

# Machine Learning

Compiled Revision Notes

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# Week 1: Introduction and Regression

## Introduction to Machine Learning

### What is Machine Learning?

- **Definition:** A field of study giving computers the ability to learn without being explicitly programmed. It is about changing behavior to improve performance in the future.
- **Core Concept:** Instead of hand-crafting complex rules (lots of `if` statements), we use data to fit parameters of a model.
  - **The Equation:** We want to find the function  $f$  in the equation  $y = f(x)$ , where we figure out the right-hand side by gathering data and fitting parameters.

### Types of Learning

- **Supervised Learning:**
  - **Definition:** Learning a function mapping inputs to outputs based on training examples where we already know the correct result (labeled data).
  - **Classification:** The output is a category or discrete label (e.g., Face/No Face, Digit 0–9).
  - **Regression:** The output is a continuous value (e.g., Stock prices, Turkey cooking time).
- **Unsupervised Learning:**
  - Techniques where there is no “right” answer known; the algorithm tries to find structure or patterns in the data.
  - Examples: Clustering (grouping data), Dimensionality Reduction.
- **Reinforcement Learning:** Learning through interaction (e.g., AlphaGo playing games against itself).

### The ML Pipeline

To perform Machine Learning, you need 4 components:

1. **The Task:** Define or limit what you are trying to do.
  2. **The Experience:** The data (more data = more experience).
  3. **The Performance Measure:** A way to measure success.
  4. **The Learning Algorithm:** The recipe by which we will improve our performance.
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## Linear Regression

### Variables

- **Independent Variable ( $x$ ):** The input. It changes independently (e.g., Time).
- **Dependent Variable ( $y$ ):** The output. It depends on the input (e.g., House Value).
- **Visualizing:** Plot independent variables on the horizontal axis ( $x$ ) and dependent on the vertical axis ( $y$ ).

### Linear Relationships

- **Definition:** A linear relationship means a change in  $x$  always produces the same proportionate change in  $y$ .

- **School Math Formula:**  $y = mx + c$ , where  $m$  is the slope and  $c$  is the y-intercept.
- **Machine Learning Notation:**  
We scale this up for larger models using **Weights** ( $w$ ). Weights are the parameters or coefficients that the model learns during training.

$$y = w_0 + w_1x$$

- $w_0$  = bias or intercept (previously  $c$ ).
- $w_1$  = weight or slope (previously  $m$ ).

### The Turkey Example

- **Scenario:** Predicting cooking time ( $t$ ) based on weight ( $w$ ).
- **Linear Model:**  $t = mw + c$  (Rule of thumb: 20 mins per pound + 20 mins).
  - *Critique:* Implies you cook a 0 lb turkey for 20 mins (the y-intercept).
- **Power Model (Pief Panofsky):**

$$t = \frac{w^{2/3}}{1.5}$$

- *Comparison:* Linear works well for small weights (1–6 lbs) but diverges significantly at higher weights.
- **Lesson:** Data points might follow a curve. If data is scattered on a curve, a simple linear model is an **inappropriate fit** as it assumes values keep increasing indefinitely.

### Training the Model

- **Goal:** Find the best parameters ( $w_0, w_1$ ) that minimize the error for our training sample.
- **Prediction vs. Observation:**
  - $y$  (**Observation**): The actual observed data point.
  - $\hat{y}$  (**Prediction**): The value predicted by the function.
  - **Residual:** The difference between the prediction ( $\hat{y}$ ) and the observation ( $y$ ).
- **Cost Function (Mean Squared Error, MSE):**

$$L = \frac{1}{2m} \sum_{i=0}^m (\hat{y}_i - y_i)^2$$

- $m$ : number of samples.
- Note: The  $\frac{1}{2m}$  term is for mathematical convenience to make derivatives simpler.
- **Gradient Descent:**
  - The algorithm typically used to solve for the parameters ( $w$ ).
  - It performs multiple iterations to find the parameters that give the smallest loss ( $L$ ).

## Multiple Linear Regression

Real-world problems have more than one input feature.

- **Polynomial Regression:**  $y = w_0 + w_1x + w_2x^2 + \dots$  (fits curves).
- **Multiple Linear Regression:** Input  $x$  is a vector of features  $(x_1, x_2, \dots)$ .

$$y = w_0 + w_1x_1 + w_2x_2 + w_3x_3 + \dots$$

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## Week 2: Generalisation and Model Evaluation

### Generalisation

#### The Goal of Machine Learning

- **Definition:** Generalisation is the model's ability to give sensible outputs to sets of input that it has never seen before.
- It is not enough to perform well on training data; the model must perform well on **previously unseen data**.
- **Measurement:** We often use root-mean-squared (RMS) error to measure performance, but calculating this on training data is misleading because the model might be overfit.

#### Underfitting vs. Overfitting

- **Underfitting (High Bias):**
  - Occurs when the model is too simple to capture the underlying trend of the data.
  - **Symptoms:** Poor performance on both the training data and the test data. The model has not learned enough.
- **Overfitting (High Variance):**
  - Occurs when the model fits the training data too well, capturing noise rather than the signal.
  - **Symptoms:** Very low training error, but high test error. The model is unreliable on new data.
  - **Confidence:** Overfit models often predict incorrect results with very high confidence.

#### Bias and Variance Trade-off

- **Bias:** Making assumptions about the underlying model. High bias leads to underfitting.
  - **Variance:** Sensitivity to training data. High variance leads to overfitting.
  - **The Goal:** Find the sweet spot between high bias and high variance to ensure good generalisation.
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## Testing and Validation Procedures

### Train and Test Split

- To test a model, we split available data into two distinct sets:

1. **Training Set:** Used to fit the model and learn parameters such as weights.
  2. **Test Set:** Used only to evaluate performance and acts as unseen data.
- **Typical Splits:** 80/20 or 75/25 (Train/Test).
  - **Crucial Rule:** The test set must be guarded carefully and used sparingly/carefully. If you use it to make decisions such as choosing model complexity, it is no longer unseen and the evaluation becomes invalid.

## Data Leakage

- **Definition:** Leakage occurs when information from the test or validation set unintentionally influences the training process. This leads to overly optimistic performance estimates that fail in the real world.
  - **The Cause:** Often caused by non-independent samples. If correlated data appears in both training and testing sets, the model effectively memorizes the answer via hidden context.
  - **Example: Bird Call Recordings**
    - *Scenario:* Recordings from Jan 1st (Recording A, Recording B), Jan 2nd, etc.
    - *Bad Split:* Randomly assigning files. Recording A goes to Train, Recording B goes to Test. The model learns background noise rather than bird species.
    - *Correct Approach: Group-based splitting.* Split by day or week. If Jan 1st is in Test, all recordings from Jan 1st must be in Test.
  - **Key Takeaway:** Ensure split groups are meaningful, such as blocks of time, to test true generalisation.
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## Model Selection and Hyperparameters

### Hyperparameters

- **Definition:** Parameters that are chosen by the engineer, not learned by the algorithm.
- **Examples:**
  - Degree of polynomial (linear vs quadratic vs cubic).
  - Learning rate ( $a$ ).
  - Number of layers in a neural network.

### The Validation Set

- We cannot use the **test set** to choose hyperparameters.
- **Solution:** Split training data further into training and validation sets (often 70/30).
- **Procedure:**
  1. Train different models on the training portion.
  2. Check error on the validation portion.
  3. Pick the hyperparameter with the lowest validation error.
  4. **Final Step:** Evaluate the chosen model on the test set, which has remained hidden.

### Cross-Validation (K-Fold)

- **Problem:** A single validation split might be biased.
- **Solution (K-Fold):**
  1. Split data into  $k$  equal folds (e.g.,  $k = 5$  or  $k = 10$ ).

2. Train on  $k - 1$  folds and validate on the remaining fold.
  3. Repeat  $k$  times so each fold is used as validation once.
  4. Average the error across all runs to obtain a robust metric.
- **Benefit:** Reduces the risk that a specific random split skews results.

## Polynomial Regression

- Complex curved data can be modeled by adding powers of  $x$  (e.g.,  $x^2, x^3$ ).
- **Degree ( $M$ ):** The hyperparameter controlling complexity.
  - Low  $M$  (e.g., 1): High bias, underfitting.
  - High  $M$  (e.g., 9): High variance, overfitting.
- Cross-validation is used to find the optimal  $M$ .

## Week 3: Classification & Logistic Regression

### Introduction to Classification

#### What is Classification?

- **Definition:** Unlike regression which predicts continuous values, classification predicts which **category** or group a sample belongs to.
- **Outputs:** The output is restricted to a limited set of possible classes (e.g., 0 or 1).
- **Examples:** Spam detection (Spam/Not Spam), Fraud detection, Medical diagnosis (Malignant/Benign).

#### Binary Classification

- **Definition:** A problem with only two classes:
  - **Negative Class (0):** The absence of the event (e.g., Benign).
  - **Positive Class (1):** The presence of the event (e.g., Malignant).
- **Categorical Data:** We represent categorical outcomes numerically, typically as 0 and 1.

**Lab Note: Encoding Categorical Features** When converting text labels to numbers (Encoding), be careful: - **Label Encoding:** Assigning numbers (0, 1, 2) can mislead the model into thinking there is an order or hierarchy (e.g.,  $2 > 1$ ), which might not exist. - **One-Hot Encoding:** A safer approach for non-ordinal data. It splits one feature into multiple binary features (e.g., `Color_Red`, `Color_Blue`), preventing the model from assuming false relationships.

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## Logistic Regression & The Logit Function

Logistic Regression is a **classification algorithm**, named “regression” only because of its mathematical roots. Despite its name, we are not trying to predict a continuous value. The response variable  $y$  is either 0 or 1.

We do predict a continuous value between 0 and 1, but we interpret it as a probability ( $p$ ) and then apply a threshold to obtain a discrete class label.

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## The Core Problem with Linear Regression

With standard linear regression:

$$\hat{y} = w_0 + w_1 x_1$$

- Predictions range from  $-\infty$  to  $+\infty$ .
- For binary classification,  $\hat{y}$  can easily be  $< 0$  or  $> 1$ .
- We want an estimate of probability  $p$  strictly between 0 and 1.

Linear regression therefore does not naturally constrain outputs to the valid probability range.

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## The Sigmoid Function

The **sigmoid function**, also called the **logistic function**, takes any real-valued number and maps it into the range  $(0, 1)$ .

$$y = f(x) = \frac{1}{1 + e^{-x}}$$

- As  $x \rightarrow +\infty$ ,  $y \rightarrow 1$ .
- As  $x \rightarrow -\infty$ ,  $y \rightarrow 0$ .
- The function maps values from  $(-\infty, +\infty)$  to  $(0, 1)$ .

Since our linear model output

$$\hat{y} = w_0 + w_1 x_1 + \dots + w_n x_n$$

also ranges from  $-\infty$  to  $+\infty$ , we apply the sigmoid to map it into a probability:

$$p = \frac{1}{1 + e^{-(w_0 + w_1 x_1 + \dots + w_n x_n)}}$$

This is the **logistic regression function**. The weights  $w_0, \dots, w_n$  are often written as  $\beta_0, \dots, \beta_n$  in the literature.

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## Odds and the Logit Function

The term

$$\frac{p}{1 - p}$$

is known as the **odds**.

Examples: - If  $p = 0.5$ :  $\frac{0.5}{0.5} = 1 : 1$  - If  $p = 0.8$ :  $\frac{0.8}{0.2} = 4 : 1$  - If  $p = 0.05$ :  $\frac{0.05}{0.95} \approx 0.053 : 1$



The odds function is asymmetrical: - If  $0 < p < 0.5$ , odds lie between 0 and 1. - If  $0.5 < p < 1$ , odds lie between 1 and  $\infty$ .

To address this asymmetry, we take the natural logarithm of the odds:

$$\ln\left(\frac{p}{1-p}\right)$$

This is called the **logit function**:

$$\text{logit}(p) = \ln\left(\frac{p}{1-p}\right)$$

The logit function forms the basis of logistic regression.

The linear model in logistic regression is therefore written as:

$$\ln\left(\frac{p}{1-p}\right) = w_0 + w_1x_1 + \dots + w_nx_n$$

## Logit vs. Logistic Function

The logit and logistic functions are inverses of each other.

Feature	Logistic (Sigmoid) Function	Logit Function
<b>Formula</b>	$f(x) = \frac{1}{1+e^{-x}}$	$\text{logit}(p) = \ln\left(\frac{p}{1-p}\right)$
<b>Purpose</b>	Maps log-odds ( $x$ ) to probability ( $p$ )	Maps probability ( $p$ ) to log-odds ( $x$ )
<b>Input Range</b>	$-\infty < x < \infty$	$0 < p < 1$
<b>Output Range</b>	$0 < p < 1$	$-\infty < x < \infty$
<b>Use in Logistic Regression</b>	Converts linear model output to probability	Converts probability to a linear form

## Decision Boundaries

- **Thresholding:** The model outputs a probability (e.g., 0.7). We must choose a threshold (e.g., 0.5) to classify it as Class 1 or Class 0.
- **Trade-off:** This threshold is technically a hyperparameter, often chosen based on the problem (e.g., lowering the threshold for cancer diagnosis to minimize False Negatives).

**Is Threshold a Hyperparameter? - Short Answer:** It is complicated. Technically yes, but it is often determined by **human decision** and domain constraints rather than just data. - **Example:** In cancer diagnosis, you might lower the threshold (e.g., to 0.1) to catch more cases. You would rather tolerate False Positives (scaring a healthy patient) than False Negatives (missing cancer).

## Training & Loss Functions

### Why MSE Fails for Classification

- **Non-Convexity:** If you use Mean Squared Error (MSE) with the Sigmoid function, the resulting cost function is **non-convex**.
- **Result:** The graph looks “wavy” with many local minima, making it impossible for Gradient Descent to reliably find the global minimum (the best weights).

### Log Loss (Binary Cross-Entropy)

- We use **Log Loss** instead. It is **convex**, ensuring a single global minimum that makes optimization efficient.
- **The Logic:**
  - If correct answer is 1: We want predicted  $p$  to be close to 1. If  $p$  is low, error is massive ( $-\log(p)$ ).
  - If correct answer is 0: We want predicted  $p$  to be close to 0. If  $p$  is high, error is massive ( $-\log(1 - p)$ ).
- **Formula:**

$$L(w) = -\frac{1}{n} \sum_{i=1}^n [y_i \cdot \log(\hat{y}_i) + (1 - y_i) \cdot \log(1 - \hat{y}_i)]$$

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## Metrics & Evaluation

### L1 vs. L2 Norms

These are ways to measure the “magnitude” or distance of a vector, often used in calculating errors.

- **L1 Norm (Manhattan):** The sum of absolute values.  $\|x\|_1 = \sum |x_i|$
- **L2 Norm (Euclidean):** The square root of the sum of squared values (straight line distance).  
 $\|x\|_2 = \sqrt{\sum x_i^2}$

### Regression Metrics

When evaluating regression models (predicting continuous values), we use several key metrics:

- **MSE (Mean Squared Error):**
  - **Formula:**  $\frac{1}{n} \sum (y_i - \hat{y}_i)^2$
  - **Use:** Standard for **Training** loss because it is differentiable (convex).
  - **Pros/Cons:** Highly sensitive to outliers because it squares the error (large errors become huge).
- **RMSE (Root Mean Squared Error):**
  - **Formula:**  $\sqrt{MSE}$
  - **Use:** **Model Evaluation**.
  - **Pros:** It returns the error to the same units as the target variable (e.g., dollars, minutes), making it easier to interpret.
- **MAE (Mean Absolute Error):**

- **Formula:**  $\frac{1}{n} \sum |y_i - \hat{y}_i|$
- **Use: Model Evaluation.**
- **Pros/Cons:** Less sensitive to outliers than MSE. However, it is **not differentiable** at 0 (has a sharp “kink”), so it cannot be used as a loss function for training algorithms like Gradient Descent.
- **$R^2$  (Coefficient of Determination):**
  - **Formula:**  $1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2}$
  - **Interpretation:** Represents the proportion of variance in the dependent variable explained by the model (Unitless, max value is 1).

## Classification Metrics

- **Accuracy:** Fraction of correct predictions. Good for balanced classes, misleading for imbalanced ones.
- **Confusion Matrix:** A table comparing Actual vs. Predicted values (TP, TN, FP, FN).
- **Precision:**  $\frac{TP}{TP+FP}$  (Accuracy of positive predictions).
- **Recall:**  $\frac{TP}{TP+FN}$  (Ability to find all positive instances).
- **F1-Score:** Harmonic mean of Precision and Recall. Best for imbalanced datasets.

**Trade off between Precision and Recall (PR Curve and PR AUC)** Precision and Recall usually trade off. Increasing the threshold increases Precision but lowers Recall (and vice versa). The PR Curve and the Area under the curve (AUC), can also be a good single number estimator of model performance.

**Note on Optimization** We typically **train** using one metric (like Log-Loss for classification or MSE for regression because they are differentiable/convex) but **evaluate** using others (like Accuracy, F1-Score, or MAE) that are more interpretable for humans.

## Week 4: k-Nearest Neighbours, Feature Engineering & Tree Ensembles

### k-Nearest Neighbours (kNN)

#### The Algorithm

- **Definition:** kNN is a simple, two-part algorithm used for either classification or regression.
- **Procedure:**
  1. Given a target instance ( $x_j$ ), calculate the distance to all recorded training cases ( $x_i$ ).
  2. Retrieve the  $k$  most similar (nearest) recorded cases.
  3. **For Classification:** Take the maximum of  $k$  votes (the most common category among the neighbors).
  4. **For Regression:** Calculate the “average” across these  $k$  cases.

#### Distance Metrics

- We typically use **Euclidean distance** to calculate the “nearest” neighbor.
- **Formula:**  $d(t, s) = \sqrt{(t_1 - s_1)^2 + \dots + (t_p - s_p)^2}$ .

- **The Scale Problem:** Scale matters significantly. If one predictor/feature has a much larger value range than another, it will disproportionately influence the distance measurement.

### Choosing $k$

- $k = 1$  (**1-Nearest Neighbour**): Looking at only the single closest point tends to overfit the training data and captures noise.
- **Higher  $k$  (e.g.,  $k = 5$ )**: Taking a vote among multiple neighbors smooths out the decision boundary and reduces overfitting.
- **The Trade-off**: If  $k$  is too small, the model overfits. If  $k$  is too large, the model underfits reality.
- **How to choose**: We treat  $k$  as a hyperparameter and select the best value using cross-validation (e.g., 10-fold cross-validation).

### Lazy vs. Eager Learning

- **Lazy Learning (e.g., kNN)**: Defers computation until a prediction is needed.
  - *Pros*: Very quick to train (it just stores the data), less memory usage during training.
  - *Cons*: Prediction is slow, relies heavily on training data during prediction, uses more memory during prediction.
- **Eager Learning (e.g., SVM, Neural Networks, Decision Trees)**: Precomputes a model during the training phase.
  - *Pros*: Faster predictions, less memory usage during prediction, less dependent on original data once trained.
  - *Cons*: Slower and more memory-intensive during the training phase.

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## Feature Engineering & Preprocessing

### Feature Scaling

Because distance metrics like Euclidean distance are heavily influenced by the scale of the data, we must bring features into a similar range.

### Normalization vs. Standardization

Feature	Min-Max Scaling (Normalization)	Standardization
<b>Output Range</b>	Fixed (0 to 1)	Not bounded
<b>Outlier Handling</b>	Very sensitive	More robust
<b>Distribution</b>	Changes the shape	Maintains shape (mostly)
<b>Common Use Case</b>	When you need exact boundaries from min to max value	When you need a “standard normal curve” (Mean 0, Std Dev 1)

### Pipelines

- We should avoid altering the entire raw dataset directly before training, as future data would also need to be manually transformed.

- **Solution:** Build the transformation directly into the model using `make_pipeline`.
- Any data that goes into the pipeline automatically passes through the transformation step (e.g., `StandardScaler()`) before reaching the classifier step.

## Feature Engineering & Custom Transforms

The features we provide to a model drastically dictate what it can learn. We can design custom features to give the model better predictive power.

- **Custom Calculations:** Using tools like `FunctionTransformer`, we can add derived features, such as calculating a point's radius/distance from the center (0,0) to help classify circular data.
- **1D to 2D Signals:** Converting 1-dimensional signals into 2-dimensional representations. For example, converting audio data or stock market data into spectrograms allows models (especially computer vision models) to find complex visual patterns in the data.

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## The Curse of Dimensionality

### The Problem with High Dimensions

- **Sparsity:** As the number of dimensions (features) increases, data points spread out, increasing sparsity.
- **Failing Distance Metrics:** In high dimensions (e.g.,  $>10$ ), Euclidean distance becomes unhelpful because all vectors become almost equidistant from the search query vector. This misleads nearest-neighbor algorithms.

### The Bioinformatics Problem

- In fields like bioinformatics (e.g., genome sequencing), datasets often have very few subjects (e.g., 1000) but millions of features (genes).
- This creates a mathematical problem similar to simultaneous equations: if you have millions of unknown variables (features) but only 1000 equations (subjects), you cannot reliably solve the system.
- **The Solution:** This issue is typically addressed using **Regularization** (especially L1 Regularization, which forces the model to ignore irrelevant features by shrinking their weights to zero).

## Dimensionality Reduction Techniques

To fix the curse of dimensionality before applying algorithms like kNN, we can use:

- **Feature Grouping:** Grouping common features based on domain knowledge (e.g., averaging 365 daily weather readings into 12 monthly averages).
- **Extraction/Embedding Algorithms:** Using techniques like Principal Component Analysis (PCA) or Linear Discriminant Analysis (LDA) to compress the data into a lower-dimensional space.

## Decision Trees & Ensembles

### Decision Trees

- **How it works:** Decision Trees mimic human decision-making by incrementally splitting a dataset into smaller subsets based on feature values (e.g., “Is it a mammal? -> Does it have stripes? -> Tiger”).
- **Anatomy of a Tree:**
  - **Root Node:** First split, entire dataset.
  - **Decision Node:** Internal split based on a feature condition.
  - **Leaf Node (Terminal Node):** Final node that outputs a prediction.
  - **Depth:** Number of split layers.

### How Trees Learn: Splitting & Purity

- At each node, the algorithm selects the feature and threshold that produce the **purest** child nodes.
- It evaluates all possible splits and chooses the one that minimises impurity.

### Impurity Measures:

- **Gini Impurity**
- **Entropy (Information Gain)**

### Gini Index (Binary Case):

$$\text{Gini} = 1 - (p_{yes}^2 + p_{no}^2)$$

- $0 \rightarrow$  perfectly pure node.
- $0.5 \rightarrow$  maximum impurity (50/50 split).
- Lower Gini = better split.
- For a full split, compute the **weighted average** of child-node Gini values and choose the lowest.

### Continuous Features:

1. Sort feature values.
2. Use midpoints as candidate thresholds.
3. Compute impurity for each.
4. Select threshold with minimum impurity.

### Overfitting:

- Without limits, trees split until leaves are perfectly pure.
  - Leads to memorisation and poor generalisation.
  - Controlled using hyperparameters such as:
    - `max_depth`
    - `min_samples_split`
    - `min_samples_leaf`
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## Ensemble Learning

- **Concept:** Combine multiple models instead of relying on a single tree.
  - Leverages the “wisdom of the crowd” for improved accuracy and robustness.
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## Bagging & Random Forests

- **Structure:** Models trained in **parallel**.
  - **Bagging:**
    - Train models on bootstrap samples (random samples with replacement).
    - Aggregate via majority vote (classification) or averaging (regression).
    - Primarily **reduces variance**.
  - **Random Forests:**
    - Bagging + random subset of features at each split.
    - Decorrelates trees so they do not all make the same mistakes.
  - **Goal:** Strong variance reduction, robust, hard to overfit.
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## Boosting

- **Structure:** Models trained **sequentially**.
  - **How it works:**
    - Tree 1 makes predictions.
    - Tree 2 focuses more on misclassified samples.
    - Tree 3 focuses on remaining errors, and so on.
  - **Popular Algorithms:** AdaBoost, Gradient Boosting, XGBoost, LightGBM.
  - **Goal:** Primarily **reduces bias**.
  - Can overfit if not properly tuned.
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## Bagging vs. Boosting

- **Bagging:** Parallel, reduces variance, resistant to overfitting.
- **Boosting:** Sequential, reduces bias, more prone to overfitting but often higher performance when tuned well.