

IN402

# Machine Learning

CHAPTER

# 0

## Introduction & Foundations

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*These notes extend course materials taught by Prof. Ahmad Faour with additional content from textbooks and supplementary resources.*

***Disclaimer:** This is not an official course document.*

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## 1 What is Machine Learning?

Machine Learning (ML) represents a fundamental shift in how we approach problem-solving with computers. Rather than explicitly programming every rule and decision, we create systems that can **learn from data** and improve their performance through experience.

### 1.1 Historical Perspective

The concept of machine learning has evolved significantly since its inception. One of the earliest and most influential definitions came from a pioneer in the field:

#### Arthur Samuel's Definition (1959)

*"Machine Learning is the field of study that gives computers the ability to learn without being explicitly programmed."*

This elegant definition captures the essence of ML: moving beyond hard-coded rules toward algorithms that discover patterns and behaviors directly from data. Samuel's work on computer checkers in the 1950s demonstrated this principle—his program improved its gameplay through self-play, without being told explicitly how to evaluate board positions.

### 1.2 A Formal Definition

As the field matured, more rigorous definitions emerged. Tom Mitchell provided a mathematical framework that has become the standard for formally describing machine learning systems:

#### Tom Mitchell's Definition (1997)

*"A computer program is said to learn from **Experience (E)** with respect to some class of **Tasks (T)** and a **Performance measure (P)**, if its performance at tasks in T, as measured by P, improves with experience E."*

This definition provides a structured way to think about any machine learning problem by identifying three key components:

**Task (T):** The specific problem the system aims to solve (e.g., classifying emails, predicting prices, recognizing faces).

**Experience (E):** The data or interactions the system learns from (e.g., labeled examples, past observations, trial-and-error).

**Performance (P):** The metric used to evaluate success (e.g., accuracy, error rate, reward).

#### Email Spam Detection

Let's apply Mitchell's framework to a familiar problem:

- ▶ **Task (T):** Classify incoming emails as either "spam" or "not spam"

- ▶ **Experience (E):** A dataset of emails that have been manually labeled by users
- ▶ **Performance Measure (P):** The percentage of emails correctly classified on new, unseen emails

The system “learns” if its classification accuracy improves as it processes more labeled examples. Initially, it might achieve 70% accuracy, but after training on thousands of examples, it could reach 95% or higher.

## 2 The Motivation Behind Machine Learning

Traditional software engineering follows a paradigm where developers write explicit rules for every situation the program might encounter. While this approach works well for many problems, it fundamentally breaks down in several important scenarios.

### 2.1 Limitations of Traditional Programming

Consider the following challenges:

- ▶ **Complex Rules:** How would you write explicit rules to recognize a cat in an image? The cat could be sitting, standing, or lying down; facing any direction; in various lighting conditions; partially hidden; with different fur colors and patterns. The rule set would be impossibly large and fragile.
- ▶ **Unknown Rules:** For some tasks, we simply don't know what the rules are. How exactly do experts diagnose diseases from medical images? Much of this knowledge is implicit and cannot be easily codified.
- ▶ **Changing Patterns:** In fraud detection, attackers constantly evolve their tactics. Hard-coded rules become obsolete quickly and require continuous manual updates.

### 2.2 The Machine Learning Advantage

Machine learning offers a fundamentally different approach that addresses these limitations:

**Adaptability:** Models continuously improve as they encounter new data, automatically adjusting to changing patterns without manual reprogramming.

**Pattern Discovery:** Algorithms can discover complex, subtle patterns that humans might miss or find difficult to articulate explicitly.

**Scalability:** ML systems can process and learn from massive datasets—millions or billions of examples—extracting insights that would be impossible for humans to find manually.

**Automation:** Once trained, models can make predictions on new data instantly, handling volumes far beyond human capacity.

#### 💡 Intuition

Think of machine learning as teaching by example rather than by instruction. Instead of giving a computer a detailed recipe (traditional programming), we show it many

examples of inputs and desired outputs, allowing it to infer the underlying patterns and rules on its own.

## 3 Machine Learning in the AI Ecosystem

Machine Learning does not exist in isolation—it is part of a broader landscape of interconnected fields. Understanding these relationships provides important context for where ML fits in the bigger picture.

### 3.1 Defining the Landscape

**Artificial Intelligence (AI):** The broadest concept, encompassing any system that can perform tasks requiring human-like intelligence. This includes reasoning, problem-solving, perception, natural language understanding, and decision-making. AI is the overarching goal: creating intelligent machines.

**Machine Learning (ML):** A subset of AI focused specifically on algorithms that learn from data. Rather than being explicitly programmed for every scenario, ML systems improve their performance through experience. ML is the primary approach currently driving AI progress.

**Deep Learning (DL):** A specialized subset of ML using artificial neural networks with multiple layers (hence “deep”). Deep learning has achieved breakthrough results in computer vision, natural language processing, and game playing.

**Data Science (DS):** An interdisciplinary field that combines multiple domains to extract knowledge from data:

- ▶ **Statistics & Mathematics:** For rigorous inference, hypothesis testing, and modeling.
- ▶ **Computer Science:** For efficient algorithms, data structures, and implementation.
- ▶ **Domain Expertise:** To understand context, ask the right questions, and interpret results meaningfully.

Data science encompasses the entire lifecycle: data collection, cleaning, exploration, visualization, modeling, and communication of insights.

**Data Mining:** The process of discovering previously unknown patterns, anomalies, and relationships in large datasets. It draws from statistics, ML, and database systems to extract actionable knowledge.

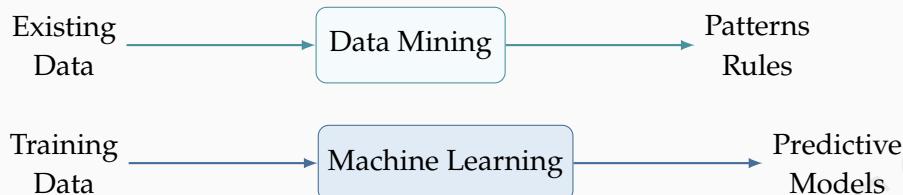
### 3.2 Machine Learning vs. Data Mining

While ML and data mining share many techniques, their primary objectives differ:

#### Contrasting Goals

- ▶ **Data Mining:** Focuses on *exploration and discovery*—finding interesting patterns and rules in existing data that were previously unknown.  
*Example:* Discovering that customers who buy bread often buy milk (market basket analysis).

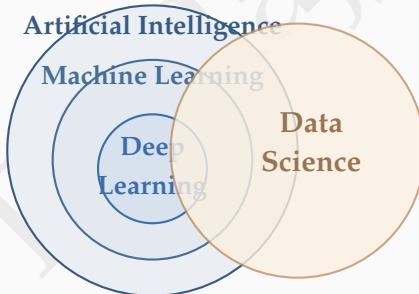
- ▶ **Machine Learning:** Focuses on building *predictive models*—learning patterns from training data to make accurate predictions on new, unseen data.  
*Example:* Building a model that predicts whether a new customer will buy milk based on their shopping history.



**Figure 1:** Contrasting objectives: Data Mining discovers patterns in existing data, while Machine Learning builds models to predict future outcomes.

### 3.3 Visualizing the Relationships

Figure 2 illustrates how these fields relate to one another. AI serves as the overarching discipline, with ML as its primary methodology. Deep Learning represents the cutting edge of ML techniques. Data Science overlaps significantly with AI and ML but also extends into areas like data engineering, business intelligence, and communication.



**Figure 2:** The AI ecosystem showing the relationships between Artificial Intelligence, Machine Learning, Deep Learning, and Data Science.

## 4 Types of Machine Learning

Machine learning algorithms can be categorized based on the nature of the learning signal and the structure of the learning task. The three primary paradigms are:

**Supervised Learning:** Learning from labeled examples—a teacher provides correct answers during training.

**Unsupervised Learning:** Finding structure in unlabeled data—no teacher, the algorithm discovers patterns independently.

**Reinforcement Learning:** Learning through trial and error—an agent receives rewards or penalties based on its actions.

Additionally, there exist hybrid approaches:

**Semi-Supervised Learning:** Combines a small amount of labeled data with a large amount of unlabeled data, leveraging both sources of information.

Each paradigm addresses different types of problems and requires different algorithmic approaches. The following sections explore each in detail.

## 5 Supervised Learning

Supervised learning is the most common machine learning paradigm. It involves learning a mapping from inputs to outputs using a dataset where each input is paired with the correct output label.

### Definition

**Supervised Learning:** The task of learning a function  $f$  that maps an input  $x$  to an output  $y$ , given a training set of labeled examples  $\{(x_i, y_i)\}_{i=1}^n$ .

$$f : x \rightarrow y$$

The objective is to find a function that not only fits the training data well but also **generalizes** to make accurate predictions on new, unseen inputs.

### 5.1 The Core Concept

#### Learning with a Teacher

The fundamental idea of supervised learning is that we have a “teacher” who provides correct answers. During training, the algorithm sees input-output pairs and learns to predict the output from the input.

Formally, we work with a dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$  where:

- ▶  $x_i \in \mathbb{R}^d$  is the feature vector (input) for the  $i$ -th example
- ▶  $y_i$  is the corresponding label (output)
- ▶  $n$  is the number of training examples
- ▶  $d$  is the number of features

The data can be organized into matrix form:

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nd} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

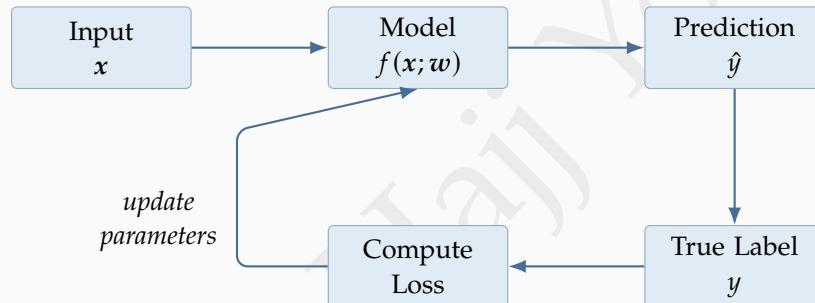
where  $X \in \mathbb{R}^{n \times d}$  contains all feature vectors and  $y \in \mathbb{R}^n$  contains all labels.

## 5.2 The Learning Process

Supervised learning follows an iterative optimization process where the model progressively improves its predictions:

### The Training Loop

1. **Forward Pass:** The model receives an input  $x$  and produces a prediction  $\hat{y}$  based on its current parameters (weights and biases).
2. **Error Computation:** The prediction  $\hat{y}$  is compared to the true label  $y$  to compute a loss or error measure (e.g., mean squared error, cross-entropy).
3. **Parameter Update:** An optimization algorithm (typically gradient descent) uses the computed error to update the model's parameters, adjusting them to reduce the error.
4. **Iteration:** This cycle repeats for many examples and multiple passes through the dataset (epochs) until the model converges or reaches satisfactory performance.



**Figure 3:** The supervised learning feedback loop showing how errors drive parameter updates during training.

### Important Note

**Critical Distinction:** Parameter updates occur *only during training*. Once training is complete, the parameters are fixed, and the model makes predictions without further modification.

## 5.3 Classification: Predicting Categories

Classification is the task of predicting a *discrete categorical label* from a finite set of classes.

### Classification

Given an input  $x$ , predict which category or class it belongs to:

$$f(x) \rightarrow y \in \{c_1, c_2, \dots, c_k\}$$

where  $k$  is the number of possible classes.

### ❖ Email Spam Detection

**Task:** Determine whether an incoming email is spam or legitimate.

**Input Features ( $x$ ):**

- ▶  $x_1$ : Word frequencies (counts of words like "free," "winner," "urgent")
- ▶  $x_2$ : Presence of links or attachments (binary: 0 or 1)
- ▶  $x_3$ : Email length (number of characters)
- ▶  $x_4$ : Sender reputation score
- ▶  $x_5$ : Ratio of uppercase to lowercase letters

**Output:** A binary label  $y \in \{\text{spam, not spam}\}$ , often encoded as  $y \in \{1, 0\}$ .

**Learning Objective:** After training on thousands of labeled emails, the model learns patterns like: "Emails with many promotional words, excessive capitalization, and unknown senders are likely spam."

### ⓘ Remark

Classification can be binary (two classes) or multi-class (more than two classes). Examples include:

- ▶ **Binary:** Disease diagnosis (positive/negative), sentiment analysis (positive/negative)
- ▶ **Multi-class:** Digit recognition (0-9), animal species identification, language detection

## 5.4 Regression: Predicting Continuous Values

Regression is the task of predicting a *continuous numerical value* rather than a discrete category.

### 📘 Regression

Given an input  $x$ , predict a real-valued output:

$$f(x) \rightarrow y \in \mathbb{R}$$

The output can be any number within a continuous range.

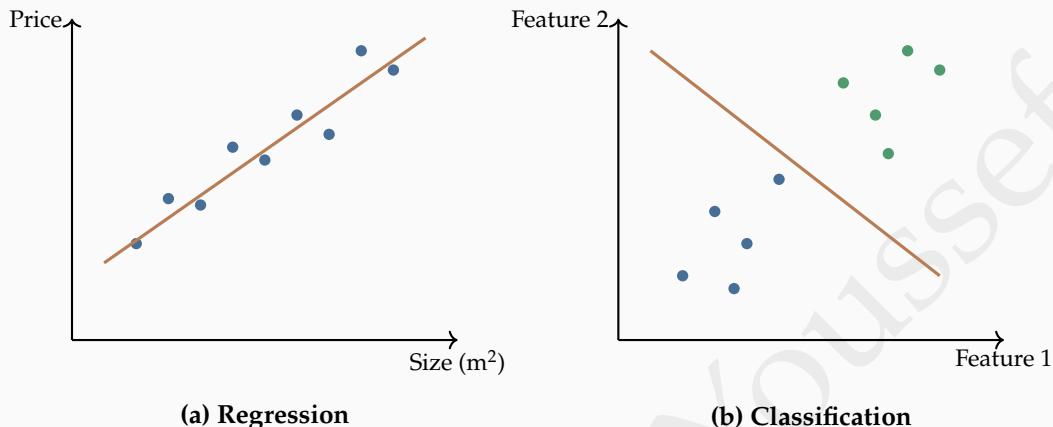
### ❖ House Price Prediction

**Task:** Estimate the selling price of a house based on its characteristics.

**Input Features ( $x$ ):**

- ▶  $x_1$ : Size in square meters
- ▶  $x_2$ : Number of bedrooms
- ▶  $x_3$ : Age of the house (years)
- ▶  $x_4$ : Distance to city center (km)
- ▶  $x_5$ : Neighborhood average income

**Output:** A continuous value  $y \in \mathbb{R}^+$  representing the predicted price (e.g., \$350,000).  
**Learning Objective:** The model learns relationships like: “Larger houses in affluent neighborhoods close to the city center command higher prices, while older homes decrease in value.”



**Figure 4:** Visual comparison: (a) Regression fits a continuous function to predict numerical values. (b) Classification finds a decision boundary to separate discrete classes.

## 5.5 Common Supervised Learning Algorithms

A rich variety of algorithms exist for supervised learning, each with different assumptions, strengths, and use cases:

- ▶ **Linear Regression:** Models linear relationships; simple and interpretable
- ▶ **Logistic Regression:** Despite its name, used for classification; models probability of class membership
- ▶ **Decision Trees:** Learns hierarchical rules; highly interpretable
- ▶ **Support Vector Machines (SVM):** Finds optimal decision boundaries; effective in high dimensions
- ▶ **K-Nearest Neighbors (KNN):** Makes predictions based on similar examples; non-parametric
- ▶ **Naive Bayes:** Probabilistic classifier based on Bayes’ theorem; fast and simple
- ▶ **Neural Networks:** Flexible function approximators; can model complex non-linear relationships

## 6 Unsupervised Learning

Unlike supervised learning, unsupervised learning works with data that has no predefined labels. The goal is to discover inherent structure, patterns, or organization within the data itself.

**Definition**

**Unsupervised Learning:** The task of finding hidden patterns, structures, or representations in an unlabeled dataset  $\{x_i\}_{i=1}^n$  without any explicit guidance about what to look for.

**Learning Without a Teacher**

In unsupervised learning, there is no “correct answer” provided during training. The algorithm must identify interesting structures on its own. This makes unsupervised learning both more challenging (no clear objective) and more exploratory (can discover unexpected patterns).

Common objectives include:

- ▶ Grouping similar data points together (clustering)
- ▶ Reducing data complexity while preserving information (dimensionality reduction)
- ▶ Finding anomalies or outliers (anomaly detection)
- ▶ Discovering latent factors or hidden variables

## 6.1 Clustering: Discovering Groups

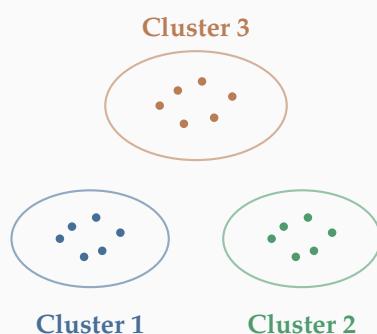
Clustering is one of the most fundamental unsupervised learning tasks.

**Clustering**

**Clustering** partitions a dataset into groups (clusters) such that:

- ▶ Data points within the same cluster are *similar* to each other
- ▶ Data points in different clusters are *dissimilar* from each other

Formally, given  $\{x_i\}_{i=1}^n$ , find a partition  $\{C_1, C_2, \dots, C_k\}$  where each  $C_j$  is a subset of the data.



**Figure 5:** Clustering groups similar data points together without predefined labels.

### ❖ Customer Segmentation

**Task:** Divide customers into distinct segments for targeted marketing strategies.

**Input Features ( $x$ ):**

- ▶  $x_1$ : Age
- ▶  $x_2$ : Annual income
- ▶  $x_3$ : Purchase frequency (transactions per month)
- ▶  $x_4$ : Average transaction value
- ▶  $x_5$ : Time since last purchase

**Output:** Cluster assignments revealing natural customer segments such as:

- ▶ *High-value regulars*: Frequent purchases, high spending
- ▶ *Budget shoppers*: Frequent but low-value purchases
- ▶ *Occasional luxury buyers*: Infrequent but very high-value purchases

**Business Value:** Each segment can receive tailored marketing campaigns, product recommendations, and retention strategies.

### ❖ Document Topic Discovery

**Task:** Automatically identify topics in a large collection of news articles.

**Input:** Thousands of unlabeled news articles represented as term frequency vectors.

**Process:** Clustering algorithms group articles with similar vocabulary and themes.

**Discovered Topics:** The algorithm might identify clusters corresponding to:

- ▶ Politics (words like: election, government, policy)
- ▶ Sports (words like: game, team, championship)
- ▶ Technology (words like: software, AI, innovation)
- ▶ Health (words like: medicine, treatment, disease)

This enables automated organization and navigation of large document collections.

## 6.2 Dimensionality Reduction: Simplifying Data

Real-world datasets often have many features, but not all features are equally informative. Dimensionality reduction techniques compress data into fewer dimensions while preserving essential information.

### ❖ Dimensionality Reduction

Transform high-dimensional data  $X \in \mathbb{R}^{n \times d}$  into a lower-dimensional representation  $Z \in \mathbb{R}^{n \times k}$  where  $k \ll d$ , while preserving as much relevant structure as possible.

#### Common Techniques:

- ▶ **Principal Component Analysis (PCA):** Finds orthogonal directions of maximum variance

- ▶ **t-SNE:** Creates 2D or 3D visualizations that preserve local structure
- ▶ **Autoencoders:** Neural networks that learn compressed representations

### Applications:

- ▶ *Visualization:* Plotting high-dimensional data in 2D or 3D for human interpretation
- ▶ *Noise reduction:* Removing irrelevant variations while keeping signal
- ▶ *Preprocessing:* Reducing computational burden for subsequent algorithms
- ▶ *Feature extraction:* Discovering meaningful latent factors

#### Important Note

**Challenge:** Unsupervised learning is inherently more difficult than supervised learning because there is no clear “correct answer” to validate against. Success depends heavily on domain knowledge, careful interpretation of results, and choosing appropriate evaluation metrics for the specific use case.

## 7 Semi-Supervised Learning

In many real-world scenarios, obtaining labeled data is expensive, time-consuming, or requires specialized expertise, while unlabeled data is abundant and cheap. Semi-supervised learning bridges this gap by combining both types of data.

#### Semi-Supervised Learning

**Semi-Supervised Learning (SSL)** is a learning paradigm that leverages both a small set of labeled examples  $\{(x_i, y_i)\}_{i=1}^{n_l}$  and a large set of unlabeled examples  $\{x_j\}_{j=1}^{n_u}$  where typically  $n_u \gg n_l$ .

The labeled data guides the learning of correct mappings, while the unlabeled data helps the model learn general features and understand the underlying data distribution.

#### Two Approaches to SSL

**Sequential Approach:** The model first learns general representations from the unlabeled data using unsupervised techniques (e.g., clustering, autoencoders), then fine-tunes these representations using the labeled data.

**Joint Approach:** Both labeled and unlabeled data are used simultaneously from the beginning. The model learns to classify the labeled examples while also discovering structure in the unlabeled examples, with both objectives informing each other.

#### Medical Image Analysis

**Task:** Detect tumors in MRI brain scans.

**Challenge:** Labeling MRI scans requires expert radiologists, making it expensive and time-consuming. However, unlabeled MRI scans are readily available from hospitals.

**Data Available:**

- ▶ 500 MRI scans labeled by radiologists (tumor/no tumor)
- ▶ 10,000 unlabeled MRI scans

**SSL Approach:**

1. The model first learns general visual features (edges, textures, shapes) from all 10,500 scans
2. These learned features are then specialized using the 500 labeled examples to distinguish tumor patterns
3. The result is a model that performs better than using only 500 labeled examples

**Benefit:** Achieves near-expert performance while requiring far fewer labeled examples than pure supervised learning.

 **Remark**

Semi-supervised learning is not limited to classification. It can be applied to regression, ranking, anomaly detection, and other tasks where the cost of labeling is a bottleneck.

## 8 Reinforcement Learning

Reinforcement learning (RL) represents a fundamentally different learning paradigm. Instead of learning from labeled examples or discovering patterns in data, RL agents learn through *interaction with an environment*, receiving feedback in the form of rewards or penalties.

 **Reinforcement Learning**

**Reinforcement Learning** is a framework where an **agent** learns to make sequential decisions by taking **actions** in an **environment**, observing the resulting **states**, and receiving **rewards** as feedback. The goal is to learn a **policy**—a strategy for choosing actions—that maximizes cumulative reward over time.

### 8.1 Core Components

 **The RL Framework**

**Agent:** The learner or decision-maker (e.g., a robot, game player, or trading algorithm).

**Environment:** The external world with which the agent interacts (e.g., a physical space, game board, or market).

**State ( $s$ ):** A representation of the current situation or configuration of the environment (e.g., board position in chess, sensor readings for a robot).

**Action ( $a$ ):** A choice the agent can make that affects the environment (e.g., move a piece, turn left, buy a stock).

**Reward ( $r$ ):** A scalar feedback signal indicating the immediate value of an action. Rewards can be:

- ▶ **Positive:** Encouraging desirable behaviors
- ▶ **Negative:** Penalizing undesirable behaviors
- ▶ **Zero:** Neutral outcomes

**Policy ( $\pi$ ):** The agent's strategy mapping states to actions:  $\pi(s) \rightarrow a$ . This is what the agent learns and improves over time.

## 8.2 The Learning Loop

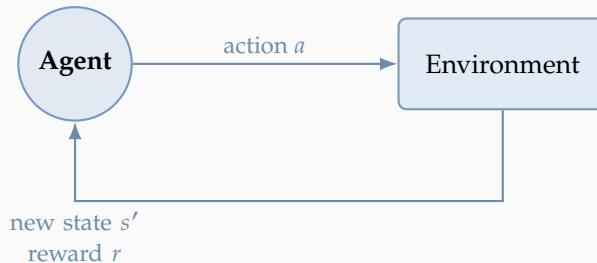
Unlike supervised learning where parameter updates happen through backpropagation, RL agents learn by experiencing consequences of their actions:

### The RL Cycle

1. **Observe:** The agent perceives the current state  $s$  of the environment.
2. **Decide:** Following its current policy  $\pi$ , the agent selects an action  $a$ .
3. **Act:** The agent executes action  $a$  in the environment.
4. **Transition:** The environment changes to a new state  $s'$ .
5. **Receive Feedback:** The environment provides a reward  $r$  (positive, negative, or zero) indicating the quality of the action.
6. **Learn:** The agent updates its policy  $\pi$  based on the experience  $(s, a, r, s')$  to make better decisions in similar future situations.
7. **Repeat:** The cycle continues, with the agent's goal being to maximize the cumulative reward over many time steps.

### Important Note

**Critical Insight:** In RL, rewards are not always immediate. An action might seem suboptimal in the short term but lead to much larger rewards later. This temporal credit assignment problem—figuring out which past actions led to current rewards—is one of RL's central challenges.



**Figure 6:** The agent-environment interaction loop: the agent takes actions and learns from environmental feedback.

### 8.3 Applications of Reinforcement Learning

#### Game Playing

**Task:** Learn to play chess at a superhuman level.

**Components:**

- ▶ *State:* Current board configuration
- ▶ *Actions:* All legal moves available
- ▶ *Rewards:* +1 for winning, -1 for losing, 0 for draws

**Learning:** The agent plays millions of games against itself, gradually learning which moves lead to victory and which lead to defeat. Systems like AlphaZero have surpassed human grandmasters using this approach.

#### Robot Navigation

**Task:** Teach a robot to navigate through a building while avoiding obstacles.

**Components:**

- ▶ *State:* Sensor readings (cameras, LIDAR, position)
- ▶ *Actions:* Move forward, turn left/right, stop
- ▶ *Rewards:* Positive for moving toward goal, negative for collisions or inefficient paths

**Learning:** Through trial and error, the robot learns safe and efficient navigation strategies without explicit programming of obstacle-avoidance rules.

#### Autonomous Driving

**Task:** Learn to drive a vehicle safely and efficiently.

**Components:**

- ▶ *State:* Road conditions, nearby vehicles, traffic signals, speed
- ▶ *Actions:* Accelerate, brake, steer, change lanes
- ▶ *Rewards:* Large positive for reaching destinations safely, large negative for accidents or violations, small negative for fuel consumption

**Learning:** The agent learns complex driving behaviors—when to yield, how to merge, optimal speeds—through experience rather than hand-coded rules.

## 9 The Machine Learning Workflow

Successfully deploying a machine learning solution requires following a systematic process. While the specific steps may vary by application, the general workflow provides a robust framework for any ML project.

### The ML Project Lifecycle

1. **Problem Definition:** Clearly articulate the problem and define success criteria. What are we trying to predict? What decisions will be made based on the model? Is this a classification, regression, or clustering task? What is the business value?
2. **Data Collection:** Gather relevant data from all available sources: databases, APIs, files, sensors, web scraping, or third-party datasets. Consider both structured data (tables) and unstructured data (text, images, audio).
3. **Data Exploration & Understanding:** Perform exploratory data analysis (EDA) to understand the data's characteristics, distributions, relationships, and potential issues. Visualize patterns and identify anomalies.
4. **Data Preprocessing:** Clean and transform the data to make it suitable for modeling:
  - ▶ Handle missing values (imputation, deletion)
  - ▶ Remove or correct errors and outliers
  - ▶ Normalize or standardize numerical features
  - ▶ Encode categorical variables (one-hot encoding, label encoding)
  - ▶ Engineer new features from existing ones
  - ▶ Balance classes if needed
5. **Data Splitting:** Divide the dataset into training, validation, and test sets. This critical step prevents overfitting and enables unbiased evaluation.
6. **Model Selection:** Choose appropriate algorithms based on the problem type, data characteristics, interpretability requirements, and computational constraints.
7. **Model Training:** Fit the selected model(s) to the training data using optimization algorithms like gradient descent. Monitor training progress and convergence.
8. **Hyperparameter Tuning:** Use the validation set to optimize hyperparameters—configuration settings that control the learning process but are not learned from data (e.g., learning rate, regularization strength, tree depth).
9. **Model Evaluation:** Assess performance on the test set using appropriate metrics. Compare against baseline models and business requirements.
10. **Deployment:** Integrate the trained model into production systems where it can make predictions on new data.

- 11. Monitoring & Maintenance:** Continuously monitor model performance in production. Retrain periodically as data distributions change over time (concept drift).

## 9.1 The Critical Role of Data Splitting

Proper data splitting is fundamental to building reliable ML systems. It ensures that we can accurately estimate how well our model will perform on new, unseen data.

### Three-Way Data Split

A typical dataset is divided into three distinct subsets, each serving a specific purpose:

**Training Set (typically 60-70%):** Used to train the model by updating its internal parameters (weights, biases). This is where the actual learning happens through optimization algorithms.

**Validation Set (typically 15-20%):** Used for model selection and hyperparameter tuning. The validation set guides decisions about model architecture and configuration but does *not* update model parameters.

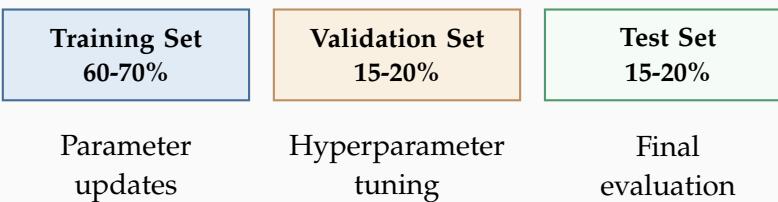
**Test Set (typically 15-20%):** Reserved for final, unbiased evaluation after all development is complete. The test set should never influence any decisions during model development.

### Critical Distinction

**Three Purposes, Three Sets:**

- ▶ **Training:** Parameter updates occur here. The model learns patterns by minimizing loss on this data.
- ▶ **Validation:** No parameter updates. Used only to compare different models or hyperparameter configurations and select the best one.
- ▶ **Testing:** No parameter updates, no model selection. Provides an honest estimate of how the model will perform in the real world.

**Why this matters:** If we use the test set during development (even just to check performance), we risk overfitting to it, leading to overly optimistic performance estimates that don't reflect real-world behavior.



**Figure 7:** The three-way data split and the distinct purpose of each subset.

## 9.2 Error Measurement and Model Evaluation

The availability of true labels in supervised learning enables systematic error measurement—a key advantage that guides both training and evaluation.

### Error Measurement Process

#### During Training:

- ▶ Model makes predictions  $\hat{y}_i$  on training inputs  $x_i$
- ▶ Predictions are compared with true labels  $y_i$  to compute loss:  $\mathcal{L}(\hat{y}_i, y_i)$
- ▶ The loss gradient guides parameter updates to improve predictions

#### During Validation:

- ▶ Model makes predictions on validation data (parameters fixed)
- ▶ Predictions are compared with validation labels to assess generalization
- ▶ Results guide hyperparameter selection and model architecture choices

#### During Testing:

- ▶ Model makes final predictions on test data (parameters fixed)
- ▶ Predictions are compared with test labels for unbiased performance evaluation
- ▶ Results determine if the model is ready for deployment

This error measurement capability is what distinguishes supervised from unsupervised learning and enables the iterative improvement of models.

## 9.3 Evaluation Metrics

Choosing the right metrics is crucial for properly assessing model performance:

#### Classification Metrics:

- ▶ *Accuracy*: Proportion of correct predictions
- ▶ *Precision*: Of predicted positives, how many are actually positive
- ▶ *Recall*: Of actual positives, how many were correctly identified
- ▶ *F1-Score*: Harmonic mean of precision and recall
- ▶ *ROC-AUC*: Area under the receiver operating characteristic curve

#### Regression Metrics:

- ▶ *Mean Squared Error (MSE)*: Average squared difference between predictions and true values
- ▶ *Mean Absolute Error (MAE)*: Average absolute difference
- ▶ *R-squared ( $R^2$ )*: Proportion of variance explained by the model
- ▶ *Root Mean Squared Error (RMSE)*: Square root of MSE, in original units

## 10 Common Challenges in Machine Learning

Building effective ML systems involves navigating a complex landscape of technical and ethical challenges. Understanding these challenges early is crucial for developing robust, responsible

solutions.

1. **Data Quality:** The maxim “garbage in, garbage out” is especially true in ML. Poor data quality manifests as:

- ▶ Missing values that require careful imputation strategies
- ▶ Noisy measurements that obscure true patterns
- ▶ Inconsistent formatting or encoding across sources
- ▶ Duplicate or contradictory entries

*Solution:* Invest significant time in data cleaning, validation, and preprocessing. Quality data is more valuable than quantity.

2. **Overfitting:** The model learns the training data too well, including noise and random fluctuations, resulting in excellent training performance but poor generalization to new data.

- ▶ *Symptoms:* Large gap between training and validation performance
- ▶ *Solutions:* Regularization, cross-validation, early stopping, simpler models, more training data

3. **Underfitting:** The model is too simple to capture the underlying patterns, performing poorly on both training and test data.

- ▶ *Symptoms:* Poor performance across all datasets
- ▶ *Solutions:* More complex models, better features, longer training

4. **Bias and Fairness:** Models trained on biased data can perpetuate or amplify societal biases, leading to discriminatory outcomes in sensitive domains like hiring, lending, or criminal justice.

- ▶ *Challenge:* Historical data often reflects past discrimination
- ▶ *Approaches:* Fairness constraints, bias detection, diverse teams, careful auditing

5. **Interpretability:** Complex models, especially deep neural networks, can act as “black boxes,” making it difficult to understand why they make specific predictions.

- ▶ *Impact:* Critical in healthcare, finance, and legal applications where explanations are required
- ▶ *Trade-off:* Often tension between accuracy and interpretability
- ▶ *Approaches:* Feature importance, attention mechanisms, surrogate models, LIME, SHAP

6. **Scalability:** As datasets grow to millions or billions of examples with thousands of features, computational and memory requirements explode.

- ▶ *Solutions:* Distributed computing, efficient algorithms, model compression, cloud infrastructure

7. **Concept Drift:** The statistical properties of the target variable change over time, causing model performance to degrade.

- ▶ *Example:* A spam detector becomes less effective as spammers adapt their tactics
- ▶ *Solutions:* Continuous monitoring, periodic retraining, online learning

8. **Ethics and Privacy:** ML systems often process sensitive personal data, raising concerns

about:

- ▶ Data privacy and security
- ▶ Consent and transparency
- ▶ Potential for misuse
- ▶ Long-term societal impacts

*Imperative:* Develop AI responsibly with strong ethical guidelines, privacy protection, and stakeholder involvement.

#### The Importance of Domain Expertise

Many of these challenges—particularly data quality, feature engineering, bias detection, and interpretation—require deep domain knowledge. Successful ML projects are collaborations between data scientists and domain experts, not purely technical endeavors.

## 11 Chapter Summary

### Key Takeaway

- ▶ **Core Concept:** ML enables computers to learn from data, defined through Task (T), Experience (E), and Performance (P). It's a subset of AI driving current progress.
- ▶ **Supervised Learning:** Uses labeled data to learn input-output mappings. Classification predicts categories; regression predicts continuous values.
- ▶ **Unsupervised Learning:** Discovers patterns in unlabeled data through clustering (grouping) and dimensionality reduction (simplification).
- ▶ **Semi-Supervised & Reinforcement Learning:** Semi-supervised combines labeled/unlabeled data. Reinforcement learns through trial-and-error with rewards.
- ▶ **Data Splitting:** Three-way split—Training (learn parameters), Validation (select models), Testing (final evaluation).
- ▶ **Error Measurement:** Supervised learning enables systematic improvement by comparing predictions with true labels.
- ▶ **Workflow:** Problem definition → Data collection → Preprocessing → Model training → Evaluation → Deployment → Monitoring.
- ▶ **Key Challenges:** Data quality, overfitting, bias/fairness, interpretability, scalability, and ethical concerns.