Machine Learning
ITCS 6156/8156

Principal Component Analysis

Whitening

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Principal Component Analysis (PCA)

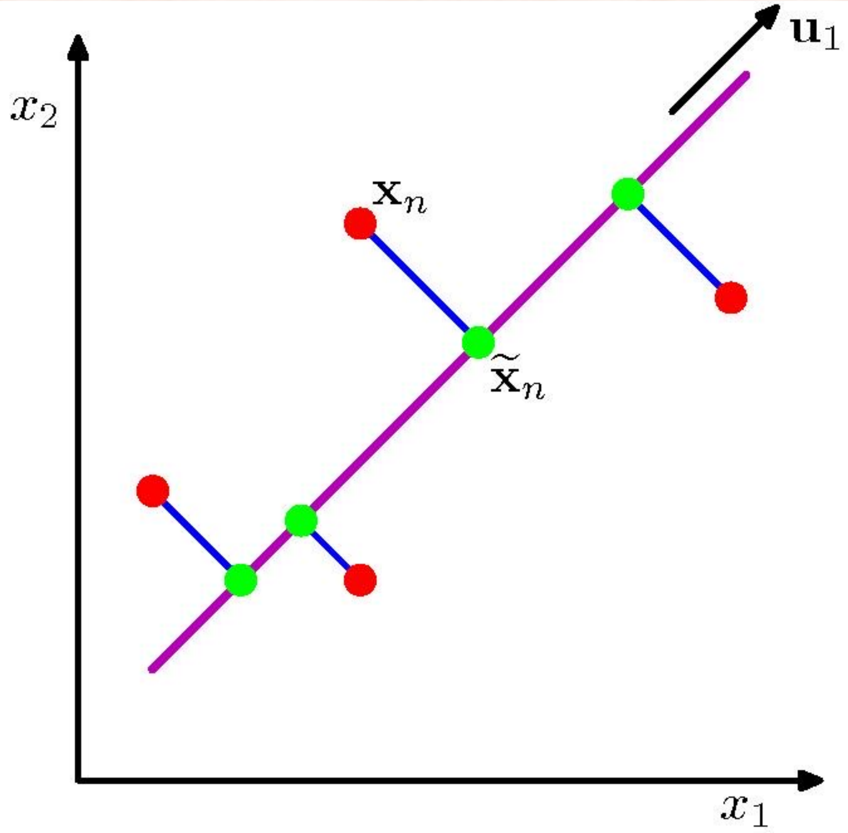
- A technique widely used for:
  - dimensionality reduction.
  - data compression.
  - feature extraction.
  - data visualization.

- Two equivalent definitions of PCA:
  1) Project the data onto a lower dimensional space such that the variance of the projected data is *maximized*.
  2) Project the data onto a lower dimensional space such that the mean squared distance between data points and their projections (average projection cost) is *minimized*.

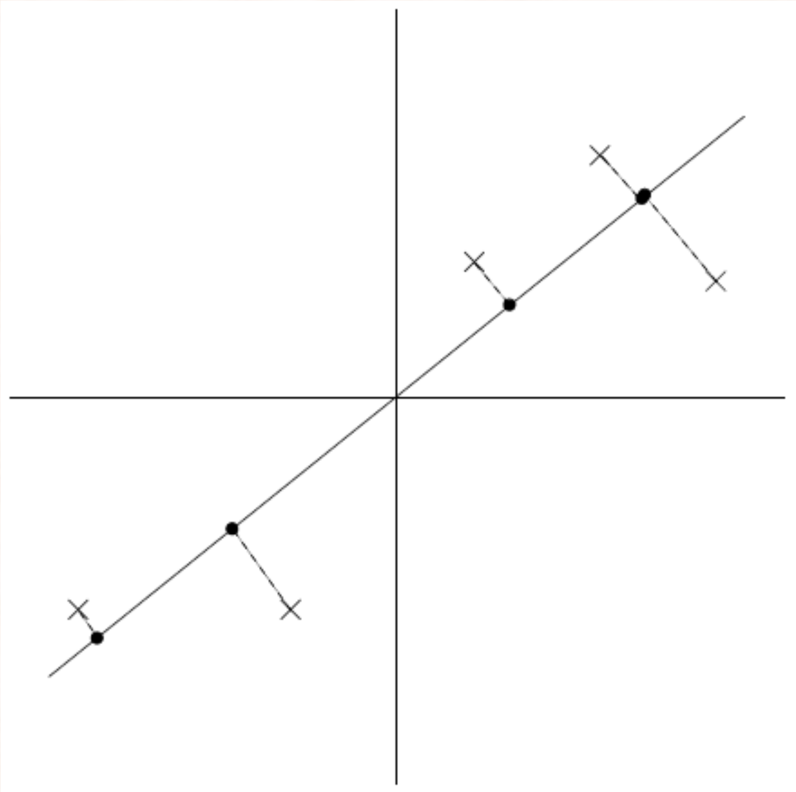
maximum variance

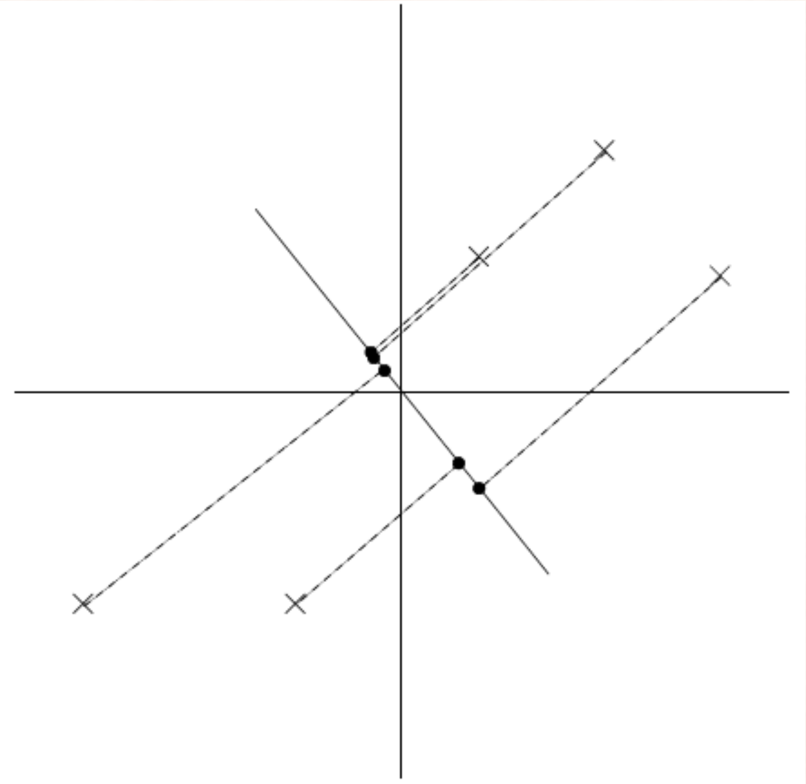
minimum error

Principal Component Analysis (PCA)



Principal Component Analysis (PCA)





PCA (Maximum Variance)

- Let X = $\{\mathbf{x}_n\}_{1 \leq n \leq N}$ be a set of observations:
  - Each $\mathbf{x}_n \in R^D$ (D is the dimensionality of $\mathbf{x}_n$).
- Project X onto an M dimensional space ($M < D$) such that the *variance* of the projected X is *maximized*.
  - Minimum error formulation leads to the same solution [PRML 12.1.2].
    - shows how PCA can be used for compression.
- Work out solution for $M = 1$, then generalize to any $M < D$.

PCA (Maximum Variance, $M = 1$)

- The lower dimensional space is defined by a vector $\mathbf{u}_1 \in R^D$.
  - Only direction is important $\Rightarrow$ choose $||\mathbf{u}_1||=1$.
- Each $\mathbf{x}_n$ is projected onto a scalar $\mathbf{u}_1^T \mathbf{x}_n$
- The (sample) mean of the data is:

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

- The (sample) mean of the projected data is $\mathbf{u}_1^T \overline{\mathbf{x}}$

PCA (Maximum Variance, $M = 1$)

- The (sample) variance of the projected data:

$$\frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{u}_1^T\mathbf{x}_n - \mathbf{u}_1^T\overline{\mathbf{x}}\right)^2 = \mathbf{u}_1^T\boldsymbol{\Sigma}\mathbf{u}_1$$

where $\boldsymbol{\Sigma}$ is the data covariance matrix:

$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{x}_n - \overline{\mathbf{x}}\right)\left(\mathbf{x}_n - \overline{\mathbf{x}}\right)^T$$

- Optimization problem is:

minimize:

$$-\mathbf{u}_1^T\boldsymbol{\Sigma}\mathbf{u}_1$$

subject to:

$$\mathbf{u}_1^T\mathbf{u}_1 = 1$$

PCA (Maximum Variance, $M = 1$)

- Lagrangian function:

$$L_P(\mathbf{u}_1, \lambda_1) = -\mathbf{u}_1^T \mathbf{\Sigma} \mathbf{u}_1 + \lambda_1(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

where λ_1 is the *Lagrangian multiplier* for constraint $\mathbf{u}_1^T \mathbf{u}_1 = 1$

- Solve:

$$\frac{\partial L_P}{\partial \mathbf{u}_1} = 0 \Rightarrow \mathbf{\Sigma}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \Rightarrow \begin{cases} \mathbf{u}_1 \text{ is an eigenvector of } \mathbf{\Sigma} \\ \lambda_1 \text{ is an eigenvalue of } \mathbf{\Sigma} \end{cases}$$

$$\Rightarrow -\mathbf{u}_1^T \mathbf{\Sigma} \mathbf{u}_1 = -\lambda_1 \mathbf{u}_1^T \mathbf{u}_1 = -\lambda_1$$

$\Rightarrow \lambda_1$ is the largest eigenvalue of $\mathbf{\Sigma}$.

PCA (Maximum Variance, $M = 1$)

- λ_1 is the largest eigenvalue of $\boldsymbol{\Sigma}$.
- $\mathbf{u}_1$ is the eigenvector corresponding to λ_1:
  - also called the *first principal component*.

- For $M < D$ dimensions:
  - $\mathbf{u}_1\ \mathbf{u}_2 \ldots \mathbf{u}_M$ are the eigenvectors corresponding to the largest eigenvalues $\lambda_1\ \lambda_2 \ldots \lambda_M$ of $\boldsymbol{\Sigma}$.
  - proof by induction.

PCA on Normalized Data

- Preprocess data $X = \{\mathbf{x}^{(i)}\}_{1 \leq i \leq m}$ such that:
  - features have the same *mean* (0).
  - features have the same *variance* (1).

1. Let $\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$.
2. Replace each $x^{(i)}$ with $x^{(i)} - \mu$.
3. Let $\sigma_j^2 = \frac{1}{m}\sum_i (x_j^{(i)})^2$
4. Replace each $x_j^{(i)}$ with $x_j^{(i)}/\sigma_j$.

PCA on Natural Images

- **Stationarity**: the statistics in one part of the image should be the same as any other.
  - ⇒ no need for variance normalization.
  - ⇒ do mean normalization by subtracting from each image its mean intensity.

$$\mu^{(i)} := \frac{1}{n}\sum_{j=1}^{n} x_j^{(i)}$$

$$x_j^{(i)} := x_j^{(i)} - \mu^{(i)}$$

PCA on Normalized Data

- The covariance matrix is:

$$\mathbf{\Sigma} = \frac{1}{m} X X^T = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}^{(i)} \left(\mathbf{x}^{(i)} \right)^T$$

- The eigenvectors are:

$$\mathbf{\Sigma u}_j = \lambda_j \mathbf{u}_j \quad \text{where} \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_D \text{ and } u_j^T u_j = 1$$

- Equivalent with:

$$\Sigma U = U \Lambda$$

$$U = [u_1, u_2, \ldots, u_D] \qquad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_D \text{ and } U^T U = I$$

$$\Lambda = diag(\lambda_1, \lambda_2, \ldots, \lambda_D)$$

PCA on Normalized Data

- U is an orthogonal (rotation) matrix, i.e. $U^T U = I$.
- The full transformation (rotation) of $x^{(i)}$ through PCA is:

$$y^{(i)} = U^T x^{(i)}$$

$$\Rightarrow x^{(i)} = U y^{(i)}$$

- The k-dimensional projection of $x^{(i)}$ through PCA is:

$$\hat{y}^{(i)} = U_{1,k}^T x^{(i)} = [u_1, \ldots, u_k]^T x^{(i)}$$

$$\Rightarrow \hat{x}^{(i)} = U_{1,k} \hat{y}^{(i)}$$

- How many components k should be used?

How many components *k* should be used?

- Compute *percentage of variance retained* by Y = $\{y^{(i)}\}$, for each value of *k*:

$$\hat{y}^{(i)} = [u_1, \ldots, u_k]^T x^{(i)}$$

$$Var(k) = \sum_{j=1}^{k} Var\left[\hat{y}_j\right] = \sum_{j=1}^{k} Var\left[u_j^T x\right]$$

$$= \sum_{j=1}^{k} \frac{1}{m} \sum_{i=1}^{m} \left(u_j^T x^{(i)} - u_j^T \bar{x}\right)^2 = \sum_{j=1}^{k} \underbrace{\frac{1}{m} \sum_{i=1}^{m} \left(u_j^T x^{(i)}\right)^2} = \sum_{j=1}^{k} \lambda_j$$

HW: *Prove it is* $\boldsymbol{\lambda_j}$

How many components *k* should be used?

- Compute *percentage of variance retained* by Y = $\{y^{(i)}\}$, for each value of *k*:
  - Variance retained:

$$Var(k) = \sum_{j=1}^{k} \lambda_j$$

  - Total variance:

$$Var(D) = \sum_{j=1}^{D} \lambda_j$$

  - Percentage of variance retained: $P(k) = \dfrac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{D} \lambda_j}$

How many components k should be used?

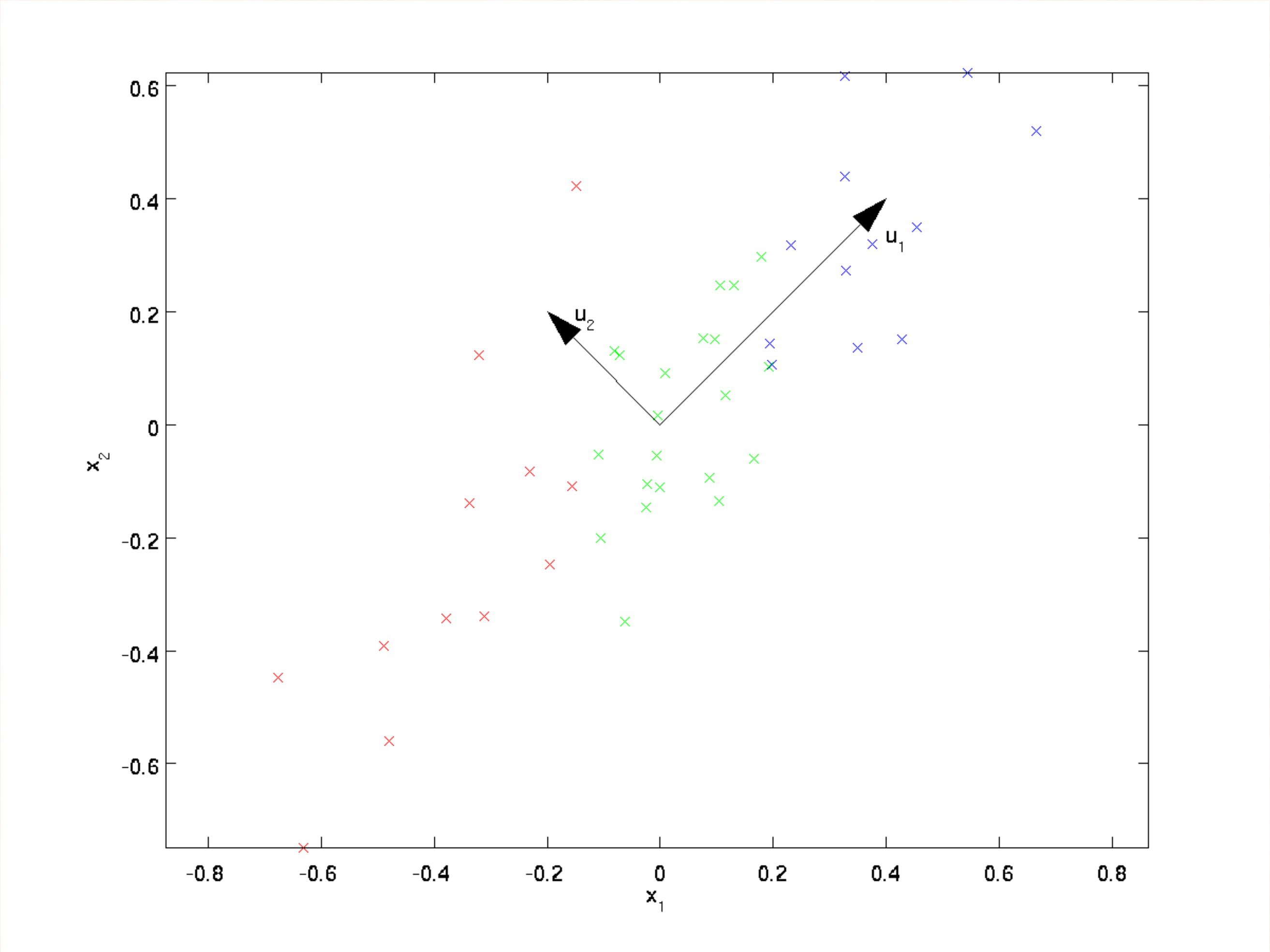
- Compute *percentage of variance retained* by $Y = \{y^{(i)}\}$, for each value of k:

$$P(k) = \frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{D} \lambda_j}$$

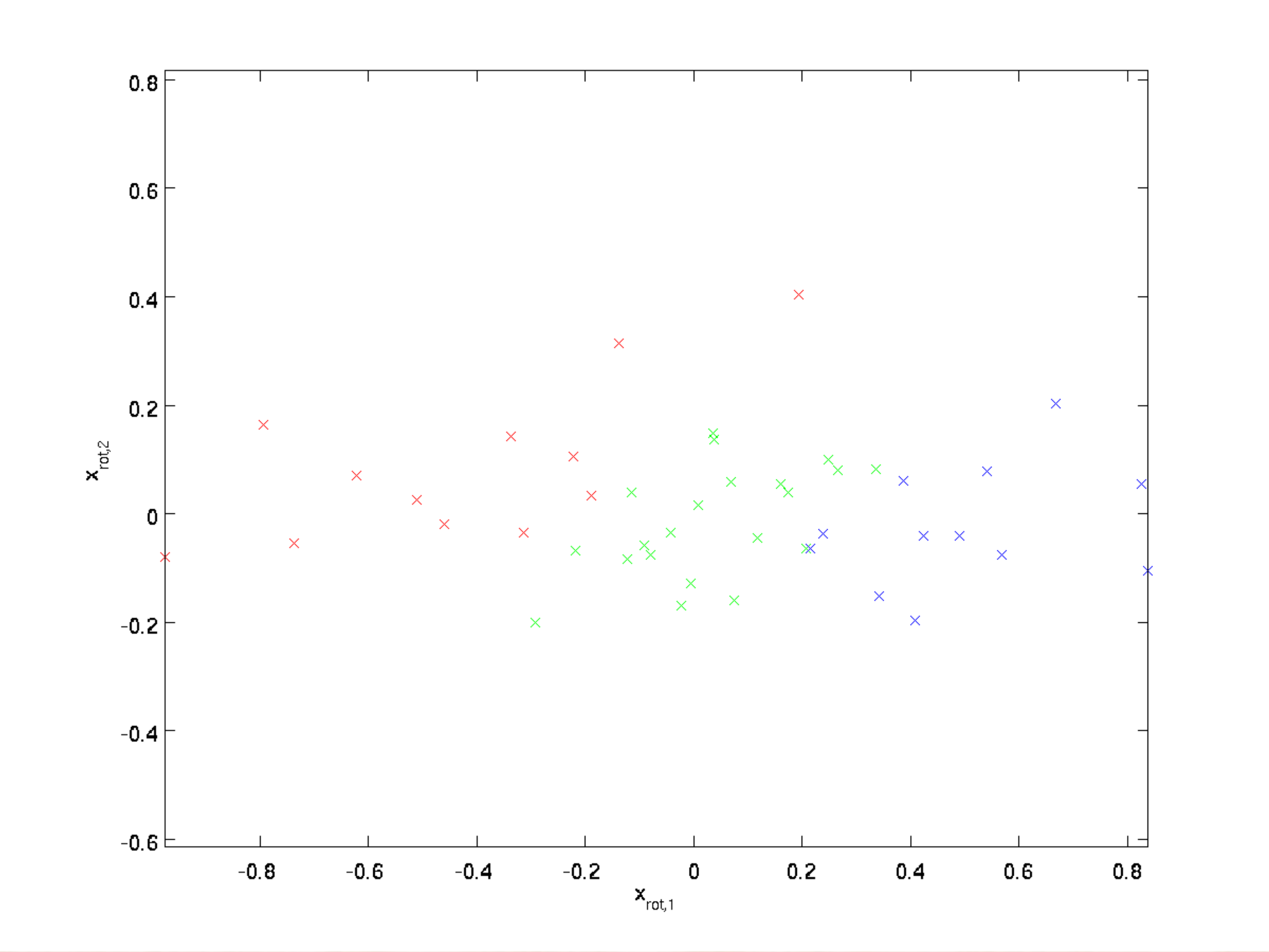
- Choose smallest k as to retain 99% of variance:

$$\hat{k} = \operatorname*{argmin}_{1 \le k \le D} \left[P(k) \ge 0.99 \right]$$

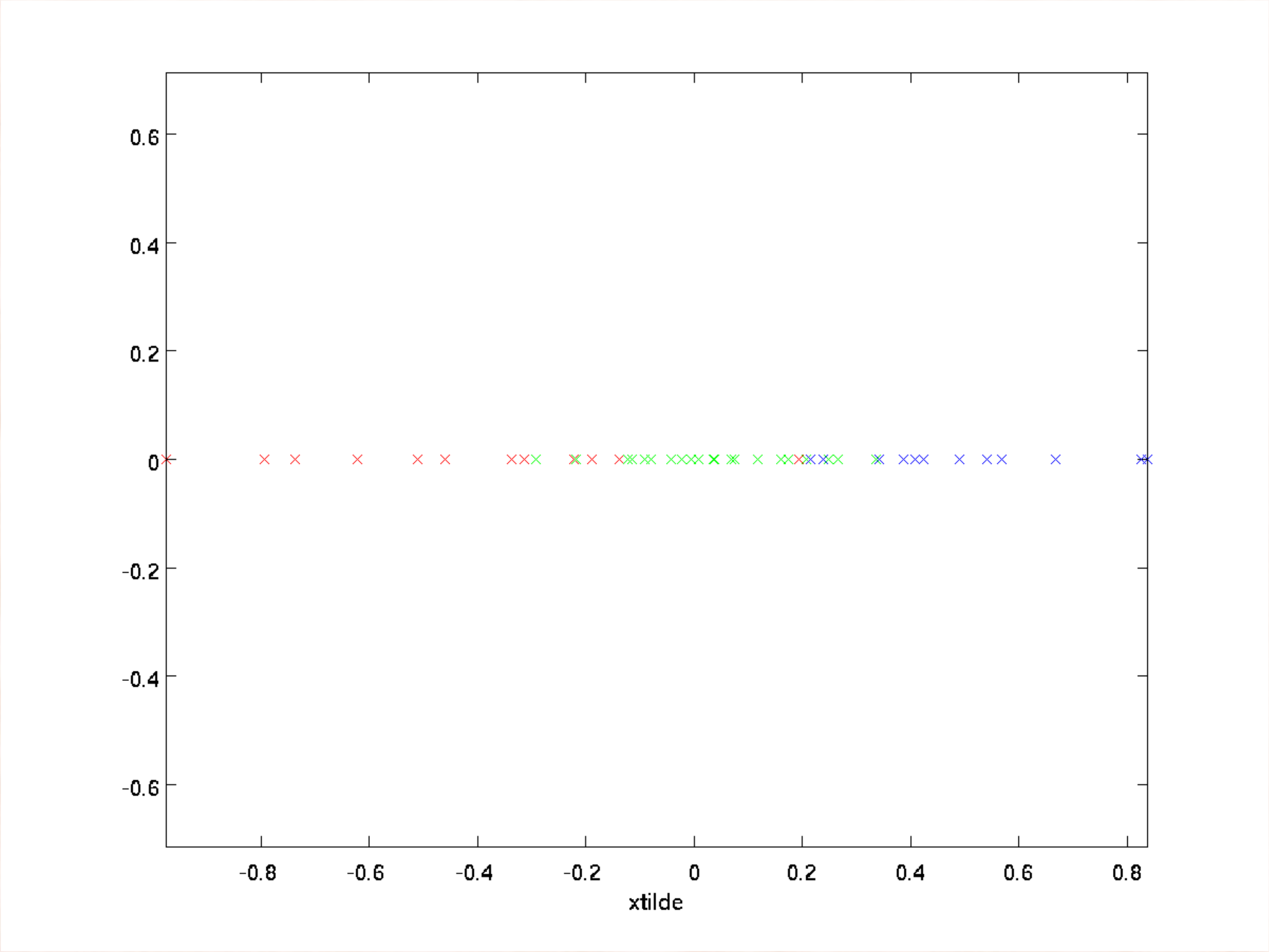
PCA on Normalized Data: $[x_1^{(i)}, x_2^{(i)}]^T$



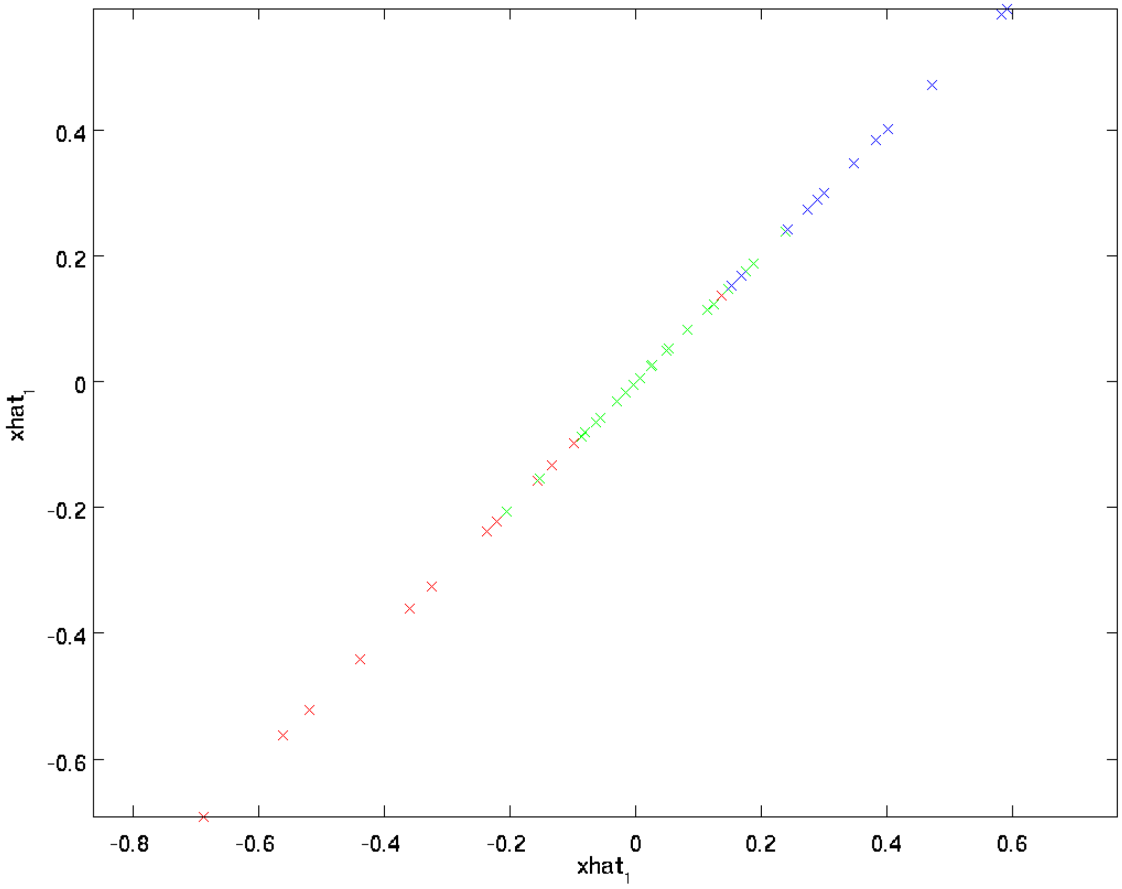
Rotation through PCA: $[u_1^T x^{(i)}, u_2^T x^{(i)}]^T$



1-Dimensional PCA Projection: $[u_1^T x^{(i)}, 0]^T$



1-Dimensional PCA Approximation: $u_1 u_1^T x^{(i)}$



PCA as a Linear Auto-Encoder

- The full transformation (rotation) of $x^{(i)}$ through PCA is:

$$y = U^T x \Rightarrow x = Uy$$

- The k-dimensional projection of $x^{(i)}$ through PCA is:

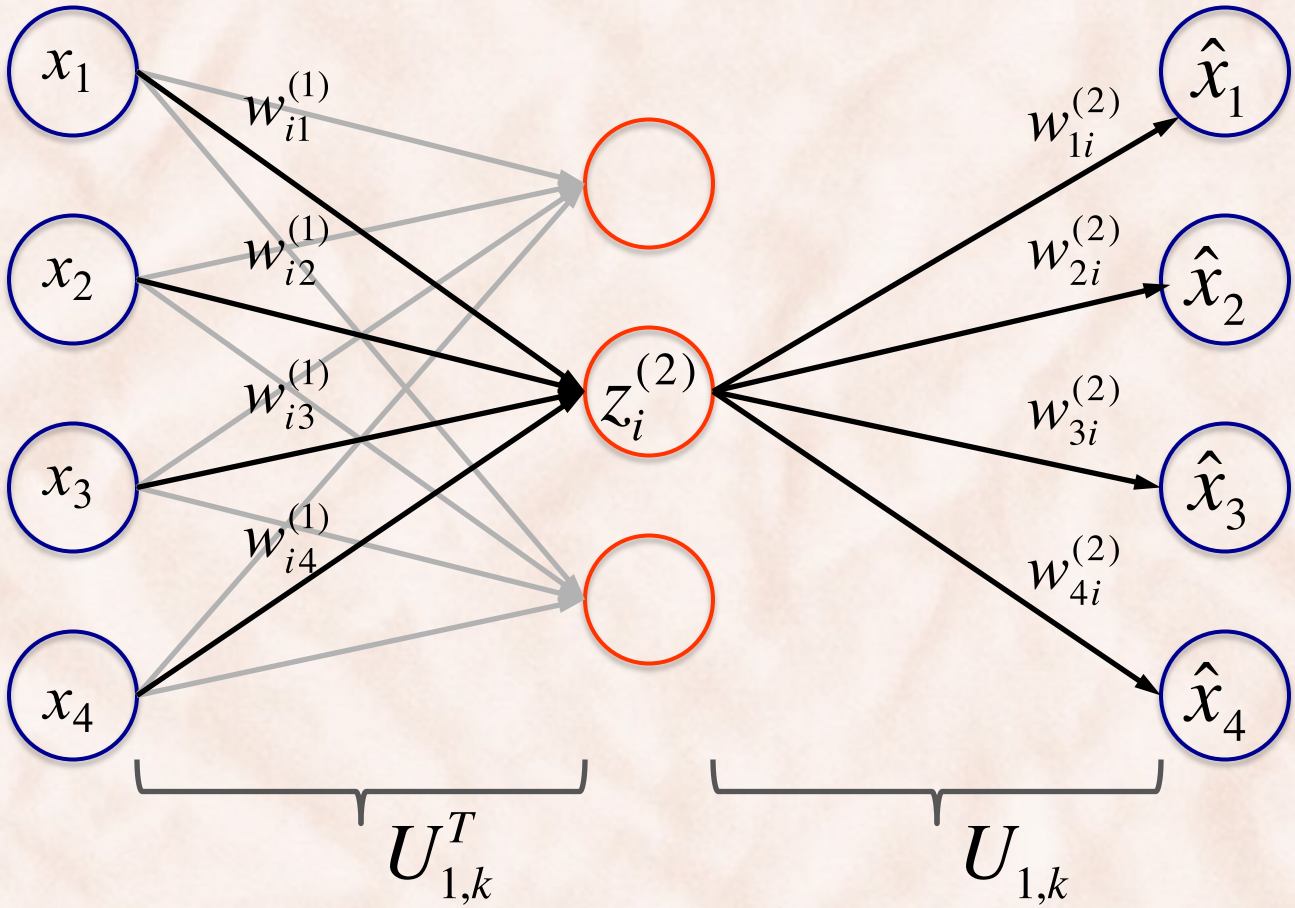
$$\hat{y} = U_{1,k}^T x = [u_1, \ldots, u_k]^T x \Rightarrow \hat{x} = U_{1,k}\hat{y} = U_{1,k}U_{1,k}^T x$$

- The minimum error formulation of PCA:

$$U_{1,k}^* = \arg\min_{U_{1,k}} \sum_{i=1}^{m} \left\| U_{1,k}U_{1,k}^T x^{(i)} - x^{(i)} \right\|^2$$

a linear auto-encoder with tied weights!

PCA as a Linear Auto-Encoder



$$u_i = \left[w_{i1}^{(1)}, w_{i2}^{(1)}, w_{i3}^{(1)}, w_{i4}^{(1)}\right]^T \qquad u_i = \left[w_{1i}^{(2)}, w_{2i}^{(2)}, w_{3i}^{(2)}, w_{4i}^{(2)}\right]^T$$

PCA and Decorrelation

- The full transformation (rotation) of $x^{(i)}$ through PCA is:

$$y^{(i)} = U^T x^{(i)} \Rightarrow Y = U^T X$$

- What is the covariance matrix of the rotated data Y?

$$\frac{1}{m} Y Y^T = \frac{1}{m} \left(U^T X\right)\left(U^T X\right)^T = \frac{1}{m} U^T X X^T U$$

$$= U^T \left(\frac{1}{m} X X^T\right) U = U^T \Sigma U = \Lambda$$

$$= diag(\lambda_1, \lambda_2, \ldots, \lambda_D)$$

=> the features in *y* are **decorrelated**!

PCA Whitening (Sphering)

- The goal of **whitening** is to make the input *less redundant*, i.e. the learning algorithm sees a training input where:
  1. The features are not correlated with each other.
  2. The features all have the same variance.

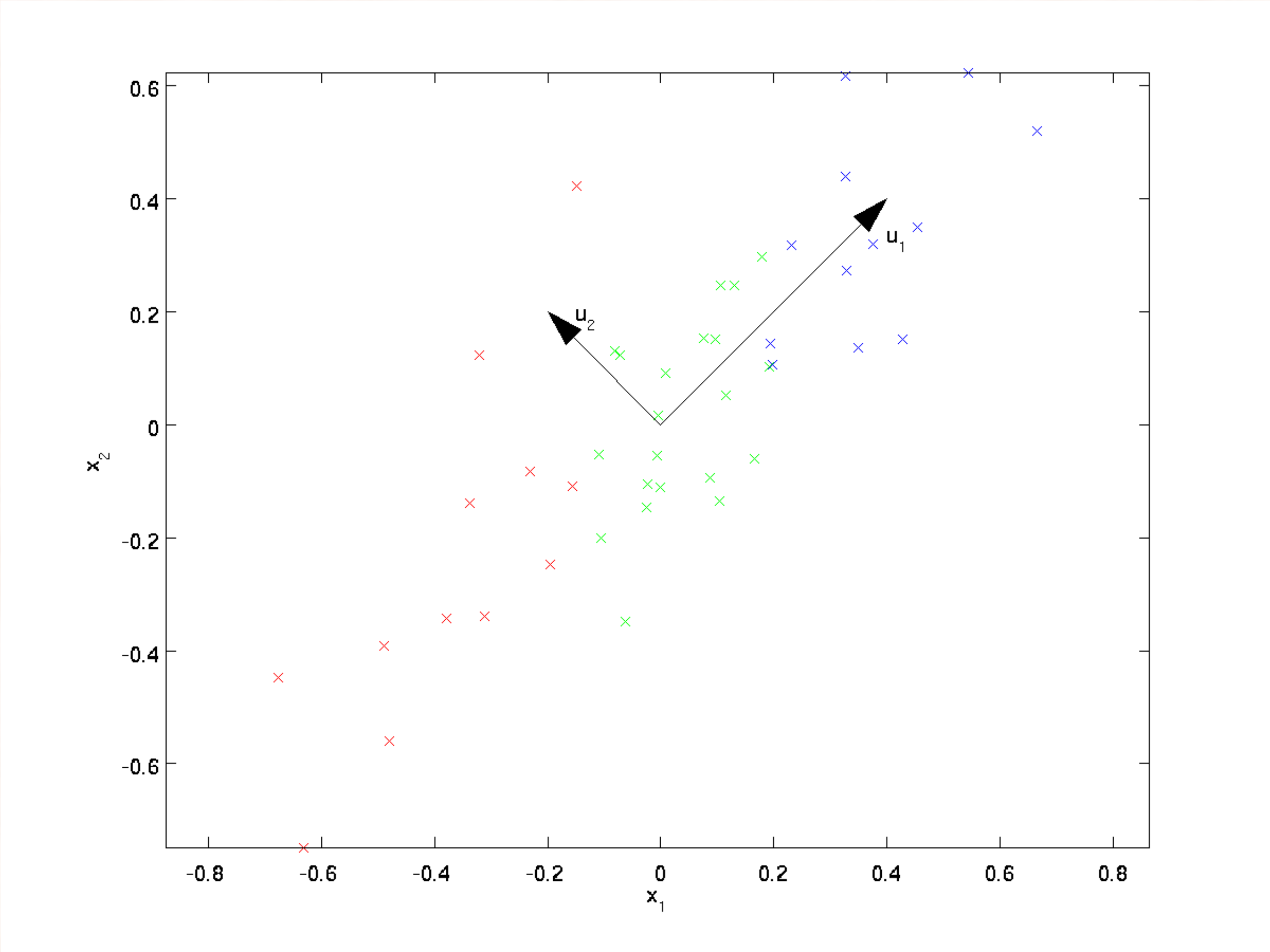
1. PCA already results in uncorrelated features:

$$y^{(i)} = U^T x^{(i)} \Leftrightarrow Y = U^T X \qquad \frac{1}{m} YY^T = diag(\lambda_1, \lambda_2, \ldots, \lambda_D)$$

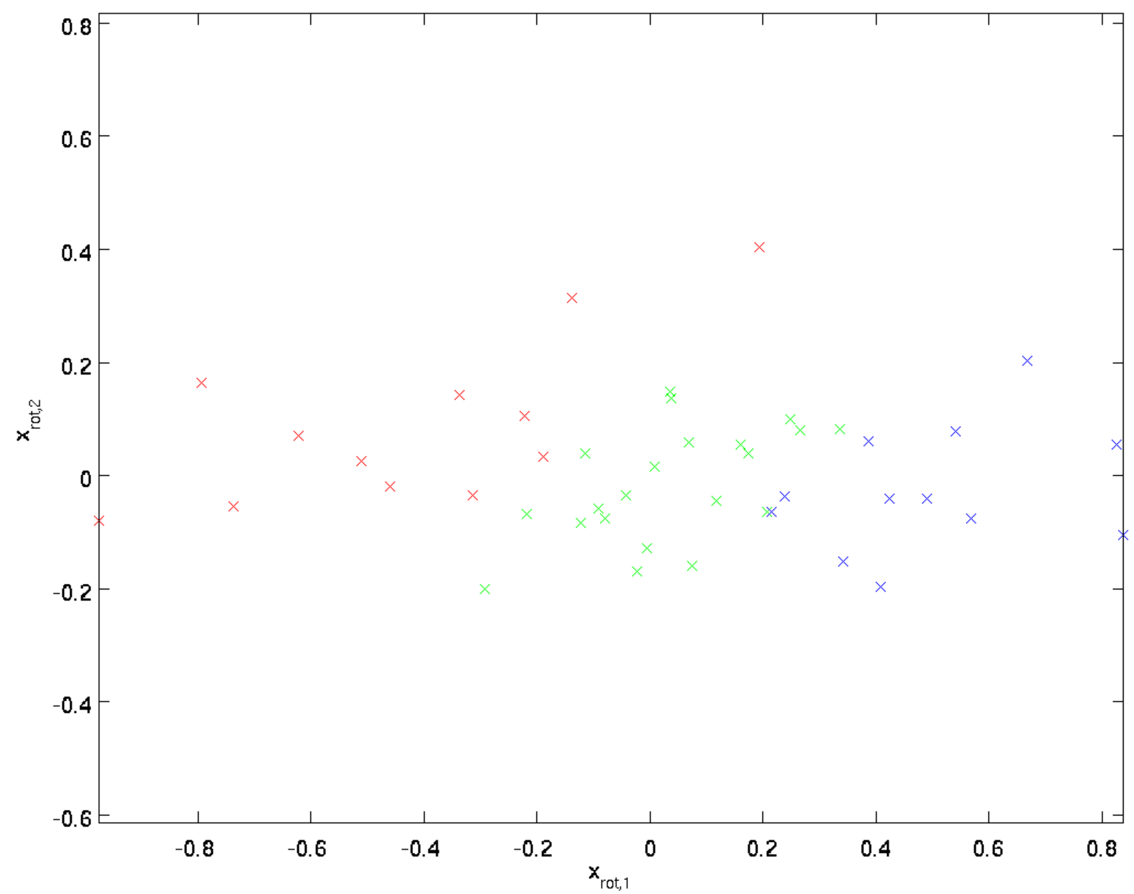
2. Transform to identity covariance (**PCA Whitening**) :

$$y_j^{(i)} = \frac{u_j^T x^{(i)}}{\sqrt{\lambda_j}} \Leftrightarrow y^{(i)} = \Lambda^{-1/2} U^T x^{(i)} \Leftrightarrow Y = \Lambda^{-1/2} U^T X$$

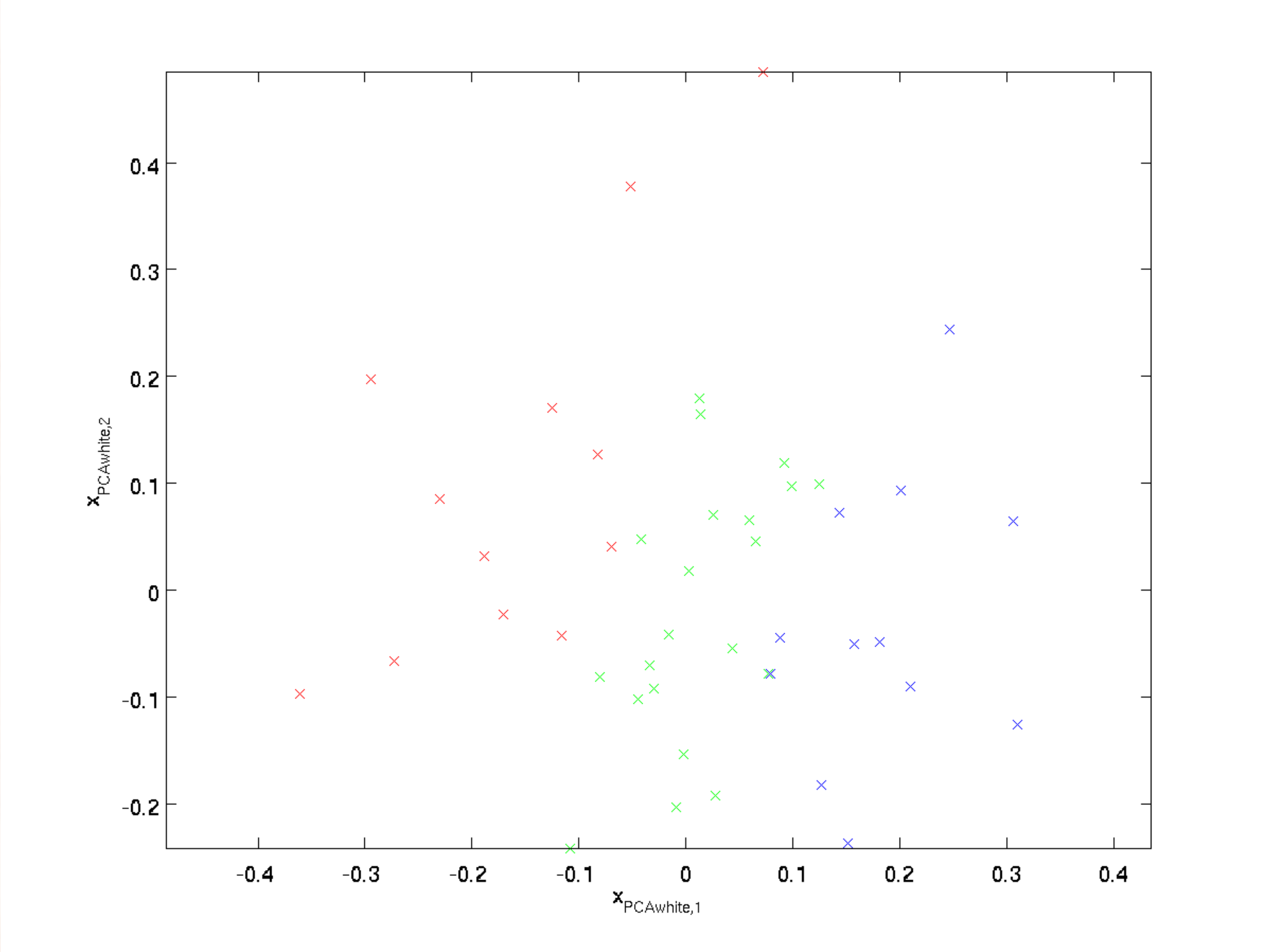
PCA on Normalized Data: $[x_1^{(i)}, x_2^{(i)}]^T$



Rotation through PCA: $[u_1^T x^{(i)}, u_2^T x^{(i)}]^T$



PCA Whitening: $\left[\frac{u_1^T x^{(i)}}{\sqrt{\lambda_1}}, \frac{u_2^T x^{(i)}}{\sqrt{\lambda_2}}\right]^T$



ZCA Whitening (Sphering)

- Observation: If Y has identity covariance and R is an orthogonal matrix, then RY has identity covariance.

1. **PCA Whitening:**

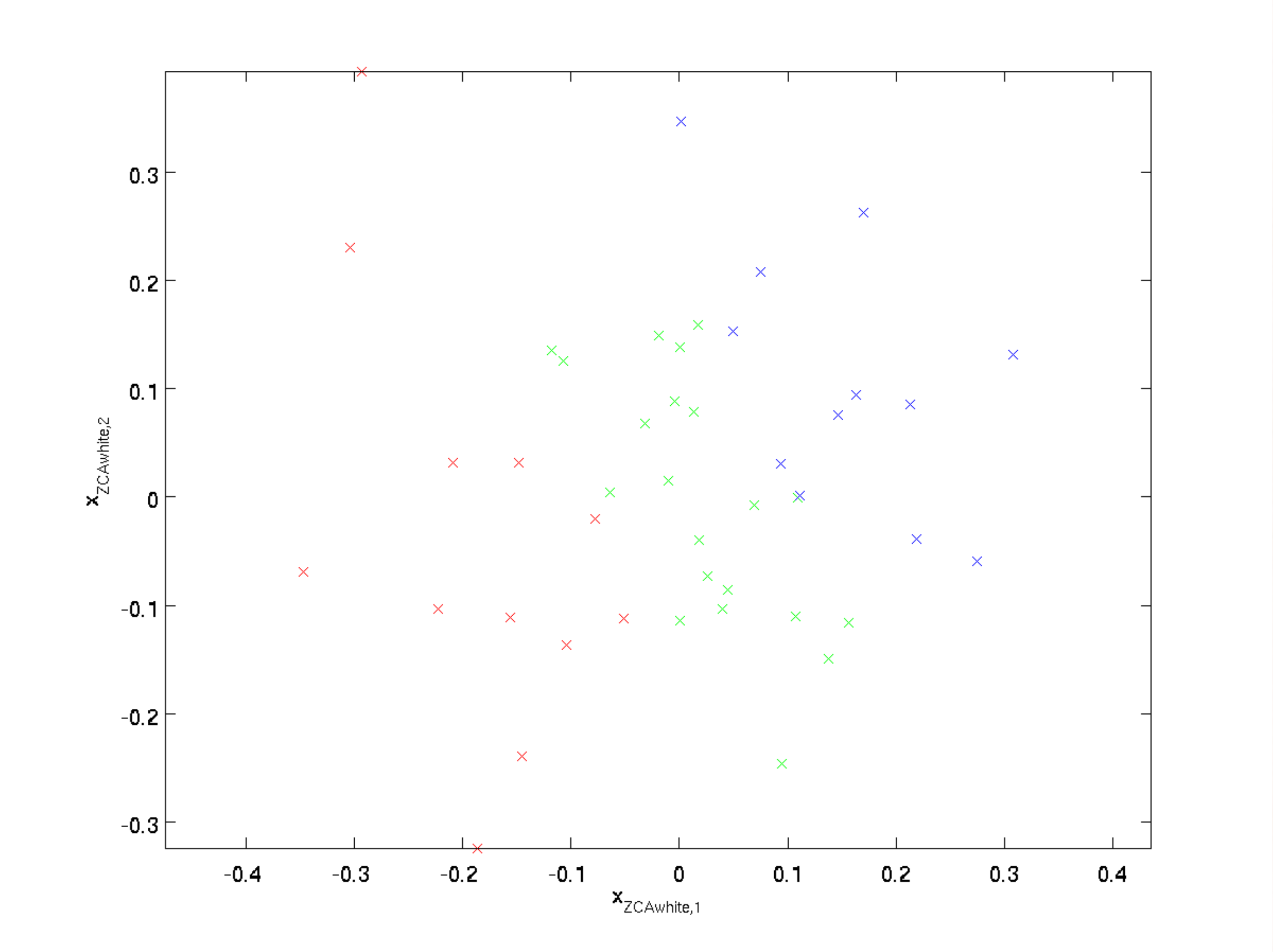
$$Y_{PCA} = \Lambda^{-1/2} U^T X$$

2. **ZCA Whitening:**

$$Y_{ZCA} = U Y_{PCA} = U \Lambda^{-1/2} U^T X$$

Out of all rotations, U makes Y_{ZCA} closest to original X.

ZCA Whitening: $Y_{ZCA} = U\Lambda^{-1/2}U^T X$



Smoothing

- When eigenvalues λ_j are very close to 0, dividing by $\lambda_j^{-1/2}$ is numerically unstable.
- **Smoothing**: add a small ε to eigenvalues before scaling for PCA/ZCA whitening:

$$y_j^{(i)} = \frac{u_j^T x^{(i)}}{\sqrt{\lambda_j + \varepsilon}} \qquad \varepsilon \approx 10^{-5}$$

- ZCA whitening is a rough model of how the biological eye (the retina) processes images (through retinal neurons).