CS 405/605 Data Science

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Big & High-Dimensional Data

- High-Dimensions = Lot of Features

Document classification

Features per document =

thousands of words/unigrams

millions of bigrams, contextual information

Surveys - Netflix

480189 users x 17770 movies

	movie 1	movie 2	movie 3	movie 4	movie 5	movie 6
Tom	5	?	?	1	3	?
George	?	?	3	1	2	5
Susan	4	3	1	?	5	1
Beth	4	3	?	2	4	2

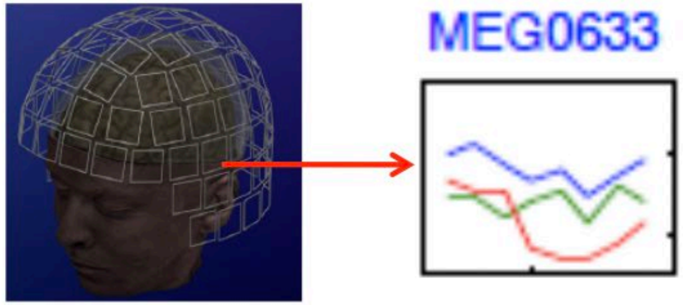
Big & High-Dimensional Data

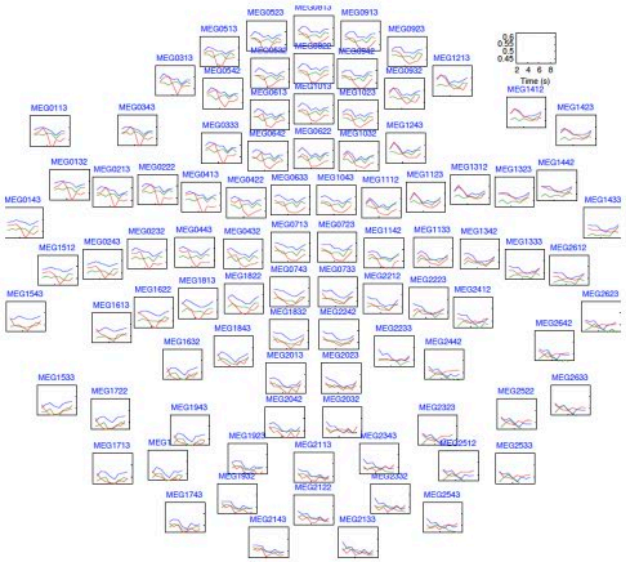
- High-Dimensions = Lot of Features

MEG Brain Imaging

120 locations x 500 time points

x 20 objects





Or any high-dimensional image data

overview

Big & High-Dimensional Data

Useful to learn lower dimensional representations of the data.

Dimensionality reduction

overview

- Today we'll cover an unsupervised learning algorithm: principal component analysis (PCA)
- Dimensionality reduction: map the data to a lower dimensional space
  - Save computation/memory
  - Reduce overfitting
  - Visualize data of high dimensionality
- PCA is a linear model, with a closed-form solution. It's useful for understanding lots of other algorithms.
  - Autoencoders
  - Matrix factorizations
  - Image compression
  - Face recognition
  - Gene expression analysis
- Today's lecture is very linear-algebra-heavy.
  - Especially orthogonal matrices and eigendecompositions.
  - Don't worry if you don't get it immediately -- next few lectures won't build on it

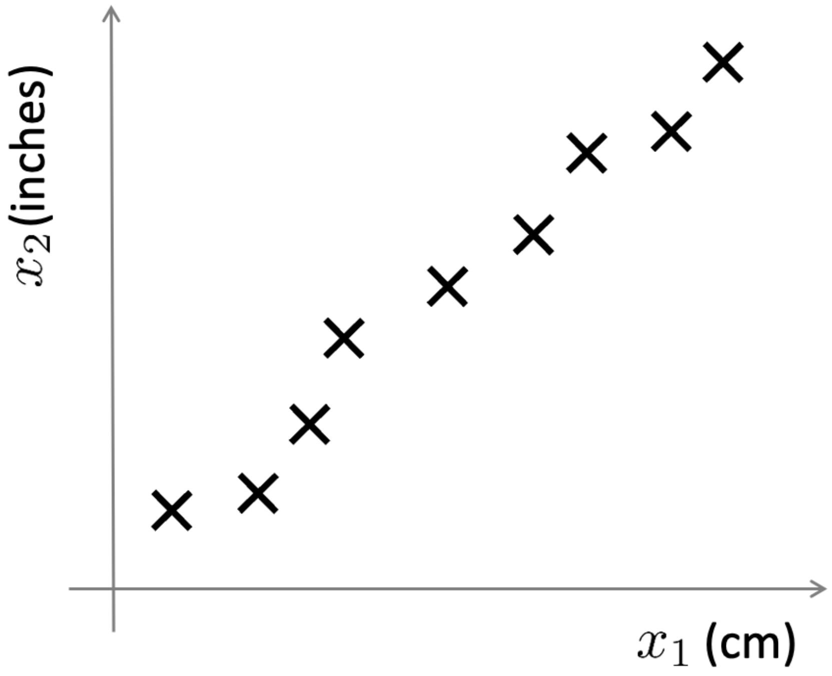
Motivation

- Dimensionality reduction
  - To simplify complex high-dimensional data
  - Summarize data with a lower dimensional real valued vector

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

Principal Components Analysis (PCA)

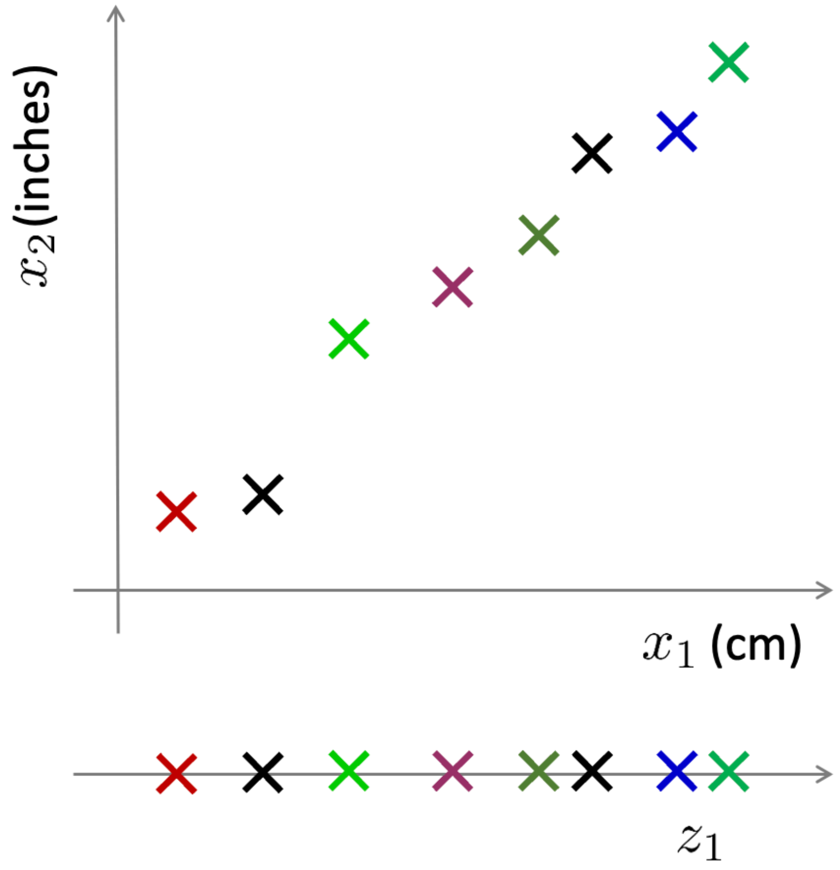
Data Compression



Reduce data from 2D to 1D

Principal Components Analysis (PCA)

Data Compression



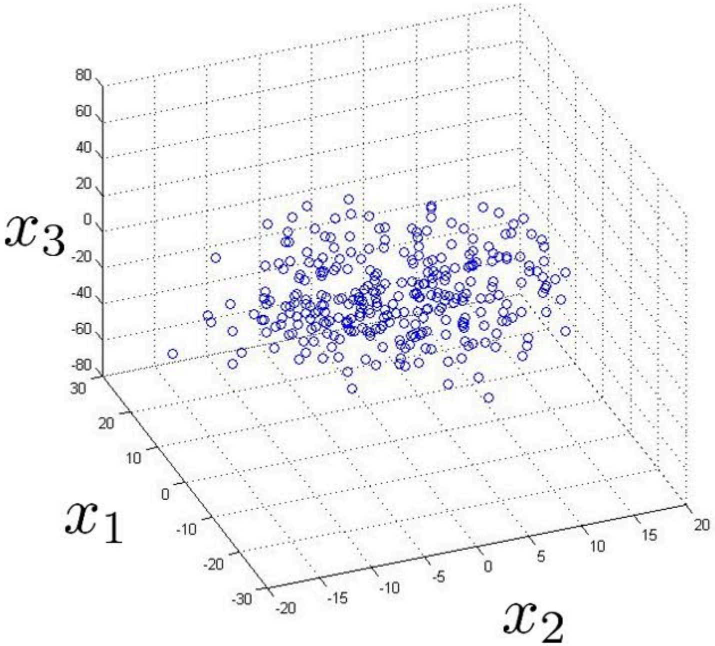
Reduce data from 2D to 1D

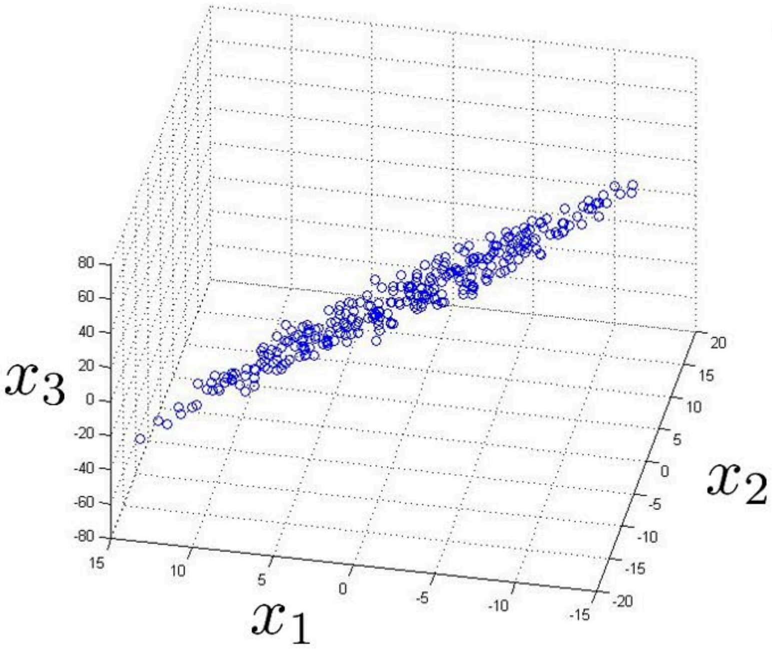
$$
\begin{aligned}
x^{(1)} &\rightarrow z^{(1)} \\
x^{(2)} &\rightarrow z^{(2)} \\
&\vdots \\
x^{(m)} &\rightarrow z^{(m)}
\end{aligned}
$$

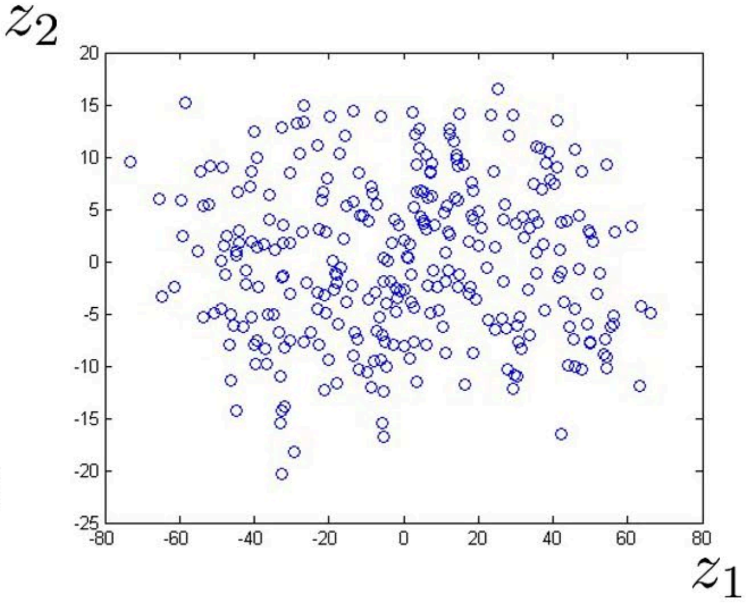
Principal Components Analysis (PCA)

Data Compression

Reduce data from 3D to 2D







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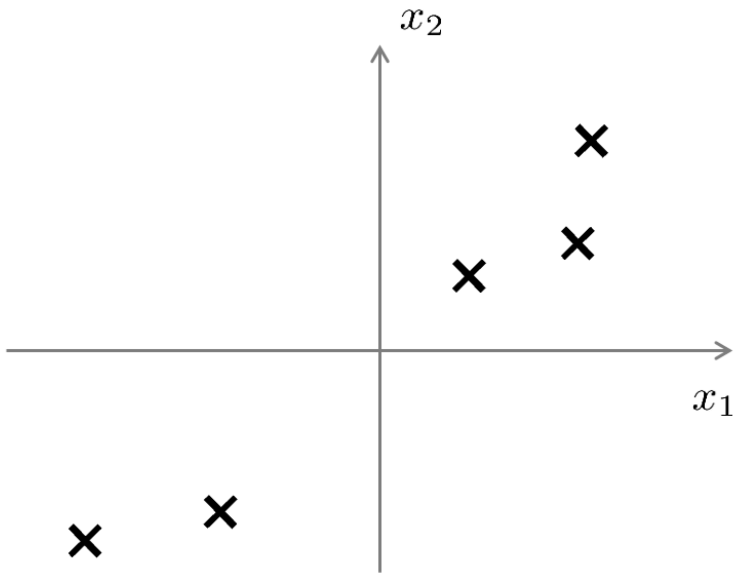
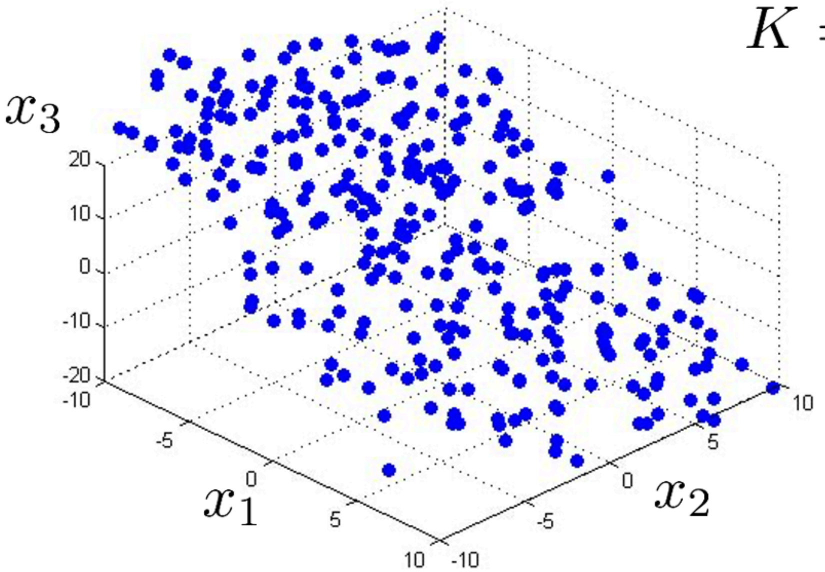
Principal Components Analysis (PCA)

Principal Component Analysis (PCA) problem formulation



$3D \rightarrow 2D$
$K = 2$



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 Components Analysis (PCA)

Definition:

Choosing a subspace to maximize the projected variance, or minimize the reconstruction error, is called principal component analysis (PCA).

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

Variance and 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**

Variance and Covariance

one attribute first

- Question: how much spread is in the data along the axis? (distance to the mean)
- Variance=Standard deviation^2

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

Temperature
42
40
24
30
15
18
15
30
15
30
35
30
40
30

Variance and Covariance

Now consider two dimensions

Covariance: measures the correlation between X and Y

- cov(X,Y)=0: independent
- Cov(X,Y)>0: move same dir
- Cov(X,Y)<0: move oppo dir

$$\mathrm{cov}(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

X=Temperature	Y=Humidity
40	90
40	90
40	90
30	90
15	70
15	70
15	70
30	90
15	70
30	70
30	70
30	90
40	70
30	90

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More than two attributes: covariance matrix

- Contains covariance values between all possible dimensions (=attributes):

$$C^{nxn} = (c_{ij} \mid c_{ij} = \text{cov}(Dim_i, Dim_j))$$

- Example for three attributes (x,y,z):

$$C = \begin{pmatrix} \text{cov}(x,x) & \text{cov}(x,y) & \text{cov}(x,z) \\ \text{cov}(y,x) & \text{cov}(y,y) & \text{cov}(y,z) \\ \text{cov}(z,x) & \text{cov}(z,y) & \text{cov}(z,z) \end{pmatrix}$$

Variance and Covariance

- Variance and Covariance:
  - Measure of the “spread” of a set of points around their center of mass(mean)
- Variance:
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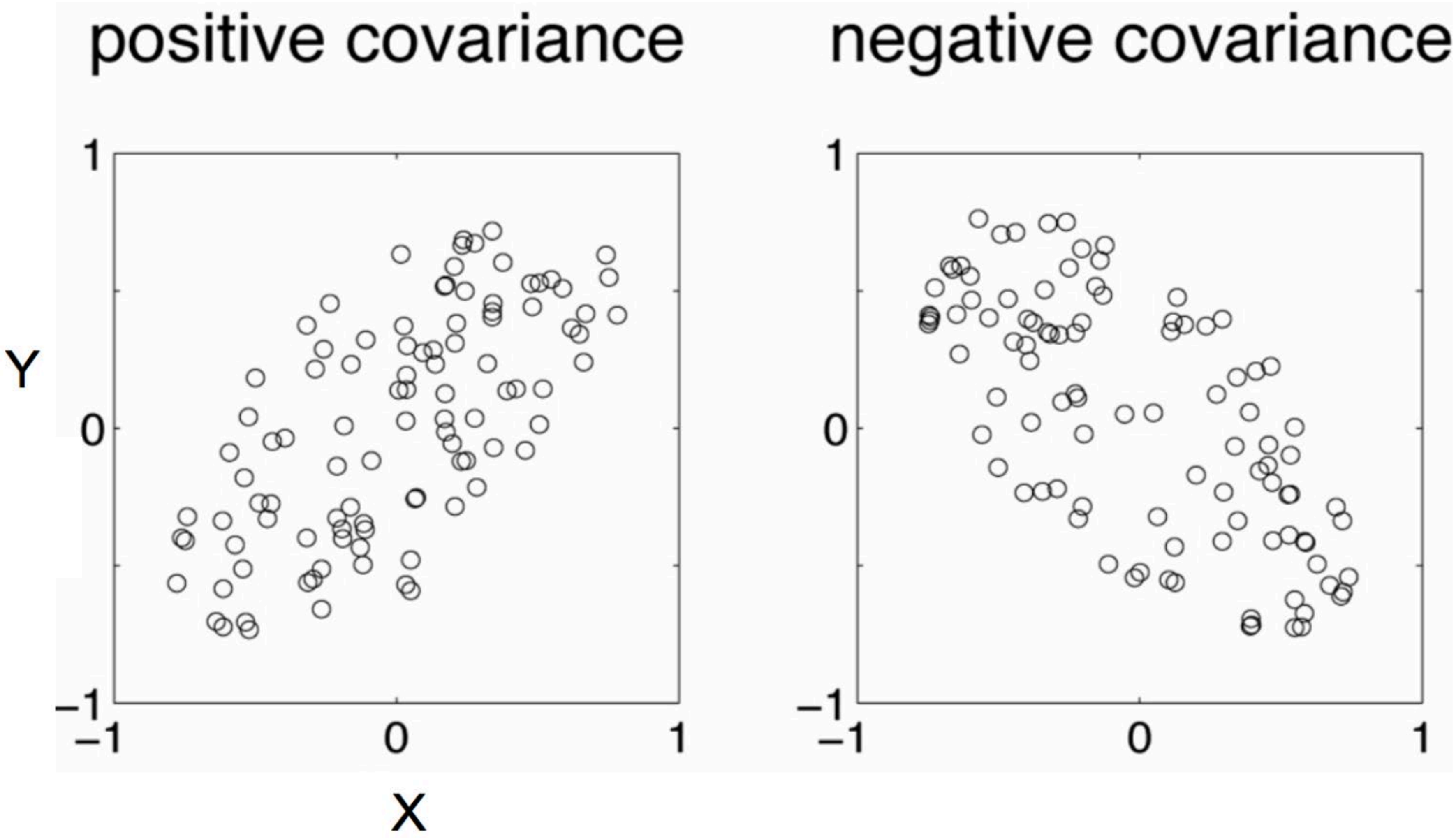
- **Covariance is measured between two dimensions**
- **Covariance sees if there is a relation between two dimensions**
- **Covariance between one dimension is the variance**

Covariance



Positive: Both dimensions increase or decrease together

Negative: While one increase the other decrease

Eigenvector and Eigenvalue

$$\mathbf{Ax = \lambda x}$$

A: Square Matrix

X: Eigenvector or characteristic vector

λ : Eigenvalue or characteristic value

- Eigenvectors having same direction as *A*

Eigenvector and Eigenvalue

$$\mathbf{Ax} = \lambda\mathbf{x}$$

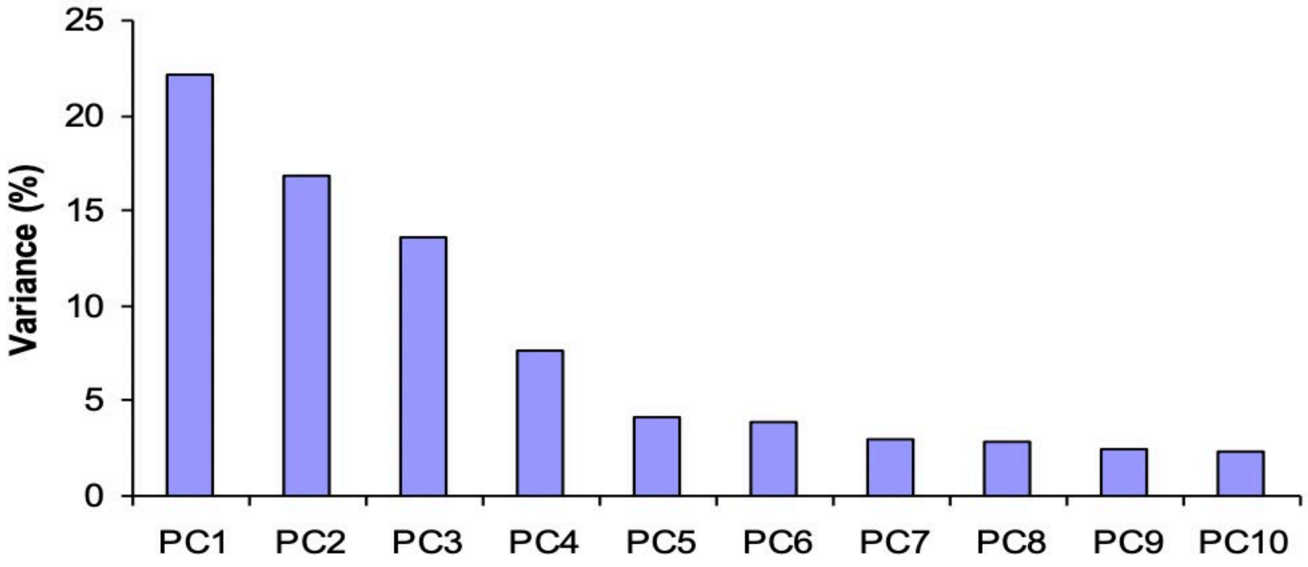
- $A\mathbf{x}=\lambda\mathbf{x} \Leftrightarrow (A-\lambda \mathrm{I})\mathbf{x}=0$
- How to calculate $\mathbf{x}$ and λ:
  - Calculate $det(A-\lambda I)$, yields a polynomial (degree n)
  - Determine roots to $det(A-\lambda I)=0$, roots are eigenvalues λ
  - Solve $(A- \lambda I)\ \mathbf{x}=0$ for each λ to obtain eigenvectors $\mathbf{x}$

Principal components

- 1. principal component (PC1)
  - The eigenvalue with the largest absolute value will indicate that the data have the largest variance along its eigenvector, the direction along which there is greatest variation
- 2. principal component (PC2)
  - the direction with maximum variation left in data, orthogonal to the 1. PC
- In general, only few directions manage to capture most of the variability in the data.

Principal components

- How many principal components?
  - For n original dimensions, sample covariance matrix is nxn, and has up to n eigenvectors. So n PCs.
- Where does dimensionality reduction come from?
  - Can ignore the components of lesser significance.



Principal components

- How many principal components?
  - For n original dimensions, sample covariance matrix is nxn, and has up to n eigenvectors. So n PCs.
- Where does dimensionality reduction come from?
  - Can ignore the components of lesser significance.
  - You do lose some information, but if the eigenvalues are small, you don't lose much
    - n dimensions in original data
    - calculate n eigenvectors and eigenvalues
    - choose only the first p eigenvectors, based on their eigenvalues
    - final data set has only p dimensions

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Principal Components Analysis (PCA)

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

Principal Components Analysis (PCA)

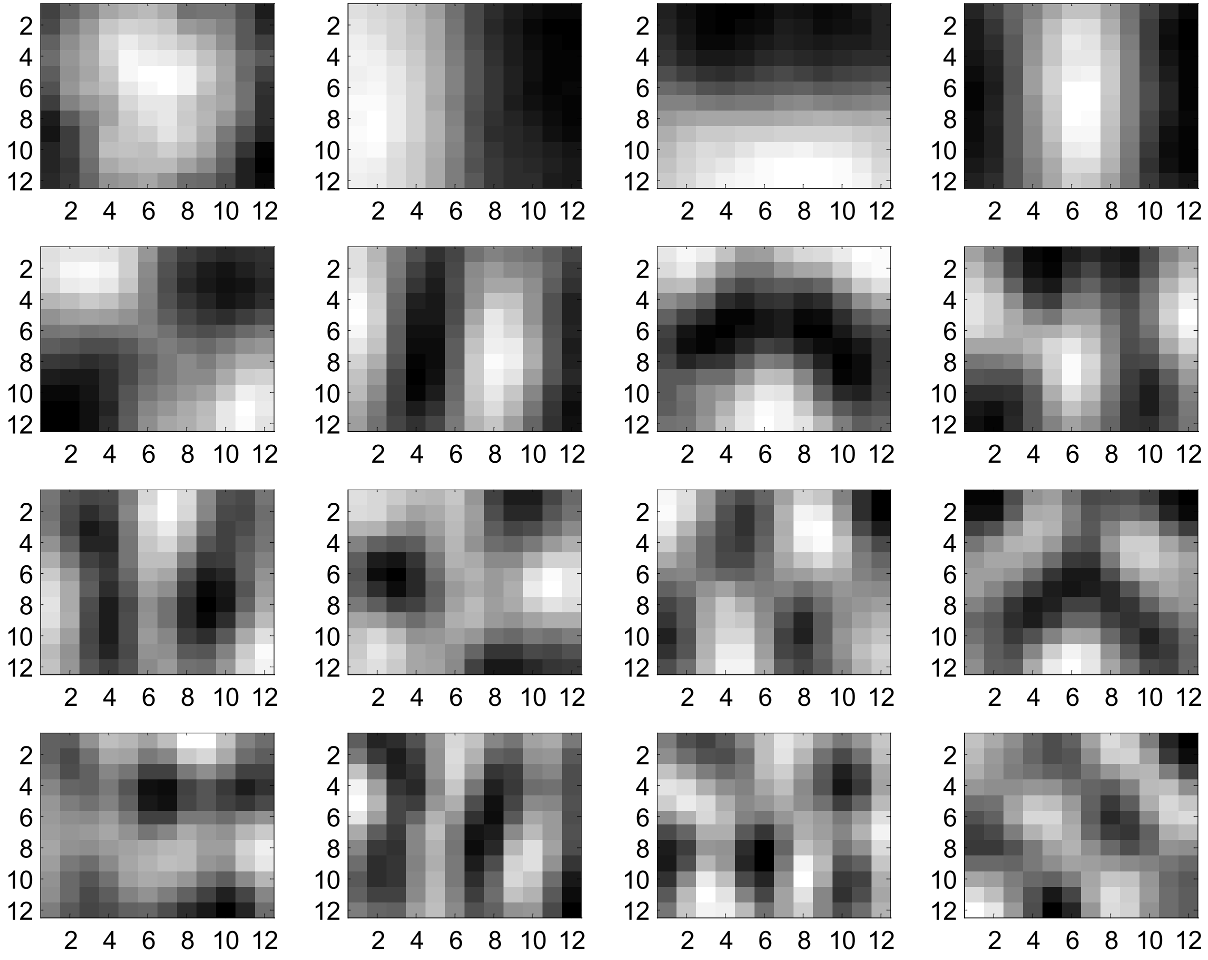
PCA compression: 144D → 60D

Principal Components Analysis (PCA)

PCA compression: 144D → 16D

Principal Components Analysis (PCA)

16 most important eigenvectors



Principal Components Analysis (PCA)

PCA compression: 144D → 6D

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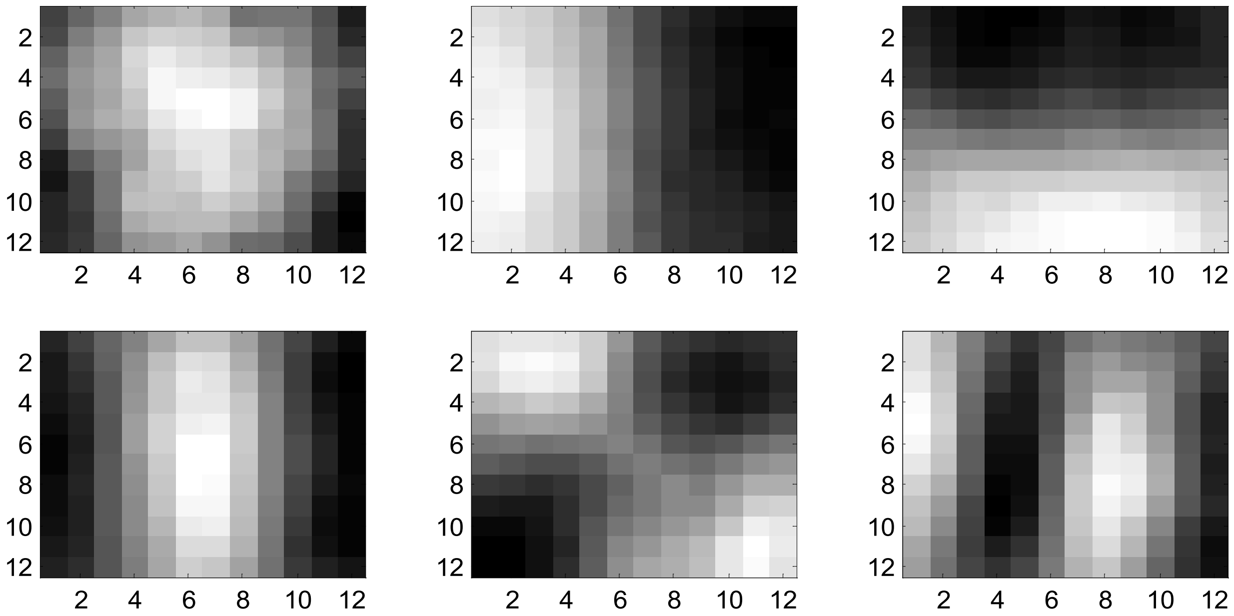
Principal Components Analysis (PCA)

6 most important eigenvectors



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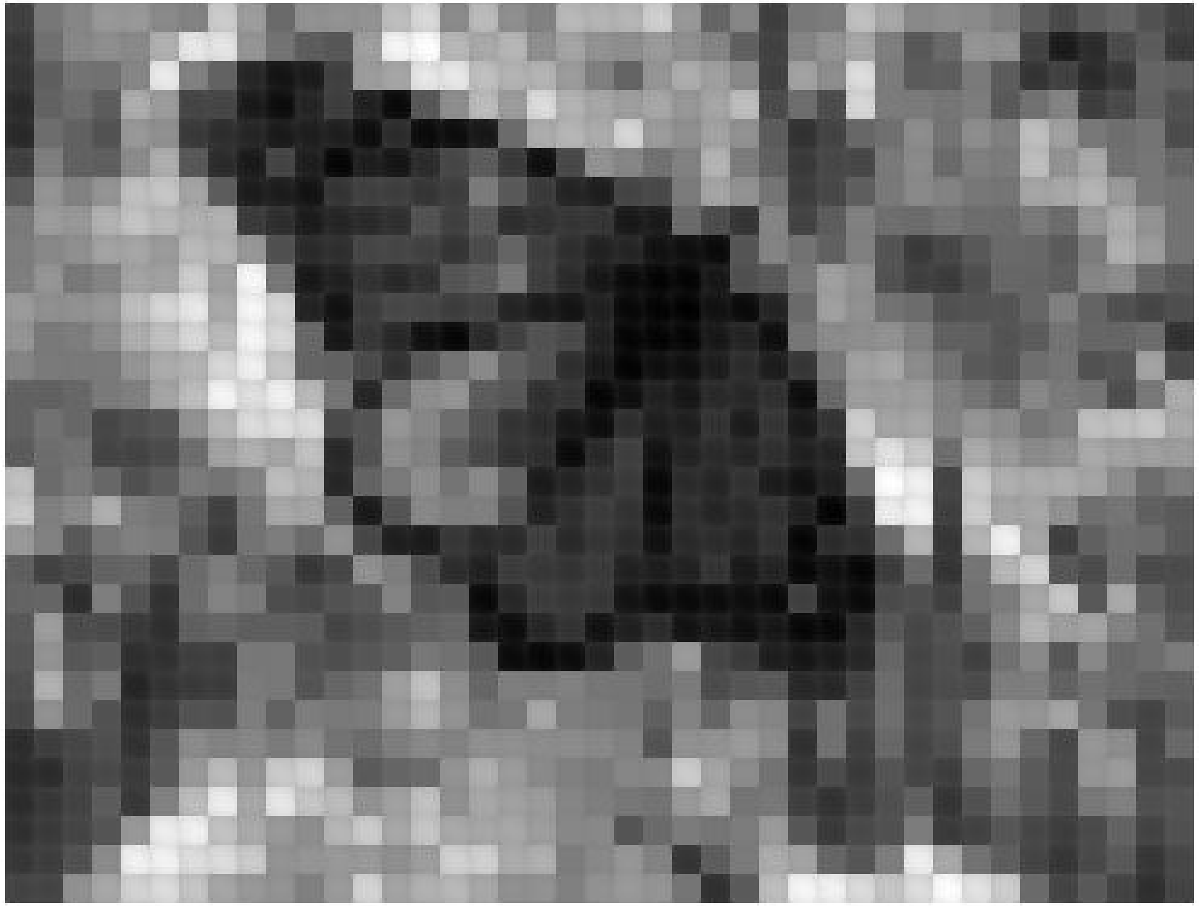
Principal Components Analysis (PCA)

PCA compression: 144D → 1D



Dimensionality reduction

Further reading:

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

Exercise (15 minutes)

- **Objective**: To understand and apply PCA for dimensionality reduction and visualize the Iris dataset in a 2D space.

1. Data loading and exploration:

```
from sklearn.datasets import load_iris
import pandas as pd
iris = load_iris()
df = pd.DataFrame(iris.data, columns=iris.feature_names)
df['species'] = iris.target
```

2. Data Standardization:

```
from sklearn.preprocessing import StandardScaler
features = iris.feature_names
x = df.loc[:, features].values
x = StandardScaler().fit_transform(x)
```

3. Applying PCA (reduce the data to 2 principal components for visualization):

```
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
principalComponents = pca.fit_transform(x)
principalDf = pd.DataFrame(data=principalComponents, columns=['Principal Component 1’, 'Principal Component 2'])
```

4. Visualization:

```
import matplotlib.pyplot as plt

fig = plt.figure(figsize=(8, 8))
ax = fig.add_subplot(1, 1, 1)
ax.set_xlabel('Principal Component 1', fontsize=15)
ax.set_ylabel('Principal Component 2', fontsize=15)
ax.set_title('2 Component PCA', fontsize=20)

targets = [0, 1, 2]
colors = ['r', 'g', 'b’]
for target, color in zip(targets, colors):
        indicesToKeep = df['species'] == target
        ax.scatter(principalDf.loc[indicesToKeep, 'Principal Component 1'], principalDf.loc[indicesToKeep,
        'Principal Component 2'], c=color, s=50)
ax.legend(iris.target_names)
ax.grid()
```