Dimensionality Reduction

Using Principal Component Analysis

Motivation

- Clustering
  - One way to summarize a complex real-valued data point with a single categorical variable

- Dimensionality reduction
  - Another way to simplify complex high-dimensional data
 - Summarize data with a lower dimensional real valued vector

Motivation

- Clustering
  - One way to summarize a complex real-valued data point with a single categorical variable

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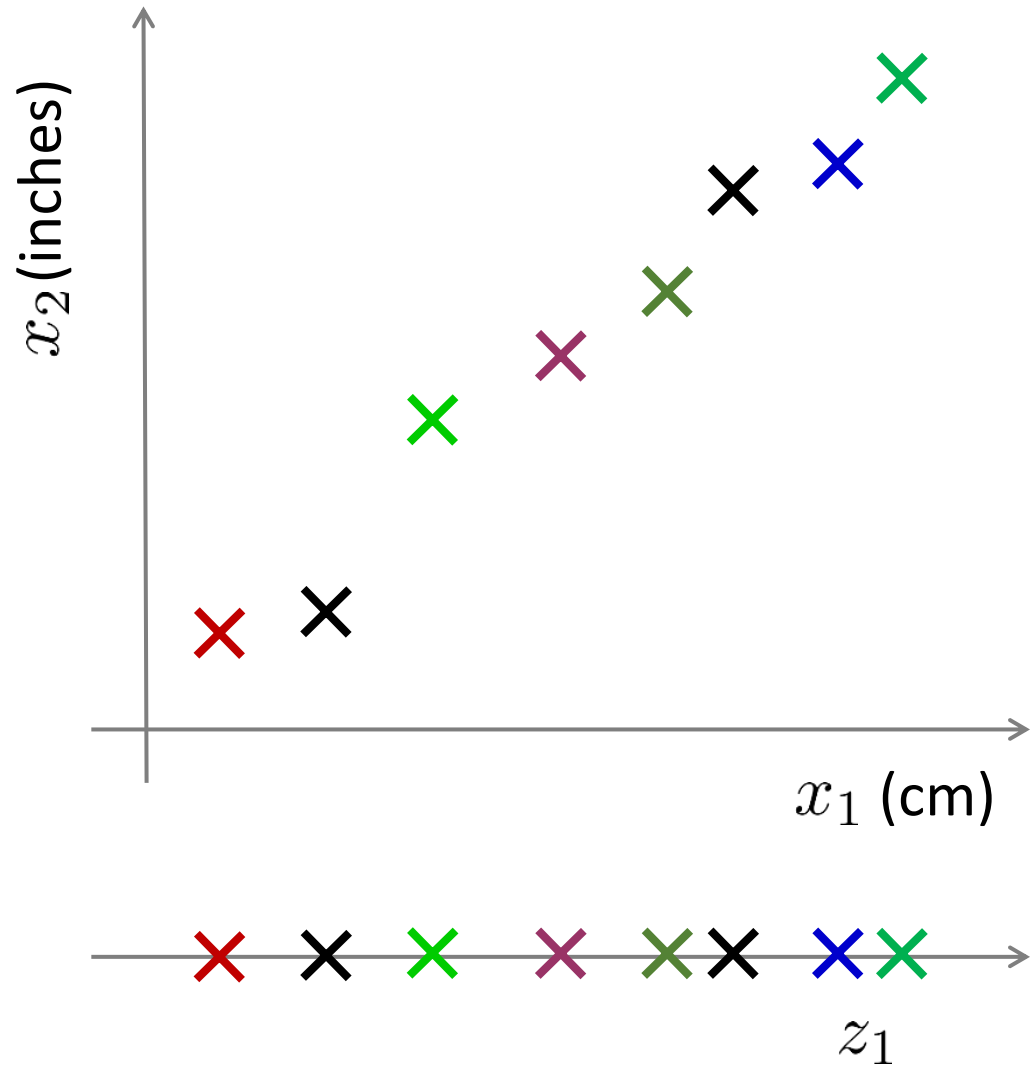 - Summarize data with a lower dimentional real valued vector

- Given data points in d dimensions
- Convert them to data points in $r<d$ dimensions
- With minimal loss of information

Data Compression
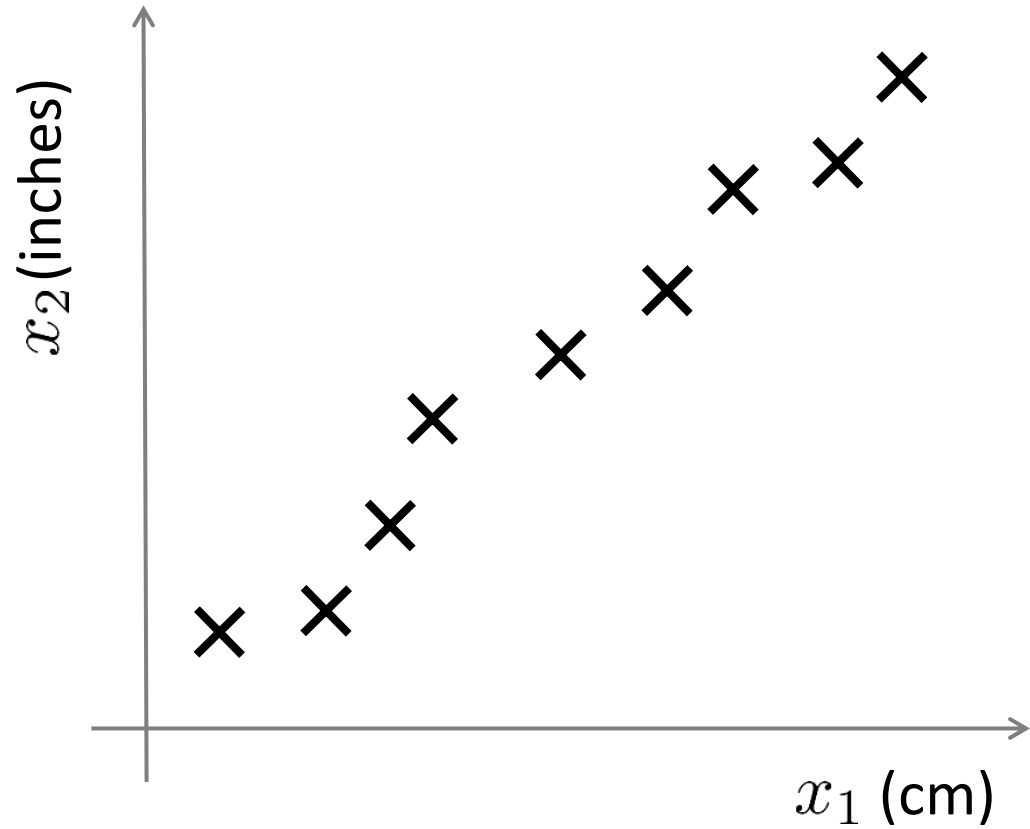
Reduce data from 2D to 1D

Data Compression
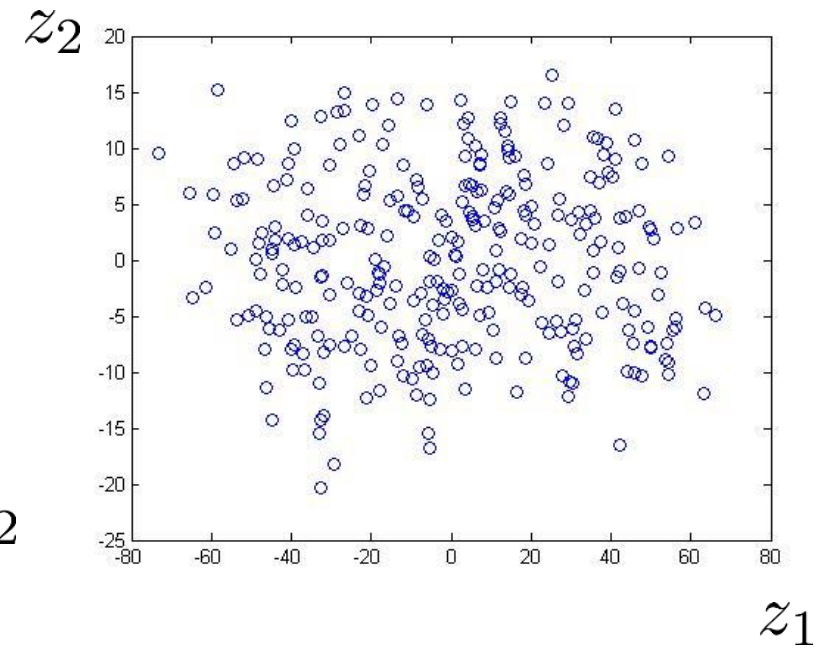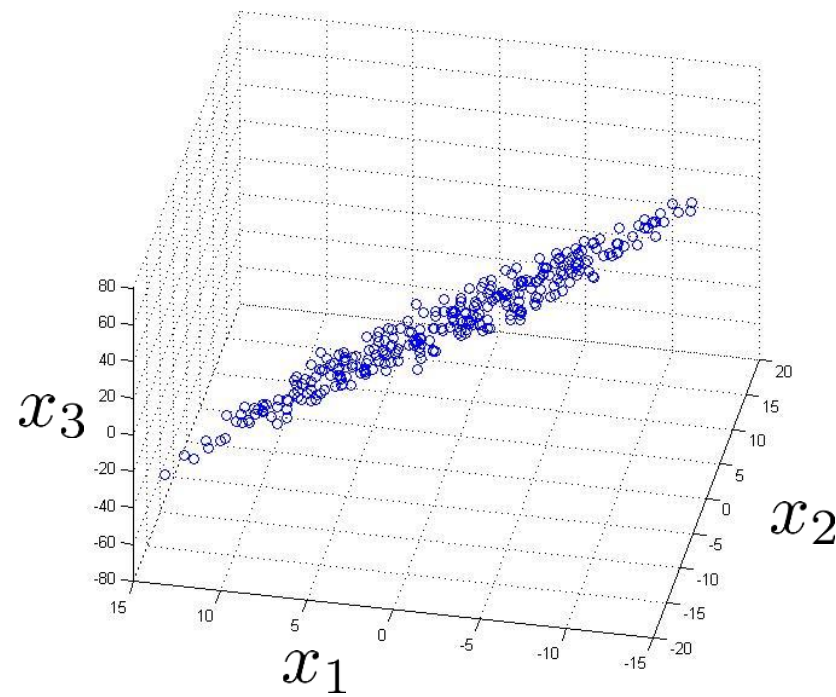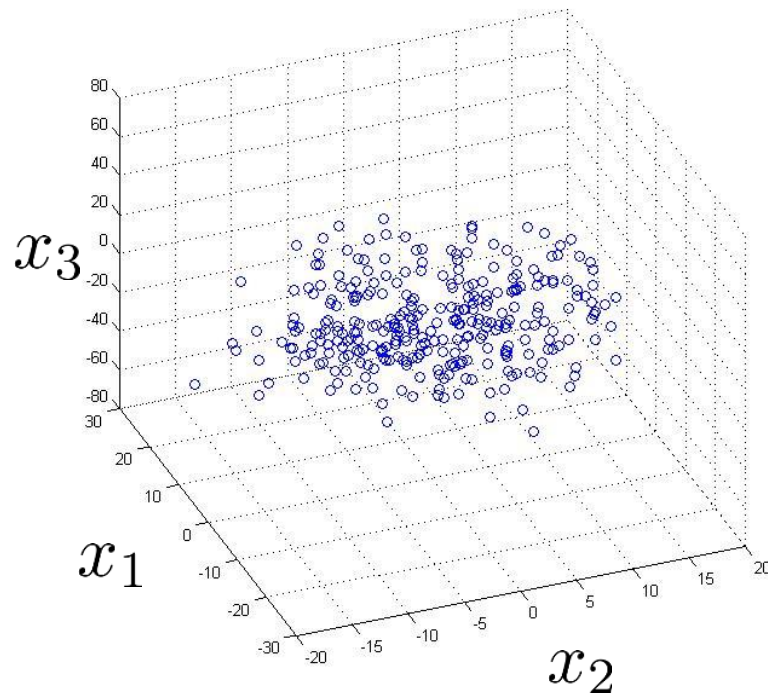

Reduce data from 2D to 1D

$$x^{(1)} \rightarrow z^{(1)}$$

$$x^{(2)} \rightarrow z^{(2)}$$

$$\vdots$$

$$x^{(m)} \rightarrow z^{(m)}$$

Data Compression

Reduce data from 3D to 2D

Principal Component Analysis (PCA) problem formulation

$$3D \to 2D$$
$$K = 2$$
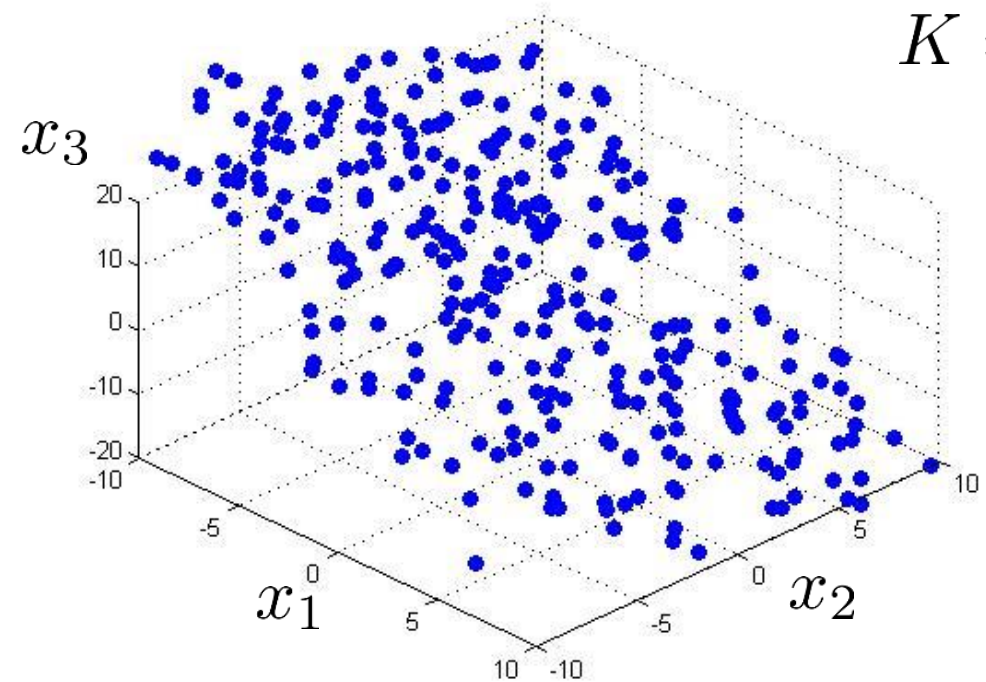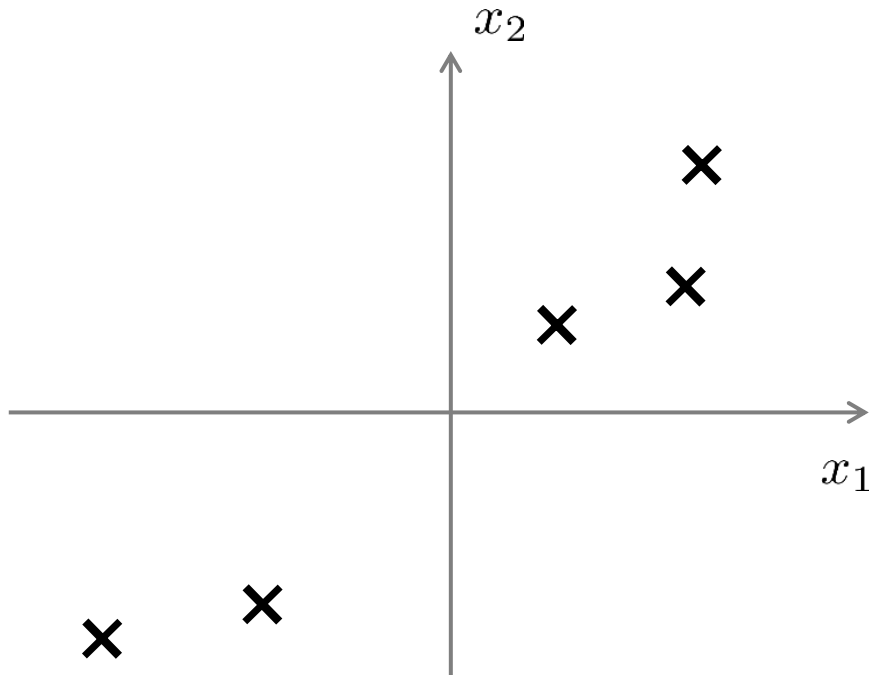
Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

Principal Component Analysis

**Goal:** Find r-dim projection that best preserves variance

1. Compute mean vector μ and covariance matrix Σ of original points

2. Compute eigenvectors and eigenvalues of Σ

3. Select top r eigenvectors

4. Project points onto subspace spanned by them:

$$y = A(x - \mu)$$

where y is the new point, x is the old one, and the rows of A are the eigenvectors

Covariance

- Variance and Covariance:
  - Measure of the "spread" of a set of points around their center of mass(mean)
- Variance:
  - Measure of the deviation from the mean for points in one dimension
- Covariance:
  - Measure of how much each of the dimensions vary from the mean with **respect to each other**
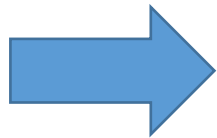
- **Covariance is measured between two dimensions**
- **Covariance sees if there is a relation between two dimensions**
- **Covariance between one dimension is the variance**

positive covariance   negative covariance
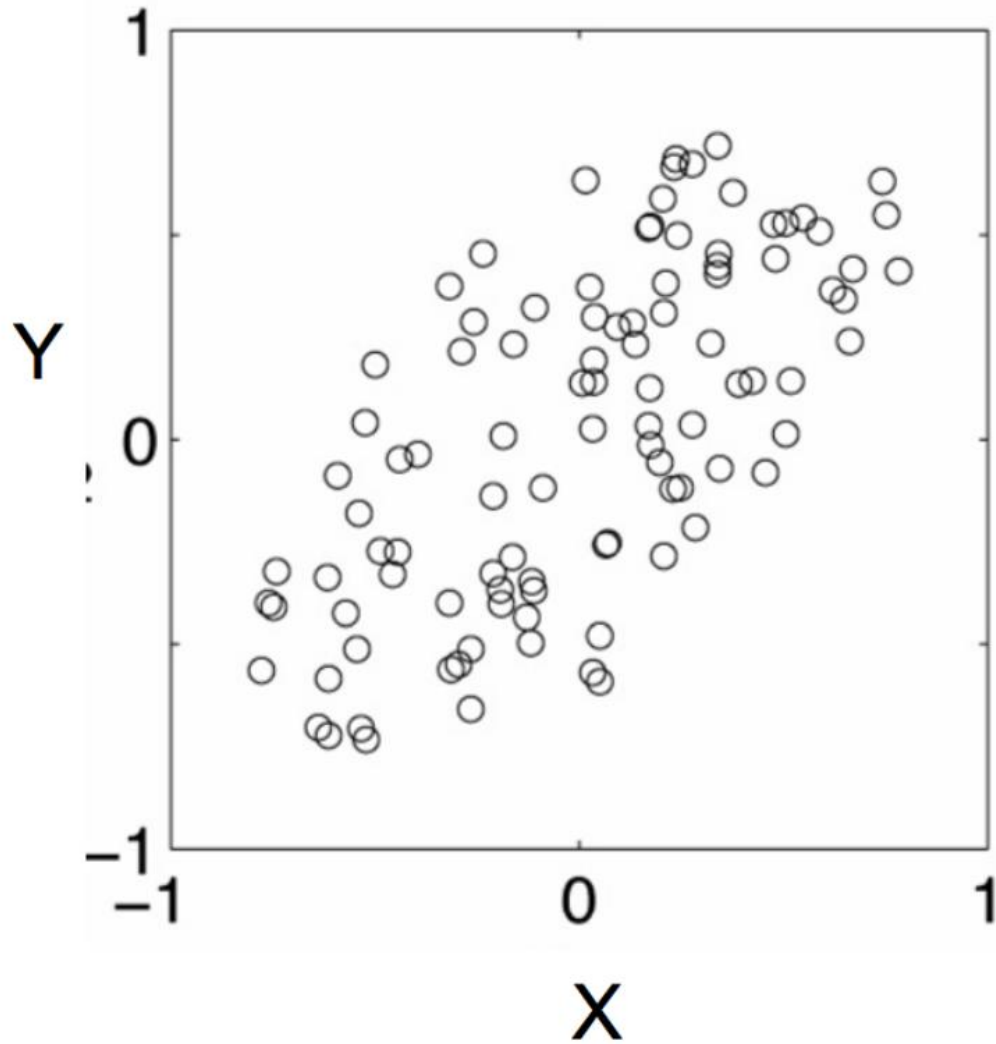
Positive: Both dimensions increase or decrease together   Negative: While one increase the other decrease
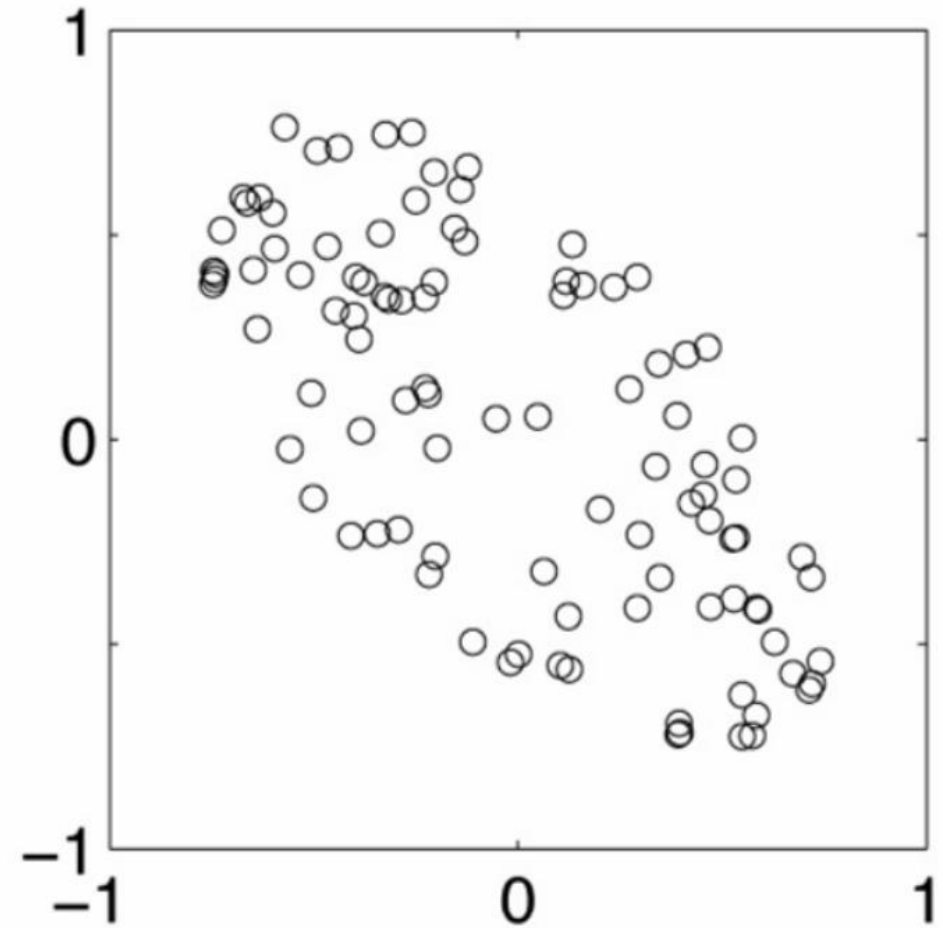
Covariance

- Used to find relationships between dimensions in high dimensional data sets

$$q_{jk} = \frac{1}{N} \sum_{i=1}^{N} (X_{ij} - E(X_j))(X_{ik} - E(X_k))$$

The Sample mean

Eigenvector and Eigenvalue

$$Ax = \lambda x$$

A: Square Matirx

λ: Eigenvector or characteristic vector

X: Eigenvalue or characteristic value
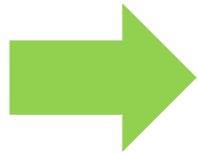
- *The zero vector can not be an eigenvector*
- *The value zero can be eigenvalue*

Eigenvector and Eigenvalue

$$Ax = \lambda x$$

A: Square Matirx

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$Show \ x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} is \, an \, eigenvector \ for \ A = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix}$

$Solution: Ax = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$But \ \ for \ \ \lambda = 0, \ \ \lambda x = 0 \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$Thus, x \, is \, an \, eigenvector \, of \ A, and \ \lambda = 0 \ is \, an \, eigenvalue.$

Example

Eigenvector and Eigenvalue

$$Ax = \lambda x$$

$$\longrightarrow$$

$$Ax - \lambda x = 0$$
$$(A - \lambda I)x = 0$$

If we define a new matrix B:

$$\longrightarrow$$

$$B = A - \lambda I$$
$$Bx = 0$$

If B has an inverse:

$$\longrightarrow$$

$$x = B^{-1}0 = 0$$
❌ **BUT! an eigenvector cannot be zero!!**
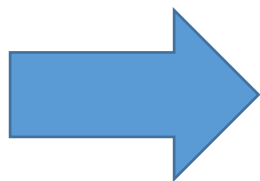
x will be an eigenvector of A if and only if B does not have an inverse, or equivalently det(B)=0 :

$$\det(A - \lambda I) = 0$$

Eigenvector and Eigenvalue

Example 1: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & -12 \\ 1 & -5 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & 12 \\ -1 & \lambda + 5 \end{vmatrix} = (\lambda - 2)(\lambda + 5) + 12$$

$$= \lambda^2 + 3\lambda + 2 = (\lambda + 1)(\lambda + 2)$$

two eigenvalues: $-1, -2$

Note: The roots of the characteristic equation can be repeated. That is, $\lambda_1 = \lambda_2 = ... = \lambda_k$. If that happens, the eigenvalue is said to be of multiplicity k.

Example 2: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & -1 & 0 \\ 0 & \lambda - 2 & 0 \\ 0 & 0 & \lambda - 2 \end{vmatrix} = (\lambda - 2)^3 = 0$$

$\lambda = 2$ is an eigenvector of multiplicity 3.

Principal Component Analysis

Input: $\mathbf{x} \in \mathbb{R}^D \colon \mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$

Set of basis vectors: $\mathbf{u}_1, \ldots, \mathbf{u}_K$

Summarize a _D_ dimensional vector _X_ with _K_ dimensional feature vector _h(x)_

$$h(\mathbf{x}) = \begin{bmatrix} \mathbf{u}_1 \cdot \mathbf{x} \\ \mathbf{u}_2 \cdot \mathbf{x} \\ \ldots \\ \mathbf{u}_K \cdot \mathbf{x} \end{bmatrix}$$

Principal Component Analysis

$$\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K]$$

Basis vectors are orthonormal

$$\mathbf{u}_i^T \mathbf{u}_j = 0$$

$$||\mathbf{u}_j|| = 1$$

New data representation *h(x)*

$$z_j = \mathbf{u}_j \cdot \mathbf{x}$$

$$h(\mathbf{x}) = [z_1, \ldots, z_K]^T$$

Principal Component Analysis

$$\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K]$$

New data representation *h(x)*

$$h(\mathbf{x}) = \mathbf{U}^T \mathbf{x}$$

$$h(\mathbf{x}) = \mathbf{U}^T (\mathbf{x} - \mu_0)$$

Empirical mean of the data $\longrightarrow$ $\mu_0 = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i$

The space of all face images

- When viewed as vectors of pixel values, face images are extremely high-dimensional
  - 100x100 image = 10,000 dimensions
  - Slow and lots of storage
- But very few 10,000-dimensional vectors are valid face images
- We want to effectively model the subspace of face images

Eigenfaces example

Top eigenvectors: $u_1, \ldots u_k$

Mean: μ
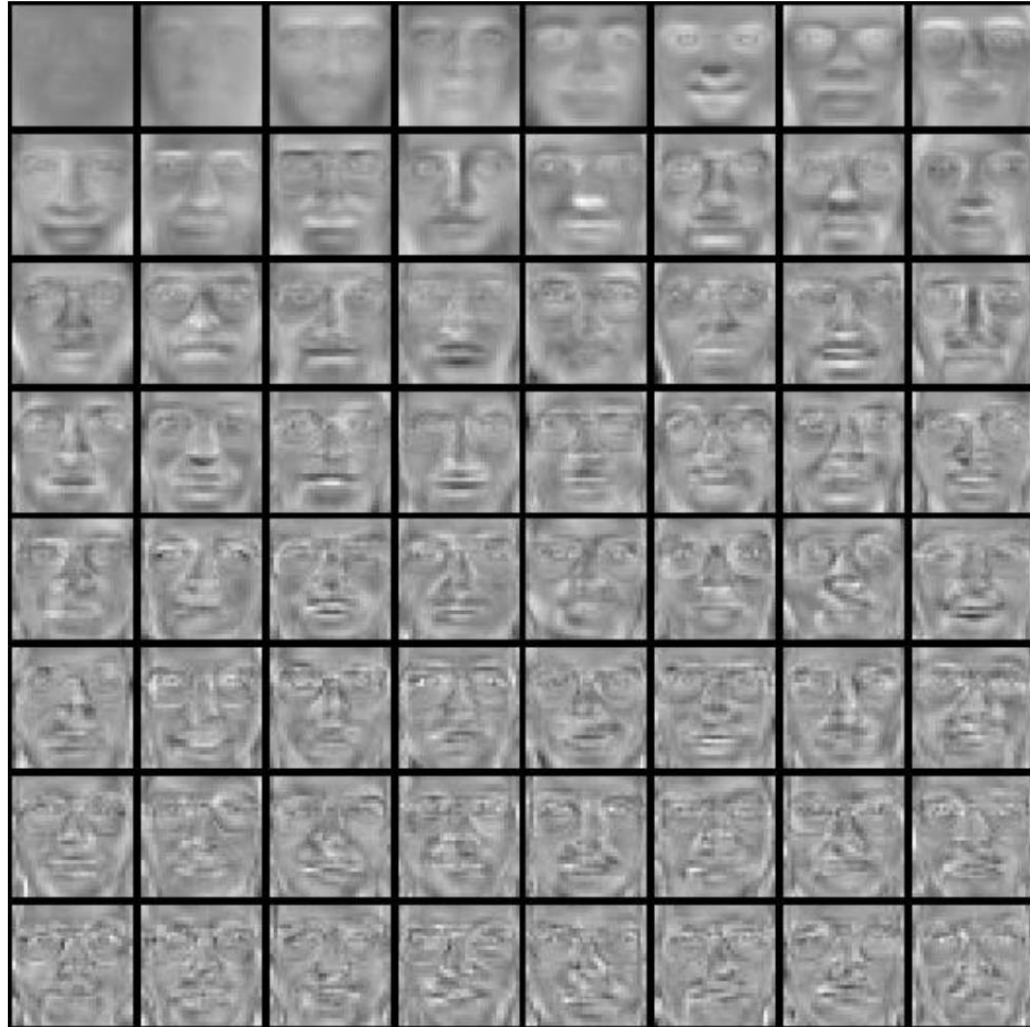
Representation and reconstruction

- Face **x** in "face space" coordinates:

$$\mathbf{x} \rightarrow \left[\mathbf{u}_1^{\mathrm{T}}(\mathbf{x} - \mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x} - \mu)\right]$$
$$= \quad w_1, \ldots, w_k$$

- Reconstruction:

$\hat{x} \quad = \quad \mu \quad + \quad w_1 u_1 + w_2 u_2 + w_3 u_3 + w_4 u_4 + \ldots$

Reconstruction

P = 4

P = 200

P = 400

After computing eigenfaces using 400 face images from ORL face database

Application: Image compression

Original Image

- Divide the original 372x492 image into patches:
  - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

PCA compression: 144D ➔ 60D

PCA compression: 144D → 16D

16 most important eigenvectors
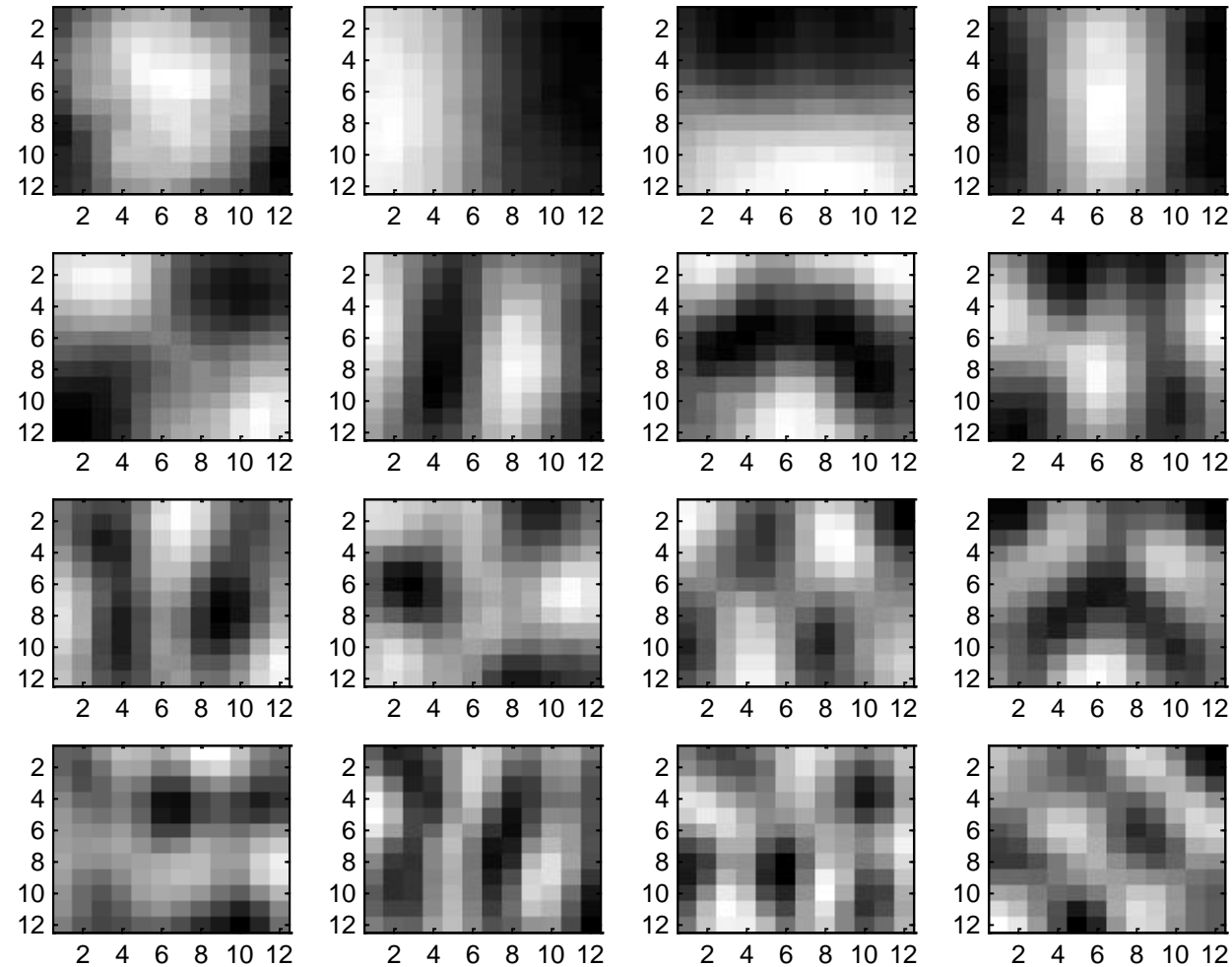
PCA compression: 144D) 6D

6 most important eigenvectors
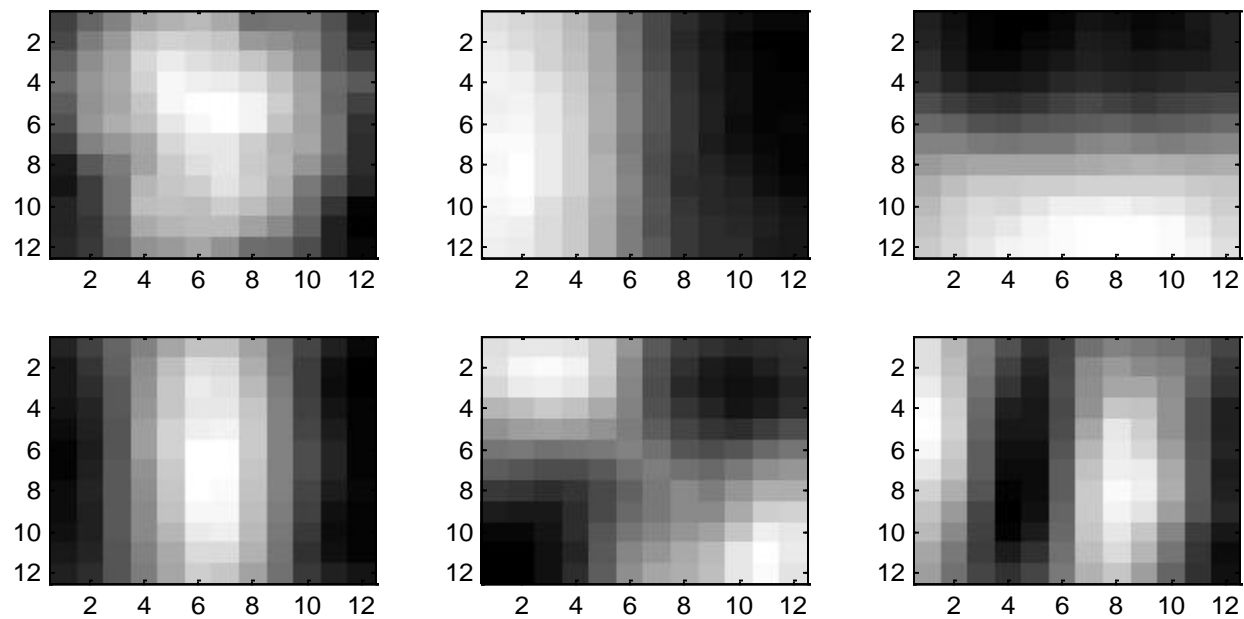
PCA compression: 144D → 3D

3 most important eigenvectors
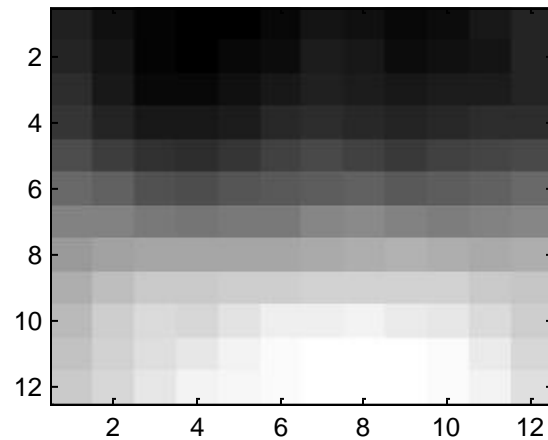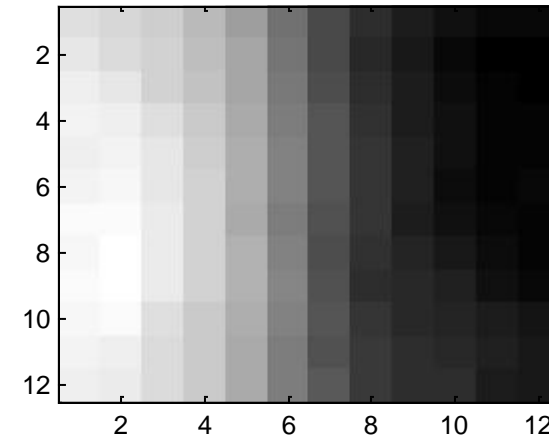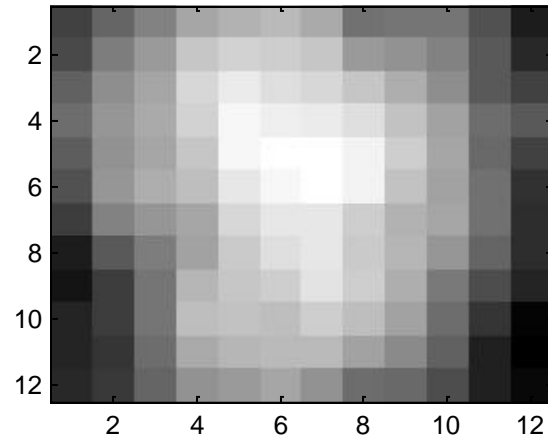
PCA compression: 144D → 1D
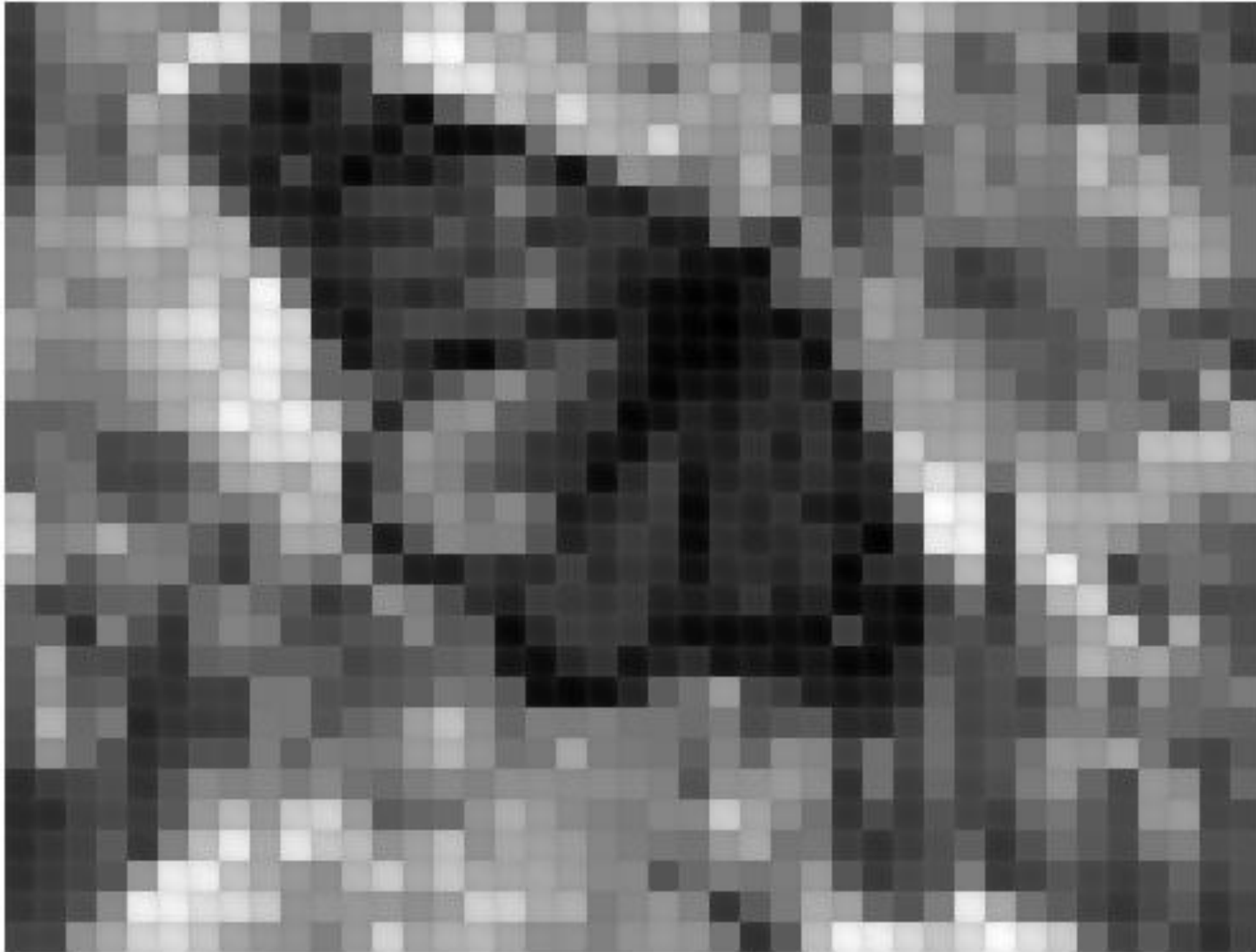
An example

Data

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

Ref: http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf

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Mean subtracted Data

x	*y*
.69	.49
-1.31	-1.21
.39	.99
.09	.29
1.29	1.09
.49	.79
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-.81	-.81
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$$cov = \begin{pmatrix} .61 & .61 \\ .61 & .71 \end{pmatrix}$$

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Eigenvalues are 1.28, 0.049

Corresponding Eigenvectors are $\begin{pmatrix} -.67 \\ -.73 \end{pmatrix}$ and $\begin{pmatrix} -.73 \\ .67 \end{pmatrix}$

What is the projection matrix?

If we are interested in 1D data

Ref: http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf

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What is the projection matrix?

$$P = \begin{pmatrix} -.67 \\ -.73 \end{pmatrix}^t$$

Transformed Data (Single eigenvector)

x
-.827970186
1.77758033
-.992197494
-.274210416
-1.67580142
-.912949103
.0991094375
1.14457216
.438046137
1.22382056

The data after transforming using only the most significant eigenvector

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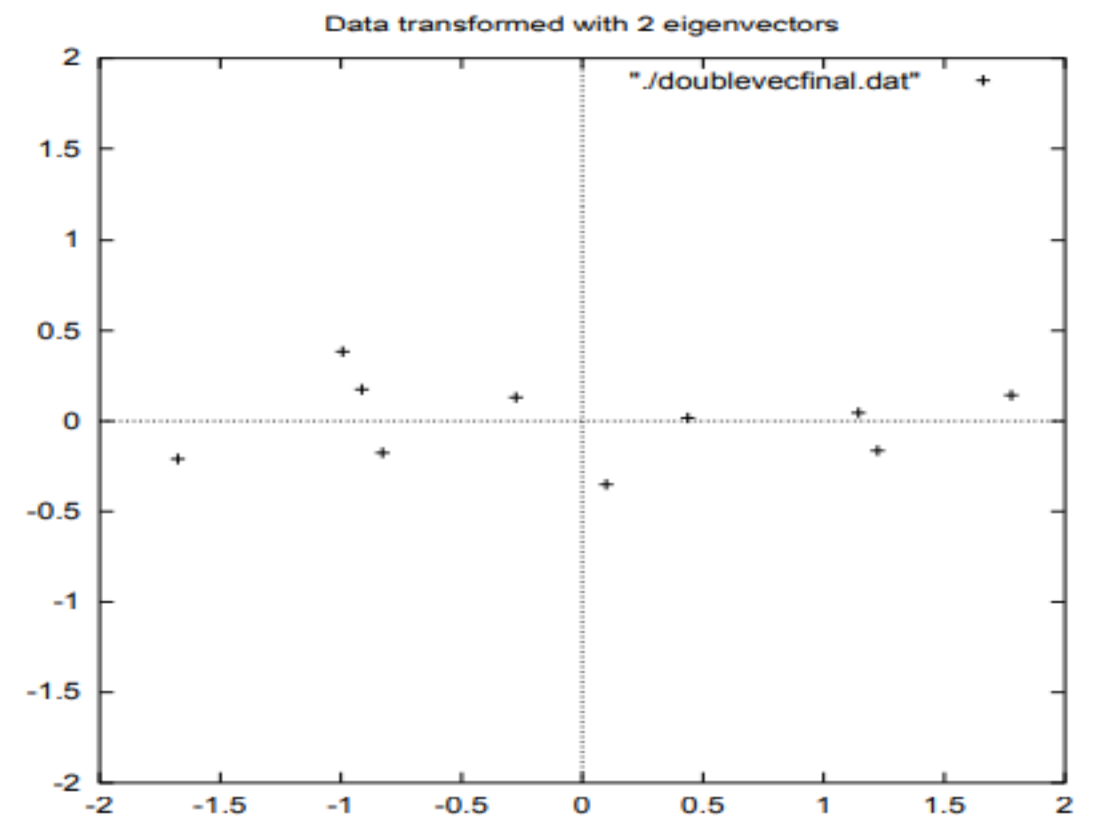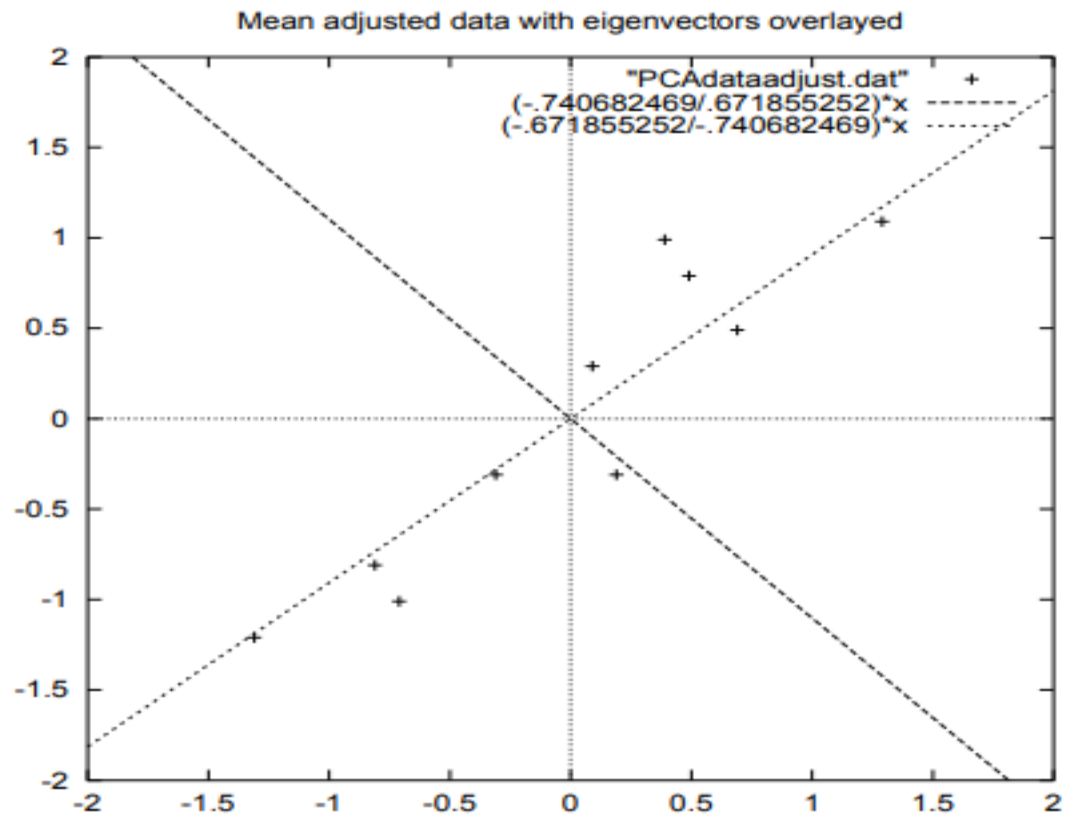| x	y
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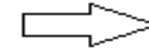
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We can get a 2D data by using both eigenvectors,

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Dimensionality reduction

- PCA (Principal Component Analysis):
  - Find projection that maximize the variance
- ICA (Independent Component Analysis):
  - Very similar to PCA except that it assumes non-Guassian features
- Multidimensional Scaling:
  - Find projection that best preserves inter-point distances
- LDA(Linear Discriminant Analysis):
  - Maximizing the component axes for class-separation
- …
- …