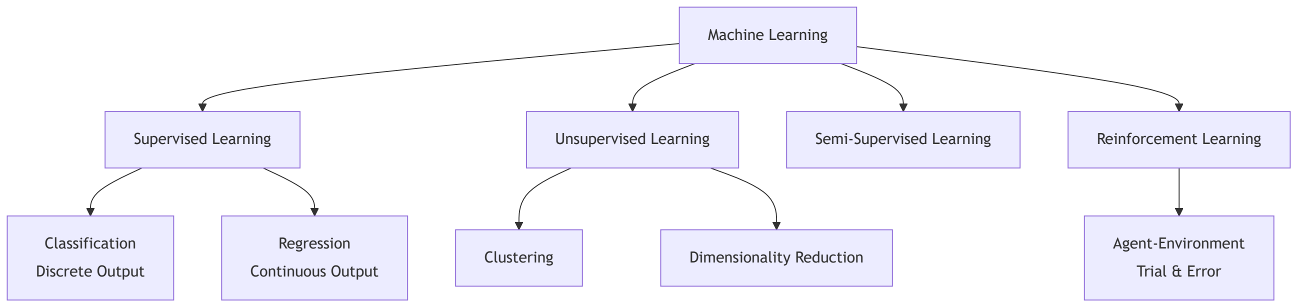
Machine Learning Course Summary

1. Introduction to Machine Learning

Types of ML



🎯 **Supervised Learning:** Learning from inputs x to output y given **labeled data**

- **Classification:** Output is discrete (e.g., spam/not spam)
- **Regression:** Output is continuous (e.g., house prices)

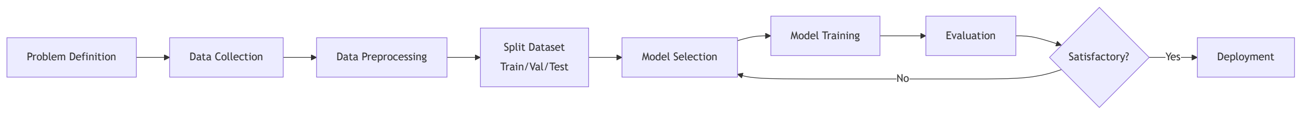
🔍 **Unsupervised Learning:** Uses **unlabeled data** to find groups, clusters, or patterns

🔄 **Semi-supervised Learning:** Uses a **small amount of labeled data** + **large amount of unlabeled data**

🎮 **Reinforcement Learning:** Learning through **trial and error** (agent-state-action-reward-environment)

ML Algorithms & Workflow

Common Algorithms: Linear regression, logistic regression, decision trees, KNN, Naïve Bayes, Neural Networks



Workflow:

1. **Problem definition** — What are we predicting?
2. **Data collection** — Gather relevant data
3. **Data preprocessing** — Clean, normalize, handle missing values
4. **Split dataset** — Training (60-70%), Validation (10-20%), Testing (10-20%)
5. **Model selection** — Choose appropriate algorithm
6. **Model training** — Fit model to training data
7. **Evaluation** — Measure performance on validation/test data

2. Linear Regression

Univariate Linear Regression

Model: $h(X) = \theta_0 + \theta_1 X$

📊 **Cost Function (MSE):** Measures the average squared difference between predicted and actual values

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} [h_\theta(x^{(i)}) - y^{(i)}]^2$$

⚡ **Gradient Descent:** Algorithm to minimize the cost function by repeating until convergence

$$\theta_j = \theta_j - \alpha \frac{\partial J(\theta_0, \theta_1)}{\partial \theta_j}$$

- α is the **learning rate** (controls step size)
- ⚠️ Update θ_0 and θ_1 **simultaneously**

Partial Derivatives:

$$\frac{\partial J}{\partial \theta_0} = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})$$
$$\frac{\partial J}{\partial \theta_1} = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

Multivariate Linear Regression

Involves **multiple independent variables** (features)

Hypothesis: $h_\theta(x) = \theta^T x = \theta_0 + \theta_1 x_1 + \ldots + \theta_n x_n$

Gradient Descent (Vectorized):

$$\theta = \theta - \frac{\alpha}{m} X^T (X\theta - y)$$

📏 **Feature Scaling:** Recommended so features are on the **same scale** for faster convergence

- Divide by max or range (max - min)
- Get features roughly in range $[-1, 1]$

Mean Normalization: Replace x_i with $\frac{x_i - \mu_i}{\sigma_i}$ (where μ is mean and σ is standard deviation)

🎯 **Normal Equation (Direct Solution):**

$$\theta = (X^T X)^{-1} X^T Y$$

Gradient Descent	Normal Equation
Need to choose α	No need for α
Needs many iterations	No iterations
Works well for large n	Slow if n is very large
$O(kn^2)$	$O(n^3)$ for matrix inversion

Polynomial Regression

Models **non-linear relationships** as an n -th degree polynomial

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + ... + \theta_n x^n$$

⚠️ **Feature scaling becomes critical** for polynomial regression!

3. Logistic Regression (Classification)

Used to predict the **probability** of a binary (0 or 1) or multi-class outcome

Binary Classification

🔵 **Sigmoid Function:** Maps output between 0 and 1

$$g(Z) = \frac{1}{1+e^{-Z}} = \frac{1}{1+e^{-\theta^T x}}$$

Key Properties:

- $g(0) = 0.5$
- $\lim_{z\to\infty} g(z) = 1$
- $\lim_{z\to-\infty} g(z) = 0$

Decision Rule:

- If $g(Z) \geq 0.5 \iff \theta^T x \geq 0$, predict **class 1**
- If $g(Z) < 0.5 \iff \theta^T x < 0$, predict **class 0**

📉 **Cost Function (Log Loss):**

$$L(\hat{y}, y) = \{\begin{matrix} -\ln(\hat{y}) & \text{if } y = 1 \\ -\ln(1-\hat{y}) & \text{if } y = 0 \end{matrix}$$

Cross-Entropy Loss (dataset):

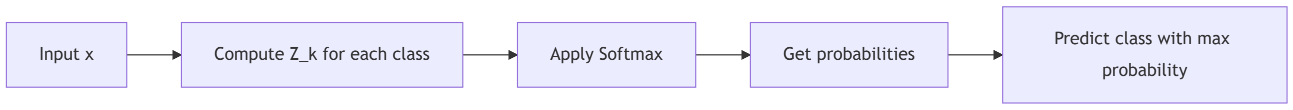
$$J(\hat{y}, y) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\ln(\hat{y}^{(i)}) + (1-y^{(i)})\ln(1-\hat{y}^{(i)})]$$

Gradient Descent Update:

$$\theta_j := \theta_j - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

⚠️ Same form as linear regression, but $h_\theta(x) = g(\theta^T x)$ is different!

Multiclass Classification


Input x
Compute Z_k for each class
Apply Softmax
Get probabilities
Predict class with max probability

For K classes:

1. Compute linear score Z_k for each class
2. Exponentiate e^{Z_k}
3. Compute probability (**Softmax**):

$$p(y=k|x) = \frac{e^{Z_k}}{\sum_{j=0}^{n} e^{Z_j}}$$

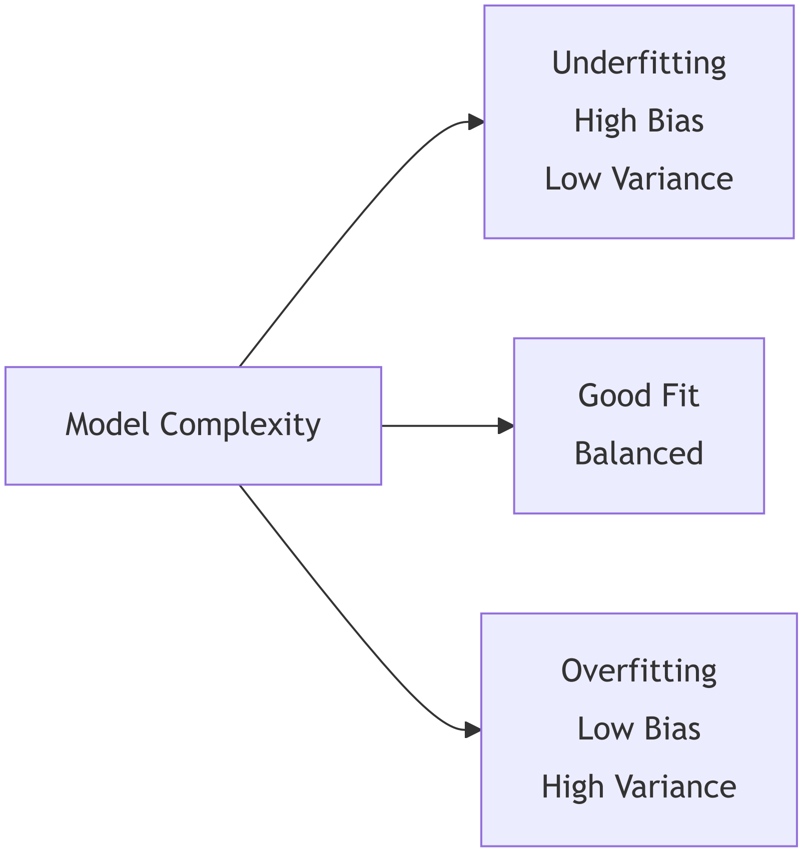
1. Prediction is the class with **max probability**

Cross-Entropy Loss (Multiclass):

$$J(\hat{y}, y) = -\frac{1}{m} \sum_{i=1}^{m} \sum_{k=0}^{K-1} y_k \ln(\hat{y}_k)$$

4. Model Evaluation & Challenges

Bias vs. Variance



🎯 **Bias:** Inability to capture the true relationship (Model **too simple** → **Underfitting**)

📊 **Variance:** Inconsistency when applied to different datasets (Model **too complex** → **Overfitting**)

Error Decomposition:

$$\text{Error} = \text{Bias}^2 + \text{Variance} + \text{Irreducible Errors}$$

Overfitting Prevention

Data Manipulation:

- ✅ Splitting (Train/Val/Test)
- ✅ Resampling
- ✅ Augmenting (rotation, scaling, flipping)
- ✅ Reducing features (feature selection)

🔒 **Regularization:** Adds a penalty to the loss function

- **L1 (Lasso):** Adds $\lambda \sum |w_i|$ → Encourages **sparsity** (some weights → 0)
- **L2 (Ridge):** Adds $\lambda \sum w_i^2$ → Encourages **small weights**

Dropout: Randomly drop units (neurons) during training

Early Stopping: Stop when validation accuracy starts to decrease

Classification Metrics

Confusion Matrix:

	Predicted Positive	Predicted Negative
Actual Positive	TP (True Positive)	FN (False Negative)
Actual Negative	FP (False Positive)	TN (True Negative)

Key Metrics:

Metric	Formula	Meaning
Accuracy	$\frac{TP+TN}{\text{Total}}$	Overall correctness
Recall (TPR)	$\frac{TP}{TP+FN}$	Coverage of actual positives
Specificity (TNR)	$\frac{TN}{FP+TN}$	Coverage of actual negatives
Precision	$\frac{TP}{TP+FP}$	Accuracy of positive predictions
F-Score	$\frac{(1+\beta^2)(P\times R)}{\beta^2 \cdot P+R}$	Harmonic mean of P & R

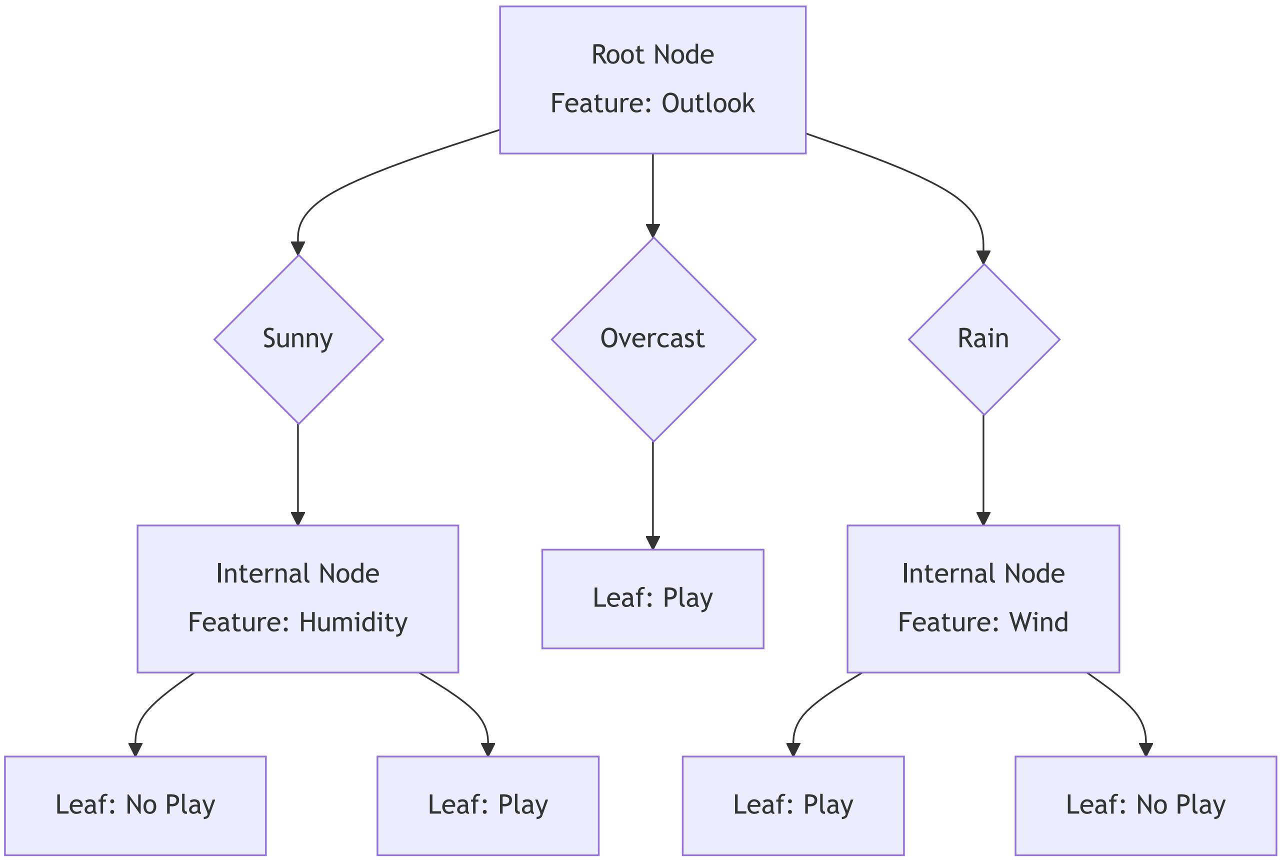
F1-Score (when $\beta = 1$):

$$F_1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

📈 **ROC Curve:** Plots TPR vs FPR

- **AUC ≈ 1** → Perfect classifier
- **AUC ≈ 0.5** → Random guessing
- **AUC < 0.5** → Worse than random

5. Decision Trees



Components

- 🌳 **Root node:** Starting point (top of tree)
- 🔀 **Internal nodes:** Decisions based on features
- 🍃 **Leaf nodes:** Final class labels/values (predictions)

Process

1. **Select** best splitting attribute (using splitting criteria)
2. **Create** branches for each value
3. **Recursively grow** subtrees until stopping condition
4. **Prune** if necessary to avoid overfitting

Splitting Criteria

ID3 (Information Gain/Entropy):

- Choose attribute with **highest Information Gain** (IG)
- $IG = E(\text{Parent}) - \sum \frac{|D_i|}{|D|} E(D_i)$
- **Entropy:** $H(D) = -\sum P_i \log_2 P_i$
  - Low entropy → High purity (homogeneous)

    - High entropy → Low purity (mixed)

C4.5 (Gain Ratio):

$$GR = \frac{IG}{\text{Split Info}}$$

Normalizes Information Gain to handle bias towards attributes with many values

CART (Gini Index): Used for classification

$$GI = 1 - \sum P_i^2$$

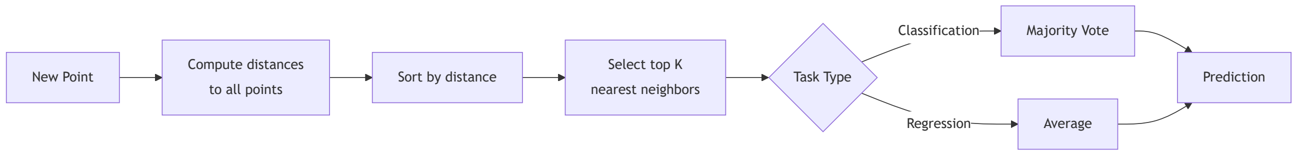
- Measures impurity
- Range: [0, 0.5] (0 = pure, 0.5 = maximum impurity)

Regression Trees: Use **Mean Squared Error (MSE) reduction** to choose splits

Criterion	Best For	Range
Entropy	ID3, C4.5	[0, 1]
Gini Index	CART (faster)	[0, 0.5]
MSE	Regression Trees	[0, ∞)

6. K-Nearest Neighbors (K-NN)

Predicts class/value based on the K **most similar** stored samples



Steps

1. **Compute** distance between new point and all training points
2. **Sort** by distance and select top K neighbors
3. **Aggregate:**
    - Classification → **Majority vote**

- Regression → **Average** (or weighted average)

Distance Metrics

Metric	Formula	Use Case
Euclidean	$d = \sqrt{\sum(x_i - x_i')^2}$	Default, measures straight-line distance
Manhattan	$d = \sum \lvert x_i - x_i' \rvert$	Grid-like paths, robust to outliers
Minkowski	$d = (\sum \lvert x_i - x_i' \rvert^p)^{1/p}$	General form ($p = 1$ Manhattan, $p = 2$ Euclidean)

⚖️ **Weighted K-NN:** Weights neighbors by **inverse distance** ($w_i = 1/d_i^2$)

- Closer neighbors have more influence

Choosing K:

- ✅ Small K → More sensitive to noise (overfitting)
- ✅ Large K → Smoother boundaries (underfitting)
- 📊 Use **cross-validation** to find optimal K
- 🔢 Often use **odd** K for binary classification (avoid ties)

7. Naïve Bayes

A **probabilistic classifier** based on Bayes' Theorem, assuming **independence** between features

Bayes' Theorem

$$P(H|D) = \frac{P(D|H) \times P(H)}{P(D)}$$

Components:

- $P(H|D)$: **Posterior** — Probability of hypothesis after seeing data
- $P(D|H)$: **Likelihood** — Probability of data given hypothesis
- $P(H)$: **Prior** — Initial probability of hypothesis
- $P(D)$: **Evidence** — Probability of data (normalizing constant)

🔑 **Naïve Assumption:** All features are **conditionally independent** given the class

$$P(x_1, x_2, \ldots, x_n|C) = P(x_1|C) \times P(x_2|C) \times \ldots \times P(x_n|C)$$

Classification Rule:

$$\hat{y} = \arg\max_c P(C = c) \prod_{i=1}^{n} P(x_i | C = c)$$

Laplace Smoothing

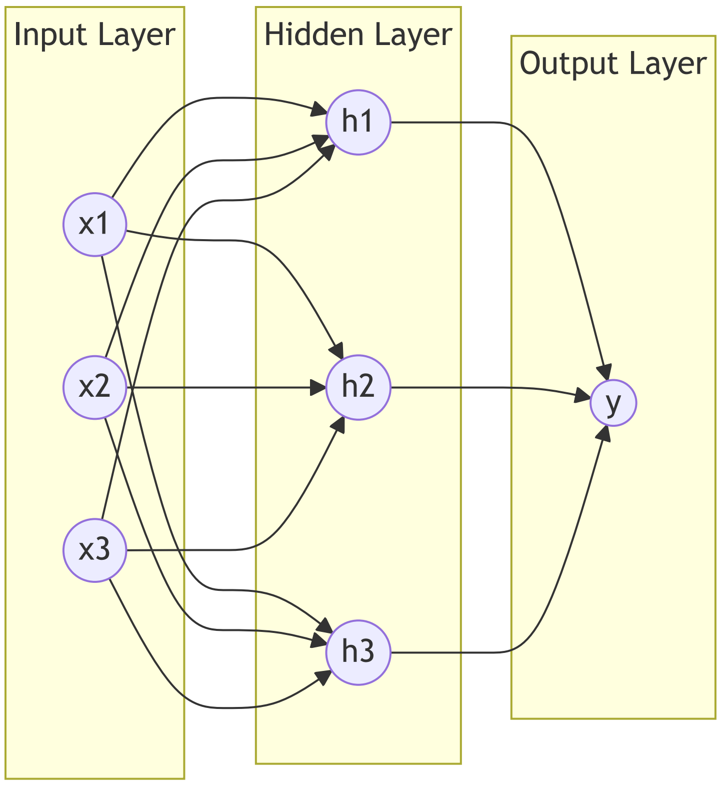
Used if a feature value **never appears** in a class to avoid **zero probability**

$$P(x_i | C) = \frac{N_{ic} + 1}{N_c + K}$$

- N_{ic} : Count of feature x_i in class C
- N_c : Total count of all features in class C
- K : Number of distinct values for feature x_i

Why needed? If $P(x_i | C) = 0$, entire product becomes 0!

8. Neural Networks



Structure

- **Input Layer:** Represents features ($x_1, x_2, \ldots, x_n$)
- **Hidden Layers:** Between input and output (can be multiple)
- **Output Layer:** Produces prediction ($\hat{y}$)

Node Computation

Linear Combination:

$$Z = \sum_{i=1}^{n} w_i x_i + b = W^T X + b$$

Activation:

$$a = f(Z)$$

where f is the **activation function**

Activation Functions

Function	Formula	Range	Use Case
Sigmoid	$\sigma(z) = \frac{1}{1+e^{-z}}$	(0, 1)	Binary classification (output)
Tanh	$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	(-1, 1)	Hidden layers (zero-centered)
ReLU	$\text{ReLU}(z) = \max(0, z)$	[0, ∞)	**Most common** for hidden layers
Leaky ReLU	$\max(0.01z, z)$	(-∞, ∞)	Fixes "dying ReLU" problem
Softmax	$\frac{e^{z_i}}{\sum e^{z_j}}$	(0, 1), sum=1	Multiclass classification

Training

🔄 **Backpropagation:** Propagates error backwards to update weights

1. **Forward pass:** Compute predictions
2. **Calculate loss:** Compare with true labels
3. **Backward pass:** Compute gradients using chain rule
4. **Update weights:** Adjust parameters

Weight Update:

$$w_{\text{new}} = w_{\text{old}} - \eta \frac{\partial L}{\partial w}$$

where η is the **learning rate**

Training Strategies (Gradient Descent)

Strategy	Batch Size	Speed	Memory	Convergence
Stochastic GD (SGD)	1	Fast per update	Low	Noisy
Batch GD	All m samples	Slow per update	High	Smooth
Mini-batch GD	k samples (32-256)	**Balanced**	Medium	**Most common**

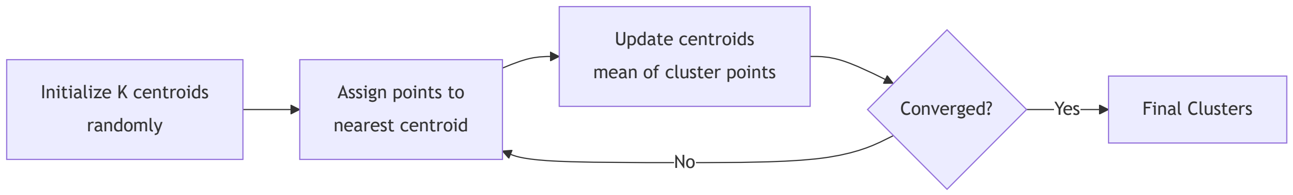
🎯 **Mini-batch GD** is the **sweet spot** — combines benefits of both!

9. Clustering

Unsupervised learning — Grouping similar data points based on **similarity/distance**

K-Means Clustering

Partitions n points into K clusters by **minimizing variance within clusters**


Initialize K centroids randomly
Assign points to nearest centroid
Update centroids mean of cluster points
Converged?
Yes
Final Clusters
No

🎯 **Objective:** Minimize Within-Cluster Sum of Squares (WCSS)

$$J = \sum_{i=1}^{K} \sum_{x \in C_i} ||x - \mu_i||^2$$

- μ_i : Centroid of cluster i
- C_i : Set of points in cluster i

Algorithm Steps:

1. **Initialize:** Randomly select K initial centroids
2. **Assignment:** Assign each point to nearest centroid
3. **Update:** Recalculate centroids as mean of assigned points
4. **Repeat:** Steps 2-3 until assignments stabilize (or max iterations)

Choosing K:

📊 **Elbow Method:**

- Plot WCSS vs K
- Look for "elbow" where decrease slows
- Trade-off between fit and complexity

📏 **Silhouette Score:**

- Measures **cohesion** (within-cluster) vs **separation** (between-cluster)
- Range: **[-1, 1]**
  - 1 → Perfect clustering
  - 0 → Overlapping clusters

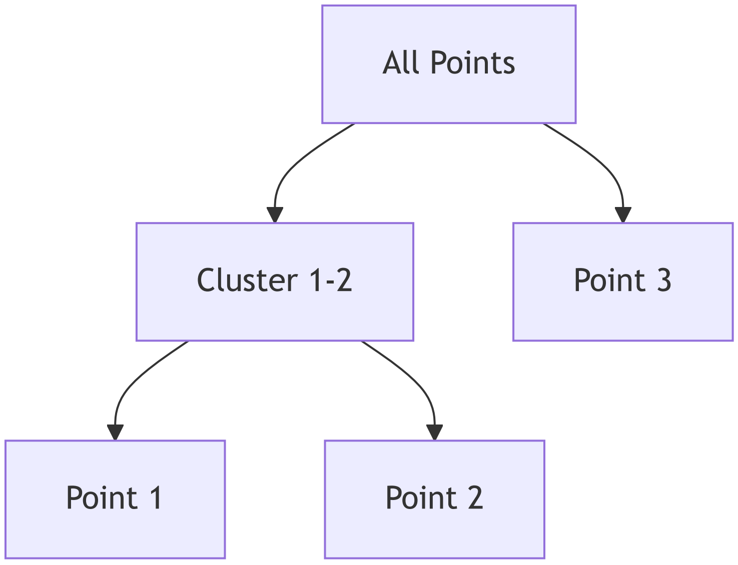
    - -1 → Misclassified points

$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

- $a(i)$: Avg distance to points in same cluster
- $b(i)$: Avg distance to points in nearest other cluster

Hierarchical Clustering

Produces a **tree-like diagram** called a **Dendrogram**



🌳 **Agglomerative (Bottom-up):**

1. Start with each point as its **own cluster**
2. **Merge** closest two clusters based on distance matrix
3. **Update** distance matrix using linkage criteria
4. **Repeat** until one cluster remains (or desired K clusters)

Linkage Criteria:

Method	Distance Between Clusters	Characteristics
Single	Min distance between any two points	Sensitive to outliers, chain effect
Complete	Max distance between any two points	Less sensitive to outliers, compact clusters
Average	Average distance between all pairs	Balanced approach
Ward's	Minimizes within-cluster variance	Produces even-sized clusters

Advantages:

- ✅ No need to specify K in advance
- ✅ Visual dendrogram for interpretation
- ✅ Captures hierarchical structure

Disadvantages:

- ❌ Computationally expensive: $O(n^2 \log n)$ or $O(n^3)$
- ❌ Cannot undo merges (greedy algorithm)

📋 Quick Reference Cheatsheet

Algorithms Comparison

Algorithm	Type	Pros	Cons	Use Case
Linear Regression	Regression	Simple, interpretable, fast	Assumes linearity	Continuous output, linear relationships
Logistic Regression	Classification	Probabilistic output, interpretable	Linear decision boundary	Binary/multiclass classification
Decision Trees	Both	Non-linear, interpretable, no scaling	Overfitting, unstable	Complex decision boundaries
K-NN	Both	Simple, no training	Slow prediction, sensitive to K	Small datasets, non-linear
Naïve Bayes	Classification	Fast, works with small data	Independence assumption	Text classification, spam detection
Neural Networks	Both	Powerful, learns complex patterns	Black box, needs large data	Image, text, complex patterns
K-Means	Clustering	Fast, scalable	Need to specify K , sensitive to init	Customer segmentation
Hierarchical	Clustering	No need for K , dendrogram	Slow, not scalable	Taxonomy, small datasets

Key Formulas

Concept	Formula	Notes
Linear Hypothesis	$h_\theta(x) = \theta^T x$	$x_0 = 1$ for bias
MSE Cost	$J = \frac{1}{2m} \sum (h_\theta(x^{(i)}) - y^{(i)})^2$	Factor of $\frac{1}{2}$ simplifies derivative
Gradient Descent	$\theta_j := \theta_j - \alpha \frac{\partial J}{\partial \theta_j}$	Update **simultaneously**
Normal Equation	$\theta = (X^T X)^{-1} X^T Y$	Direct solution, $O(n^3)$
Sigmoid	$g(z) = \frac{1}{1+e^{-z}}$	Maps to (0, 1)
Cross-Entropy	$J = -\frac{1}{m} \sum [y \log(\hat{y}) + (1-y) \log(1-\hat{y})]$	Logistic regression loss
Softmax	$p_k = \frac{e^{z_k}}{\sum_j e^{z_j}}$	Multiclass probabilities
Entropy	$H(D) = -\sum P_i \log_2 P_i$	Decision tree splitting
Gini Index	$GI = 1 - \sum P_i^2$	Alternative to entropy
Euclidean Distance	$d = \sqrt{\sum (x_i - x_i')^2}$	K-NN default metric
Bayes' Theorem	$P(H\|D) = \frac{P(D\|H)P(H)}{P(D)}$	Naïve Bayes foundation

Evaluation Metrics

Metric	Formula	When to Use
Accuracy	$\frac{TP+TN}{Total}$	Balanced classes
Precision	$\frac{TP}{TP+FP}$	Minimize false positives (spam detection)
Recall	$\frac{TP}{TP+FN}$	Minimize false negatives (disease detection)
F1-Score	$\frac{2 \times P \times R}{P+R}$	Imbalanced classes, balance P & R
MSE	$\frac{1}{m} \sum (y - \hat{y})^2$	Regression
MAE	$\frac{1}{m} \sum \|y - \hat{y}\|$	Regression, robust to outliers
R²	$1 - \frac{SS_{res}}{SS_{tot}}$	Regression, % variance explained

Hyperparameters

Algorithm	Hyperparameter	Typical Values	Impact
All GD	Learning rate α	0.001, 0.01, 0.1, 1	Speed & convergence
Regularization	λ	0.01, 0.1, 1, 10	Overfitting control
K-NN	K neighbors	3, 5, 7, 11 (odd)	Bias-variance tradeoff
Decision Tree	Max depth	3-10	Overfitting control
Neural Network	Hidden layers	1-5+	Model complexity
Neural Network	Neurons per layer	32, 64, 128, 256	Representational power
K-Means	K clusters	Use elbow/silhouette	Number of groups
Mini-batch GD	Batch size	32, 64, 128, 256	Memory vs convergence

Feature Preprocessing

Technique	Formula	Purpose
Min-Max Scaling	$\frac{x-\min}{\max-\min}$	Scale to [0, 1]
Standardization	$\frac{x-\mu}{\sigma}$	Mean=0, Std=1 (preferred for GD)
Normalization	$\frac{x}{\|x\|}$	Scale to unit norm

Model Selection Guide

Choose based on:

1. **Data size:** Small → K-NN, Naïve Bayes; Large → Neural Networks
2. **Interpretability needed:** Decision Trees, Linear/Logistic Regression
3. **Output type:** Continuous → Regression; Discrete → Classification
4. **Linearity:** Linear → Linear models; Non-linear → Trees, NN, K-NN
5. **Training speed:** Fast → Naïve Bayes, Linear; Slow → Neural Networks
6. **Prediction speed:** Fast → Linear, Trees; Slow → K-NN

💡 **Key Takeaways:**

- Always **split data** (train/val/test) to avoid overfitting
- **Feature scaling** improves gradient descent convergence
- **Regularization** helps prevent overfitting
- Choose **metrics** based on problem (accuracy vs precision vs recall)

- **Cross-validation** for reliable model selection
- Start **simple**, add complexity only if needed