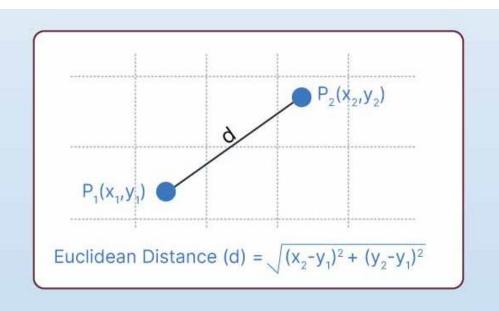
# COMP30027 MACHINE LEARNING TUTORIAL

Workshop - 5

# Distance Measures, KNN & SVM

- How to implement distance measures (Euclidean, Manhattan, etc.)
- How to implement K-NN
- How to implement SVM
- Design decisions involved in K-NN and SVM classification



# Euclidean Distance



### Formula

 $\sqrt{(\Sigma(xi-y_i)^2)}$  calculates the straight-line distance between points.



Ideal for continuous numerical features

### Limitation

Highly sensitive to feature scaling. Normalization is essential.

# Euclidean Distance

Emp	Age	Salary
Emp1	44	73000
Emp2	27	47000
Emp3	30	53000
Emp4	38	62000
Emp5	40	57000
Emp6	35	53000
Emp7	48	78000
	Emp1 Emp2 Emp3 Emp4 Emp5 Emp6	Emp1 44 Emp2 27 Emp3 30 Emp4 38 Emp5 40 Emp6 35

Distance between Emp2 and Emp1 =  $\sqrt{(27-44)^2+(47000-73000)^2}$  = 31.06 Distance between Emp2 and Emp3 =  $\sqrt{(30-27)^2+(53000-47000)^2}$  = 6.70



 $\sqrt{(\Sigma(xi-y_i)^2)}$  calculates the straight-line distance between points.

### Best Use

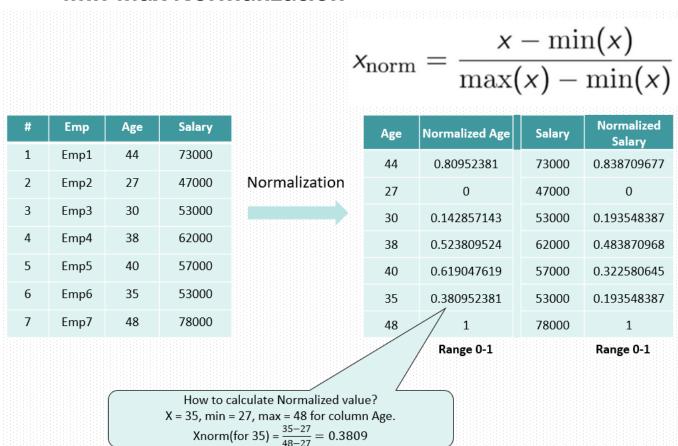
Ideal for continuous numerical features

### Limitation

Highly sensitive to feature scaling. Normalization is essential.

## **Feature Scaling Techniques**

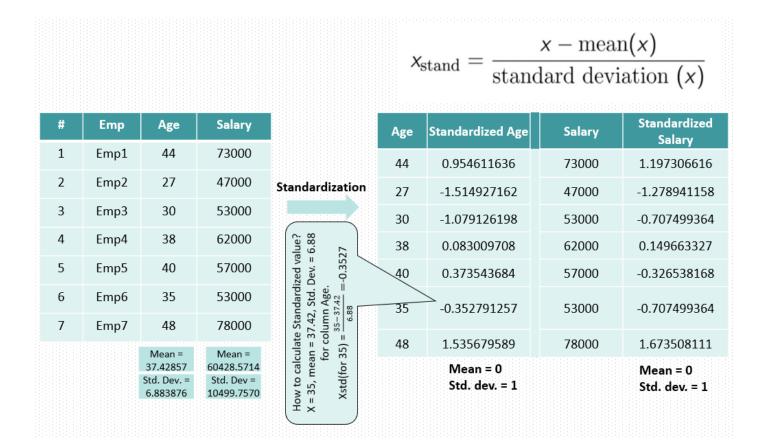
### **Min-Max Normalization**

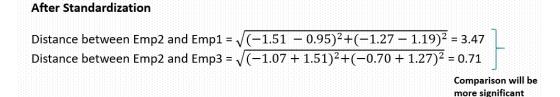


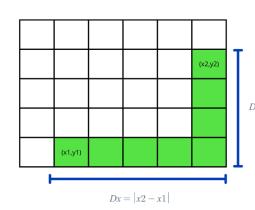
### After Normalization

Distance between Emp2 and Emp1 =  $\sqrt{(0-.80)^2+(0-.83)^2}$  = 1.15 Comparison will be more significant

### **Standardization**







### **Manhattan Distance**

$$D = Dx + Dy$$

$$D_{Dy = |y2 - y1|} D = |x2 - x1| + |y2 - y1|$$

# Manhattan Distance

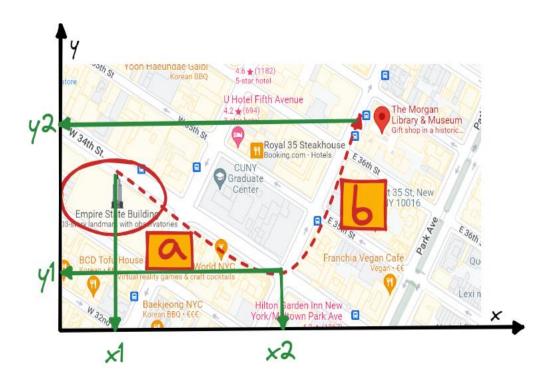
### What Is It?

Manhattan distance measures the sum of absolute differences between coordinates.

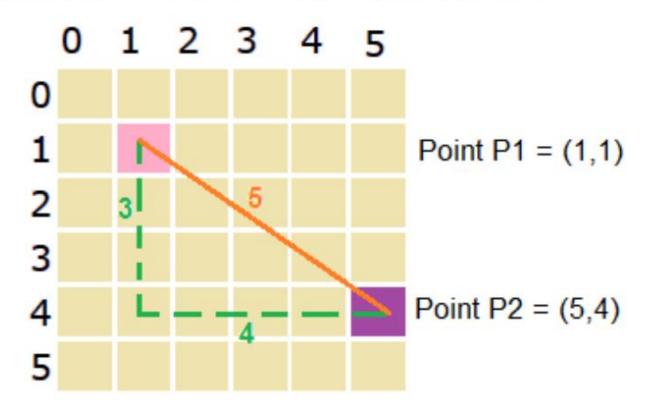
It follows grid-like paths similar to navigating city blocks.

### Formula

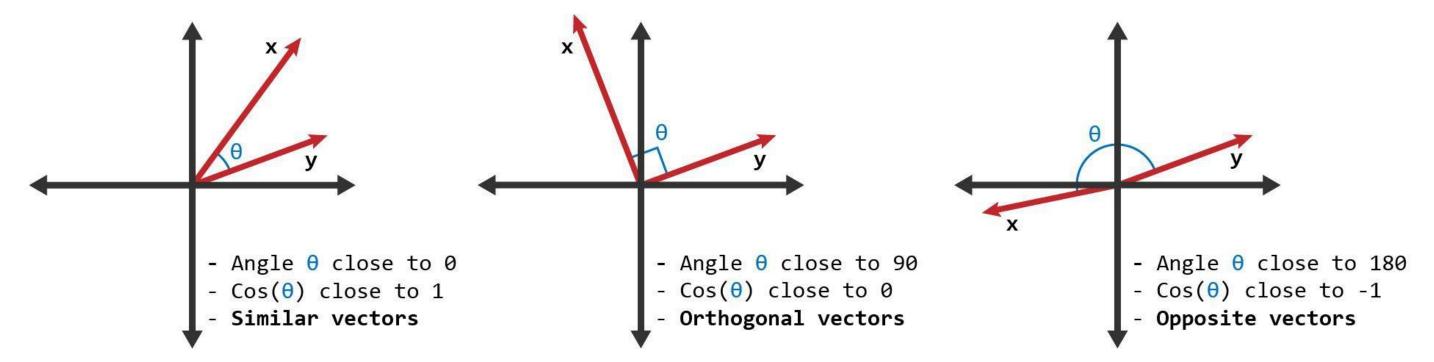
 $\Sigma |x_i - y_i|$  for all coordinates in the feature vectors.



Manhattan Distance vs Euclidean Distance



Euclidean distance = 
$$\sqrt{(5-1)^2 + (4-1)^2} = 5$$

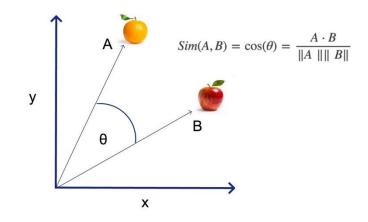


# Cosine Similarity



### Angle-Based Measurement

Measures the cosine of the angle between two non-zero vectors.





### Formula Application

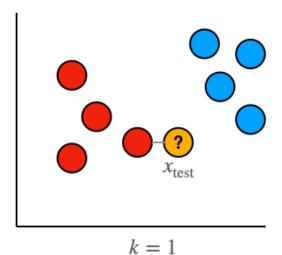
$$\cos( heta) = rac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = rac{\sum\limits_{i=1}^n A_i B_i}{\sqrt{\sum\limits_{i=1}^n A_i^2} \sqrt{\sum\limits_{i=1}^n B_i^2}}$$



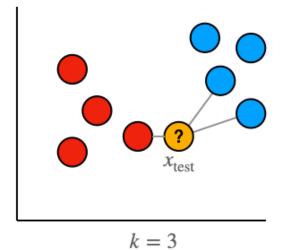
### High-Dimensional Data

Excels with sparse vectors like TF-IDF representations.

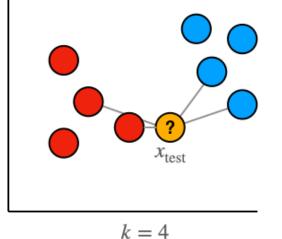
# K-Nearest Neighbors



Nearest point is red, so  $x_{test}$  classified as red



Nearest points are {red, blue, blue} so  $x_{\text{test}}$  classified as blue



Nearest points are {red, red, blue, blue} so classification of  $x_{\text{test}}$  is not properly defined

# K-Nearest Neighbors Overview

### Classification

Predicts class based on majority vote of nearest neighbors

### Regression

Predicts values using averages of nearest neighbors

### Storage

Stores all training examples as reference points

K-NN is intuitive and versatile, requiring no training phase beyond storing examples. It's memory-intensive but highly flexible for various problem types.

# Category B New data point assigned to Category A Category A X1 X2 After K-NN Category B New data point assigned to Category 1 Category A

# K-NN Implementation Steps

### Choose Value of K

Select an optimal K value through cross-validation. K should be odd to avoid ties.

### Calculate Distances

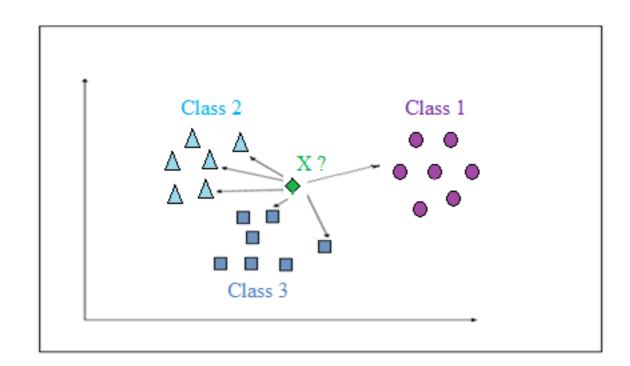
Compute distances between test example and all training examples. Use Euclidean, Manhattan, or Cosine metrics.

### Find K Nearest Neighbors

Sort distances and identify the K closest training examples. This subset determines the classification.

### Apply Voting Mechanism

Use **majority** or **weighted voting** to determine the predicted class. Return the result.



# Majority Voting in K-NN

### How It Works

Each of the K nearest neighbours casts one equal vote. The class with the most votes wins.

Simple to implement and explain, requiring only vote counting.

### Implementation

Count occurrences of each class among K neighbors. Return the most frequent class.

### Challenges

Ties can occur with even K values.
Solution: use odd K or add
tiebreaker rule.

All neighbors have equal influence regardless of distance.

# Weighted Voting Technique

By the inverse linear distance from the test instance to instance j

$$w_j = \frac{d_{max} - d_j}{d_{max} - d_{min}}$$

where  $d_{min}$  is for the nearest neighbour of the test instance, and  $d_{max}$  is for the furthest neighbour of the test instance

• By the inverse distance from the test instance to instance j

$$w_j = \frac{1}{d_j + \epsilon}$$

### Vote Calculation

Sum weights for each class; highest weighted class wins

# What is the class label using different weighting strategies?

Instance	Class	Distance
$d_1$	no	0
$d_2$	yes	1
$d_3$	yes	1.5
$d_4$	yes	2

Equal weight (majority voting):

Inverse linear distance voting:

$$d_{min} = 0, d_{max} = 2,$$
  
 $yes = (\frac{1}{2} + \frac{0.5}{2} + 0) = \frac{3}{4}$   
 $no = 1$ 

• Inverse distance voting ( $\epsilon = 0.5$ )

yes = 
$$(\frac{1}{1.5} + \frac{1}{2} + \frac{1}{2.5}) = 1.57$$
  
no =  $\frac{1}{0.5} = 2$ 

K-NN classification

Consider the following dataset Training set:

CLASS	SUN	LEMON	IBM	APPLE
fruit	1	1	0	4
fruit	2	5	0	5
computer	0	0	5	2
computer	7	1	2	1

Test set:

CLASS	SUN	LEMON	IBM	APPLE
?	1	3	0	2
Ş	0	1	2	1

### Q1

Classify the test instances using 1-NN and 3-NN with various distance measures (Euclidean distance, Manhattan distance, cosine similarity). For 3-NN, consider both majority vote and weighted voting (cosine similarity can be weighted by simply summing the similarities of the 3 neighbours). Complete the tables below. How does the classification of each test instance change with different parameters?

### Euclidean distance

The Euclidean distances to the neighbors for test instance 1 are:

A. 
$$\sqrt{(2-4)^2+(0-0)^2+(3-1)^2+(1-1)^2}=\sqrt{8}=2.828$$
 (class = fruit)

B. 
$$\sqrt{(2-5)^2 + (0-0)^2 + (3-5)^2 + (1-2)^2} = \sqrt{14} = 3.742$$
 (class = fruit)

C. 
$$\sqrt{(2-2)^2 + (0-5)^2 + (3-0)^2 + (1-0)^2} = \sqrt{35} = 5.916$$
 (class = computer)

D. 
$$\sqrt{(2-1)^2 + (0-2)^2 + (3-1)^2 + (1-7)^2} = \sqrt{45} = 6.708$$
 (class = computer)

The Euclidean distances to the neighbors for test instance 2 are:

A. 
$$\sqrt{(1-4)^2 + (2-0)^2 + (1-1)^2 + (0-1)^2} = \sqrt{14} = 3.742$$
 (class = fruit)

B. 
$$\sqrt{(1-5)^2 + (2-0)^2 + (1-5)^2 + (0-2)^2} = \sqrt{40} = 6.325$$
 (class = fruit)

C. 
$$\sqrt{(1-2)^2 + (2-5)^2 + (1-0)^2 + (0-0)^2} = \sqrt{11} = 3.317$$
 (class = computer)

D. 
$$\sqrt{(1-1)^2 + (2-2)^2 + (1-1)^2 + (0-7)^2} = \sqrt{49} = 7$$
 (class = computer)

### Inverse distance

fruit: 
$$\frac{1}{2.828+\epsilon} + \frac{1}{3.742+\epsilon} = 0.621$$

computer: 
$$\frac{1}{5.916+\epsilon}=0.169$$

and the test instance 1 label is fruit.

Inverse linear distance

if using inverse linear distance to classify test instance 1, the weights are:

fruit: 
$$\frac{5.916-2.828}{5.916-2.828} + \frac{5.916-3.742}{5.916-2.828} = 1.704$$

computer: 
$$\frac{5.916-5.916}{5.916-2.828} = 0$$

and the test instance 1 label is fruit.

### Manhattan distance

The Manhattan distances to the neighbors for test instance 1 are:

A. 
$$|2-4| + |0-0| + |3-1| + |1-1| = 4$$
 (class = fruit)

B. 
$$|2-5| + |0-0| + |3-5| + |1-2| = 6$$
 (class = fruit)

C. 
$$|2-2| + |0-5| + |3-0| + |1-0| = 9$$
 (class = computer)

D. 
$$|2-1|+|0-2|+|3-1|+|1-7|=11$$
 (class = computer)

The Manhattan distances to the neighbors for test instance 2 are:

A. 
$$|1-4|+|2-0|+|1-1|+|0-1|=6$$
 (class = fruit)

B. 
$$|1-5|+|2-0|+|1-5|+|0-2|=12$$
 (class = fruit)

C. 
$$|1-2|+|2-5|+|1-0|+|0-0|=5$$
 (class = computer)

D. 
$$|1-1|+|2-2|+|1-1|+|0-7|=7$$
 (class = computer)

(cosine similarity can be weighted by simply summing the similarities of the 3 neighbours)

### Cosine similarity

Cosine similarity between two vectors A, B is  $\frac{(A \cdot B)}{\|A\| \|B\|}$ 

The cosine similarities to the neighbors for test instance 1 are:

A. 
$$((2*4) + (0*0) + (3*1) + (1*1))/(\sqrt{4+0+9+1}*\sqrt{16+0+1+1}) = 0.756$$
 (class = fruit)

B. 
$$((2*5) + (0*0) + (3*5) + (1*2))/(\sqrt{4+0+9+1}*\sqrt{25+0+25+4}) = 0.982$$
 (class = fruit)

C. 
$$((2*2) + (0*5) + (3*0) + (1*0))/(\sqrt{4+0+9+1}*\sqrt{4+25+0+0}) = 0.199$$
 (class = computer)

D. 
$$((2*1) + (0*2) + (3*1) + (1*7))/(\sqrt{4+0+9+1}*\sqrt{1+4+1+49}) = 0.432$$
 (class = computer)

The cosine similarities to the neighbors for test instance 2 are:

A. 
$$((1*4) + (2*0) + (1*1) + (0*1))/(\sqrt{1+4+1+0}*\sqrt{16+0+1+1}) = 0.481$$
 (class = fruit)

B. 
$$((1*5) + (2*0) + (1*5) + (0*2))/(\sqrt{1+4+1+0}*\sqrt{25+0+25+4}) = 0.556$$
 (class = fruit)

C. 
$$((1*2) + (2*5) + (1*0) + (0*0))/(\sqrt{1+4+1+0}*\sqrt{4+25+0+0}) = 0.910$$
 (class = computer)

D. 
$$((1*1) + (2*2) + (1*1) + (0*7))/(\sqrt{1+4+1+0}*\sqrt{1+4+1+49}) = 0.330$$
 (class = computer)

A value of 1 indicates perfect similarity, 0 indicates orthogonality (no similarity), -1 indicates perfect dissimilarity.

Test instance 1

APPLE	IBM	LEMON	SUN	CLASS
2	0	3	1	?

Measure	K	Weight	Prediction
Euclidean	1	N/A	fruit
Euclidean	3	Majority vote	fruit
Euclidean	3	Inverse dist	fruit
Euclidean	3	Inverse linear dist	fruit
Manhattan	1	N/A	fruit
Manhattan	3	Majority vote	fruit
Manhattan	3	Inverse dist	fruit
Manhattan	3	Inverse linear dist	fruit
Cosine	1	N/A	fruit
Cosine	3	Majority vote	fruit
Cosine	3	Sum	fruit

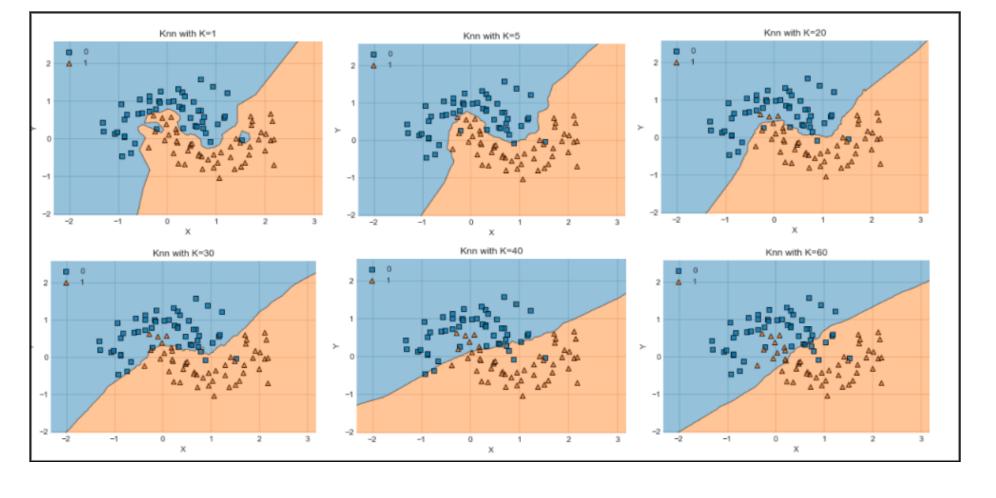
### Test instance 2

APPLE	IBM	LEMON	SUN	CLASS
1	2	1	0	?

Prediction	Weight	K	Measure
computer	N/A	1	Euclidean
fruit	Majority vote	3	Euclidean
fruit	Inverse dist	3	Euclidean
computer	Inverse linear dist	3	Euclidean
computer	N/A	1	Manhattan
computer	Majority vote	3	Manhattan
computer	Inverse dist	3	Manhattan
computer	Inverse linear dist	3	Manhattan
computer	N/A	1	Cosine
fruit	Majority vote	3	Cosine
fruit	Sum	3	Cosine

# Impact of K Value

K directly controls decision boundary complexity. Lower K creates irregular boundaries sensitive to local patterns. Higher K produces smoother boundaries capturing general trends.



### Small K Values (K=1, 3)

Creates complex, highly flexible decision boundaries.

Fits training data closely but risks overfitting to noise.

### Large K Values (K=10+)

Creates smoother, more generalized boundaries.

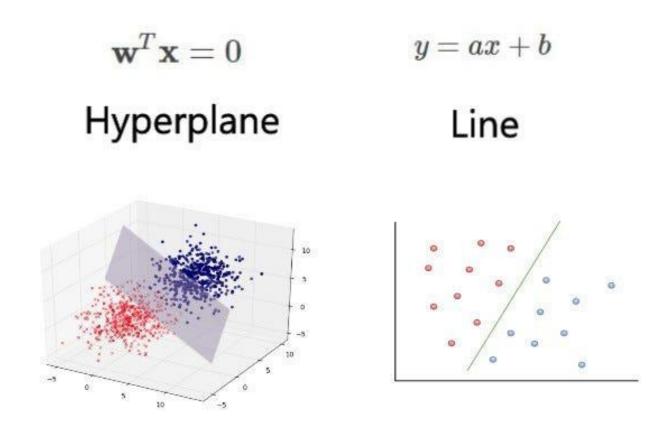
If the dataset has high class imbalance, setting k to a high value may make the classifier unable to recognize the rare classes.

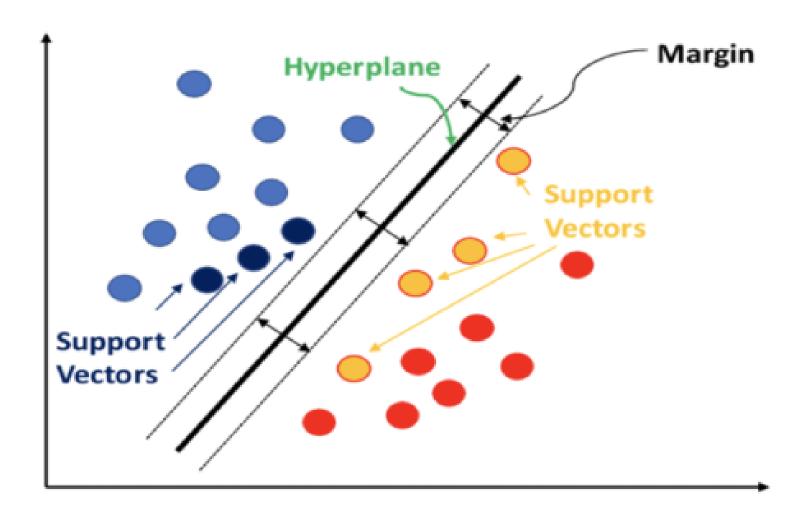
### Finding Optimal K

Use cross-validation to test different K values.

# Support Vector Machines Introduction

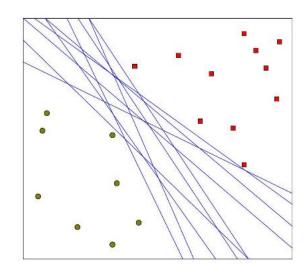
SVM tries to find the best boundary (hyperplane) that separates data points of different classes.





- •Hyperplane Hyperplane is the decision boundary that aids in classifying the data points.
- •Support Vectors Support Vectors are the data points that are on or nearest to the hyperplane and influence the position of the hyperplane.
- •Margin Margin is the gap between the hyperplane and the support vectors.
- •**Kernel function** These are the functions used to determine the shape of the hyperplane. Transforms data to handle non-linear classification.

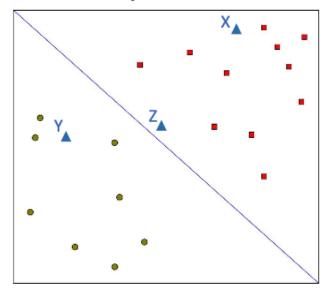
# Support Vector Machines Introduction



### Hyperplane Optimization

Finds optimal decision boundary with maximum margin

Consider the distance from a data point to the boundary

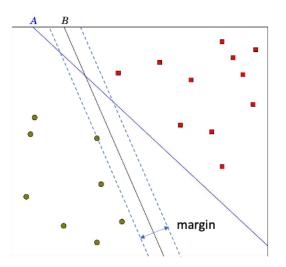


- For point X, we should be quite confident about the prediction of its class.
- For point Z, a small change to the decision boundary might change our decision to change; we are less confident in the prediction.

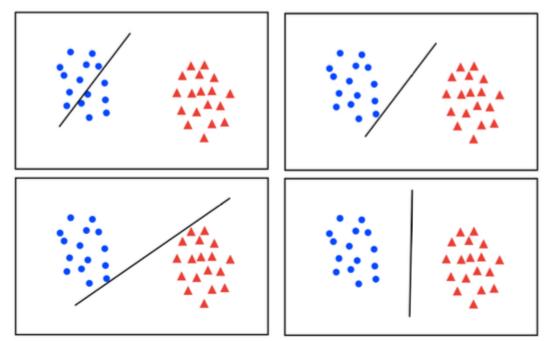
# Hyperplane Optimization

- Aim: find a decision boundary that allows to make all correct and confident (far from the decision boundary) predictions for a given training set.
- SVM finds an optimal solution
  - Maximises the distance between the hyperplane and the difficult points close to decision boundary

Margin: 2 x the minimum distance between boundary and data points



What is the best hyperplane?

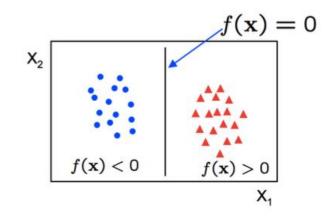


### Linear Classifier

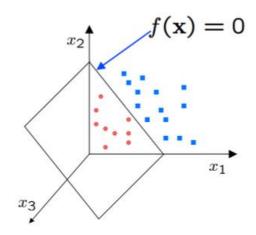
- A separating hyperplane in  ${\cal D}$  dimensions can be defined by a normal  ${\bf w}$  and an intercept  ${\bf b}$
- The hyperplane passing a point  $x = \begin{bmatrix} x_1 \\ x_2 \\ ... \\ x_D \end{bmatrix}$  is:

$$\begin{aligned} \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b &= 0 \\ w_1 x_1 + ... + w_D x_D + b &= 0 \end{aligned}$$

- Linear classifier takes the form  $f(x) = \mathbf{w}^{T}x + b$
- In 2D space, this is a straight line



- Linear classifier takes the form  $f(x) = w^{T}x + b$
- In 3D space, this is a plane



# Linearly Separable Classification

PerfectSeparation

Classes can be completely divided by a linear

hyperplane.

MaximumMargin

SVM finds the widest possible gap between classes.

Support Vectors

Only points
nearest to
boundary
influence the

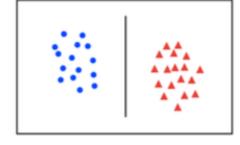
result.

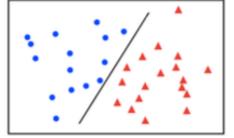
Robustness

Maximum margin provides better generalization.

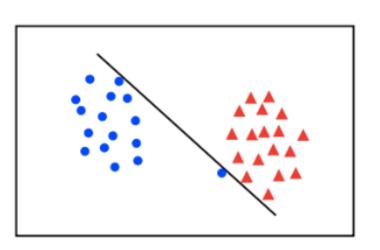
### Linear separability

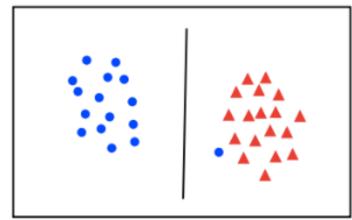
linearly separable



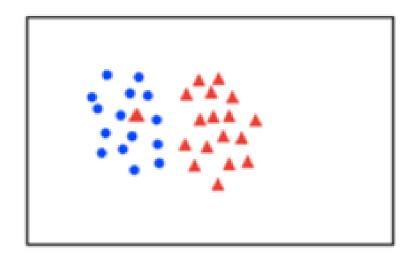


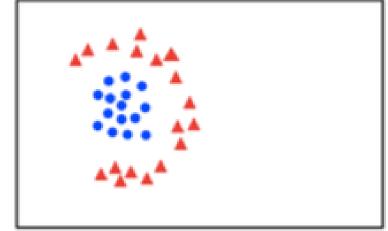
# But What if Data is Not Linearly Separable?





not linearly separable





# Two Solutions



### Allow Soft Margin (C Parameter)

- •Introduce a **soft margin** to allow some **misclassifications** using the **C parameter**.
- •This lets the SVM **tolerate overlap** between classes while still finding the best possible boundary.

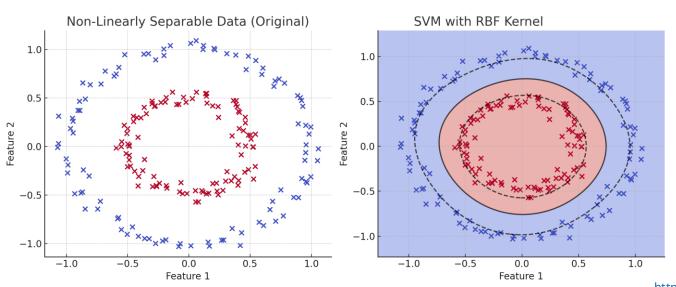


### Use the Kernel Trick

•Apply a non-linear kernel function to map the data into a higher-dimensional space where it

becomes linearly separable.

- •Common kernels:
  - RBF (Gaussian)
  - Polynomial
  - Sigmoid



Decision

boundary

Hard margin

Margin

Decision

boundary

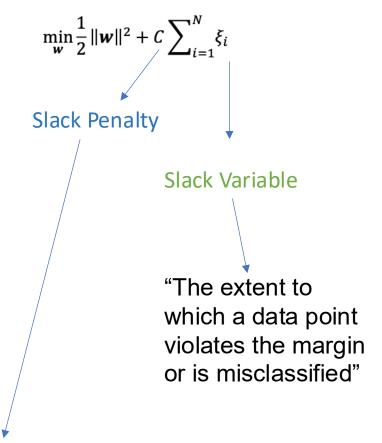
Sample violating constraint

Support vector

Soft margin

### Soft Margins

- Introduce slack variables  $\{\xi_1, \xi_2, ..., \xi_i, ..., \xi_N\}$ , which allows few points to be on the "wrong" side of the hyperplane at some cost
- New objective function with slack variables



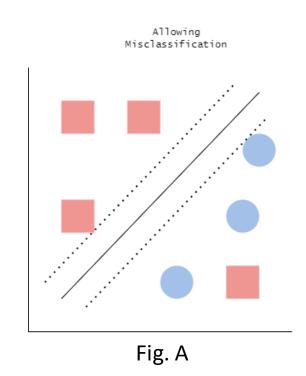
"How much should we penalize violations of the margin?"

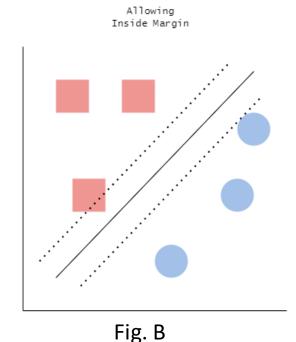
# Soft margins

In real-world datasets, classes are often **not perfectly separable**. So, SVM allows some points to:

- •Be on the wrong side of the margin (i.e., lie within the margin boundaries as in Fig. B)
- •Even be misclassified (as in Fig. A)

Using Slack variables (ξ)





### Soft Margins

- Introduce slack variables  $\{\xi_1, \xi_2, ..., \xi_i, ..., \xi_N\}$ , which allows few points to be on the "wrong" side of the hyperplane at some cost
- · New objective function with slack variables

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{N} \xi_i$$

- •Here, w is the normal vector to the hyperplane
- •||w|| controls the margin → smaller w → wider margin
- •SVM minimizes the norm of w to maximize the margin

### C is a **regularization parameter**:

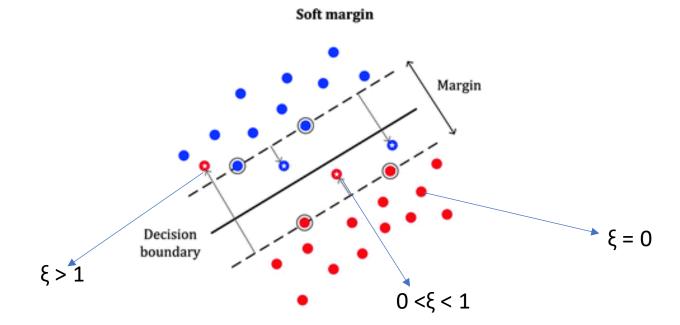
- •Low C → wider margin, more misclassifications
- •**High C**  $\rightarrow$  narrow margin, fewer violations

# Slack Variables in SVM

### What is a Slack Variable (ξ<sub>i</sub>)?

For each data point i, slack variable  $\xi_i$  tells **how much it violates** the margin:

ξ <sub>i</sub> value
$\boldsymbol{\xi}_i = \boldsymbol{0}$
$0 < \xi_i < 1$
$\xi_i > 1$



### Slack Penalty

$$C = 0.1$$

Low Penalty

Allows many violations, creating smoother boundaries

$$C = 1.0$$

Balanced Penalty

Moderate trade-off between errors and margin width

$$C = 10$$

**High Penalty** 

Strict boundaries with fewer misclassifications allowed

$$C = 100$$

**Extreme Penalty** 

Nearly rigid separation, risking overfitting

Large C → hard margin behaviour

Small C → soft margin behaviour (more forgiving)

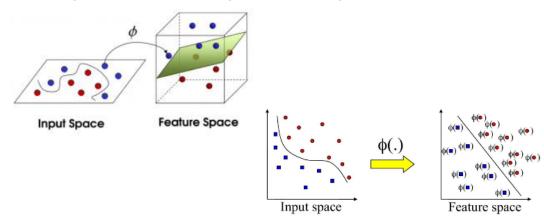
- A hard margin requires perfect separation (no misclassified points).
- A **soft margin** allows:
  - Some points to lie inside the margin.
  - Some points to be misclassified.

# Kernal Methods

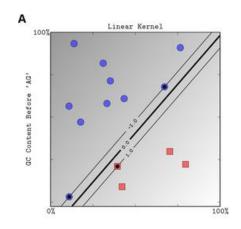
Transform the input data into a higher-dimensional space using kernel functions

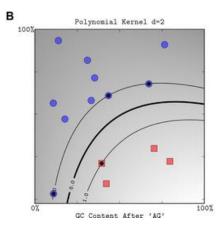
- •Common kernels:
  - RBF (Gaussian): For circular or complex boundaries.
  - Polynomial: Captures curved decision boundaries.
  - Sigmoid: Similar to neural networks.

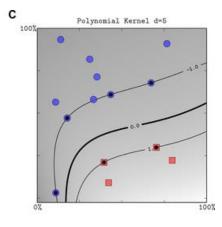
- Make non-linearly separable problem separable
- Map data into better representation space

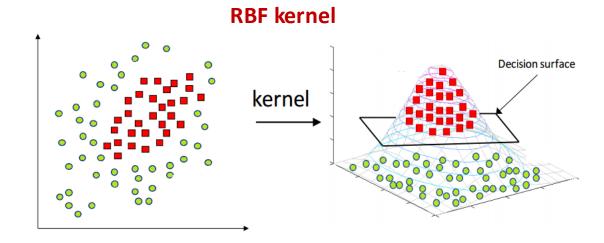


### **Polynomial Kernel**









What does it mean for a classification dataset to be "linearly separable"? If a dataset isn't linearly separable, an SVM learner has two major options. What are they, and why might we prefer one to the other?

If a dataset is "linearly separable," it is possible to completely separate the classes with a single hyperplane

If a dataset isn't linearly separable, the options for SVM are:

### 1. Soft margins

### 2. Kernel methods

Method	Purpose	Handles
Soft Margin	Allow misclassifications by maximizing margin	Noisy or almost separable data
Kernel Trick	Transform data to separable space	Complex non-linear boundaries

What is the value of slack variables for data points that are correctly classified in SVMs? What should the slack penalty C be to make a soft-margin SVM function as a hard-margin SVM?

- For data points that are correctly classified, the value of their slack variable is 0
- Hard SVM don't allow any mistakes or in other words the penalty rate for the mistakes
  is equal to infinity (∞). To make soft SVM to act like hard SVM the slack penalty C
  should be very large.

How do changes in data points affect the decision boundary of an SVM?

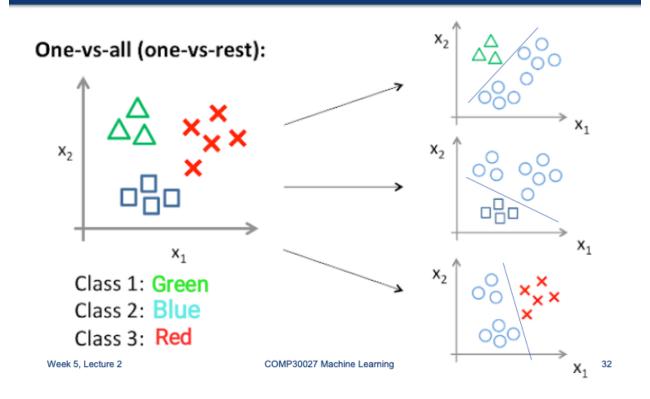
The support vectors are used to define the hyperplane that separates the classes. Changes in data points that are not support vectors have no effect on the decision boundary.

However, changes in the position or label of support vectors can have a significant impact on the decision boundary.

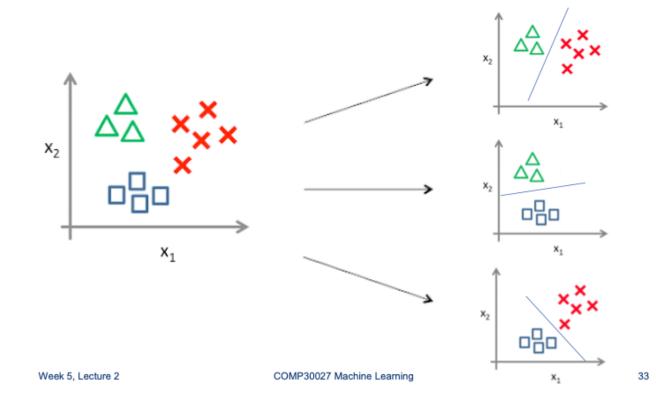
https://greitemann.dev/svm-demo

# Multi-Class SVM

### Multi-Class SVM: One-vs-All



### Multi-Class SVM: One-vs-One



How many binary classifiers are needed to classify a dataset with 4 classes using one-vs-one method?

In the one-vs-one (OvO) strategy:

You train one binary classifier for every pair of classes.

So, for C classes, the number of binary classifiers needed is:

$$ext{Number of classifiers} = rac{C(C-1)}{2}$$

### For 4 classes:

$$\frac{4(4-1)}{2} = \frac{4\times 3}{2} = 6$$

Each classifier is trained to distinguish between just two classes:

- Class 0 vs 1
- Class 0 vs 2
- Class 0 vs 3
- Class 1 vs 2
- Class 1 vs 3
- Class 2 vs 3

### Then during prediction:

- Each classifier votes for a class
- The class with the most votes wins (majority voting)

# Advantages of SVMs

### High-Dimensional Space

SVMs maintain effectiveness with many features. They avoid the curse of dimensionality.

The algorithm focuses on support vectors rather than all data points.

### Generalization Power

Maximum margin principle provides better theoretical guarantees. SVMs often outperform K-NN.

They're less prone to overfitting with proper regularization.

### Memory Efficiency

Only support vectors are stored after training. This makes prediction more efficient.

K-NN must store the entire training dataset.

Unlike other geometric methods such as K-NN, SVMs work better with large attribute sets. Why might this be true?

- 1. SVMs focus on the most important points (support vectors)
  - •SVM builds a decision boundary using only the **critical support vectors**, not all the data.
  - •In high dimensions, many features may be **irrelevant or noisy**, and SVMs **ignore non-support points** during decision making.
- **2. No need for prior feature selection;** SVMs can implicitly capture the relationships between different features and can handle interactions between them without the need for explicit feature engineering. This means that SVMs can effectively learn from a large number of features without requiring a priori knowledge about which features are most important for the classification task.