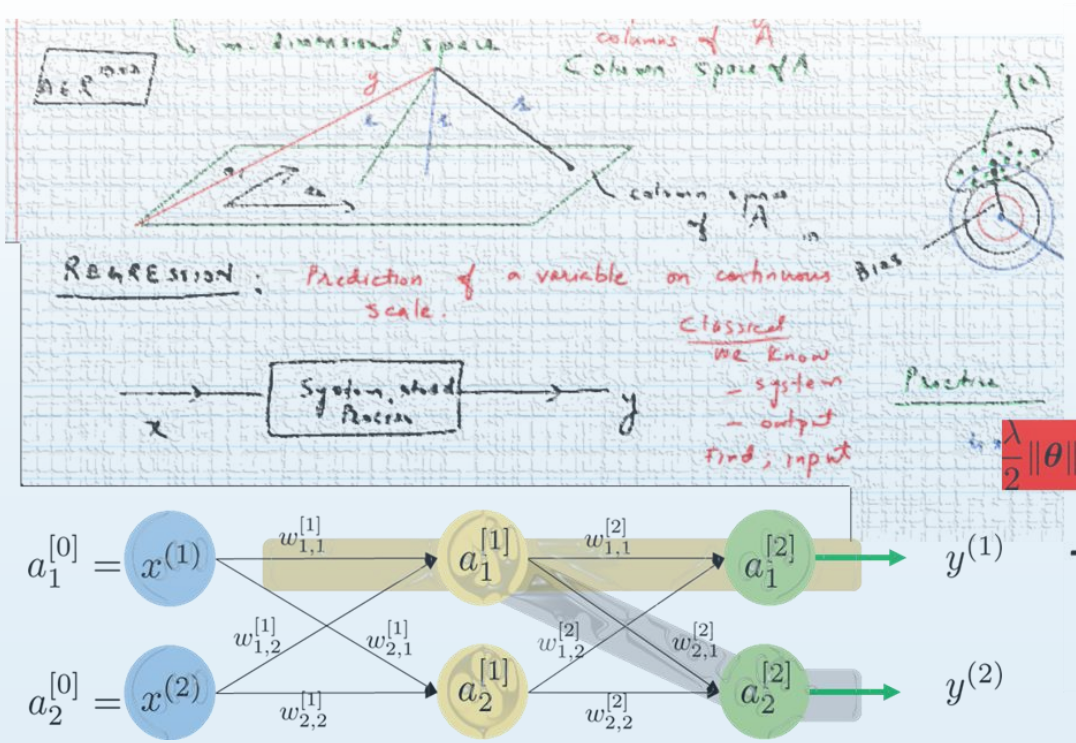
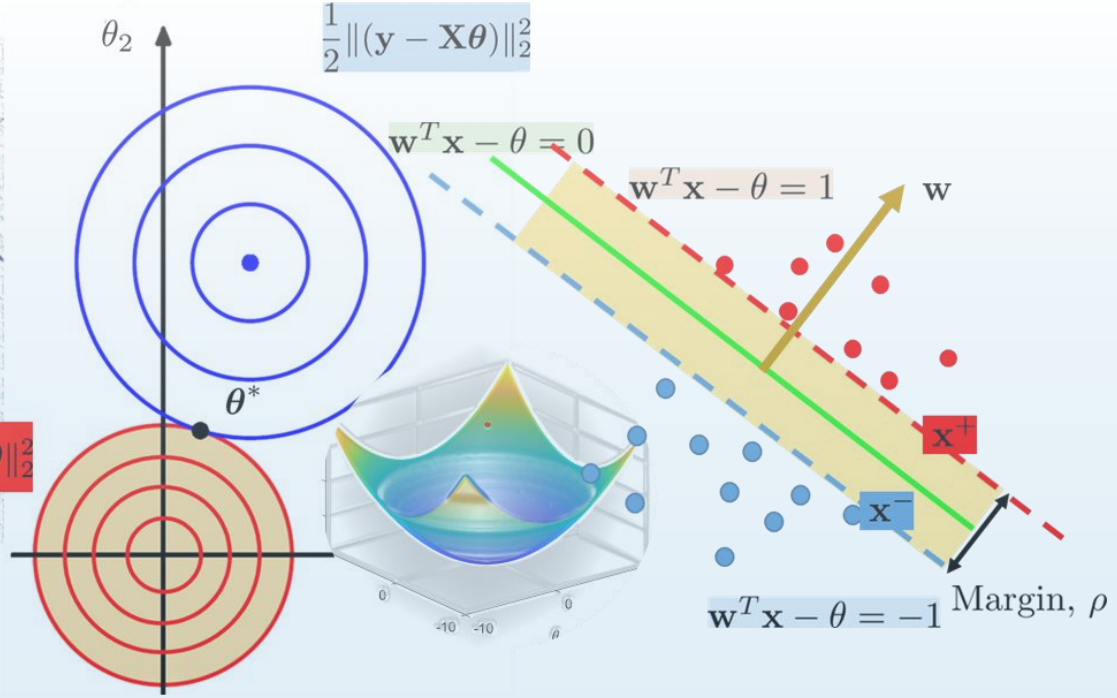




AI-501 Mathematics for AI

Principal Component Analysis

Zubair Khalid

School of Science and Engineering

LUMS
A Not-for-Profit University

https://www.zubairkhalid.org/ai501_2024.html

Outline

- The Curse of Dimensionality
- Principal Component Analysis

The Curse of Dimensionality

Concept:

- Refers to the problems or phenomena associated with classifying, analyzing and organizing the data in high-dimensional spaces that do not arise in low-dimensional settings.

- For high-dimensional datasets, the **size** of data **space** is **huge**.

- In other words, the size of the feature space grows exponentially with the number of dimensions (d) of the data sets.

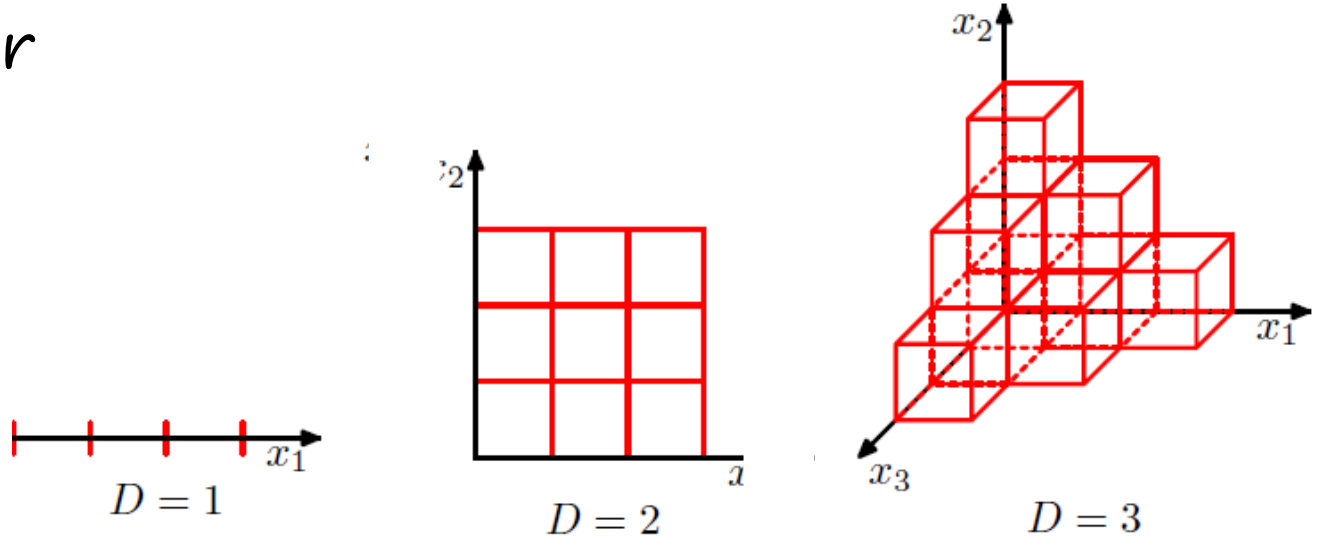
- To ensure the points stay close to each other, the size (n) of the data set must also have exponential growth. That means, we need a very large dataset to maintain the density of points in the high dimensional space.

The Curse of Dimensionality

Illustration 1:

- For high-dimensional datasets, the **size** of data **space** is **huge**.

For an exponentially large number of cells, we need an exponentially large amount of training data to ensure that the cells are not empty.



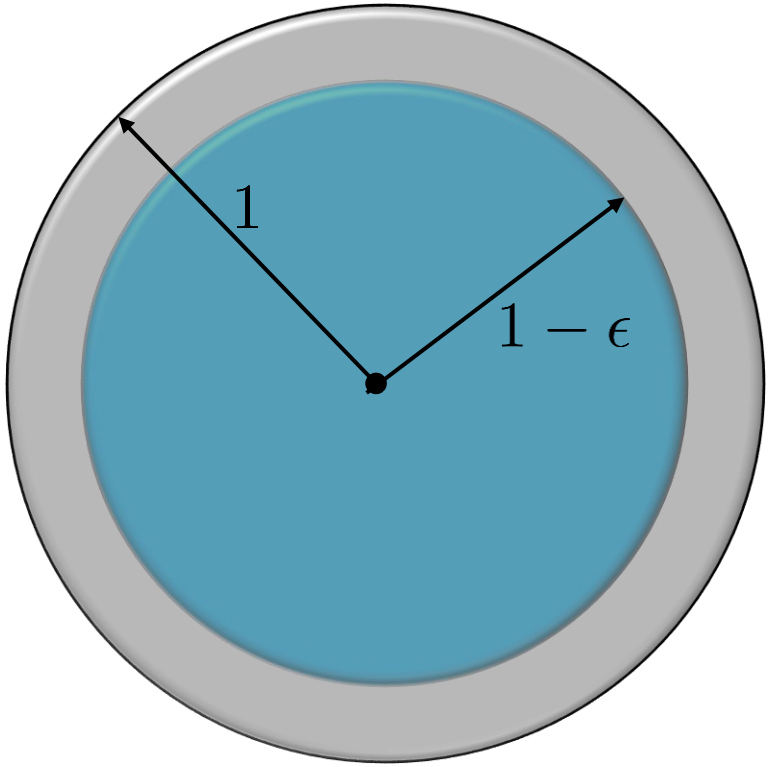
Ref: CB

The Curse of Dimensionality

Illustration 2:

Consider a ball of radius r defined as

$$B(r) = \{\|\mathbf{x}\|_2 \leq r \,|\, \mathbf{x} \in \mathbf{R}^d\}$$



Volume of a ball of radius r

$$V(d) = K_d r^d$$

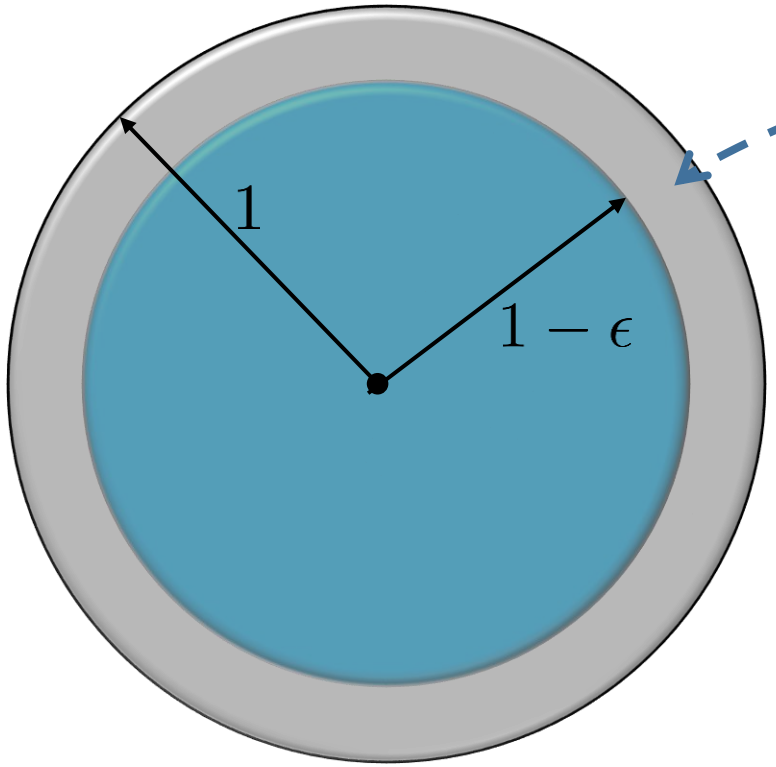
Fraction of a volume between the balls of radius 1 and radius $1-\epsilon$

$$\frac{V(1) - V(1-\epsilon)}{V(1)} = 1 - (1-\epsilon)^d$$

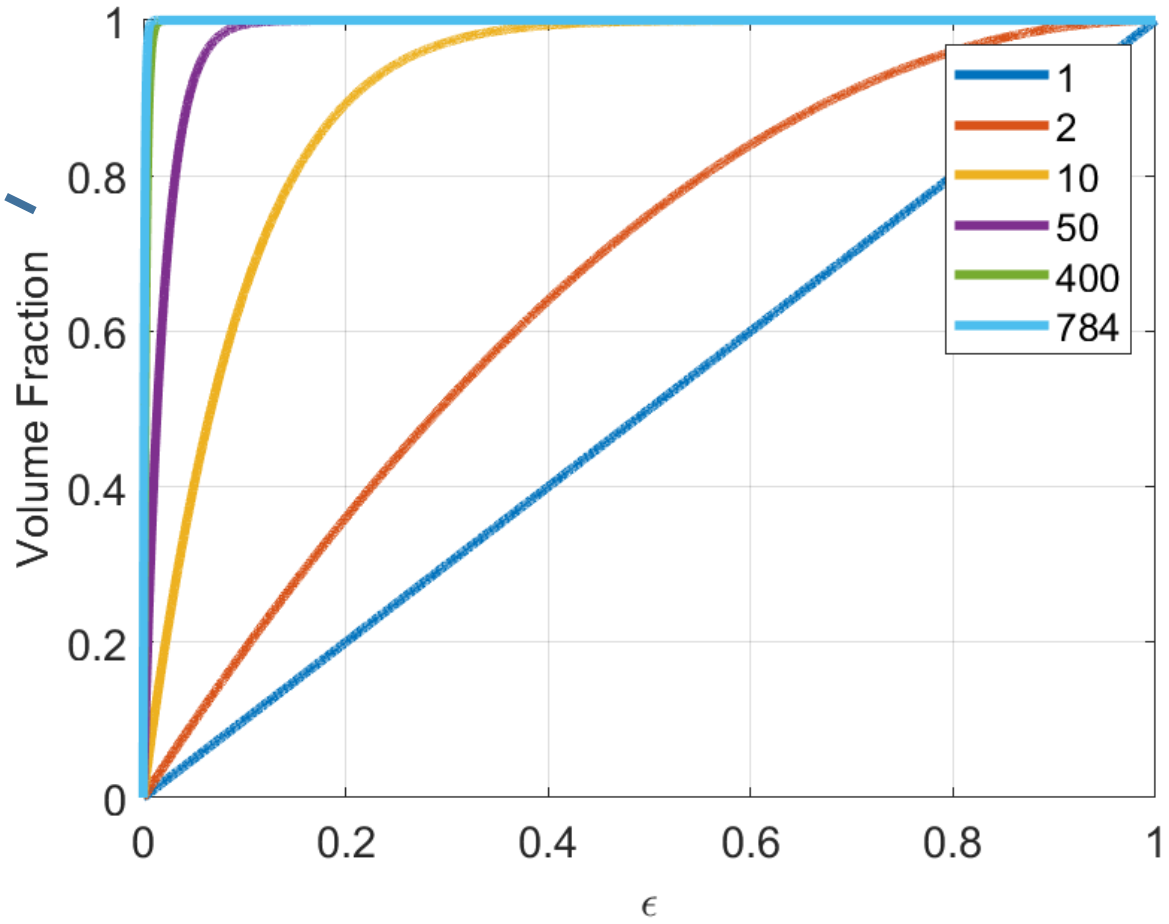
$$K_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}$$

The Curse of Dimensionality

Illustration 2:



$1-(1-\epsilon)^d$



The Curse of Dimensionality

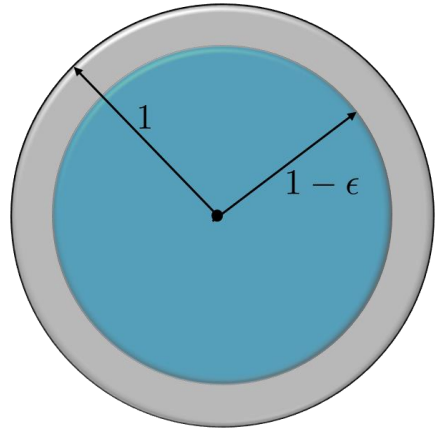


Illustration 2 (Another viewpoint):

Calculate Probabilities that a uniformly distributed point is inside

$\epsilon = 0.1$

the shell: $1 - (1 - \epsilon)^d$

the inner ball: $(1 - \epsilon)^d$

d = 1	2	10	50	400	784
0.1	0.19	0.65	0.995	1.000	1.000
0.9	0.81	0.35	0.005	0.000	0.000

For $d = 50$, 5 out of 1000 data-points would be inside the inner ball.

For $d = 400$, $(1 - \epsilon)^d = 4.9774e - 19$; almost all points lie on the surface of the ball.

If you take a test point on the origin and $d = 400$, (almost) every point is at the same (Euclidean) distance from the origin.

The Curse of Dimensionality

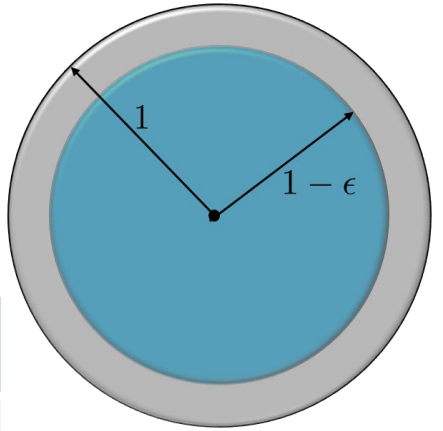


Illustration 2 (Another viewpoint):

Calculate Probabilities that a uniformly distributed point is inside

$\epsilon = 0.01$

the shell: $1-(1-\epsilon)^d$

the inner ball: $(1-\epsilon)^d$

d = 1	2	10	50	400	784
0.01	0.02	0.096	0.395	0.982	0.999
0.99	0.98	0.904	0.605	0.018	0.0004

Practical Datasets

- With the increase in the number of features or number of dimensions of the feature space, data-points are never near to one another.

- Real-world data in the higher dimensional space is confined to a region with effective lower dimensionality.
  - **Dimensionality Reduction**

- Real-world data exhibits smoothness that enables us to make predictions exploiting interpolation techniques.

- For example,
  - Data along a line or a plane in higher dimensional space
  - detection of orientation of object in an image; data lies on effectively 1 dimensional manifold in probably 1million dimensional space.
  - Face recognition in an image (50 or 71 features)

Dimensionality Reduction

Feature Extraction:

Transform existing features to obtain a set of new features using some mapping function.

$$\mathbf{x} = [x_1, x_2, \ldots, x_d]$$

$$\mathbf{z} = f(\mathbf{x})$$

$$\mathbf{z} = [z_1, z_2, \ldots, z_k]$$

- The mapping function **z**=*f*(**x**) can be **linear** or non-linear.

- Can be interpreted as projection or mapping of the data in the higher dimensional space to the lower dimensional space.

- Mathematically, we want to find an optimum mapping **z**=*f*(**x**) that preserves the desired information as much as possible.

Dimensionality Reduction

Feature Extraction:

Idea:

- Finding optimum mapping is equivalent to optimizing an **objective** function.
- We use different objective functions in different methods;
  - Minimize Information Loss: Mapping that represent the data as accurately as possible in the lower-dimensional space, e.g., Principal Components Analysis (PCA).
  - Maximize Discriminatory Information: Mapping that best discriminates the data in the lower-dimensional space, e.g., Linear Discriminant Analysis (LDA).
- Here we focus on PCA, that is, a linear mapping.
- Why Linear: Simpler to Compute and Analytically Tractable.

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

- Given features in d-dimensional space

- Project into lower dimensional space using the following linear transformation

$$\mathbf{z} = \mathbf{W}^T \mathbf{x}$$

- For example (can you tell me size of matrix **W** for the following cases),
  - find best planar approximation to 4D data
  - find best planar approximation to 100D data

- We want to find this mapping while preserving as much information as possible, and ensuring

  - ***Objective 1***: the features after mapping are uncorrelated; cannot be reduced further

  - ***Objective 2***: the features after mapping have large variance

$$\mathbf{z} = \mathbf{W}^T \mathbf{x}$$

- Can you tell the size of matrix W for the following cases

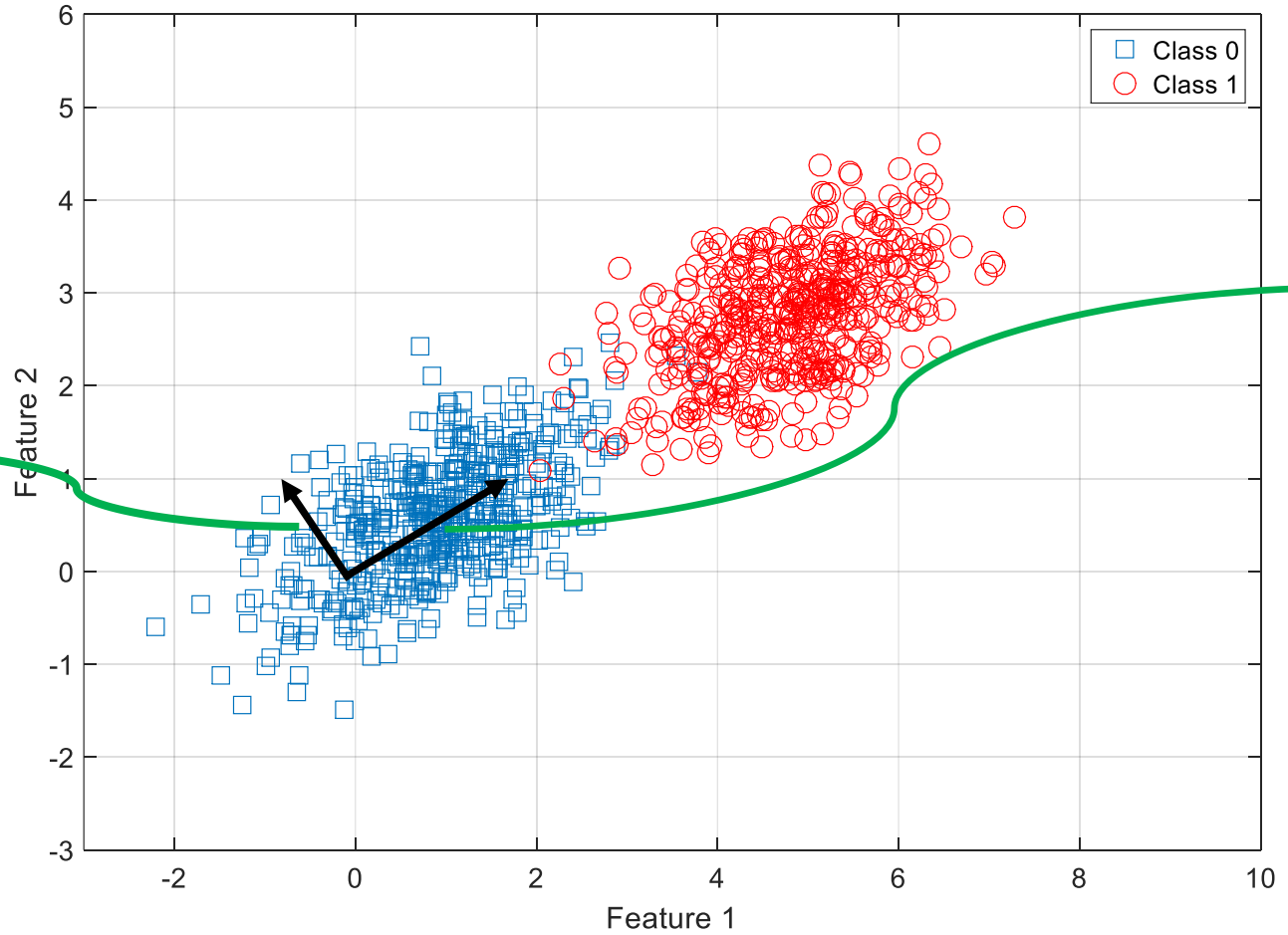
  - find best planar approximation to 4D data

  - find best planar approximation to 100D data

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Geometric Intuition:



Most contribution of each class lies in this direction

First Principal Component

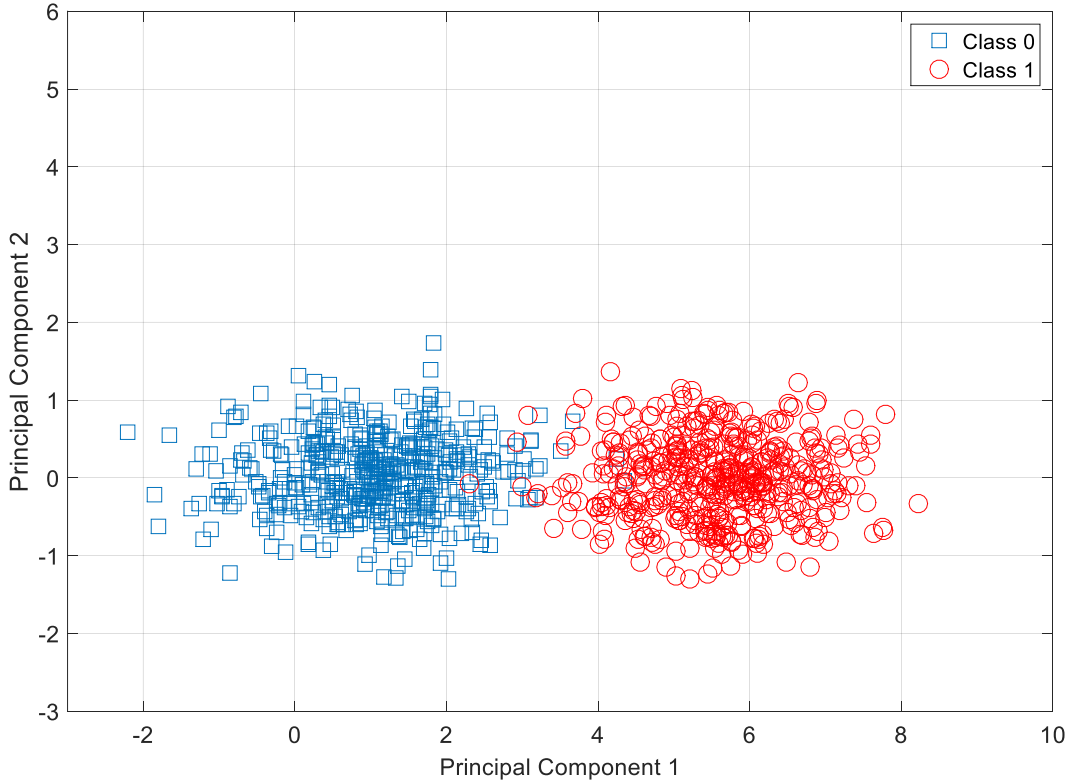
Second Principal Component

Toy Illustration in two dimensions

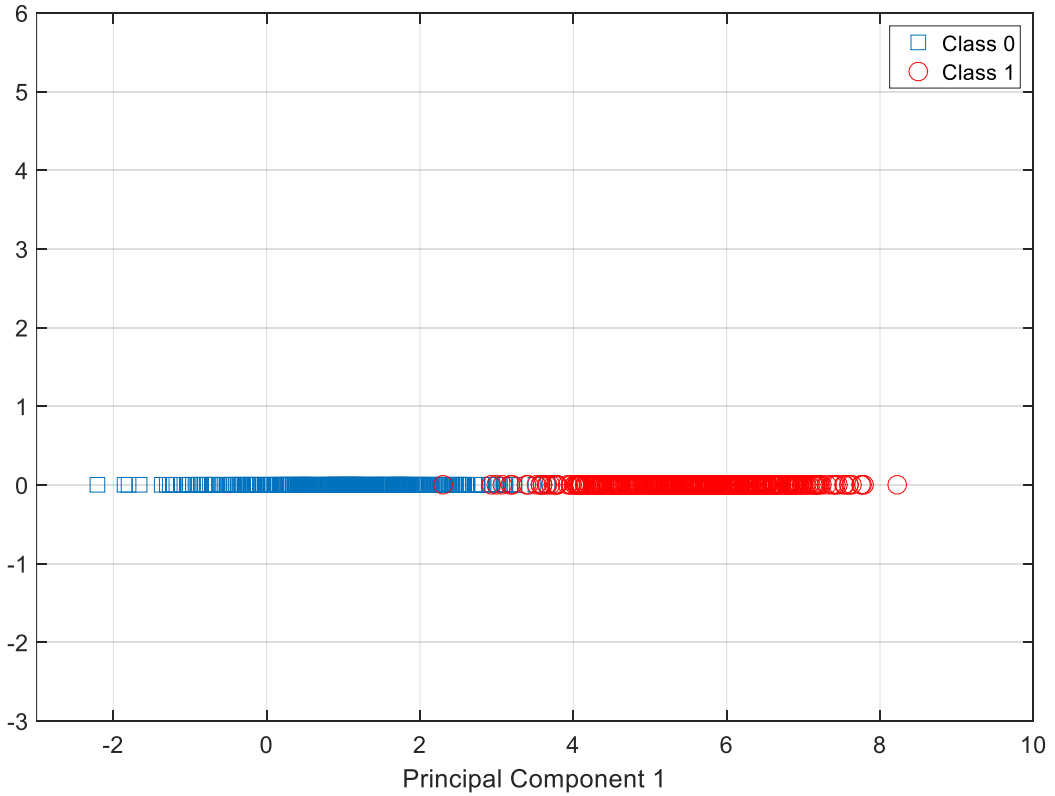
Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Geometric Intuition:



Change of coordinates: Linear combinations of features



Ignoring the Second Component/Feature

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Mathematical Formulation:

We have n feature vectors of the form $\mathbf{x} \in \mathbf{R}^d$.

Note d represents the number of features.

In PCA, we want to represent $\mathbf{x}$ in a new space of lower dimensionality using only k basis vectors ($k < d$), that is,

$$\hat{\mathbf{x}} = \sum_{i=1}^{k} z_i \mathbf{v}_i$$

such that

$$\|\mathbf{x} - \hat{\mathbf{x}}\|_2$$

is minimized.

Here $\mathbf{v}_i \in \mathbf{R}^d$ for $i = 1, 2, \ldots, k$ represent the k number of orthogonal vectors that form the basis, referred to as principal components, of the subspace of dimensionality=k.

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Mathematical Formulation:

How do we find the basis vectors $\mathbf{v}_i \in \mathbf{R}^d$ for $i = 1, 2, \ldots, k$?

Steps to find Principal Components:

We have n feature vectors $\mathbf{x}_i \in \mathbf{R}^d, \quad i = 1, 2, \ldots, n.$

Step 1: Compute Sample Mean:

Sample mean (note summtion over the number of feature vectors n)

$$\overline{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i$$

Step 2: Subtract Sample Mean:

Subtract sample mean from each feature vector $\mathbf{x}_i$ to obtain $\mathbf{s}_i$, that is,

$$\mathbf{s}_i = \mathbf{x}_i - \overline{\mathbf{x}}$$

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Mathematical Formulation:

Step 3: Calculate the Covariance Matrix:

What is special about these vectors?

Zero mean; taken along all feature vectors

Now we have n feature vectors $\mathbf{s}_i \in \mathbf{R}^d, \quad i = 1, 2, \ldots, n.$

Calculate the Covariance Matrix as follows

$$\Sigma = \frac{1}{n} \sum_{i=1}^{n} \mathbf{s}_i \mathbf{s}_i^T$$

How do you interpret the entries of the matrix? Spend some time and try to understand this!

This can also be expressed as

$$\Sigma = \frac{1}{n} \mathbf{S}\mathbf{S}^T$$

where

$$\mathbf{S} = [\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n]$$

For two vectors $\mathbf{f}, \mathbf{g} \in \mathbf{R}^n$, covariance is defined as

$$\sigma_{\mathbf{fg}} = \frac{1}{n} \sum_{i}^{n} (f_i - \text{avg}(\mathbf{f}))\,(g_i - \text{avg}(\mathbf{g}))$$

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Special about the Covariance Matrix:

The covarince matrix is symmetric, that is, $\Sigma^T = \Sigma$. (super easy to show)

The covarince matrix is positive semi-definite. (again, super easy)

Size of Σ is $d \times d$.

Step 4: Carry out Eigenvalue Decomposition of Covariance Matrix:

Carry out eigenvalue decomposition of the covarince matrix as

$$\Sigma = \mathbf{V}\mathbf{D}\mathbf{V}^T$$

Here the matrix $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_d]$ contains d orthogonal eigenvectors $\mathbf{v}_i \in \mathbf{R}^d$, referred to as principal components, that serve as the basis of $\mathbf{R}^d$.

Here the matrix $\mathbf{D}$ is a diagonal matrix with eigenvalues denoted by $\lambda_1, \lambda_2, \ldots, \lambda_d$.

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Step 5: Dimensionality Reduction

We wanted to find the basis vectors $\mathbf{v}_i \in \mathbf{R}^d$ for $i = 1, 2, \ldots, k$.

We have $\mathbf{v}_i \in \mathbf{R}^d$ for $i = 1, 2, \ldots, d$.

- *Q: How to select k out of d?*

- A: *Simple, select the ones corresponding to k largest eigenvalues.*

Construct the maapping matrix of size $d \times k$ as

$$\mathbf{W} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k]$$

to reduce the dimensionality of the feature space from $\mathbf{R}^d$ to $\mathbf{R}^k$ as

$$\mathbf{z} = \mathbf{W}^T \mathbf{x}$$

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Using $\mathbf{z}$, we can go back to $\mathbf{R}^d$ to obtain apprxoimation of $\mathbf{x}$ as

$$\hat{\mathbf{x}} = \sum_{i=1}^{k} z_i \mathbf{v}_i = \mathbf{W}\mathbf{z}$$

Connection with the Objectives:

- **Objective 1**: the features after mapping are uncorrelated; cannot be reduced further
  - Enabled by orthogonality of the principal components
- **Objective 2**: the features after mapping have large variance
  - We have used covariance matrix to define the mapping and used eigenvectors with largest eigenvalues, that is, those dimensions capturing the variations in the data.
  - **PCA maps the data along the directions where we have most of the variations in the data.**

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

How do we choose k?

- It depends on the amount of information, that is variance, we want to preserve in the mapping process.

- We can define a variable T to quantify this preservation of information

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i} > T$$

- T=1, when k=d; No reduction.
- T=0.8, interpreted as that 80% variation in the data has been preserved.

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Example: $d = 2,\ n = 10,\ k = 1$

Step 1: Compute sample mean:

$$\bar{\mathbf{x}} = [1.81, 1.91]$$

x_1	x_2	
2.5000	2.4000	$\mathbf{x}_1$
0.5000	0.7000	$\mathbf{x}_2$
2.2000	2.9000	
1.9000	2.2000	
3.1000	3.0000	
2.3000	2.7000	
2.0000	1.6000	
1.0000	1.1000	
1.5000	1.6000	
1.1000	0.9000	

Step 2: Subtract Sample Mean:

$$\mathbf{s}_i = \mathbf{x}_i - \overline{\mathbf{x}}$$

s_1	s_2	
0.6900	0.4900	$\mathbf{s}_1$
-1.3100	-1.2100	$\mathbf{s}_2$
0.3900	0.9900	
0.0900	0.2900	
1.2900	1.0900	
0.4900	0.7900	
0.1900	-0.3100	
-0.8100	-0.8100	
-0.3100	-0.3100	
-0.7100	-1.0100	

Step 3: Calculate the Covariance Matrix:

$$\mathbf{S} = [\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n]$$

$$\Sigma = \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i \mathbf{s}_i^T = \frac{1}{n}\mathbf{S}\mathbf{S}^T$$

$$\Sigma = \begin{bmatrix} 0.5549 & 0.5539 \\ 0.5539 & 0.6449 \end{bmatrix}$$

We have divided by n. Some authors divide by n-1. It won't change the principal components

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Example:

Step 4: Carry out Eigenvalue Decomposition of Covariance Matrix:

$$\Sigma = \mathbf{V}\mathbf{D}\mathbf{V}^T \qquad \mathbf{V} = \begin{bmatrix} -0.7352 & 0.6779 \\ 0.6779 & 0.7352 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 0.0442 & 0 \\ 0 & 1.1556 \end{bmatrix}$$

Step 5: Dimensionality Reduction

Use $\mathbf{W} = [\mathbf{v}_2]$ (associated with the largest eigenvalue) to reduce the dimensionality of the feature space from $\mathbf{R}^2$ to $\mathbf{R}$ as

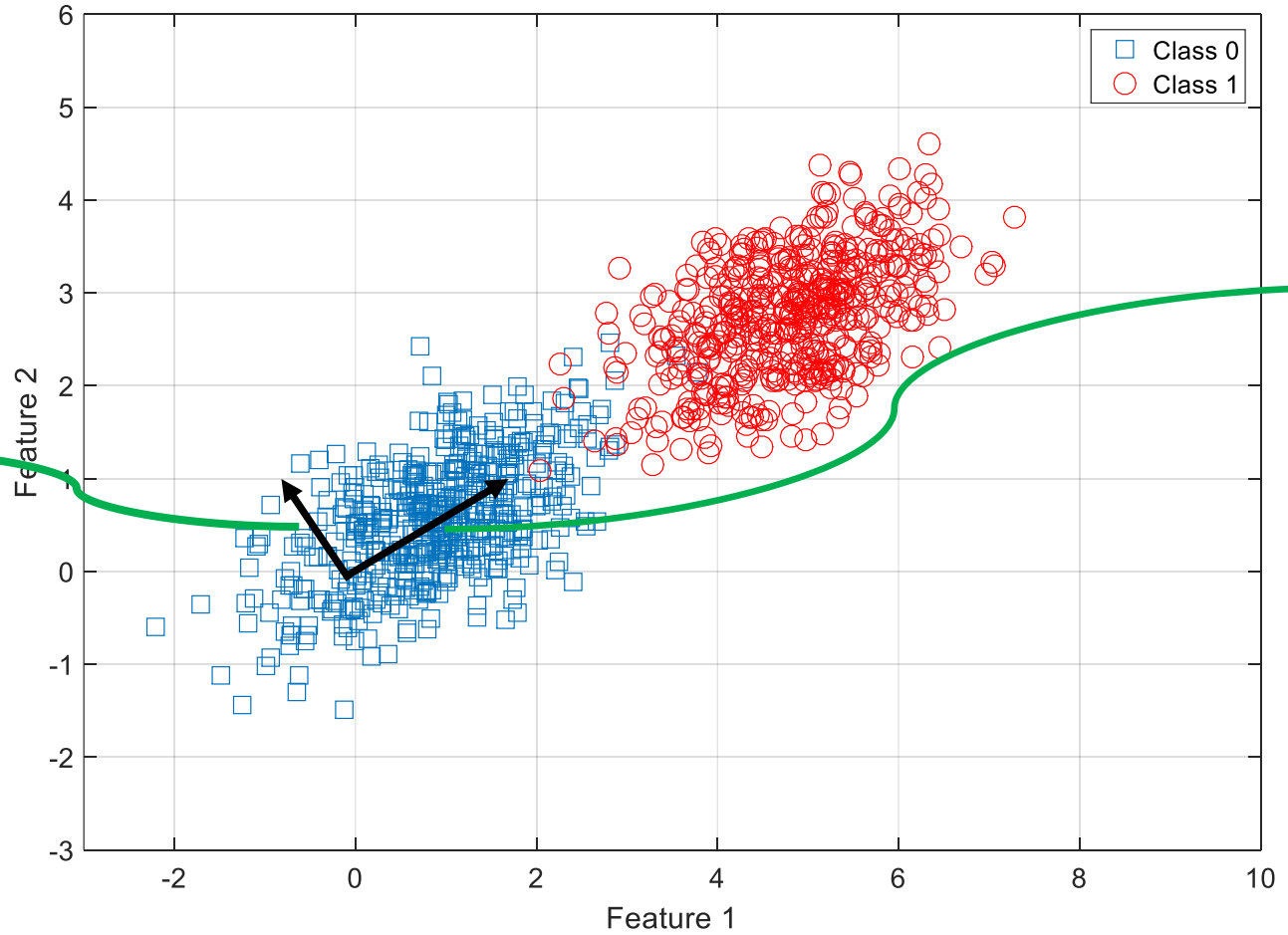
$$\mathbf{z} = \mathbf{W}^T\mathbf{x}$$

z
3.4591
0.8536
3.6233
2.9054
4.3069
3.5441
2.5320
1.4866
2.1931
1.4073

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Geometric Intuition:



Most contribution of each class lies in this direction

First Principal Component

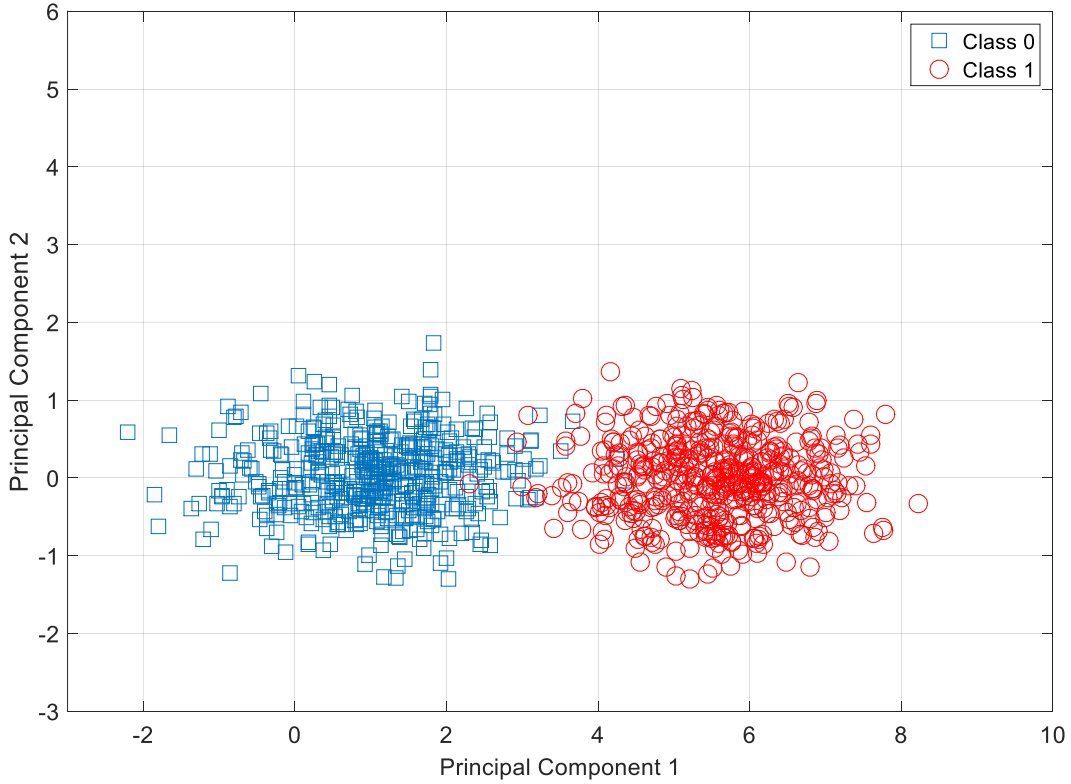
Second Principal Component

Toy Illustration in two dimensions

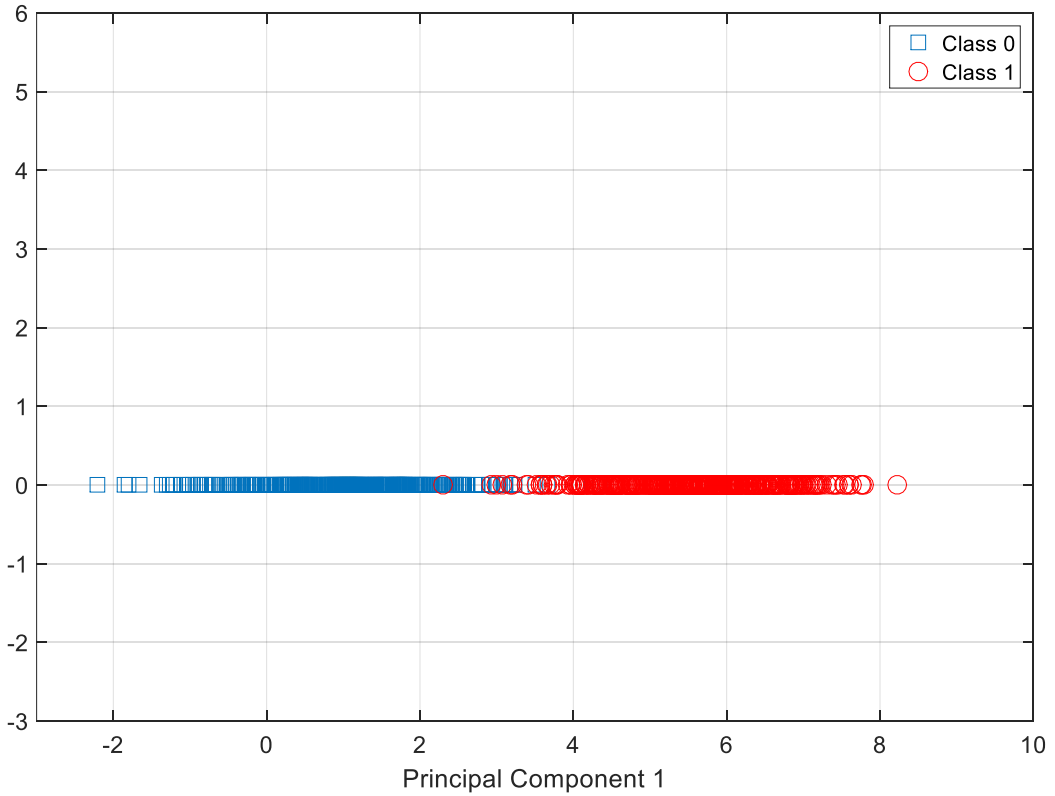
Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Geometric Intuition:



Change of coordinates: Linear combinations of features



Ignoring the Second Component/Feature

Dimensionality Reduction

Feature Extraction - Principal Component Analysis:

Practical Considerations and Limitations:

- Data should be normalized before using PCA for dimensionality reduction.

- Usually, we normalize every feature by subtracting mean of that feature followed by dividing with standard deviation of the feature.

- The covariance matrix of the reduced feature is projection along orthogonal components (directions) and therefore features are uncorrelated to each other. In other words, PCA decorrelates the features.

- ***Limitation:***
  - PCA does not consider the separation of data with respect to class label and therefore we do not have a guarantee the mapping of the data along dimensions of maximum variance results in the new features good enough for class discrimination.

  Solution: Linear Discriminant Analysis (LDA) – Find mapping directions along which the classes are best separated.