भारतीय प्रौद्योगिकी संस्थान मुंबई

Indian Institute of Technology Bombay

Artificial Intelligence and Machine Learning

Week 1: Optimization Foundations and Linear Regression

Swaprava Nath

Department of Computer Science and Engineering, IIT Bombay

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Knowledge is the supreme goal

Course Overview

What this course covers (6 weeks):

1. Optimization + Linear Regression
2. Classification + SVM
3. Neural Networks I (MLP + Backprop)
4. Neural Networks II (CNN, RNN, Transformers)
5. Classical AI Search (A* and friends)
6. Multi-Agent AI (Game Theory + Minimax)

Evaluation:

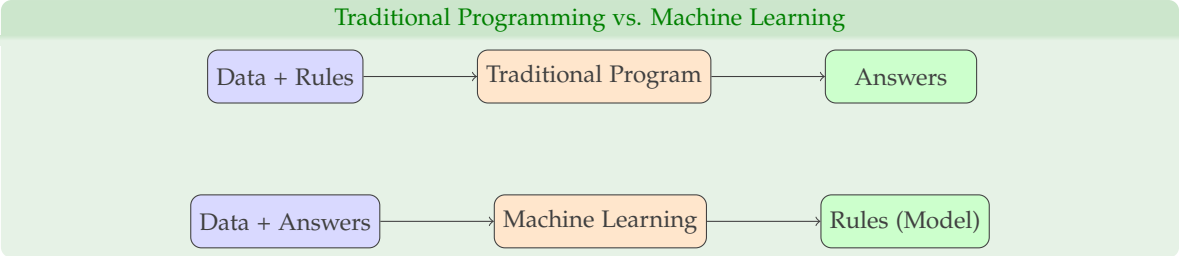
- **Programming Assignment** – end of Week 4 (in-person, proctored)
- **Written Endsem Exam** – end of Week 6 (in-person, proctored)

Prerequisites:

- Probability and statistics
- Linear algebra (matrices, eigenvalues)
- Calculus (partial derivatives)
- Basic Python programming

Contents

What is Machine Learning?



- In ML, we **learn a function** $f : \mathcal{X} \to \mathcal{Y}$ from **examples** $(x_1, y_1), \ldots, (x_n, y_n)$
- $\mathcal{X}$ is the **input space** (e.g., images, text, sensor readings)
- $\mathcal{Y}$ is the **output space** (e.g., a price, a label, a probability)

Types of Machine Learning

Supervised Learning

- Given: labeled pairs (x_i, y_i)
- Goal: learn $f(x) \approx y$
- Examples: house price prediction, spam detection

Unsupervised Learning

- Given: unlabeled data $\{x_i\}$
- Goal: discover structure
- Examples: clustering customers, topic modelling

Reinforcement Learning

- Given: environment + reward signal
- Goal: learn a policy via interaction
- Examples: game playing, robotics

This Course Focus

We cover **supervised learning** in depth (Weeks 1–4). Classical AI search (Week 5) and multi-agent game theory (Week 6) complete the picture.

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Why Optimization?

- Almost every ML algorithm reduces to: **minimize a loss function** $L(\theta)$ over parameters θ
- Example: for linear regression, $L(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^\top x_i)^2$
- We need to find $\theta^* = \arg\min_\theta L(\theta)$

Key Concept: Convexity

A function $f : \mathbb{R}^d \to \mathbb{R}$ is **convex** if for all $x, y \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$f(\lambda x + (1-\lambda)y) \leqslant \lambda f(x) + (1-\lambda) f(y)$$

- Convex functions have **no local minima other than the global minimum**
- The squared loss $L(\theta) = \|\mathbf{y} - X\theta\|^2$ is convex in θ – so gradient descent will find the global minimum
- **Intuition:** the function bowl never has false valleys

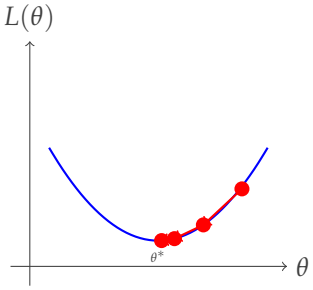
Gradient Descent

Algorithm: Gradient Descent

1. Initialize $\theta^{(0)}$ (e.g., randomly or at $\mathbf{0}$)
2. Repeat until convergence:

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \alpha \nabla_\theta L(\theta^{(t)})$$

- $\alpha > 0$ is the **learning rate** (step size)
- $\nabla_\theta L$ points in the direction of steepest **ascent**; we subtract it to descend
- Each step moves θ toward lower loss



Gradient Descent: Variants

Batch GD

- Use **all** n samples per update
- Stable, but slow for large n
- $\nabla L = \frac{1}{n} \sum_{i=1}^{n} \nabla \ell_i$

Stochastic GD (SGD)

- Use **one** random sample per update
- Fast but noisy updates
- $\nabla L \approx \nabla \ell_i$

Mini-batch GD

- Use a **batch** of B samples
- Best of both worlds
- Typical: $B \in \{32, 64, 128\}$

Learning Rate Sensitivity

- Too large α: oscillates or diverges
- Too small α: converges very slowly
- In practice: use learning rate schedules or adaptive methods (Adam, covered in Week 3)

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The Supervised Learning Setup

Formal Setup

- **Training data**: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, where $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$
- **Hypothesis class**: a family of functions $\mathcal{H} = \{f_\theta : \theta \in \Theta\}$
- **Loss function**: $\ell(f_\theta(x), y)$ measures prediction error
- **Goal**: find $\theta^* = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \ell(f_\theta(x_i), y_i)$

- **Example:** Predict a student's exam score y from hours studied x_1 and assignments completed x_2
- Features: $x = (x_1, x_2) \in \mathbb{R}^2$, label: $y \in \mathbb{R}$
- We want to find a function that generalizes to **new, unseen** students

Linear Regression: Model

- **Linear regression** assumes $f_\theta(x) = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d = \theta^\top \tilde{x}$
- where $\tilde{x} = (1, x_1, \ldots, x_d)^\top \in \mathbb{R}^{d+1}$ includes the bias term, $\theta \in \mathbb{R}^{d+1}$

Squared Error Loss (Ordinary Least Squares)

$$L(\theta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta^\top \tilde{x}_i)^2 = \frac{1}{n} \|y - X\theta\|^2$$

where $X \in \mathbb{R}^{n \times (d+1)}$ is the **design matrix** with rows $\tilde{x}_i^\top$, and $y \in \mathbb{R}^n$ is the label vector.

- This is a convex quadratic in θ
- **Why squared error?** Penalizes large mistakes more than small ones. Also arises naturally from a probabilistic model (next slide).

Closed-Form Solution: The Normal Equation

- Since $L(\theta) = \frac{1}{n}\|y - X\theta\|^2$ is convex and differentiable, set gradient to zero:

$$\nabla_\theta L = \frac{2}{n} X^\top (X\theta - y) = 0$$

- Solving: $X^\top X\theta = X^\top y$

Normal Equation

$$\hat{\theta} = (X^\top X)^{-1} X^\top y$$

provided $X^\top X$ is invertible (requires $n \geqslant d + 1$ and no redundant features).

- **Geometric interpretation:** $X\hat{\theta}$ is the **orthogonal projection** of y onto the column space of X
- $y - X\hat{\theta}$ (the **residual**) is perpendicular to every column of X
- **Limitation:** Computing $(X^\top X)^{-1}$ costs $O(d^3)$ – impractical when d is very large. Use gradient descent instead.

Probabilistic Interpretation: MLE

- Suppose the true relationship is $y_i = \theta^\top x_i + \epsilon_i$ where $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ i.i.d.
- Then $y_i \mid x_i \sim \mathcal{N}(\theta^\top x_i, \sigma^2)$, so:

$$p(y_i \mid x_i; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^\top x_i)^2}{2\sigma^2} \right)$$

Maximum Likelihood Estimation (MLE)

Maximize $\prod_{i=1}^n p(y_i \mid x_i; \theta)$ over θ. Taking log and simplifying, this is **equivalent to minimizing** $\sum_{i=1}^n (y_i - \theta^\top x_i)^2$.

- **Conclusion:** Ordinary least squares is the MLE under Gaussian noise. Minimizing squared error is not just convenient – it has a principled probabilistic justification.

Gradient Descent for Linear Regression

For $L(\theta) = \frac{1}{n}\|y - X\theta\|^2$, the gradient is:

$$\nabla_\theta L = -\frac{2}{n} X^\top (y - X\theta)$$

Update Rule

$$\theta^{(t+1)} \leftarrow \theta^{(t)} + \frac{2\alpha}{n} X^\top \left(y - X\theta^{(t)}\right)$$

Convergence:

- For a fixed step size $\alpha < \frac{1}{\lambda_{\max}(X^\top X/n)}$, batch gradient descent converges to $\hat{\theta}$
- When n and d are large, mini-batch SGD is preferred over the normal equation

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When should you use the normal equation vs. gradient descent?

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When should you use the normal equation vs. gradient descent?

Answer

Normal equation: small d (e.g., $d < 10^4$). Gradient descent: large d or large n where matrix inversion is too slow.

Basis Functions: Going Beyond Linear

- Real data is often not linearly related to raw inputs
- **Basis functions** $\phi : \mathbb{R}^d \to \mathbb{R}^p$ transform the input before fitting a linear model:

$$f_\theta(x) = \theta^\top \phi(x)$$

- The model is **linear in** θ but **non-linear in** x

Polynomial basis (for $d = 1$):

$$\phi(x) = (1, x, x^2, \ldots, x^p)^\top$$

Fits degree-p polynomial curves.

Radial Basis Functions (RBF):

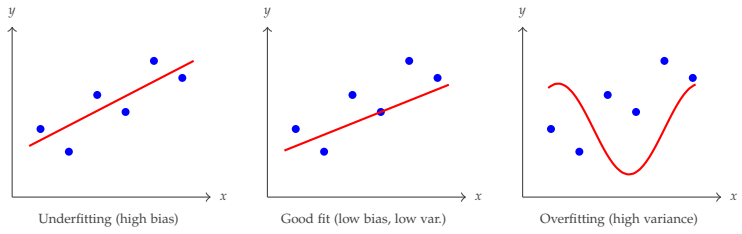
$$\phi_j(x) = \exp\left(-\frac{\|x - \mu_j\|^2}{2s^2}\right)$$

Basis function is a Gaussian with mean μ_j.

Warning: Overfitting

Using too many basis functions fits the training data exactly but generalizes poorly. This is the **bias-variance tradeoff** – a central theme in ML.

Overfitting and Model Selection



- **Bias:** error from wrong model assumptions (too simple)
- **Variance:** sensitivity to small fluctuations in training data (too complex)
- **Remedy:** use a **validation set** to choose model complexity; use **regularization**

Regularization: Ridge Regression

- Add a penalty on the magnitude of θ to the loss:

$$L_{\text{ridge}}(\theta) = \frac{1}{n}\|y - X\theta\|^2 + \lambda\|\theta\|^2$$

- $\lambda > 0$ is the **regularization strength** (a hyperparameter)
- Larger λ pulls θ toward zero, reducing variance at the cost of some bias

Closed-Form Ridge Solution

$$\hat{\theta}_{\text{ridge}} = (X^\top X + \lambda n I)^{-1} X^\top y$$

The added $\lambda n I$ ensures the matrix is always invertible (even if $n < d$).

- **Lasso** (ℓ_1 penalty): $\lambda\|\theta\|_1$ encourages **sparse solutions** – many $\theta_j = 0$
- **Elastic Net:** combines ℓ_1 and ℓ_2 penalties

Week 1 Summary

What We Learned

1. ML is about learning a function from data. Supervised learning uses labeled pairs.
2. Optimization underpins all of ML. Convex functions have global minima; gradient descent finds them.
3. Linear regression models $y = \theta^\top x$. The normal equation $\hat{\theta} = (X^\top X)^{-1} X^\top y$ gives the exact solution.
4. The squared error loss has a probabilistic justification: it is the MLE under Gaussian noise.
5. Basis functions let us fit non-linear patterns while keeping the optimization linear.
6. Overfitting arises when the model is too complex. Regularization (ridge, lasso) controls it.

Looking ahead (Week 2): When y is a discrete class label rather than a real number, we need **classification** methods – logistic regression and support vector machines.

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