



K-Nearest Neighbors (KNN) – Full Notes

1 Definition

K-Nearest Neighbors (KNN) is a **supervised machine learning algorithm** used for **classification and regression**, based on the idea that **similar data points exist close to each other**.

KNN predicts the label of a new sample by looking at the ‘K’ closest labeled points in training data.

2 Real-Life Intuition

Imagine you moved to a new city and want to predict your personality type.

You look at **your 5 nearest neighbors (K=5)**—if **3 are extroverts** and **2 are introverts**, you say **you are extrovert**.

Example:

```
Nearest neighbors labels = [1, 1, 1, 0, 0]  
Prediction = majority vote = 1
```

3 Why do we need KNN?

Reason	Explanation
Easy & intuitive	Based on similarity concept
Works without assumptions	Non-parametric → no underlying distribution
Good baseline model	Simple, interpretable
Real world is similarity-based	Example: recommendation systems, medical diagnosis

4 When did KNN come / why was it introduced?

KNN originated in **1951 (Fix & Hodges)** as a statistical method for **pattern classification**. It was introduced because many datasets do **not fit linear equations** like regression or SVM — **we need similarity-based models**.

5 How KNN works (Step by Step)

Given: New data point x

1. **Choose K** (number of neighbors)
 2. **Calculate distance** between x and all points
 3. **Sort distances** in ascending order
 4. **Pick first K nearest points**
 5. **Majority vote** → classification
or **mean of neighbors** → regression
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6 Mathematical Explanation

Distance Formula Used

Most common distance: **Euclidean Distance**

$$d(x,y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}$$

Other distances:

Metric	Formula	Use Case
Manhattan	$\sum x_i - y_i $	

Minkowski $(\sum |x_i - y_i|)$

Cosine similarity $(\frac{A \cdot B}{\|A\| \|B\|})$

7 Example Calculation

Assume we want to classify a new point $X = (3, 4)$ with 3 nearest neighbors ($K=3$)

Point	Class	Distance
(2,2)	0	$\sqrt{(3-2)^2 + (4-2)^2} = \sqrt{5}$
(4,4)	1	$\sqrt{(3-4)^2 + (4-4)^2} = 1$
(3,7)	1	3

Nearest 3 classes = [1, 1, 0]

Prediction = 1

8 Hyperparameters

Parameter	Meaning
K	number of neighbors
distance	euclidean, manhattan,
metric	cosine
weights	uniform / distance weighted
algorithm	brute, kd_tree, ball_tree

How to Choose the Best K in KNN

A commonly used **rule of thumb** is:

$$K = \sqrt{N}$$

Where:

- K = number of nearest neighbors
 - N = total number of training samples
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Simple Example

If you have:

$N = 100$ samples

Then:

$$K=100=10K = \sqrt{100} = 10K=100=10$$

So you should start with $K = 10$ and then test other values near it (like 9, 11, 12).

Why this rule exists

- If K is too small, model becomes **noisy & overfits**
→ sensitive to outliers
- If K is too large, model becomes **too simple / underfits**
→ loses important patterns

Choosing K around \sqrt{N} gives a **balanced starting point**.

Then you test 5–10 values near it using **cross-validation**.

Final Notes

- \sqrt{N} is **only a starting point**, not exact best value always
 - You still tune K using **accuracy scores & validation curve**
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One-line exam answer

We usually select K by starting around \sqrt{N} (square root of total samples), because too small K causes overfitting and too large K causes underfitting, and \sqrt{N} gives a balanced choice.

Errors:

K small	K large
Overfitting	Underfitting
Highly sensitive to noise	Too generalized

10 Advantages & Disadvantages

✓ Advantages

- Simple to understand & implement
- Non-parametric (no assumption)
- Works well with small, clean datasets
- Flexible for classification & regression

✗ Disadvantages

- Slow prediction for large data
- Sensitive to irrelevant features & scaling

- Memory expensive
 - Bad with high dimensional data
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11 Need for Feature Scaling

Because distance depends on value magnitude:

$$X' = X - \text{mean} \\ stdX' = \frac{X - \text{mean}}{\text{std}} \\ X' = \text{std}X - \text{mean}$$

Example:

Height range: 150-200

Weight range: 40-80

Weight becomes less important → wrong results

So use: **StandardScaler or MinMaxScaler**

12 Applications

Field	Use
Healthcare	cancer detection
Finance	credit score risk
Recommendation systems	movie similarity
Handwritten digits	MNIST dataset

13 Python Code

```
from sklearn.neighbors import KNeighborsClassifier  
from sklearn.preprocessing import StandardScaler  
  
scaler = StandardScaler()  
X_train = scaler.fit_transform(X_train)
```

```
X_test = scaler.transform(X_test)

knn = KNeighborsClassifier(n_neighbors=5)
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
```

14 When not to use KNN

- 🚫 Very large datasets
 - 🚫 High-dimensional datasets
 - 🚫 Real-time prediction required
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Summary in One Line

KNN predicts using similarity (distance) to nearest neighbors instead of learning a mathematical model.



Different Algorithms Used in KNN

When KNN predicts, it must **search for the K nearest points**.

Doing this on large datasets can be slow, so sklearn gives different search algorithms:

1 Brute Force (Exhaustive Search)

Definition

Compares the distance from the query point to **every other point** in the dataset.

Time Complexity

$O(n \times d)$

n = number of samples

d = number of dimensions

When to Use

- Small datasets
- Low dimensions
- Very accurate results

Example

```
KNeighborsClassifier(algorithm='brute')
```

2 KD-Tree (K-Dimensional Tree)

Definition

A **binary tree structure** that divides data space into halves recursively.

Used for **fast nearest neighbor search**.

Time Complexity

Average:

$O(\log n)$

Worst case:

$O(n)$

When to Use

Requirements	Reason
Numeric data	KD tree works only for numeric values
Low dimensions ($d < 30$)	Performance decreases when dimensions increase

Example

```
KNeighborsClassifier(algorithm='kd_tree')
```

3 Ball Tree

Definition

Divides space into **hyperspheres (balls)** instead of splitting along axes (like KD-tree).
Better for **high-dimensional and complex data**.

Time Complexity

Better performance than KD-tree when dimensions are high.

When to Use

Condition	Why
High-dimensional data	handles spherical clusters better
Mixed type distributions	more stable

Example

```
KNeighborsClassifier(algorithm='ball_tree')
```

4 Auto (Default)

Definition

Automatically selects the best algorithm among:

`kd_tree → ball_tree → brute`

depending on data size & dimension.

Example

```
KNeighborsClassifier(algorithm='auto')
```

🏆 Which algorithm is best?

Data Type	Best Algorithm
Small dataset	brute
Low dimensions ($d < 30$)	kd_tree
High dimensions	ball_tree
Not sure	auto

🎯 Why do we need these algorithms?

Because KNN is **slow during prediction**

$O(n)$ per prediction

To improve **speed / runtime**, we need efficient searching structures (KD tree, Ball tree).

🔍 Summary Table

Algorithm	Works How	Best Use	Weakness
Brute	checks every point	small dataset	slow for large data
KD-tree	axis split tree	low-d high speed	bad when dims high
Ball-tree	spherical clustering	high-dimensional	complex
Auto	auto selection	general usage	none



KNN Parameters Recap

```
KNeighborsClassifier(  
    n_neighbors=5,  
    weights='uniform',  
    metric='minkowski',  
    algorithm='auto'  
)
```



Interview Question

Q: Why is KNN called a lazy learner?

Because it does **not train a model** — it stores data and **waits until prediction time**, where it performs heavy computation.



Final Answer (Simple)

KNN is called a lazy learner because it does not build a model during training. Instead, it waits until prediction time and then performs all computations (like finding distances) to make a prediction.