

YZM2011

Introduction to Machine Learning

Week 1: Introduction to Machine Learning and Fundamental Concepts

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Course Content

What Will We Learn?

- **Foundations:** ML intro, probability & statistics, linear algebra for ML
- **Supervised learning:** Linear & logistic regression, model evaluation, regularization
- **Decision trees, LDA, Naive Bayes:** Information theory, generative vs discriminative
- **Support vector machines:** Maximum margin, kernels, soft margin
- **Unsupervised & ensembles:** Clustering (K-means, GMM, etc.), PCA, bagging, boosting, random forests
- **Probabilistic models:** Bayesian networks, sampling (MCMC, Gibbs), hidden Markov models

Textbook

Christopher M. Bishop — *Pattern Recognition and Machine Learning*

Additional Resources

- Andrew Ng, CS229 Stanford (<https://www.youtube.com/playlist?list=PLoROMvodv4rMiGQp3WXShMGgzqpfVfbU>)
- Aurelien Geron, Hands-on ML (<https://github.com/ageron/handson-ml3>)

Grading

Assessment

- Project: 30%
- Midterm Exam: 30%
- Final Exam: 40%

Exam Approach

All exams are open-book:

- Internet access allowed
- LLM tools (ChatGPT, Claude, etc.) allowed
- Lecture notes and materials allowed
- **Focus:** Problem-solving ability, not memorization



Course Policies

Lecture Format

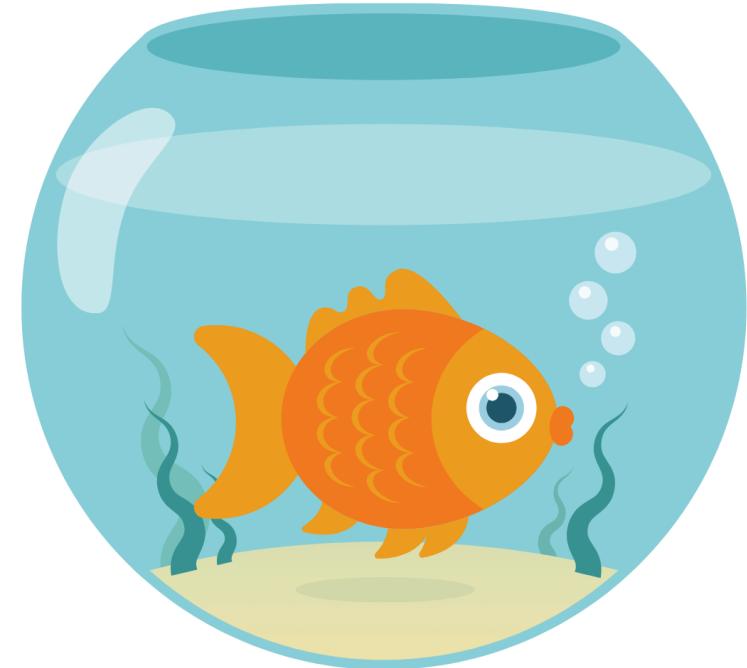
Pomodoro Lectures:

- 20-minute sessions + 5-minute breaks
- During breaks: stretch, chat, check your phone — completely **your choice**
- **Why?** We all have the attention span of a goldfish

Attendance Policy

Not mandatory - You are adults making your own educational decisions

- You can leave if the class doesn't suit you
- No explanation required, no penalty
- You should be here **by choice, not by obligation**



Weekly Schedule

Weeks 1-8: Fundamentals

Week	Topic	Key Concepts
1	Introduction to ML and Fundamental Concepts	Types, terminology, bias–variance
2	Probability Theory and Statistical Foundations	Bayes, distributions, MLE
3	Linear Algebra for Machine Learning	Matrices, eigenvectors, SVD
4	Linear Regression Models	OLS, gradient descent, regularization
5	Logistic Regression and Classification	Sigmoid, cross-entropy, multiclass
6	Model Evaluation and Regularization	Metrics, cross-validation, L1/L2
7	Decision Trees and Information Theory	Entropy, information gain, pruning
8	Midterm Exam	Weeks 1–7 topics

Weekly Schedule

Weeks 9-16: Advanced Topics

Week	Topic	Key Concepts
9	Linear Discriminant Analysis (LDA) and Naive Bayes	Generative vs discriminative
10	Support Vector Machines	Kernel trick, margin, soft margin
11	Clustering Algorithms	K-means, hierarchical, DBSCAN, GMM/EM
12	Dimensionality Reduction	PCA, curse of dimensionality
13	Ensemble Learning Models	Bagging, boosting, random forest
14	Bayesian Networks and Graphical Models	Factorization, d-separation, inference
15	Sampling Methods and Hidden Markov Models	MCMC, Gibbs, forward–backward, Viterbi
16	Final Exam	All topics

What is Machine Learning?

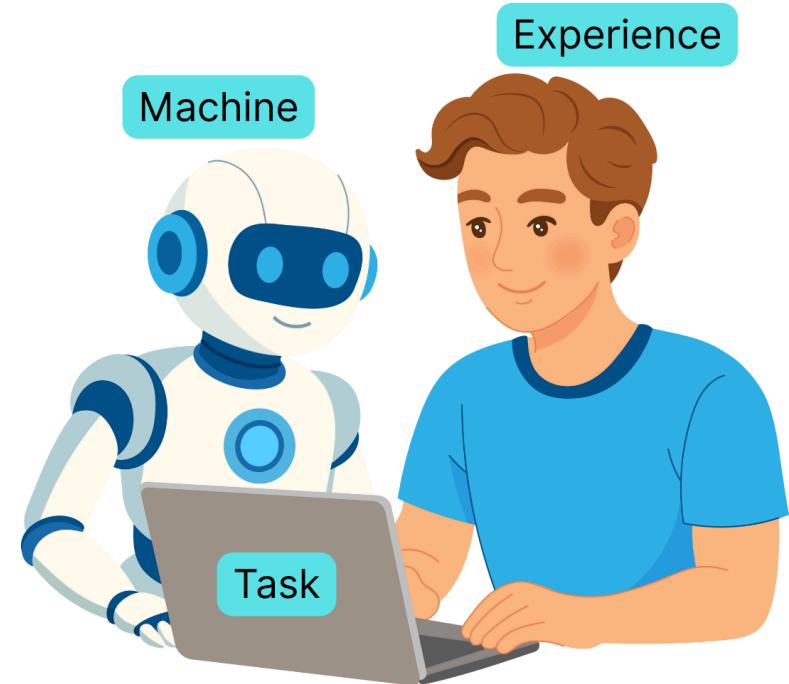
Machine Learning: Formal Definition

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

— Tom Mitchell, 1997

Breaking Down This Definition

Component	Description	Example (Spam Detection)
Task (T)	The task to be performed	Classify emails
Experience (E)	Learning data	Labeled email examples
Performance (P)	Success metric	Accuracy



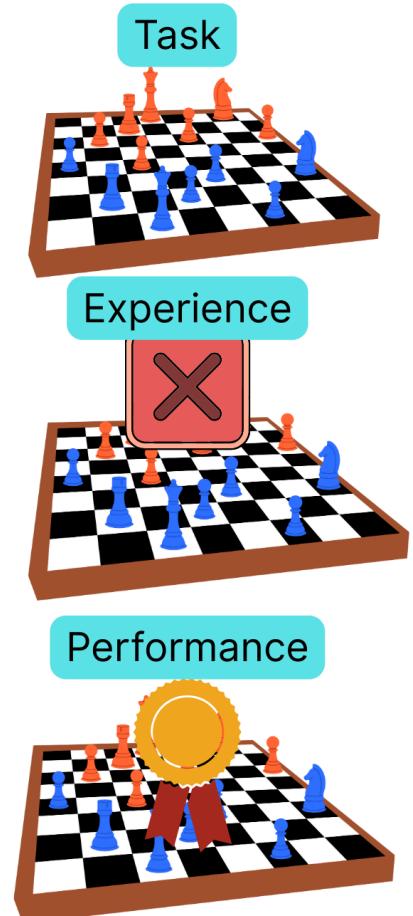
Machine Learning - Example

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

— Tom Mitchell, 1997

Chess Example

Component	Description	Example (Spam Detection)
Task (T)	The task to be performed	Win the chess game
Experience (E)	Learning data	Playing the game over and over again
Performance (P)	Success metric	How many games are won



Machine Learning - Simplified

Traditional Programming

Data + Rules = Output

Example: "If sender is not in the list AND
subject contains 'free' = SPAM"

Machine Learning

Data + Output = Rules (Model)

Example: "Learn spam/ham patterns
from these 10,000 emails"

Why Do We Need Machine Learning?

1. Complex Rules

Writing rules for face recognition:

```
if (eye_distance == X AND  
    nose_angle == Y AND  
    jaw_structure == Z AND  
    ...1000 more rules...)
```

2. Changing Environments

- Spam techniques constantly evolve
- Updating rules is difficult
- ML models can adapt

Why Do We Need Machine Learning?

3. Big Data

- Too much data for human analysis
 - e.g., what is the optimal move in a chess game in a given board ?
- Hard to see patterns
- ML discovers automatically

4. Personalization

- Separate rules for each user?
- ML adapts to each user
- Netflix, Spotify, Temu recommendations

5. Too Many Unknowns

- Stock price prediction
- Weather forecasting
- Traffic flow

ML vs Traditional Programming

Problem: Handwritten Digit Recognition

Traditional Approach

```
def recognize_digit(image):
    if has_closed_loop_top(image):
        if has_closed_loop_bottom(image):
            return 8
        else:
            if has_tail_right(image):
                return 9
            else:
                return 6
    elif is_vertical_line(image):
        return 1
    # ... 100+ more rules
```

ML Approach

```
from sklearn.neural_network import MLPClassifier

# Load data
X, y = load_mnist()

# Create model
model = MLPClassifier()

# Learn!
model.fit(X, y)

# Predict
prediction = model.predict(new_image)
```

Problem: Every handwriting is different, very difficult/impossible to generalize.

Result: 98%+ accuracy (magic black box a.k.a. sklearn)

Practice - ML or Traditional?

Which approach is more suitable for the following problems? Why?

1. Determining if a number is prime
2. Sentiment analysis from customer reviews
3. Playing chess
4. Validating required fields in a form
5. Face recognition from photos

Two Central Problems in ML

What we need to solve

Problem	Question
Estimation	We have noisy data about some quantity. How do we aggregate the data and make reliable estimates or predictions ? How do we predict how well an estimate will do on future data?
Generalization	How do we predict well on situations we have never seen in our training set?

Operational assumption

We **operationalize** generalization by assuming:

- Training data are **i.i.d.** (independent, identically distributed) from some distribution.
- **Test queries** (or future data) are drawn from the **same** distribution.

Without some such assumption, we cannot justify generalizing from **past to future**.

Describing ML Problems and Solutions

Six characteristics - three for the **problem**, three for the **solution**

#	Characteristic	Meaning
1	Problem class	Nature of training data and of queries at test time (e.g. supervised classification, regression)
2	Assumptions	What we assume about the data source or form of the solution (e.g. i.i.d., linear model)
3	Evaluation criteria	How we score individual predictions (loss) and overall performance (risk, test error)
4	Model type	Will we build an intermediate model ? How is it used to predict? (e.g. prediction rule $h(\mathbf{x}; \theta)$)
5	Model class	Which class of models? What criterion to pick one from the class? (e.g. linear, minimize training error)
6	Algorithm	Computational process to fit the model and/or make predictions (e.g. gradient descent, closed-form least squares)

ML Paradigms - Overview

1. Supervised Learning

Learning with a teacher

- Training with labeled data
- Learns input-output relationship
- Classification, regression

2. Unsupervised Learning

Learning without a teacher

- Unlabeled data
- Discovers hidden structures
- Clustering, dimensionality reduction

3. Reinforcement Learning

Learning through trial and error

- Learns through rewards/penalties
- Trial-and-error
- Games, robotics, language

Other Types

- **Semi-supervised:** Few labeled + many unlabeled
- **Self-supervised:** Data generates its own labels
- **Transfer learning:** Reuse experience from related tasks
- **Density estimation:** Estimate $p(\mathbf{x})$ from unlabeled samples
- **Sequence learning:** Map input sequences to output sequences
- **Active learning:** Algorithm chooses which inputs to get labeled

Supervised Learning

Analogy: Student-Teacher

1. Teacher asks a question (Input)
2. Student gives an answer (Prediction)
3. Teacher gives the correct answer (Label)
4. Student learns from their mistake
5. Repeat...

Mathematical Formulation

$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

- \mathcal{X} : input space (e.g. \mathbb{R}^d); each input is a feature vector \mathbf{x}
- \mathcal{Y} : output space (e.g. \mathbb{R} for regression, $\{1, \dots, K\}$ for classification)
- f : unknown target function to be **approximated** from data \mathcal{D}

We do not know f ; we learn an approximation from the labeled pairs in \mathcal{D} , so we can predict y for new inputs \mathbf{x} .

Expert



Habitable



Non-habitable



Supervised Learning

Training Data

$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

Example	Input (X)	Label (Y)
1	[120m ² , 3 rooms, Kadikoy]	2.5M TL
2	[80m ² , 2 rooms, Bagcilar]	1.2M TL
3	[150m ² , 4 rooms, Besiktas]	4.0M TL

Goal

Predict y for new x : we want the model to **generalize**—to perform well on inputs it has not seen during training.

[100m², 3 rooms, Uskudar] \rightarrow ? TL

Supervised Learning - Task Types

Regression

Continuous value prediction

Examples

- House price prediction -> 2,450,000 TL
- Temperature prediction -> 23.5°C
- Sales volume -> 1,234 units
- Stock price -> \$142.50

Algorithms

- Linear Regression
- Polynomial Regression
- Ridge/Lasso Regression
- Random Forest Regressor
- Neural Networks

Classification

Categorical value prediction

Examples

- Email -> Spam / Ham
- Disease -> Present / Absent
- Image -> Cat / Dog / Bird
- Credit -> Approved / Denied

Algorithms

- Logistic Regression
- Decision Trees
- Random Forest Classifier
- SVM
- Neural Networks

Regression in Detail

Problem Definition

Input: Feature vector $\mathbf{x} = [x_1, x_2, \dots, x_n]$

Output: Continuous value $y \in \mathbb{R}$

In **regression**, we predict a numeric value from inputs.

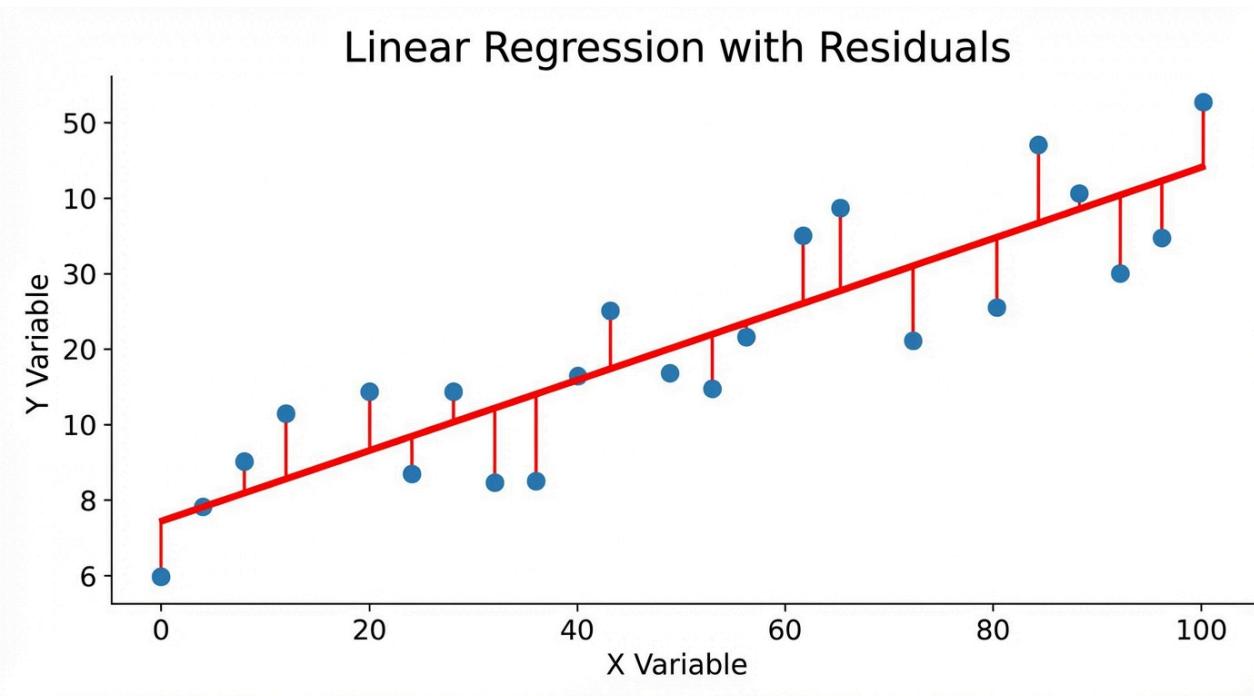
- Each input is described by a set of **features** (the vector \mathbf{x}).
- The goal is to learn a function that maps these features to a real number y
 - e.g., a price, a temperature, or a score.

Simple Linear Regression

$$y = w_0 + w_1 x$$

The simplest form is **one input, one output**: we fit a straight line.

- Here w_0 is the **intercept** (value when $x = 0$) and w_1 is the **slope** (how much y changes per unit change in x).
- Learning the model means estimating w_0 and w_1 from data so the line best fits the observed points.



Regression in Detail

Example - House Price

$m^2 (x)$	Price TL (y)
100	1,500,000
120	1,800,000
150	2,200,000

Model

$$Price = 100,000 + 15,000 \times m^2$$

Here the **intercept** is 100,000 TL (base price) and the **slope** is 15,000 TL per m^2 : each extra square meter adds 15,000 TL to the predicted price.

Prediction:

- $110 m^2 \rightarrow 1,750,000$ TL
- $130 m^2 \rightarrow 2,050,000$ TL



Christian Keil
@pronounced_kyle

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⋮

My 3-month-old son is now TWICE as big as when he was born.

He's on track to weigh 7.5 trillion pounds by age 10



9:41 AM · 16 Mar 24 · 279K Views

Practice - Simple Regression

Find the linear regression model for the following data:

Study Hours (x)	Exam Score (y)
1	50
2	60
3	70
4	80

Questions:

1. Estimate the values of w_0 and w_1 in the formula $y = w_0 + w_1x$
2. What is the predicted score for a student who studies 5 hours?
3. Is this model realistic? What are its limitations?

Classification in Detail

Problem Definition

Input: Feature vector \mathbf{x}

Output: Class label $y \in \{C_1, C_2, \dots, C_k\}$

In **classification**, we predict a **category** (class label) from inputs. Each input is again described by features \mathbf{x} . The output y is one of k possible classes. The model learns a decision boundary (or score per class) so we can assign new inputs to the most likely category.

Classification in Detail

Binary Classification

Two classes: e.g. Positive / Negative. The model often outputs a probability for one class; we then apply a threshold (e.g. 0.5) to get a final label.

Examples:

- Spam / Ham
- Sick / Healthy
- Pass / Fail

Output:

- Probability: $P(y = 1|x) = 0.87$
- Decision: "Spam" (threshold > 0.5)

Multiclass Classification

More than two classes. The model typically outputs a probability (or score) for each class; we predict the class with the highest probability or score.

Examples:

- Digit recognition: 0, 1, 2, ..., 9
- Sentiment analysis: Positive, Negative, Neutral
- Image: Cat, Dog, Bird, Fish

Output:

$$\begin{aligned} P(\text{Cat}) &= 0.75 \\ P(\text{Dog}) &= 0.20 \\ P(\text{Bird}) &= 0.05 \end{aligned}$$

Prediction: Cat

Classification Example: Spam Detection

Features

Feature	Description	Example Value
word_count	Number of words	45
has_free	Contains "free" word	1 (yes)
exclamation_count	Number of exclamation marks	5
link_count	Number of links	3
capital_ratio	Ratio of capital letters	0.35
sender_known	Is sender known	0 (no)

Model Decision

```
features = [45, 1, 5, 3, 0.35, 0]
probability = model.predict_proba(features) # [0.15, 0.85]
prediction = "SPAM" if probability[1] > 0.5 else "HAM"
# → SPAM (85% confidence)
```

Unsupervised Learning

Analogy: Exploration

1. We have data but **no labels** (no teacher to correct us)
2. We ask: "What structure is in this data?"
3. The system discovers groups, patterns, or a compact representation on its own
4. No right or wrong answer, we **explore** rather than predict a target

Mathematical Formulation

$$\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}, \quad \mathbf{x}_i \in \mathcal{X}$$

- \mathcal{X} : input space (e.g. \mathbb{R}^d); each \mathbf{x}_i is a feature vector
- **No labels** y_i , we do not have a target to predict
- **Goal:** Find hidden structure: groups (clustering), low-dimensional representation (dimensionality reduction), or anomalies

We learn from the **distribution** or **geometry** of the data alone, without a performance signal tied to correct labels.

Student



Unsupervised Learning

Data

x_1, x_2, \dots, x_n (no labels y_i)

Goal

Discover **structure** in the data—e.g. group similar customers, reduce 1000 features to 2 for visualization, or flag outliers—without using any target variable.

[120, 8, 2] → Cluster 2 (e.g. "Frequent buyers")
[1000 features] → [2 components] for plotting

Two Main Categories

1. **Clustering:** Assign data points to groups so that similar points are together and different groups are separated; no predefined labels.
2. **Dimensionality Reduction:** Represent data with fewer features while preserving as much structure as possible (e.g. for visualization or efficiency).

Clustering

Group Similar Examples

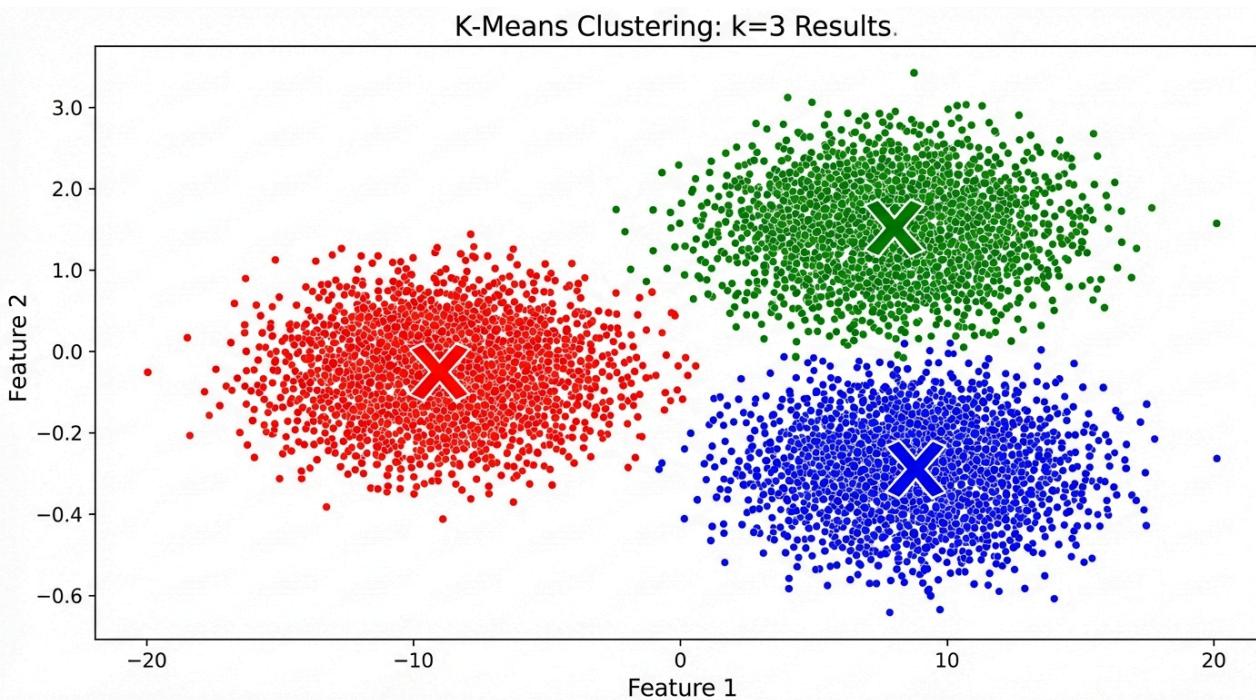
K-Means Algorithm

Idea: Partition the data into K groups by iteratively assigning each point to the nearest cluster center and then setting each center to the mean of its assigned points.

1. Choose K centers
2. Assign each point to nearest center
3. Update centers (average)
4. Repeat (stop if no change)

Use Cases

- Customer segmentation
- Image compression
- Anomaly detection
- Gene expression analysis



Clustering

Example: Customer Segmentation

Customer	Spending	Visits
A	High	Frequent
B	Low	Rare
C	High	Frequent
D	Medium	Occasional

Segment 1: VIP Customers

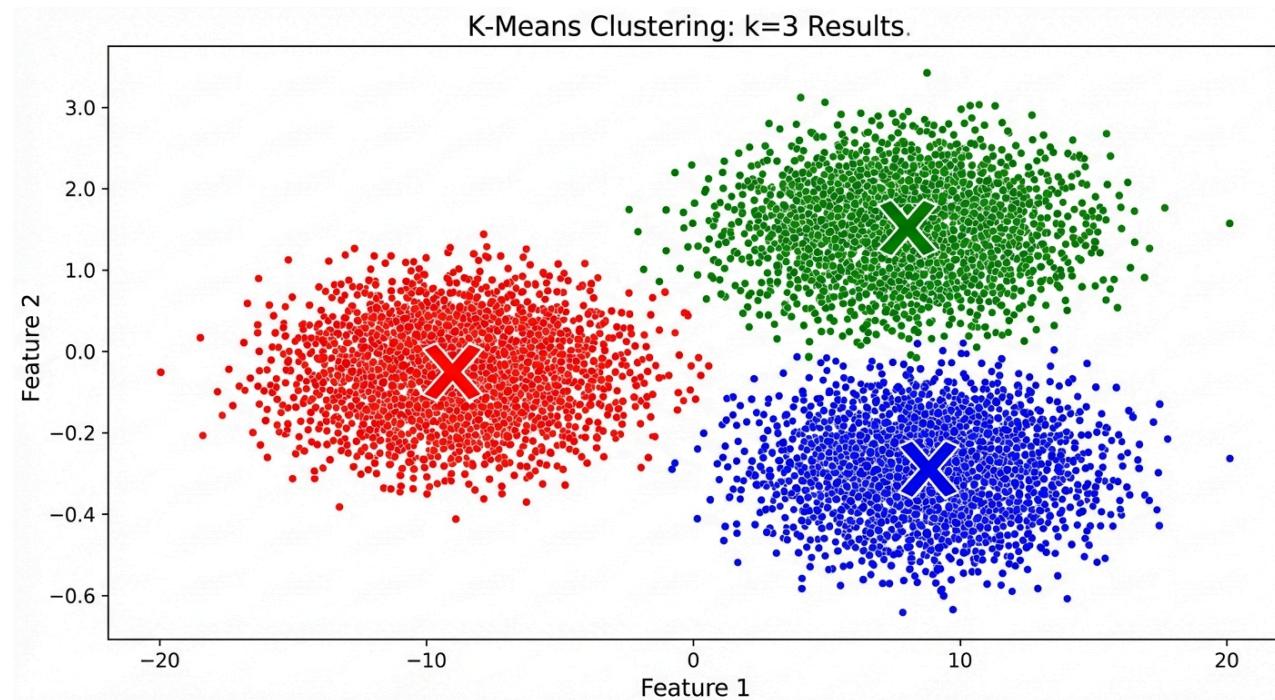
- High spending, frequent visits

Segment 2: Occasional Customers

- Medium spending, occasional

Segment 3: Passive Customers

- Low spending, rare



Curse of Dimensionality

Why High-Dimensional Spaces Are Tricky

Volume in a Thin Shell

In D dimensions, fraction of unit sphere volume between $r = 1 - \varepsilon$ and $r = 1$:

$$1 - (1 - \varepsilon)^D \rightarrow 1 \quad \text{as } D \rightarrow \infty$$

- For large D , almost all volume is in a **thin shell** near the surface
- In 100D, ~99.99% of volume is in the outer 5% shell

Implications

- Grid-based methods: number of cells grows **exponentially** with D
- "Nearest" neighbors in high-D can be far in absolute terms
- Need much more data to fill the space

Why ML Still Works

1. **Manifold hypothesis:** Real data often lies on lower-dimensional manifolds
2. **Smoothness:** Small change in input \rightarrow small change in output; we don't need to sample every cell

Gaussian in High-D (PRML Fig. 1.23)

- Most probability mass is in a shell at radius $\approx \sqrt{D} \sigma$, not at the mode
- Counterintuitive; matters for sampling (Week 15)

Dimensionality Reduction

Compress Data, Preserve Essence

Problem

With many features, data becomes sparse, computation is costly, and we cannot visualize. **Dimensionality reduction** finds a lower-dimensional representation that preserves the most important structure (and helps with the curse of dimensionality).

- Data with 1000 features
- Hard to visualize
- Slow computation
- **Curse of dimensionality**

Example: Face Recognition

Original: $64 \times 64 = 4096$ pixels

After PCA: 100 components

95% of information preserved!

Use Cases

- Visualization (reduce to 2D/3D)
- Noise reduction
- Feature extraction
- Data compression

Dimensionality Reduction

PCA (Principal Component Analysis)

Idea: Find new axes (principal components) such that projecting the data onto them preserves as much variance as possible. We keep the top few components and drop the rest, so we reduce dimensions while keeping the main structure.

- Find directions that explain most variance
- Reduce dimensions but preserve information

Why unsupervised? We use **only the inputs $\mathbf{x}_1, \dots, \mathbf{x}_n$** —no labels or target variable. PCA discovers structure (directions of maximum variance) from the **geometry of the data alone**, without any "correct" output to predict. That is exactly the unsupervised setting: learn from $\mathcal{D} = \{\mathbf{x}_i\}$ with no teacher.

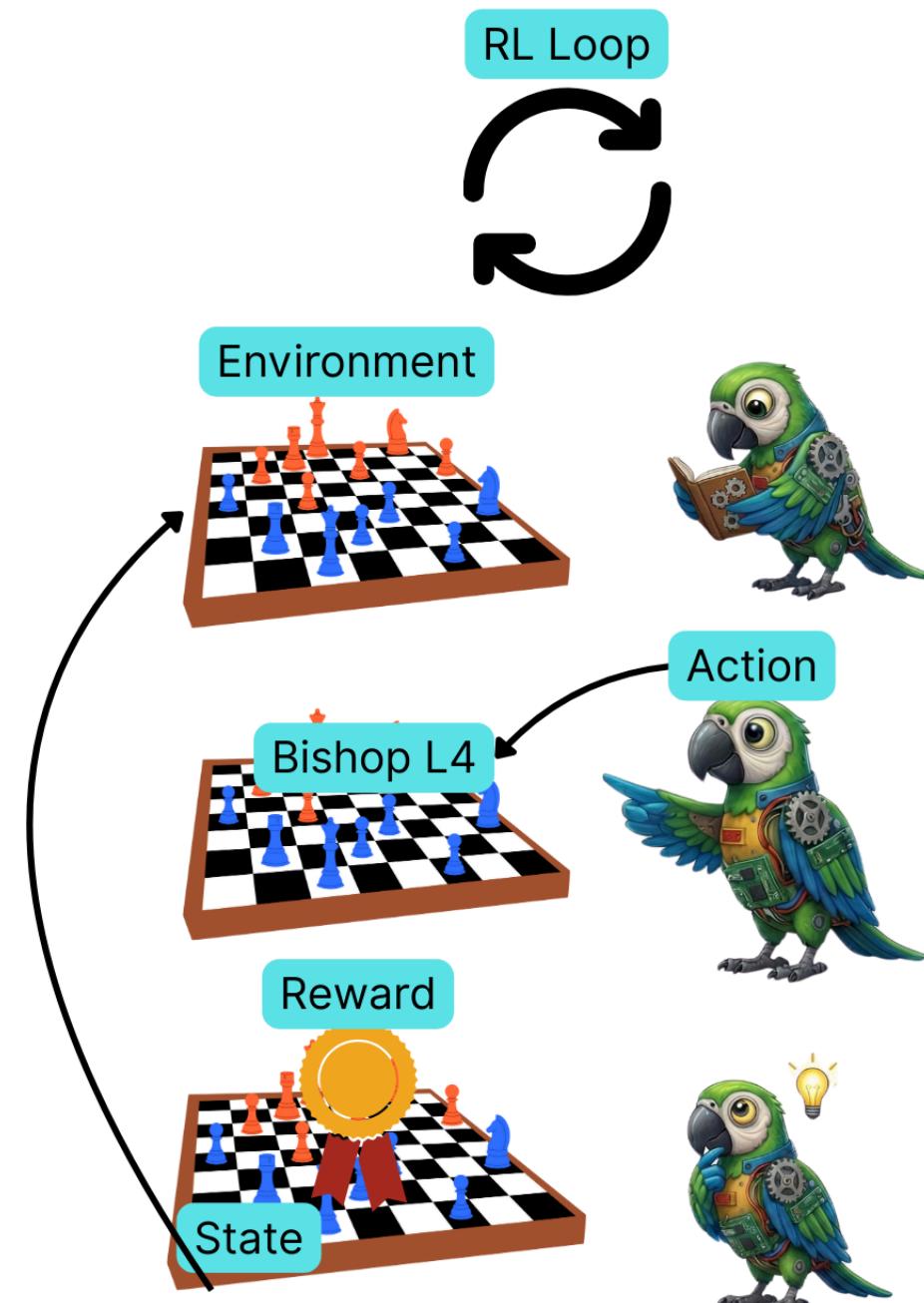
Reinforcement Learning

Learning by Trial and Error

Basic Components

The **agent** interacts with the **environment**: it observes the current **state**, chooses an **action**, and receives a **reward** (or penalty). The **policy** is the rule that maps states to actions; the goal is to learn a policy that maximizes cumulative reward over time.

Component	Description
Agent	Decision-making system
Environment	External world
State	Current situation
Action	Possible actions
Reward	Reward/penalty
Policy	Decision strategy



Reinforcement Learning

Analogy: Dog Training

1. Dog sit (action)
2. Sits -> Reward (reward +1)
3. Doesn't sit -> No reward (reward 0)
4. Dog learns to sit

Examples

- **Games:** AlphaGo, Atari, Chess
- **Robotics:** Walking, grasping
- **Autonomous vehicles:** Driving
- **Recommendation systems:** Which content?
- **Resource management:** Energy, traffic

RL Example - Playing Pac-Man

State

- Pac-Man position
- Ghost positions
- Pellet positions
- Remaining time

Actions

- Up
- Down
- Left
- Right

Rewards

Situation	Reward
Eat pellet	+10
Eat ghost	+200
Caught by ghost	-500
Take a step	-1
Game over (won)	+1000

Policy (Strategy)

Initially: Random movement

Later: "Run from ghosts, go to pellets"

RL vs Supervised vs Unsupervised

Comparison Table

Feature	Supervised	Unsupervised	Reinforcement
Data	Labeled	Unlabeled	Reward signal
Goal	Input->Output	Structure discovery	Maximize cumulative reward
Feedback	Instant (each example)	None	Delayed
Example	Spam detection	Clustering	Game playing
Challenge	Labeling cost	Hard to evaluate	Reward design

When to Use Which?

- **Supervised:** Labeled data available, clear goal
- **Unsupervised:** Data available but structure unknown
- **Reinforcement:** Sequential decisions, experimentation possible

Practice - Scenario Matching

Determine the most suitable ML type for each scenario:

#	Scenario	Type
1	Group customers by shopping habits	?
2	Determine if an email is spam	?
3	Robot learning to navigate a room	?
4	Predict house price	?
5	Visualize big data in 2D	?
6	Learn to play chess	?

Options:

Supervised (Classification / Regression), Unsupervised (Clustering / Dim. Reduction), Reinforcement

Data Terms

Basic Terms (Formal)

Term	Notation / Definition
Sample	One pair (\mathbf{x}_i, y_i) or just \mathbf{x}_i (unsupervised)
Feature	Component $x_{i,j}$ of \mathbf{x}_i ; input dimension = d
Feature vector	$\mathbf{x}_i \in \mathcal{X} \subseteq \mathbb{R}^d$
Label	$y_i \in \mathcal{Y}$ (target for sample i)
Dataset	$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$; size N

Example: House Dataset

$N = 2$ samples, $d = 4$ features (after encoding district):

Sample 1: $\mathbf{x}_1 = [120, 3, 5, \text{Kadikoy}]^T, y_1 = 2\,500\,000$

Sample 2: $\mathbf{x}_2 = [80, 2, 3, \text{Bagcilar}]^T, y_2 = 1\,200\,000$

Design matrix (numerical part):

$$\mathbf{X} = \begin{bmatrix} 120 & 3 & 5 \\ 80 & 2 & 3 \end{bmatrix}$$

Synonyms

- Sample = instance, example, data point, observation
- Feature = attribute, variable, covariate, dimension
- Label = target, output, response, dependent variable

Feature Types

Numerical (quantitative)

Type	Mathematical view	Examples
Continuous	$x_j \in \mathbb{R}$ (or an interval)	Temperature, price, distance
Discrete / count	$x_j \in \mathbb{Z}_{\geq 0}$ (or finite subset)	Number of rooms, age in years, count of events

Categorical (qualitative)

Type	Mathematical view	Examples
Nominal	$x_j \in \{c_1, c_2, \dots, c_K\}$, no order	Color, city, ID
Ordinal	Same set but with order $c_1 \prec c_2 \prec \dots$	Education level, size (S/M/L), rating

Many algorithms expect **numerical** inputs; categorical features are encoded

Feature Transformations

Why Transform?

Most ML algorithms expect **numerical** inputs - a feature vector $\mathbf{x} \in \mathbb{R}^d$

- Categorical values (e.g. city, color) must be turned into numbers in a way that does not introduce **false order**.
- For numerical features, **scale** matters
 - Distance-based methods (e.g. K-NN) and gradient-based optimization are sensitive to the range of each feature; putting all features on a comparable scale often speeds training and improves results.

One-Hot Encoding

For **nominal** categories (no natural order), we represent each category c_k as a **binary vector** $\mathbf{e}_k \in \{0, 1\}^K$ with a 1 in position k and 0 elsewhere.

- This avoids implying that one category is *larger* than another. With K categories we get K binary features; only one is 1 per sample.
- **Example:** Districts Kadıköy, Başakşehir, Esenler \rightarrow Kadıkoy $\mapsto [1, 0, 0]$, Başakşehir $\mapsto [0, 1, 0]$, Esenler $\mapsto [0, 0, 1]$.

Feature Transformations

Label Encoding

For **ordinal** categories (order is meaningful), we assign consecutive integers: $c_1 \mapsto 0, c_2 \mapsto 1$, and so on.

- We only use this only when the order is real (e.g. education level, size S/M/L)
- For purely nominal categories, one-hot encoding is safer so the model does not treat **category 2** as **twice category 1**.

Normalization

We rescale numerical features so they lie in a common range or have similar spread. Two common choices:

- **Min-max:** $x' = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \in [0, 1]$ – map the feature to $[0, 1]$ using the observed min and max. Simple but sensitive to outliers.
- **Z-score:** $x' = \frac{x - \mu}{\sigma}$ – subtract the mean μ and divide by the standard deviation σ , so the transformed feature has mean 0 and variance 1. Works well when features are roughly symmetric.

Hypothesis, Loss, and Risk

Hypothesis and Hypothesis Space

- **Hypothesis h** : a candidate function $h : \mathcal{X} \rightarrow \mathcal{Y}$ (e.g. a specific linear model).
- **Hypothesis space \mathcal{H}** : set of all candidate models we consider (e.g. all linear functions).
- **Parameterized hypothesis h_θ** : hypothesis determined by parameter vector θ ; then $\mathcal{H} = \{h_\theta : \theta \in \Theta\}$.

Learning algorithm

A **learning algorithm** is a **procedure** that takes a dataset \mathcal{D} and (optionally) a hypothesis class \mathcal{H} , and **outputs** a hypothesis $h \in \mathcal{H}$:

$$\mathcal{D} \longrightarrow \text{learning algorithm}(\mathcal{H}) \longrightarrow h$$

Restricting the **size or expressiveness** of \mathcal{H} is one way to improve generalization.

Loss and Risk

- **Loss $\ell(\hat{y}, y)$** : cost of predicting \hat{y} when true value is y .
- **Empirical risk** (training error): $\widehat{R}(\theta) = \frac{1}{N} \sum_{i=1}^N \ell(h_\theta(\mathbf{x}_i), y_i)$.
- **Training** = choose θ to minimize $\widehat{R}(\theta)$ (possibly with a regularizer).

Common Loss Functions

Classification

Loss	Formula	Use
0–1 loss	$\ell(g, a) = 1 \text{ if } g \neq a, \text{ else } 0$	Training/test error rate = average 0–1 loss; simple but not smooth (difficult to optimize for linear classifiers)
Asymmetric loss	Different cost for "predict + when –" vs "predict – when +" (e.g. medical: miss disease = 10, false alarm = 1)	When errors have different consequences; decision threshold $\neq 0.5$

Regression

Loss	Formula
Squared loss	$\ell(g, a) = (g - a)^2$
Absolute loss	$\ell(g, a) = g - a $

Risk = expected loss (over data distribution). We usually **minimize** (empirical or expected) risk.

Model Terms

Model = Parameterized Hypothesis

A model is a function from inputs to outputs, determined by parameters θ :

$$h_\theta : \mathcal{X} \rightarrow \mathcal{Y}, \quad \hat{y} = h_\theta(\mathbf{x})$$

- **Parameters** θ : learned from data (e.g. weights \mathbf{w} , bias w_0).
- **Hyperparameters**: chosen before training (e.g. learning rate η , regularization λ , model complexity). **Not** optimized by the same training procedure.

Training vs Inference

- **Training (learning)**: find $\theta^* = \arg \min_{\theta} \widehat{R}(\theta)$ (plus optional regularization). Here $\arg \min$ = the value of θ that minimizes the expression.
- **Inference (prediction)**: for new \mathbf{x} , output $\hat{y} = h_{\theta^*}(\mathbf{x})$.

Example: Linear Regression

$$h_\theta(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2, \quad \theta = (w_0, w_1, w_2)^T$$

Parameters (learned): w_0, w_1, w_2 (e.g. 500000, 15000, 50000).

Hyperparameters (user-set): learning rate, max iterations, regularization λ .

Loss (squared error): $\ell(\hat{y}, y) = (\hat{y} - y)^2$

Empirical risk: $\widehat{R}(\theta) = \frac{1}{N} \sum_{i=1}^N (h_\theta(\mathbf{x}_i) - y_i)^2$.

Model Class vs Model Fitting

Two levels of choice

Concept	Meaning	Example
Model class \mathcal{M} (or \mathcal{H})	Set of possible models (e.g. "all linear functions", "all polynomials of degree $\leq M$ ")	Linear regression: $h(\mathbf{x}; \boldsymbol{\theta}, \theta_0) = \boldsymbol{\theta}^T \mathbf{x} + \theta_0$
Model fitting	Given a class, pick one model — i.e. choose parameters Θ (e.g. $\boldsymbol{\theta}, \theta_0$) by minimizing training error or regularized loss	Find $\boldsymbol{\theta}^*, \theta_0^*$ that minimize $\hat{R}(\boldsymbol{\theta})$
Model selection	Choosing the model class (or hyperparameters like M, λ) from several candidates; often via validation or cross-validation	Pick $M = 3$ vs $M = 9$ for polynomial

Prediction rule

Typical flow: (1) **Fit** a model to training data (choose Θ). (2) **Fix** Θ and use $h(\mathbf{x}; \Theta)$ to predict for new \mathbf{x} .

Parametric models: fixed, finite number of parameters (e.g. linear, logistic). **Non-parametric** models: complexity can grow with data (e.g. nearest neighbors, some Bayesian models).

Generalization, Capacity, and Errors

Generalization vs training

We care about how the model performs on **new** data, not just on the data we used to train. The following terms make that precise:

Term	Definition
Training error	Empirical risk $\widehat{R}(\theta)$ on $\mathcal{D}_{\text{train}}$ — what we minimize
Test error	Error on $\mathcal{D}_{\text{test}}$ — unseen data; what we care about
Generalization error	Expected risk $R(\theta) = \mathbb{E}_{(\mathbf{x},y)}[\ell(h_\theta(\mathbf{x}), y)]$ — average loss on the true data distribution (Week 2)
Generalization gap	Test error — training error; large gap \Rightarrow overfitting

A model that fits the training set well but does poorly on the test set has **failed to generalize**; a large generalization gap is a sign of overfitting.

Generalization, Capacity, and Errors

Model capacity and irreducible error

Capacity (or model complexity) is how rich the hypothesis space \mathcal{H} is.

- For example, the degree M of a polynomial. More capacity lets the model fit more patterns in the data, but it also increases the risk of fitting noise (overfitting).
- We try to match capacity to the amount and quality of data we have.

Irreducible error (Bayes error) is the part of the loss that no model can remove

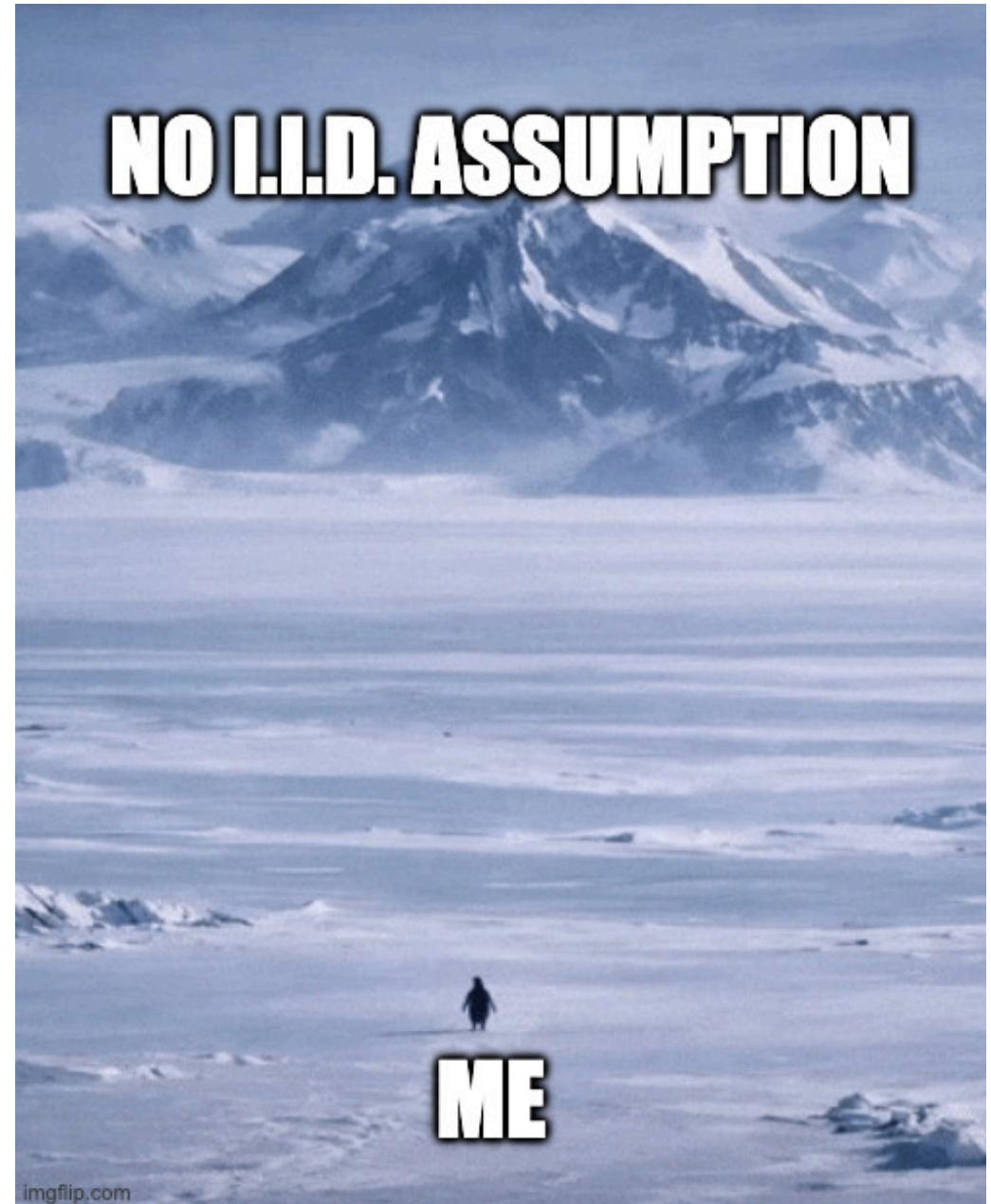
- It comes from noise in the data or from unobserved factors.
- In regression it is $\mathbb{E}[\text{var}[y \mid \mathbf{x}]]$
- In classification it is $1 - \max_k P(C_k \mid \mathbf{x})$.
- Our goal is to get as close as possible to this limit, not to beat it.

Data Assumptions and Pitfalls

Standard assumption: i.i.d.

Most theory and practice assumes that training pairs (\mathbf{x}_i, y_i) are **independent and identically distributed** (i.i.d.) draws from a fixed (unknown) joint distribution $p(\mathbf{x}, y)$.

- **Independent** means that one sample does not depend on another
- **Identically distributed** means that every sample comes from the same $p(\mathbf{x}, y)$
 - The distribution that generates the test set should be the same as the one that generated the training set.
 - When this fails standard guarantees no longer hold and we need different methods (e.g. temporal splits, domain adaptation).



imgflip.com

Data Assumptions and Pitfalls

Data leakage

Data leakage occurs when information from the **test** set influences **training** or model choice.

- The model then appears to perform better than it really will on genuinely new data.
- Common examples: normalizing features using the mean or variance of the **whole** dataset (including test), or selecting features or hyperparameters using test labels.
- The **golden rule** is that any statistic used in preprocessing or model selection must be computed only from **training** (or validation) data
- The test set must be used only once, for a final performance estimate.

Training / Validation / Test Sets

Problem: Overfitting

If we evaluate the model only on the data it was trained on, we cannot tell whether it has **generalized** or simply **memorized**.

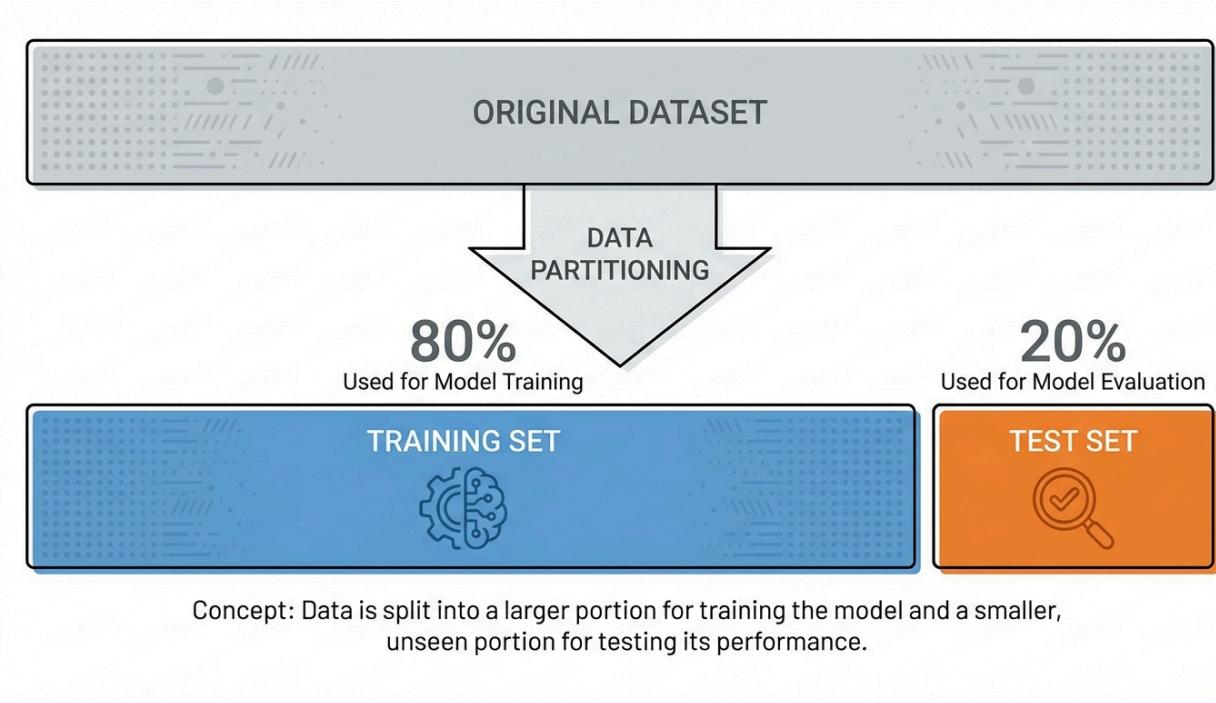
- A model that gets 99% accuracy on the training set but only 60% on new data has overfit; we would never see that if we did not hold out some data.

Solution: Separate Test Set

We split the dataset and evaluate on data the model has **never seen** during training. Typically we use three disjoint sets:

$$\mathcal{D} = \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}} \cup \mathcal{D}_{\text{test}}$$

Example: 10,000 samples -> Train: 8,000 (80%), Validation: 1,000 (10%), Test: 1,000 (10%).



Training / Validation / Test Sets

Purpose of Each Set

Set	Notation	Purpose
Training	$\mathcal{D}_{\text{train}}$	Learn θ (minimize \hat{R} on this set)
Validation	\mathcal{D}_{val}	Choose hyperparameters, model selection
Test	$\mathcal{D}_{\text{test}}$	Final performance estimate — use only once

We **fit** the model on the training set. We use the **validation** set to choose hyperparameters (e.g. λ , model complexity) or to pick among models. The **test** set is reserved for a single, final estimate of performance; once you use it to make decisions, it is no longer an unbiased estimate.



Important Rule

Never look at the test set (or tune on it) during training or model selection.

Once you do, you can no longer interpret test performance as an honest estimate of how the model will do on new data.

Cross-Validation

K-Fold Cross-Validation

When data is limited, we want a **reliable estimate** of how a learning procedure will perform without burning a separate test set.

- In **K-fold cross-validation** we split the data into K parts (folds) D_1, \dots, D_K .
- For each $i = 1, \dots, K$, we train on all folds except D_i and compute the error E_i on the withheld fold D_i .
- We then report the **average** $\frac{1}{K} \sum_{i=1}^K E_i$ (and optionally the standard deviation). Every sample is used for testing exactly once, so we get a stable estimate of performance.

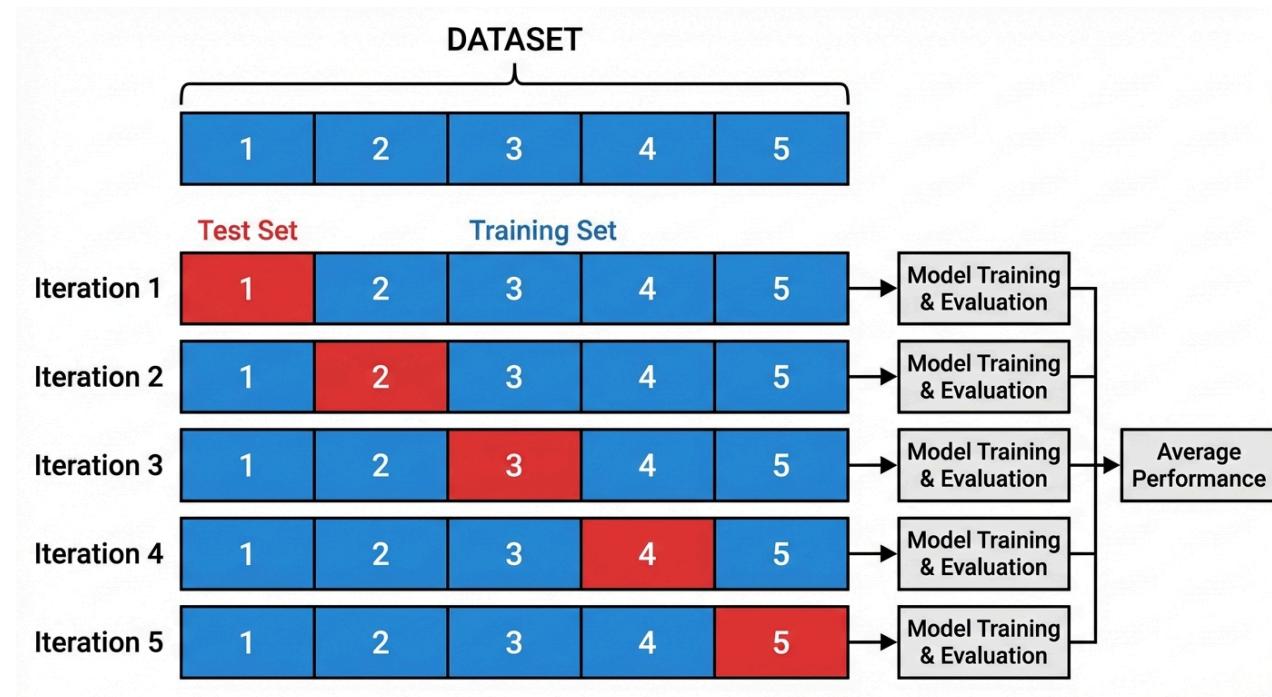


Cross-Validation

What does CV evaluate?

Cross-validation **does not** produce a single hypothesis h for deployment; it **evaluates the learning algorithm**

- How well that *procedure* tends to do when we train on one chunk and test on another.
- Variability in the reported performance can come from which examples were in each fold and from any **randomization inside the algorithm** (e.g. random initialization)
- K-fold (or repeating train–test multiple times) helps average out that variability.



Cross-Validation

Advantages

We use **all** data for both training and testing (in different folds), so the estimate is more reliable than a single train–test split, and we can report variance (e.g. 0.85 ± 0.015) to see how stable the procedure is.

Training error alone is **not** a good guide to generalization; we use **held-out data** (validation or cross-validation) to choose among models.



Evaluation Metrics — Regression

Measuring prediction error on continuous y

For regression we predict a continuous y ; we need a single number that summarizes how wrong we are on average. The **residual** for sample i is $e_i = y_i - \hat{y}_i$. Common metrics:

Metric	Formula	Interpretation
MSE	$\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$	Mean squared error; penalizes large errors more
RMSE	$\sqrt{\text{MSE}}$	Same units as y ; easier to interpret
MAE	$\frac{1}{N} \sum_{i=1}^N y_i - \hat{y}_i $	Mean absolute error; robust to outliers
R^2	$1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$	Fraction of variance explained; 1 = perfect, 0 = no better than mean

MSE is the standard loss for linear regression; RMSE is in the same units as y . MAE is less sensitive to outliers. R^2 tells us what fraction of the variance in y the model explains. We often assume residuals are i.i.d. (e.g. Gaussian) when deriving estimators (Week 4).

Evaluation Metrics — Classification

Confusion matrix

For binary classification we count how many predictions fall into each of four cells. The **confusion matrix** summarizes this:

	Predicted +	Predicted -
Actual +	TP (true positive)	FN (false negative)
Actual -	FP (false positive)	TN (true negative)

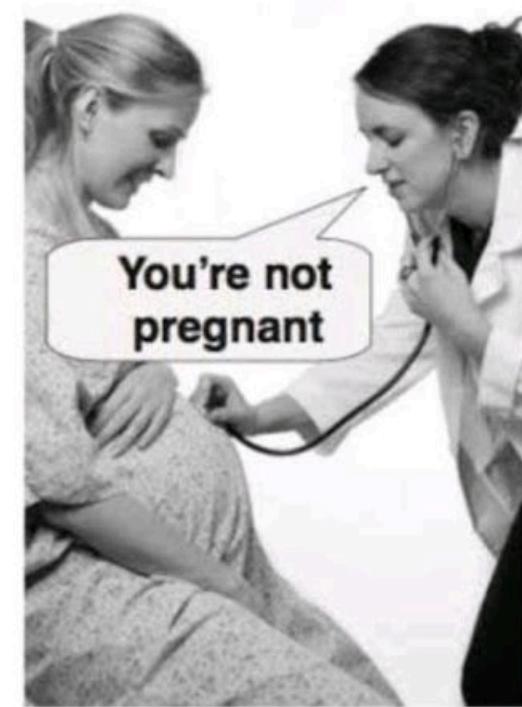
From these we define metrics that answer different questions:

- Overall correctness (accuracy)
- Correctness among positive predictions (precision)
- Coverage of actual positives (recall)
- Balance between precision and recall (F1).

Type I error
(false positive)



Type II error
(false negative)



Evaluation Metrics — Classification

Derived metrics

Metric	Formula	Meaning
Accuracy	$\frac{TP+TN}{N}$	Fraction correct (misleading if classes imbalanced)
Precision	$\frac{TP}{TP+FP}$	Of predicted +, how many are actually +
Recall (sensitivity)	$\frac{TP}{TP+FN}$	Of actual +, how many we found
Specificity	$\frac{TN}{TN+FP}$	Of actual -, how many we correctly rejected
F1 score	$2 \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$	Harmonic mean of precision and recall

Decision threshold: Many classifiers output a probability

- We assign class + when $P(+ | \mathbf{x}) > \tau$ (e.g. $\tau = 0.5$).
- Raising τ typically increases precision and lowers recall; lowering τ does the opposite
- We choose τ based on the cost of false positives vs false negatives.

Overfitting vs Underfitting

Underfitting (High Bias)

Problem: Model is too simple. It does not have enough capacity to capture the true relationship in the data.

- Couldn't even learn training data
- Both train and test error high

Symptoms:

- Training accuracy low
- Test accuracy low

Solutions:

- More complex model
- More features
- Longer training

Overfitting (High Variance)

Problem: Model is too complex. It fits the training data (including noise) so closely that it fails on new data.

- Memorized training data
- Can't generalize to new data

Symptoms:

- Training accuracy very high
- Test accuracy low

Solutions:

- Simpler model
- More data
- Regularization
- Dropout, Early stopping

Polynomial Curve Fitting

We fit a **polynomial** of order M to N noisy points drawn from $t = \sin(2\pi x) + \text{noise}$ (e.g. $N = 10$). Changing M will illustrate underfitting (M too low) and overfitting (M too high).

Data: N points generated from $t = \sin(2\pi x) + \text{noise}$ (e.g. $N = 10$)

Model

$$y(x, \mathbf{w}) = w_0 + w_1x + w_2x^2 + \cdots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

We predict y as a **polynomial in x** of order M , with weights \mathbf{w} . The model is **linear in \mathbf{w}** (so we can optimize easily) even though it is nonlinear in x . Higher M means more flexibility (and risk of overfitting).

- **Linear in \mathbf{w}** (linear model) even though nonlinear in x
- M = polynomial order (model complexity)

Polynomial Curve Fitting

Error Function

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{y(x_n, \mathbf{w}) - t_n\}^2$$
$$E_{\text{RMS}} = \sqrt{2E(\mathbf{w}^*)/N}$$

We fit \mathbf{w} by **minimizing** the sum of squared differences between predictions $y(x_n, \mathbf{w})$ and targets t_n . E_{RMS} is the root-mean-square error at the optimum, so we can compare across different dataset sizes N .

- Sum-of-squares; E_{RMS} comparable across different N

Overfitting Visualization

$N = 10$ training points, polynomial of order M .

- As M grows, the model fits the data more closely, **but** past a point it fits **noise** instead of the true curve.

$M = 0$ (constant)

- Underfitting and cannot capture the curve

$M = 1$ (linear)

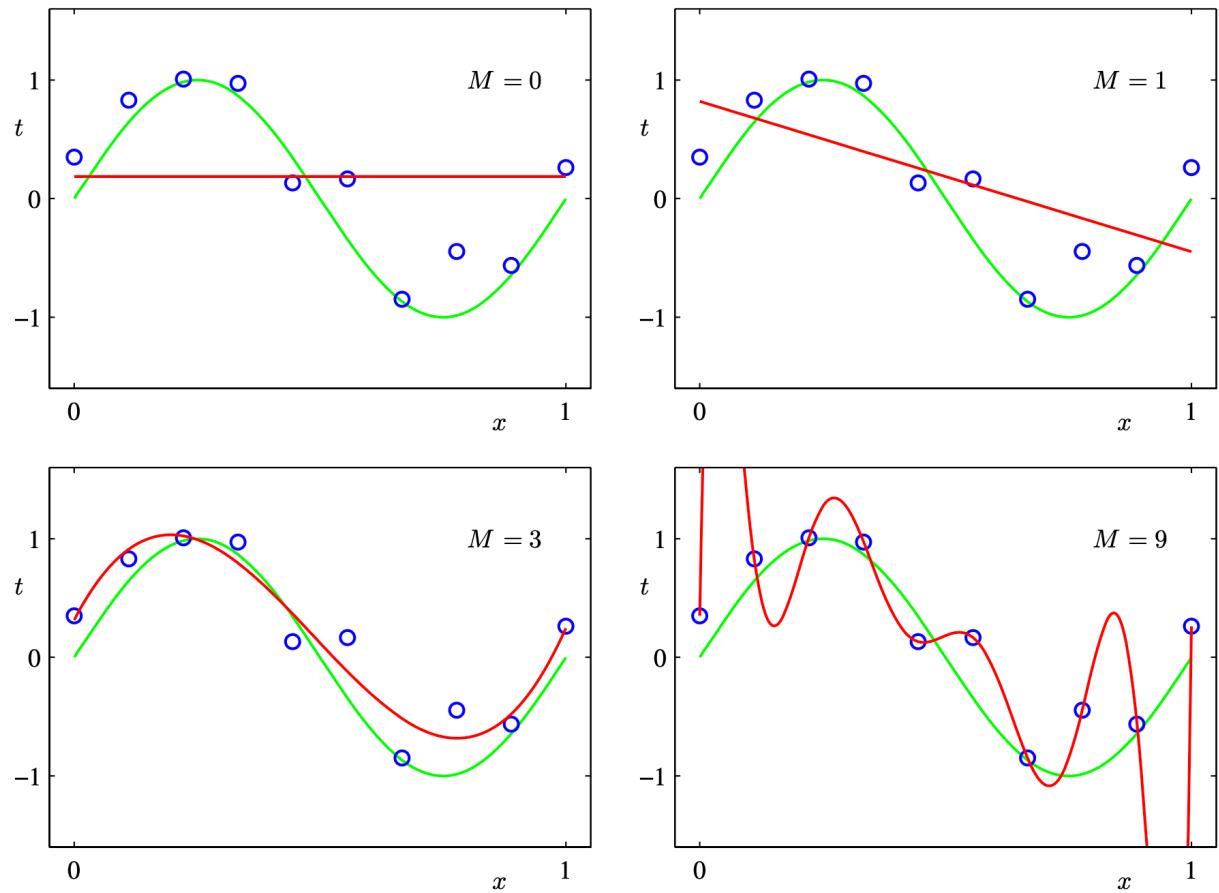
- Still underfitting

$M = 3$

- Good fit**, captures signal, not noise

$M = 9$

- Overfitting** passes through every point
- Huge oscillations between points
- Memorized the noise**



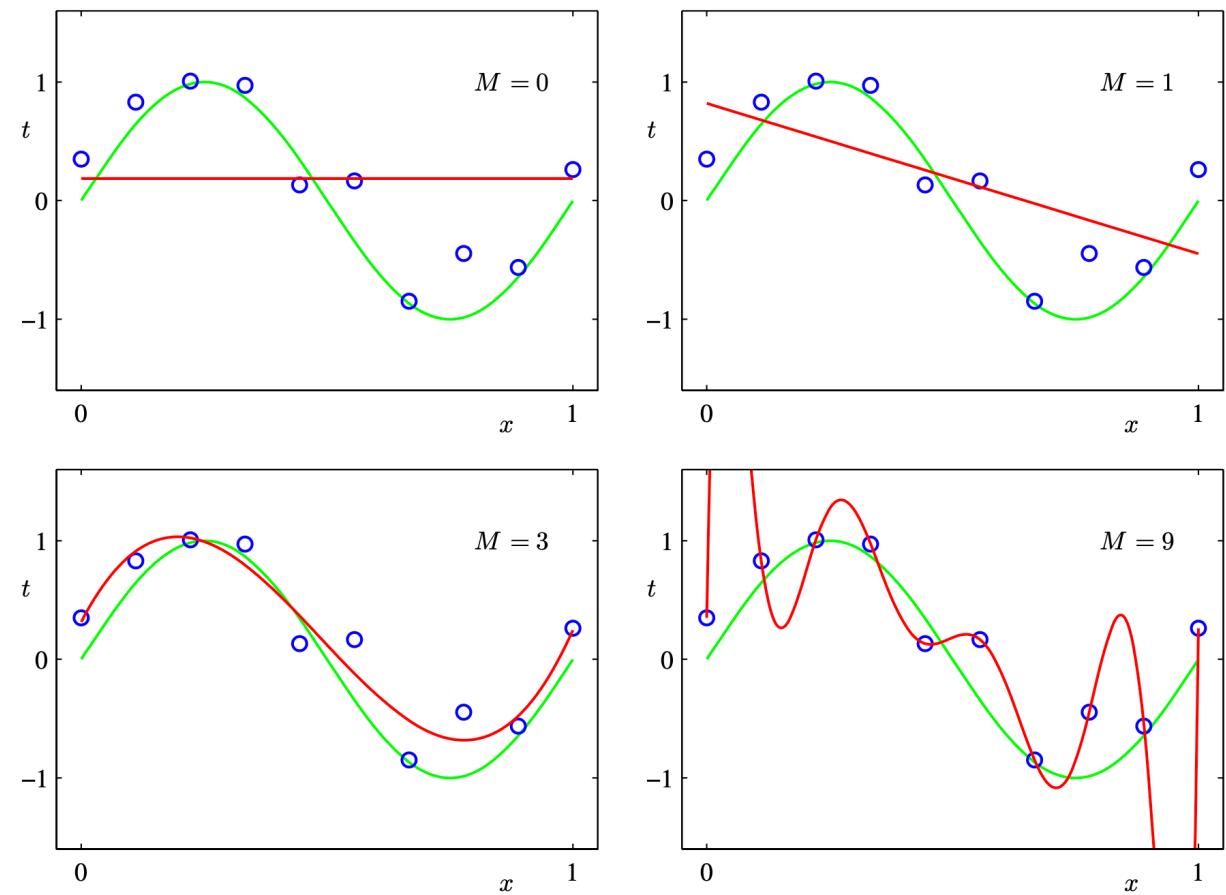
Overfitting Visualization

Key Insight

- Training error decreases as M increases (can always fit better)
- Test error has a U-shape \rightarrow minimum around $M = 3\text{--}8$
- $M = 9$ with 10 points: zero train error, high test error

"The model has memorized the noise."

Use held-out data (test set) to choose M .



Why Overfitting Happens

Coefficient Explosion and Data Size

In the polynomial example, when M is large and data is limited, the fitted curve passes through every point including noise.

Two things explain this: **huge coefficients** and **too few data points** for the number of parameters.

Coefficient Magnitudes

For high M , the fitted coefficients become huge (e.g. $\pm 10^6$):

- Large positive and negative values cancel to fit noise
- Small changes in $x \rightarrow$ wild swings in y

Heuristic

- Number of data points \gtrsim (e.g. 5–10) \times number of parameters
- Not a perfect rule; model complexity is subtler

More Data Helps

- $M = 9, N = 15$: still overfits, but less
- $M = 9, N = 100$: overfitting much reduced

"The larger the data set, the more complex the model we can afford to fit."

Takeaway

Overfitting = model too flexible for the amount of data.

- **Fixes:** use a simpler model (lower M), collect **more data**, or add **regularization**

Regularization

Instead of lowering M or waiting for more data, we can **keep** a flexible model (e.g. high M) and **penalize large weights** so the solution stays smooth. We add a penalty term to the error function:

$$\tilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

with $\|\mathbf{w}\|^2 = \mathbf{w}^T \mathbf{w} = w_0^2 + w_1^2 + \dots + w_M^2$. The hyperparameter λ controls how strongly we penalize complexity.

Regularization

Effect of λ

- λ small: close to least squares; can still overfit
- λ large: weights shrunk \rightarrow underfitting (too smooth)
- Good λ : balances fit and complexity (e.g. cross-validation)

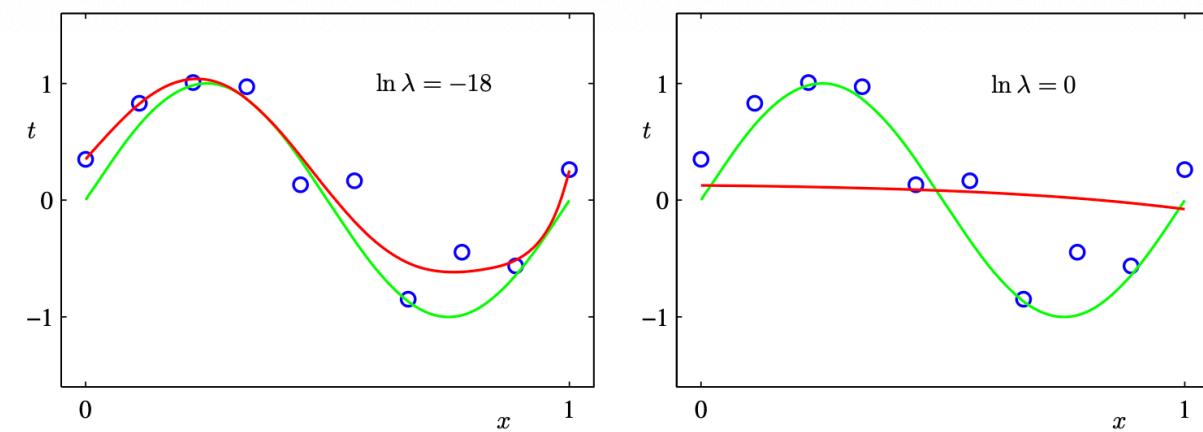
Names

- Ridge regression (statistics)
- Weight decay (neural networks)

Intuition

"We add a penalty that says large weights are unlikely."

- Same idea will reappear as **Bayesian prior** (spoiler)
- λ controls **effective complexity**



Practice - Overfitting Analysis

Using the ideas from this section (train vs test error, underfitting vs overfitting), classify each scenario:

#	Train Acc	Test Acc	Status
A	65%	63%	?
B	99%	72%	?
C	45%	43%	?
D	88%	85%	?
E	100%	55%	?

Options: Underfitting, Overfitting, Good Model

Loss Functions

Training a model means **choosing parameters** so that predictions match the data as well as possible.

- We need a way to measure **how wrong** a prediction is: that is the **loss** (or error) for one example.
 - For example, in the polynomial curve-fitting example we **minimized the sum of squared differences** between predictions $y(x_n, \mathbf{w})$ and targets t_n —so the loss there was **squared error** per point.
- **Loss** $\ell(\hat{y}, y)$: how bad it is to predict \hat{y} when the true value is y .
- **Training** = minimize the **average** loss over the training set (empirical risk). The choice of loss (squared, absolute, cross-entropy, etc.) defines what **best** means.

Loss vs Cost

Loss function $L(y_i, \hat{y}_i)$ (or ℓ): the error for a **single** example, how wrong we were on one prediction.

Cost function $J(\theta)$ (or empirical risk $\widehat{R}(\theta)$): the **average** loss over all training examples. We choose parameters θ to minimize $J(\theta)$:

$$J(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \hat{y}_i) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h_\theta(\mathbf{x}_i))$$

Loss = per-example; **cost** = what we actually minimize during training. Gradient descent (and other optimizers) reduce $J(\theta)$ step by step.

Common Loss Functions

Regression (continuous y)

Loss	Formula $\ell(\hat{y}, y)$	Notes
Squared (MSE)	$(\hat{y} - y)^2$	Standard for linear regression; penalizes large errors more; smooth.
Absolute (MAE)	$ \hat{y} - y $	Robust to outliers; not differentiable at 0.

Classification (discrete y)

Loss	Idea	Use
0–1 loss	1 if $\hat{y} \neq y$, else 0	Error rate; not smooth, hard to optimize with gradient methods.
Cross-entropy	$-\sum_k y_k \log \hat{p}_k$ (for probabilities \hat{p}_k)	Standard for classification; smooth; used with logistic regression, neural nets.

We will see these again when we formalize **hypothesis space**, **risk**, and **optimization** (Mathematical Foundations and later weeks).

Mathematical Foundations

Scalars, Vectors, Matrices

Symbol	Meaning	Example
x, y	Scalars (single numbers)	$x = 3, y = 2.5$
\mathbf{x}, \mathbf{w}	Vectors (bold lowercase)	$\mathbf{x} = [x_1, x_2, \dots, x_d]^T \in \mathbb{R}^d$
\mathbf{X}	Matrix (bold uppercase)	$\mathbf{X} \in \mathbb{R}^{N \times d}$ – N rows, d columns
x_i or $x^{(i)}$	i -th component of \mathbf{x} , or i -th sample	Context-dependent

Conventions in This Course

- N = number of samples (data points)
- d = number of features (input dimension)
- n sometimes used for sample index; j for feature index
- Vectors are **column vectors** by default: $\mathbf{x} = (x_1, \dots, x_d)^T$

Spaces and Dataset

Input and Output Spaces

- **Input space \mathcal{X} :** set of all possible inputs
 - Regression: often $\mathcal{X} \subseteq \mathbb{R}^d$
 - Classification: same, but **output** is discrete
- **Output space \mathcal{Y} :**
 - Regression: $\mathcal{Y} \subseteq \mathbb{R}$ (continuous)
 - Classification: $\mathcal{Y} = \{1, 2, \dots, K\}$ or class labels

Dataset (Supervised)

Training set — a finite collection of input–output pairs:

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_N, y_N)\}$$

- Each $\mathbf{x}_i \in \mathcal{X}$ is a **feature vector** (one sample)
- Each $y_i \in \mathcal{Y}$ is the **label** (target) for \mathbf{x}_i
- **Design matrix:** stack inputs as rows: $\mathbf{X} = [\mathbf{x}_1^T; \dots; \mathbf{x}_N^T] \in \mathbb{R}^{N \times d}$

Feature Map

Real-world inputs are rarely vectors

- Inputs are often **songs, images, text, persons** - not vectors of numbers.
- We define a **feature map** ϕ that maps each raw input to a vector in \mathbb{R}^d :

$$\phi : (\text{raw input}) \rightarrow \mathbb{R}^d$$

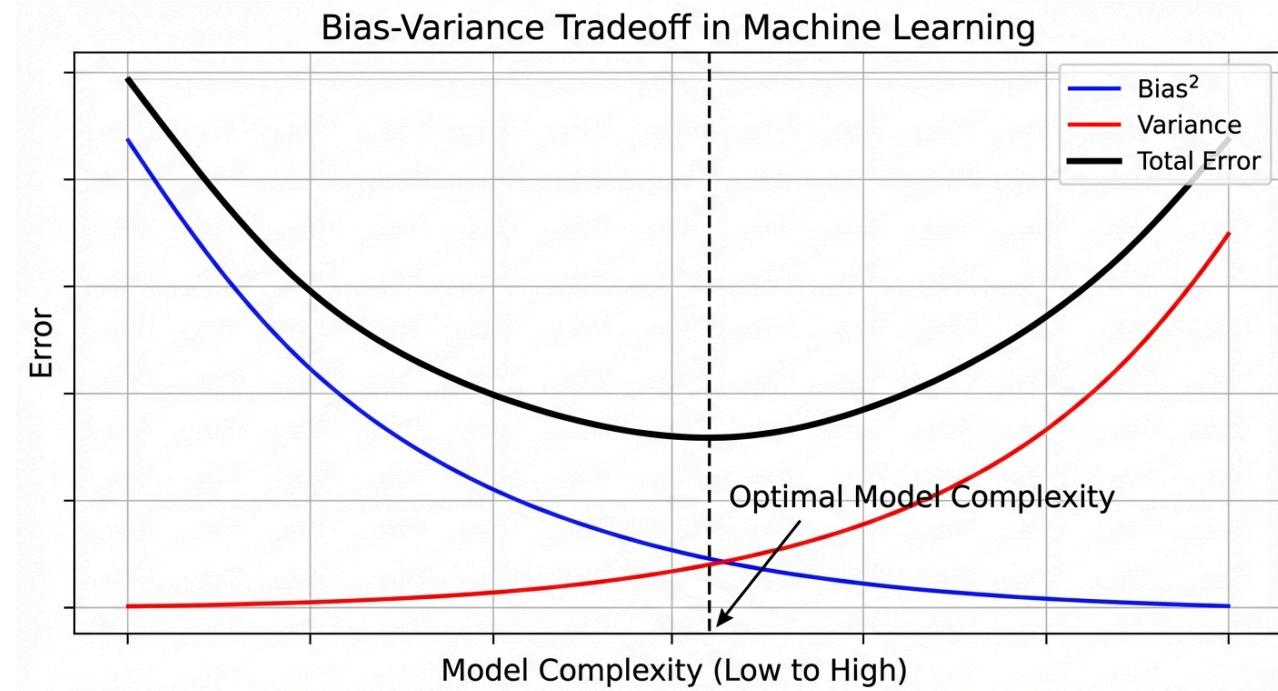
- **Examples:** height/weight of a person; pixel intensities of an image; TF-IDF of a document; **amount of bass** in a song.
- The model then sees $\mathbf{x} = \phi(\text{raw input})$; we often write $h(\mathbf{x})$ and omit ϕ , but it is almost always there in practice.
- **Feature engineering** = designing a good ϕ (and the set of features) for the task.

Bias-Variance Tradeoff

The total error of a model can be split into **bias** and **variance** (plus noise). Choosing model complexity is a tradeoff:

- Simpler models tend to have high bias and low variance
- More complex models tend to have low bias but high variance.

We want **balance**



Bias-Variance Tradeoff

Bias

Bias is error due to the model **oversimplifying** reality.

- Systematically wrong because the model class cannot represent the true relationship (e.g. a straight line when the true curve is wavy).

High bias: The model is too simple and misses important patterns.

- Both training and test error stay high (underfitting).

Low bias: The model is flexible enough to capture the true structure

- We need enough capacity without overfitting.

Variance

Variance is error due to the model being **too sensitive** to the particular training set

- If we retrain on a different sample, we get a very different model and different predictions.

High variance: Different training sets give very different fits

- The model is learning noise and overfitting.

Low variance: The model is stable

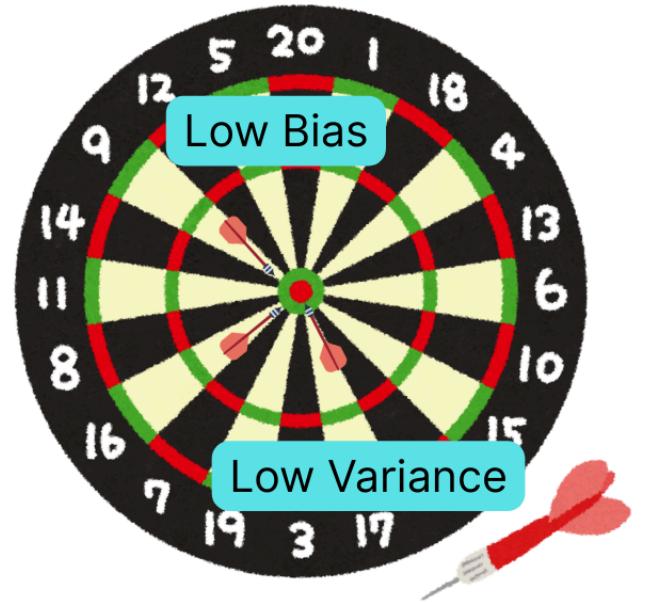
- Small changes in the training data do not change the learned model much.

Bias-Variance Tradeoff

Think of the **bullseye** as the true prediction $f(x)$ and each **throw** as a model \hat{f} trained on a different random sample.

- **Bias** is the average distance of the throws from the center (systematic error).
- **Variance** is how spread out the throws are (sensitivity to the training set).

We want **low bias** and **low variance**



Bias-Variance Tradeoff

Low Bias, Low Variance

Ideal. Predictions are centered on the truth and consistent across training sets, model has enough capacity and does not overfit.

High Bias, Low Variance

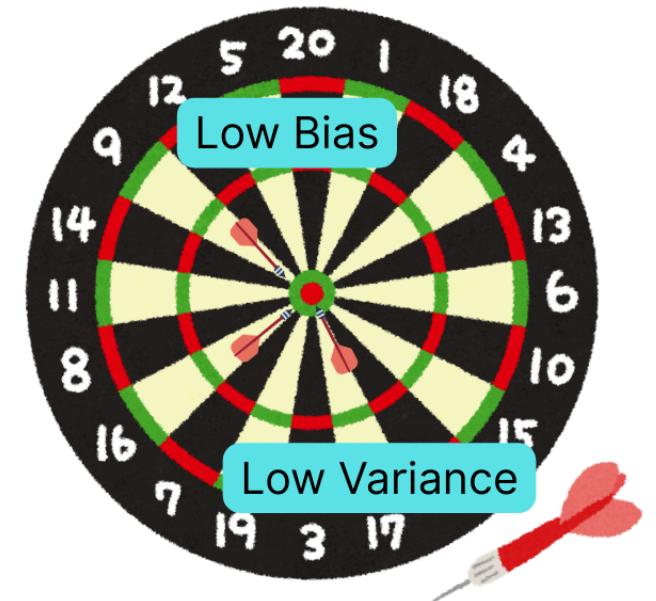
Consistent but wrong. The model is stable (low variance) but systematically off (high bias). **Underfitting.**

Low Bias, High Variance

Right on average, but unstable. Averaged over many training sets we would be correct (low bias), but each individual model is scattered (high variance). **Overfitting.**

High Bias, High Variance

Worst case. Predictions are both off-center and highly variable (e.g. a very flexible model with too little data). We get neither stability nor accuracy.



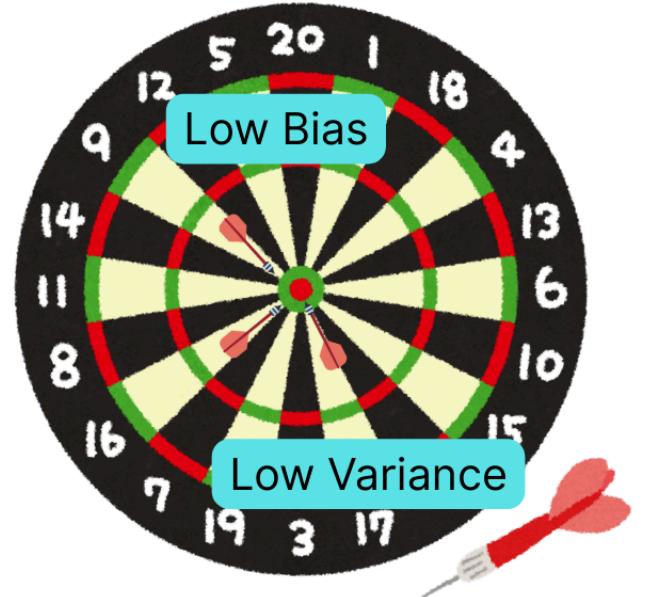
Bias-Variance Tradeoff

Effect of Model Complexity

As we move from **simple** to **complex** models: **bias** tends to go down, while **variance** tends to go up. So we cannot simply *add more capacity without cost*.

Sweet Spot

The **best generalization** usually comes from a model that balances bias and variance—not too simple (high bias), not too complex (high variance). We find this **sweet spot** in practice using a validation set or cross-validation to choose complexity (e.g. M , λ).



Course Project

Course Projects Details

3 Projects — 30% of Grade (One Problem, Three Aspects)

You choose one real-world problem and one dataset

- The **same** problem and dataset are used across all three projects
- Each project focuses on a **different aspect** of the ML pipeline.
- Together, the three deliverables form a **complete, real-world ML execution** from data understanding to modeling and evaluation.

Pick a problem you care about, use a dataset you create or adapt, or put a new twist on an existing dataset.

- Standard public datasets are allowed only if you clearly customize the problem or add a localized angle.

There will be **3 deliverables** (P1, P2, P3), each focusing on a different aspect of your chosen problem:

#	Project	Due	Focus
P1	Problem & EDA	Week 6	Problem formulation, data cleaning, exploration, visualization
P2	Regression	Week 10	Linear/polynomial regression, feature engineering, evaluation
P3	Classification or Beyond	Week 15	Classification/Regression, model selection, report

Course Projects Details

Submission Format

- Jupyter Notebook (.ipynb) per project
- GitHub repository (one repo for all three)
- README.md with problem description, dataset source, and how the three projects connect
- Clean, commented code
- Working prototype in the end

Thank You!

Contact Information

- Email: ekrem.cetinkaya@yildiz.edu.tr
- Office Hours: Wednesday 13:30-15:30 - Room C-120
- Book a slot before coming: [Booking Link](#)
- Course Repository: [GitHub](#)

Next Week

Week 2: Probability Theory and Statistics Fundamentals