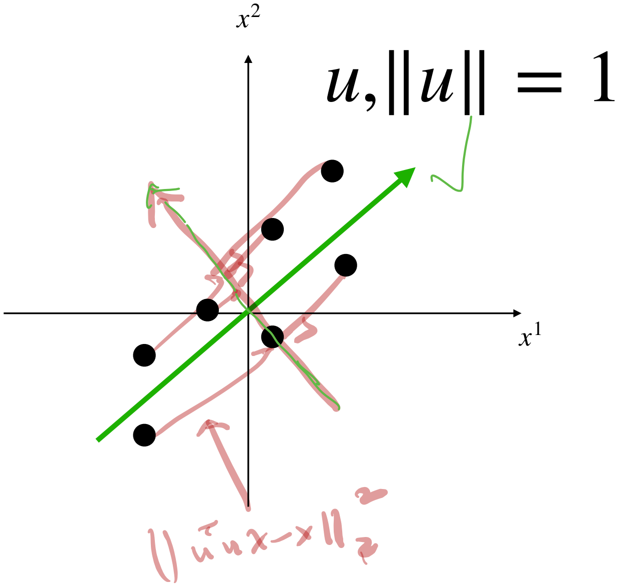

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PCA first principle component procedure : find u that minimizes the total reconstruction error

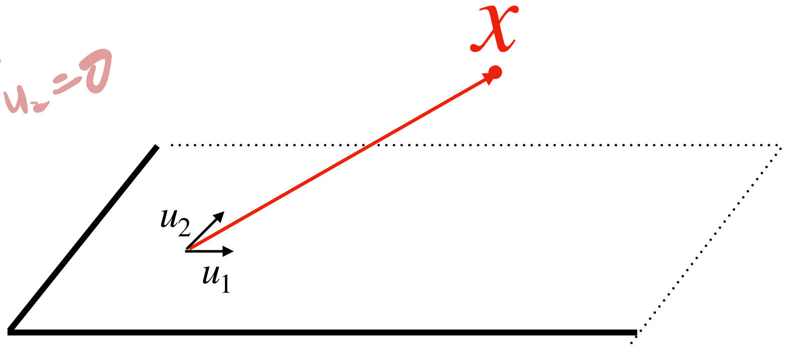
$$\arg\min_{u:\|u\|_2=1} \sum_{i=1}^{n} \|uu^\top x_i - x_i\|_2^2$$

projected point of Xi on U

Think about PCA from a data re-construction perspective

$x \in R^3$

$u_1^T u_2 = 0$



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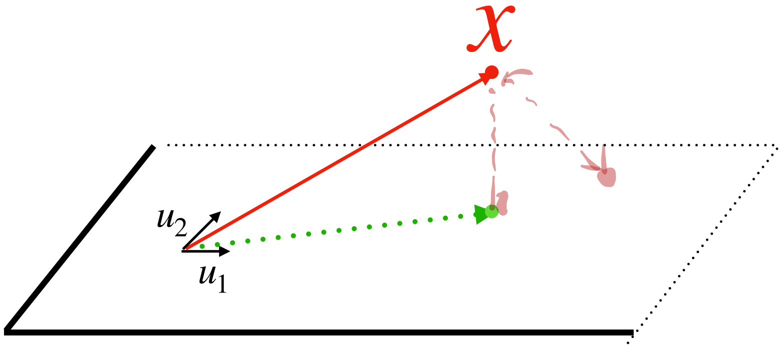

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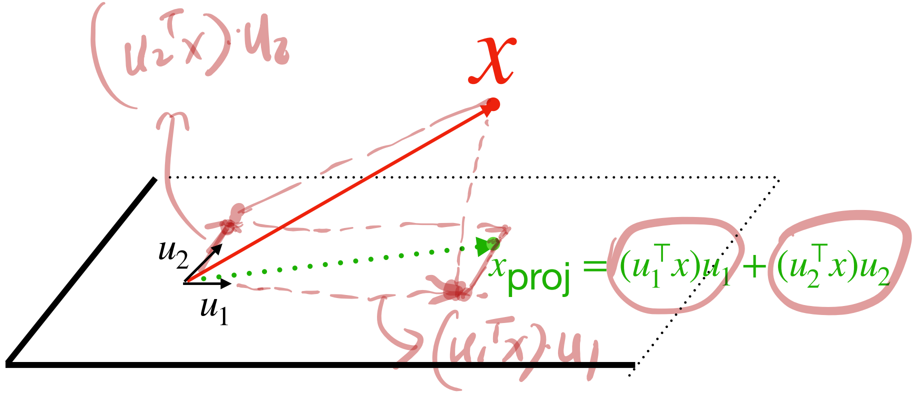
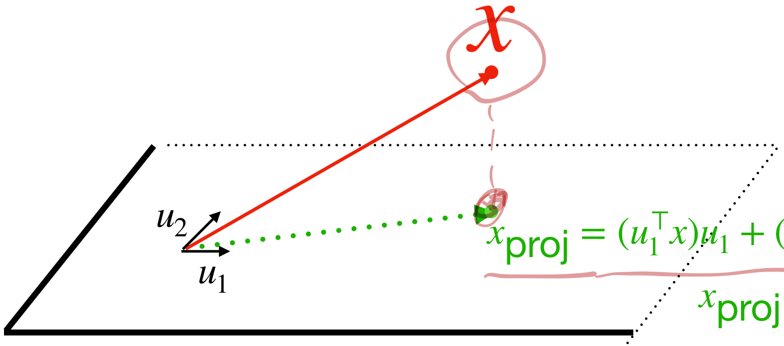


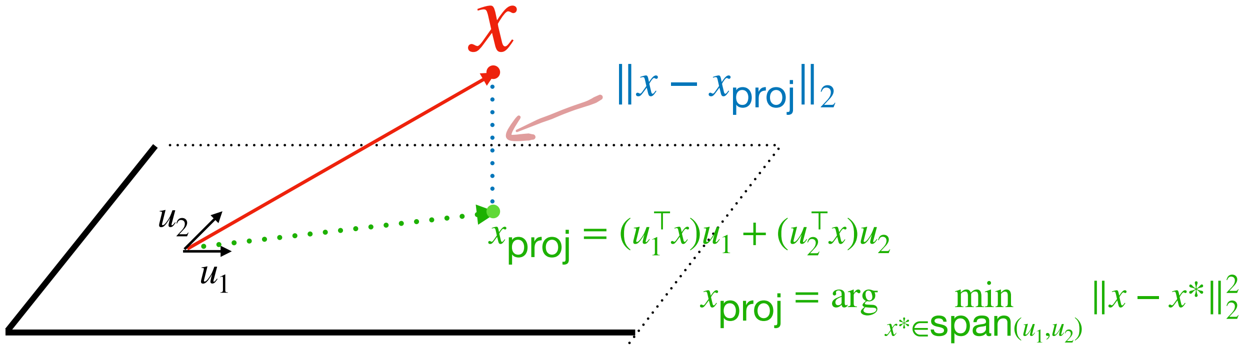
Think about PCA from a data re-construction perspective



$$x_{\text{proj}} = (u_1^\top x)u_1 + (u_2^\top x)u_2$$

$$x_{\text{proj}} = \arg \min_{x^* \in \text{span}(u_1, u_2)} \|x - x^*\|_2^2$$

Think about PCA from a data re-construction perspective



Think about PCA from a data re-construction perspective

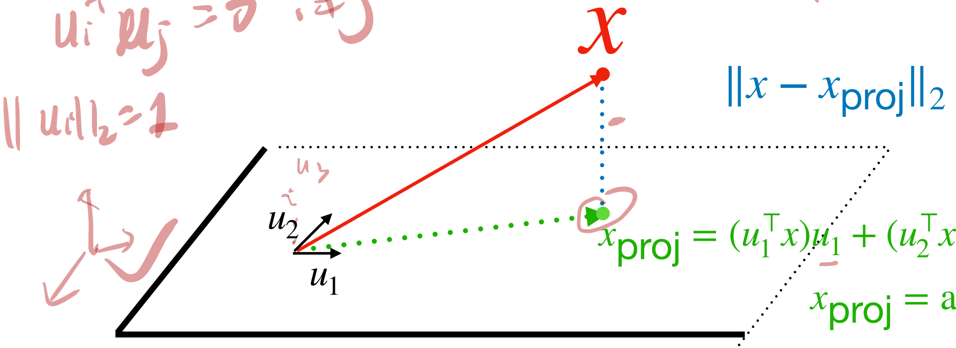
Another way to think about PCA is to find $u_1, u_2, \ldots, u_k$ to minimize re-construction error

$$\min_{u_1, u_2, \ldots, u_k} \sum_{i=1}^{n} \left\| \sum_{j=1}^{k} (u_j^\top x_i) u_j - x_i \right\|_2^2, \text{ s.t. } \forall i : u_i^\top u_i = 1, \text{ and } u_i^\top u_j = 0, \forall i \neq j$$

$\to \|x_i - x_{i,proj}\|_2^2$

$u_i^\top u_j = 0 \quad i \neq j$

$\|u_i\|_2 = 1$



$$x_{\text{proj}} = (u_1^\top x) u_1 + (u_2^\top x) u_2$$

$$x_{\text{proj}} = \arg \min_{x^* \in \text{span}(u_1, u_2)} \|x - x^*\|_2^2$$

Outline for today:

1. Intro of PCA

2. PCA via eigendecomposition

3. Example of PCA: eigenfaces

Application of PCA: Eigenfaces

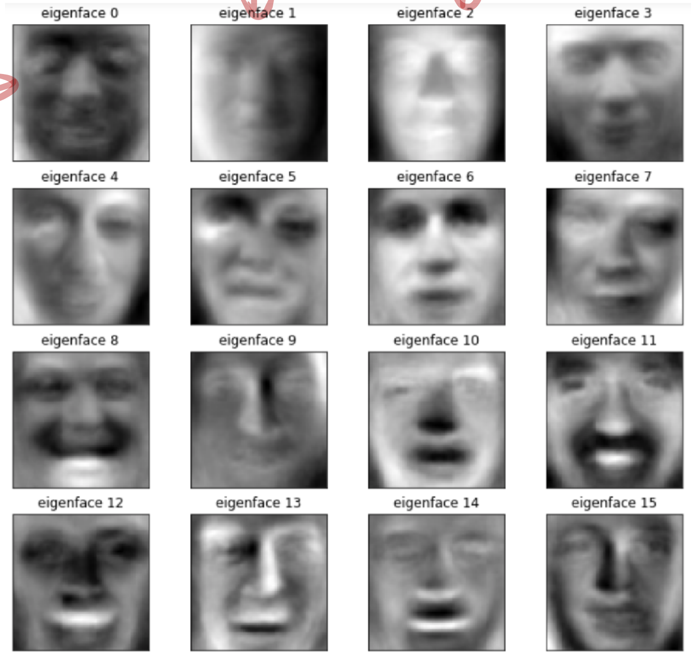
$$\mathcal{D} = \{x_1, \ldots, x_n\}, x_i \in \mathbb{R}^{64^2}$$

64×64

→ reshape 2-d image to 1-d vector

Application of PCA: Eigenfaces

The top 15 Eigenfaces (top 15 eigenvectors reshaped into 64×64 matrices)



Application of PCA: Eigenfaces

Reconstruct original images using Eigenfaces

Application of PCA: Eigenfaces

Reconstruct original images using Eigenfaces

Given $x \in \mathbb{R}^{64^2}$, and top K eigenvectors $u_1, \ldots, u_k$, we can approximate x as follows:

$$x' = (x^\top u_1)u_1 + (x^\top u_2)u_2 + \ldots + (x^\top u_k)u_k$$

projection of x on span$\{u_1, \ldots, u_k\}$

Application of PCA: Eigenfaces

Reconstruct original images using Eigenfaces

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(Q: when $k \to 64^2$, we should expect $x' \to x$, why?)

Application of PCA: Eigenfaces

Reconstruct original images using Eigenfaces

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(Q: when $k \to 64^2$, we should expect $x' \to x$, why?)

Recall that PCA is about finding $u_1, u_2, \ldots, u_k$ to minimize re-construction error

$$\min_{u_1, u_2, \ldots, u_k} \sum_{i=1}^{n} \left\| \sum_{j=1}^{k} (u_j^\top x_i) u_j - x_i \right\|_2^2, \text{ s.t. } \forall i : u_i^\top u_i = 1, \text{ and } u_i^\top u_j = 0, \forall i \neq j$$

project in on span$\{u_1, u_2 \dots u_{50}\}$

Application of PCA: Eigenfaces

Reconstruct images using top 50 eigenfaces

projection

Application of PCA: Eigenfaces

projecting it on span{$u_1, \ldots, u_{200}$}

Reconstruct images using top 200 eigenfaces

$k = 200$

Summary

1. The PCA algorithm: Eigendecomposition on $XX^\top$

2. Dimensionality reduction and Data reconstruction via PCA