Basic Optimization

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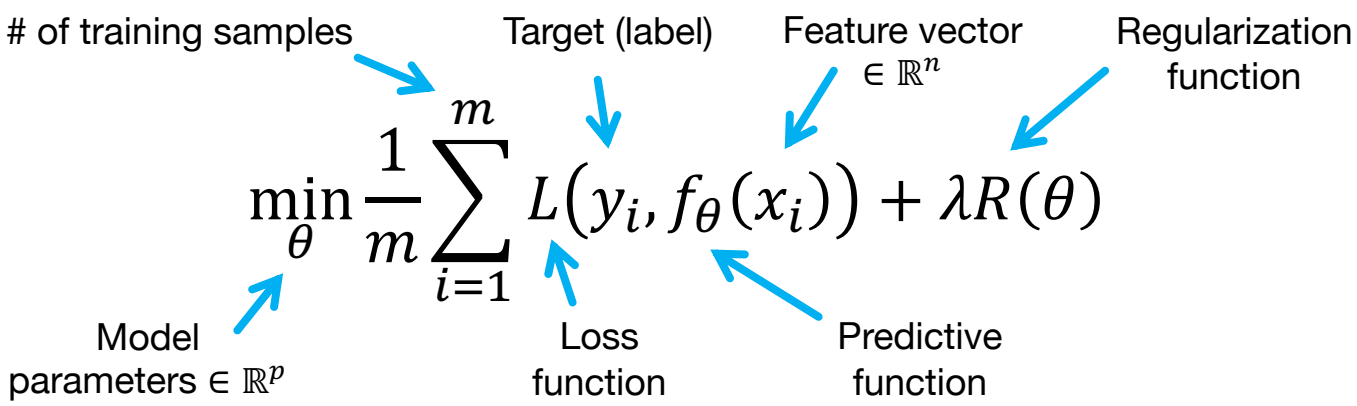
Learning Outcomes

- Formulate machine learning problems as optimization problems and explain the role of objectives, variables, and constraints
- Distinguish convex and non-convex problems and explain why convexity enables global optimality
- Recognize common convex functions and sets arising in machine learning models
- Apply gradient-based methods, including batch and stochastic gradient descent, to empirical risk minimization
- Select step-size strategies and stopping criteria for practical optimization
- Express optimization problems in matrix–vector form for efficient computation
- Formulate constrained optimization problems using the Lagrangian and interpret duality and KKT conditions in machine learning contexts

Motivation & Fundamentals

Why Optimization in ML?

Most ML problems can be written as:



Three components:

- Decision variables
- Constraints
- Objective function

Convex/nonconvex optimization

Modeling

- Statistics and geometric models
- Clustering
- PCA
- MLE
- Regression
- Support vector machine
- Deep learning

Solution Methods

- Heuristics (e.g., K-means)
- Special methods (e.g., PCA, EM)
- General methods (e.g., gradient descent, SGD)

Convex Optimization

Definition: An optimization problem specified by:

$$\begin{aligned} \text{minimize} \quad & f_0(x) && && \leftarrow \text{Convex objective function} \\ \text{subject to} \quad & f_i(x) \leq 0, && i = 1, \ldots, m && \leftarrow \text{Convex inequality constraints} \\ & h_i(x) = 0, && i = 1, \ldots, p && \leftarrow \text{Affine equality constraints} \end{aligned}$$

ML mapping:

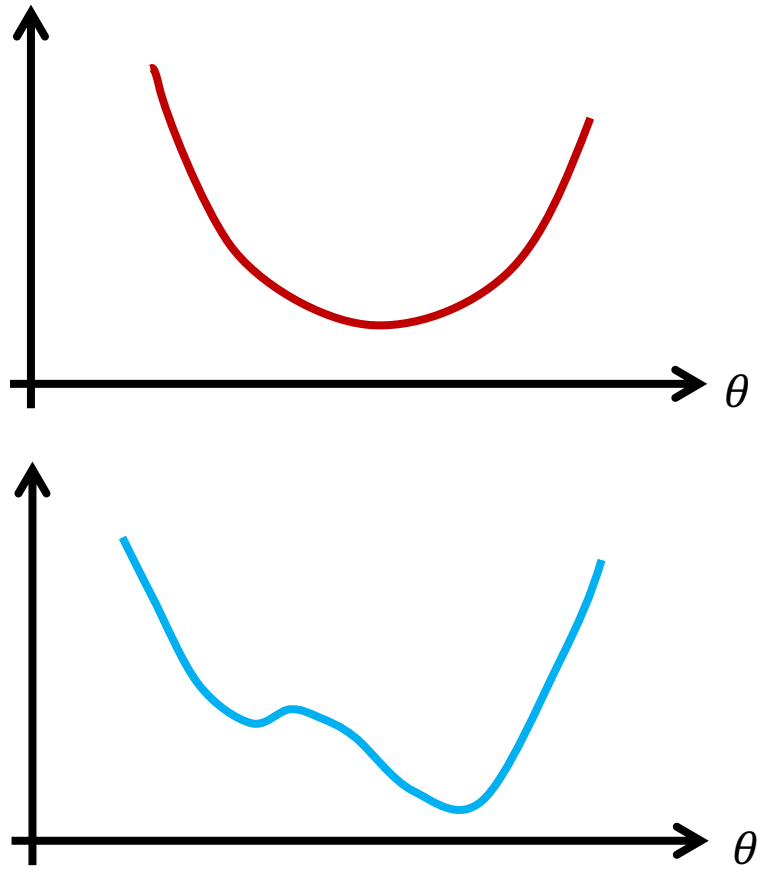
- Objective function → loss function
- Constraints → regularization or feasibility
- Decision variables → model parameters

Convex optimization problems are attractive because they have no "bad" local minima

Unconstrained Optimization

In ML, unconstrained problems are the most common case:

$$\text{minimize}_x \ f_0(x)$$



- **Examples:** Linear and logistic regression
- Constraints are often absorbed into the objective via **regularization**
- First order optimality condition:

$$\nabla f_0(x) = 0$$

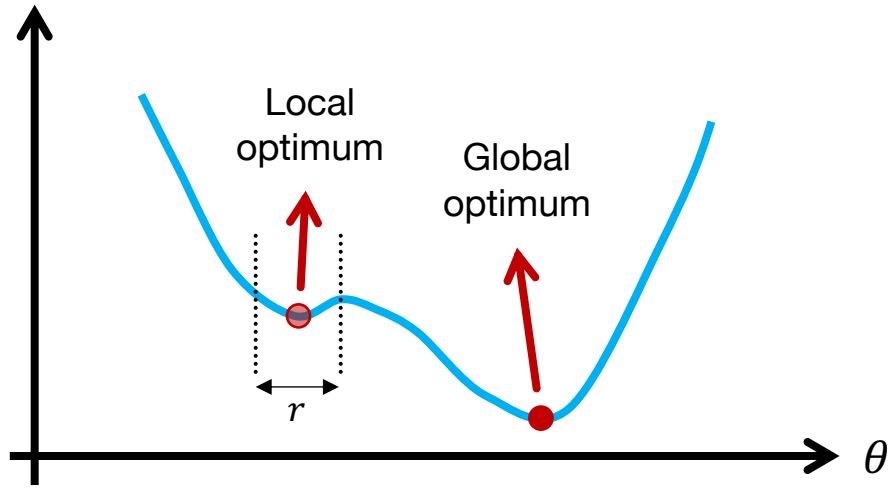
If $\nabla f_0(x) = 0$, does that guarantee we found the best solution?

Global vs Local Optimum

Global optimum: A point x^* in the feasible set is global optimum iff

$$f_0(x^*) \leq f_0(x)$$

for all x in the feasible set



Local optimum: A point x^* in the feasible set is local optimum iff there exists $r > 0$ such that for all $x \in \{x \mid \|x - x^*\| \leq r\}$ and also in the feasible set, we have

$$f_0(x^*) \leq f_0(x)$$

For convex optimization problem, any local optimum is also a global optimum

Constrained vs Unconstrained

Clustering: Unconstrained

- Optimization variables = cluster centers c
- Each cluster center is free to move anywhere in $\mathbb{R}^n$

$$\min_{c,\pi} \frac{1}{m}\sum_{i=1}^{m}\left\|x^i - c^{\pi(i)}\right\|^2$$

Regression: Unconstrained

- Parameter θ lives in $\mathbb{R}^n$ with no explicit constraint
- Regularization (Ridge/LASSO) is usually added

$$\min_{\theta} \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2$$

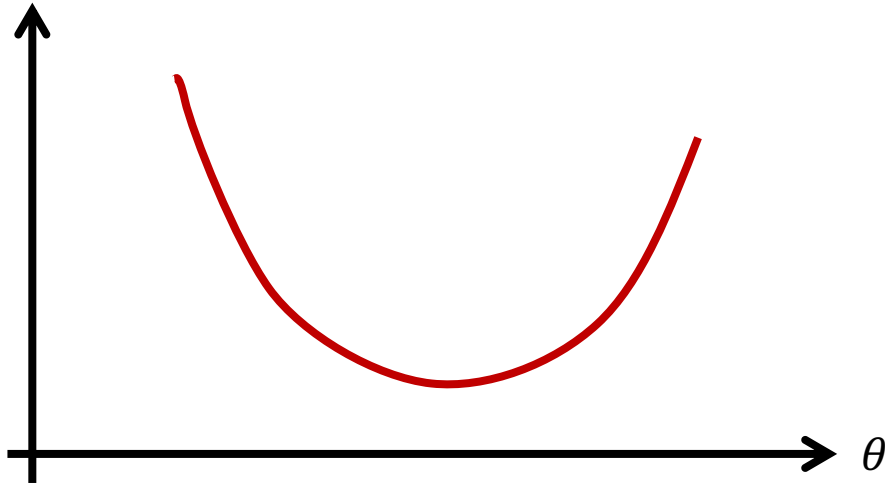
PCA: Constrained; $\|w\| = 1$ serves as an essential, **hard constraint**

$$\max_{w:\|w\|\leq 1} \frac{1}{m}\sum_{i=1}^{m}\left(w^\top x^i - w^\top \mu\right)^2$$

Convex vs Non-Convex

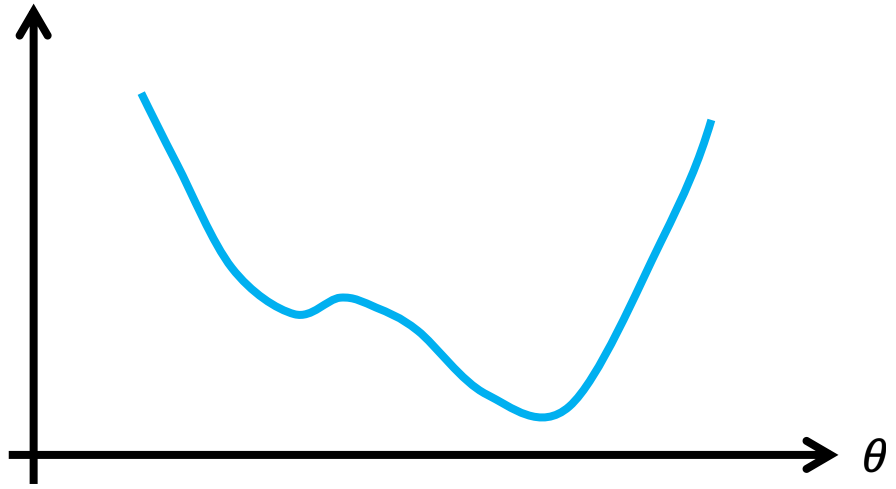
Convex Problem

- e.g., linear regression
- Can be solved efficiently (find global optimal solution) in polynomial time
- Gradient descent (or many acceleration methods; e.g., Newton method) can converge to global solution



Non-Convex Problem

- e.g., clustering, PCA
- Cannot find global solution in polynomial time (NP-hard)
- Use heuristics to find local optimal solution
- “Non-convex” does not mean “unsolvable,” but it does mean we rely on heuristics and initialization



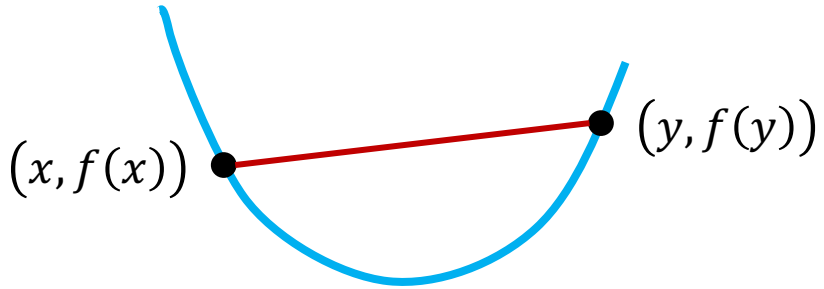
Convex Functions & Sets

Convex Functions

Definition: A function $f: \mathbb{R}^n \to \mathbb{R}$ is **convex** if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$ and $0 \leq \alpha \leq 1$, we have

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y)$$

Geometrically, the line segment between $\big(x, f(x)\big)$ and $\big(y, f(y)\big)$ lies **above** the graph of f



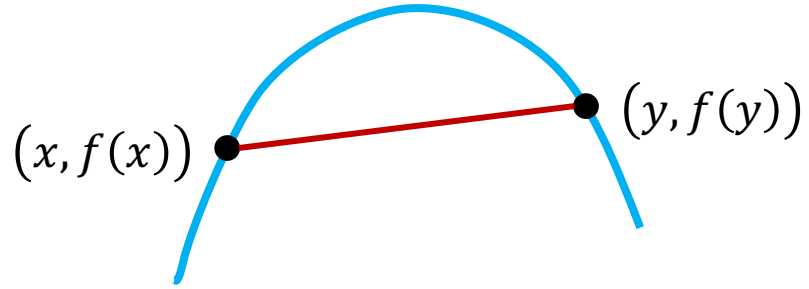
A convex function has a single "bowl-shaped" landscape

Concave Functions

Definition: A function $f: \mathbb{R}^n \to \mathbb{R}$ is **concave** if the domain $\mathbf{dom} f$ is a convex set and if for all $x, y \in \mathbf{dom} f$ and $0 \leq \alpha \leq 1$, we have

$$f(\alpha x + (1-\alpha)y) \geq \alpha f(x) + (1-\alpha) f(y)$$

Geometrically, the line segment between $\big(x, f(x)\big)$ and $\big(y, f(y)\big)$ lies **below** the graph of f



Maximizing a concave function is equivalent to minimizing a convex function

Examples

Function	Convex?	Concave?
Exponential	$f(x) = e^{ax}$ for any $a \in \mathbb{R}$	–
Powers	$f(x) = x^a$ on $\mathbb{R}_{++}$ when $a \geq 1$ or $a \leq 0$	$f(x) = x^a$ on $\mathbb{R}_{++}$ when $0 \leq a \leq 1$
Powers of absolute value	$f(x) = \lvert x \rvert^p$ for $p \geq 1$	–
Logarithm	–	$f(x) = \log x$ on $\mathbb{R}_{++}$
Negative entropy	$f(x) = x \log x$ on $\mathbb{R}_{++}$	–
Norms	All norms	–
Max function	$f(x) = \max\{x_1, \ldots, x_n\}$	–
Log-determinant	$f(x) = -\log \det X$	$f(x) = \log \det X$

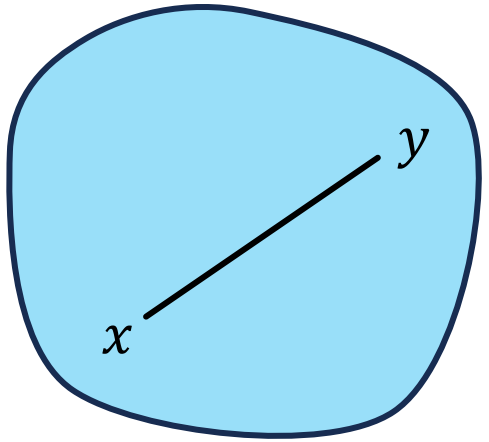
Convex Sets

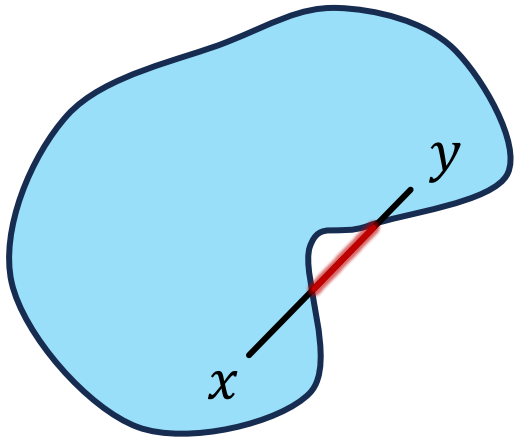
Definition: A set A is convex, if for every $0 \leq \alpha \leq 1$ it satisfies

$$\forall x, y \in A \quad \Leftrightarrow \quad \alpha x + (1-\alpha) y \in A$$

The line segment between any two points is also in the set

Convex set





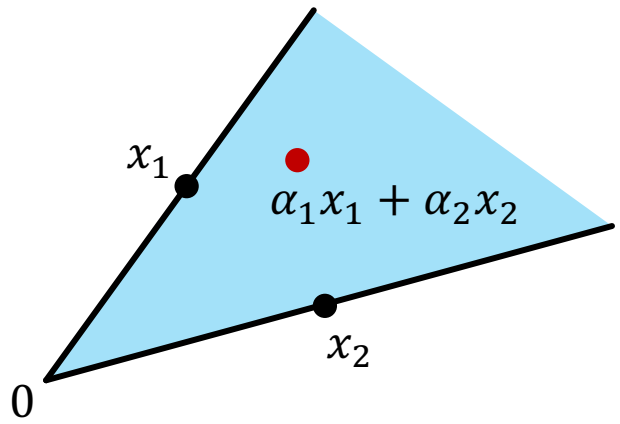
Non-convex set

Convex sets ensure feasibility regions without "holes"

Common Convex Sets

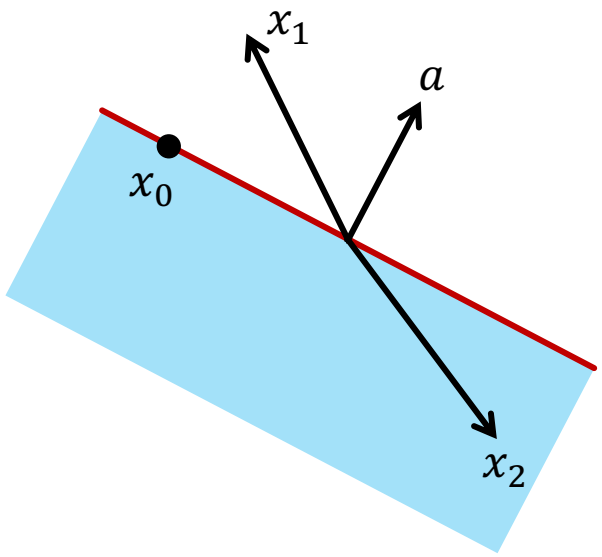
Cones: A set C is a convex cone, if for any $x_1, x_2 \in C$ and $\alpha_1, \alpha_2 \geq 0$, we have

$$\alpha_1 x_1 + \alpha_2 x_2 \in C$$



Hyperplanes: A set is hyperplane if

$$\{x \mid a^\top (x - x_0) = 0, a \neq 0\}$$



Halfspaces: A set is halfspace if

$$\{x \mid a^\top (x - x_0) \leq 0, a \neq 0\}$$

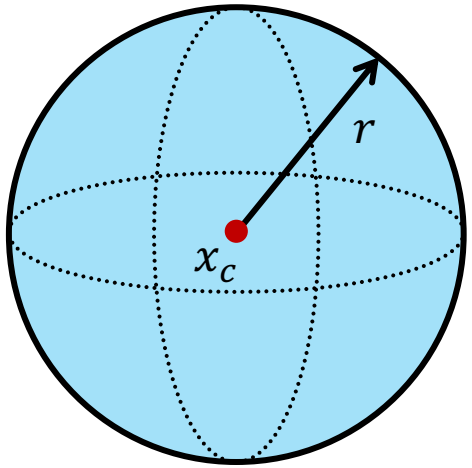
Is a hyperplane itself a feasible region or a boundary?

Common Convex Sets (cont.)

Euclidean balls: A Euclidean ball has the form

$$B(x_c, r) = \{x \mid \|x - x_c\|_2 \leq r\}$$

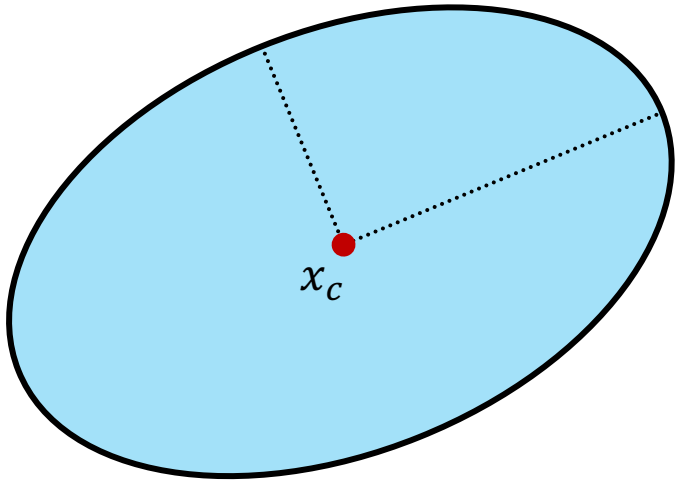
ℓ_2 regularization corresponds to Euclidean balls



Ellipsoids: Used in support vector novelty detection

$$E = \{x \mid (x - x_c)^\top P^{-1}(x - x_c) \leq r\}$$

The eigenvectors and eigenvalues determine the direction and shape of the semi-axes

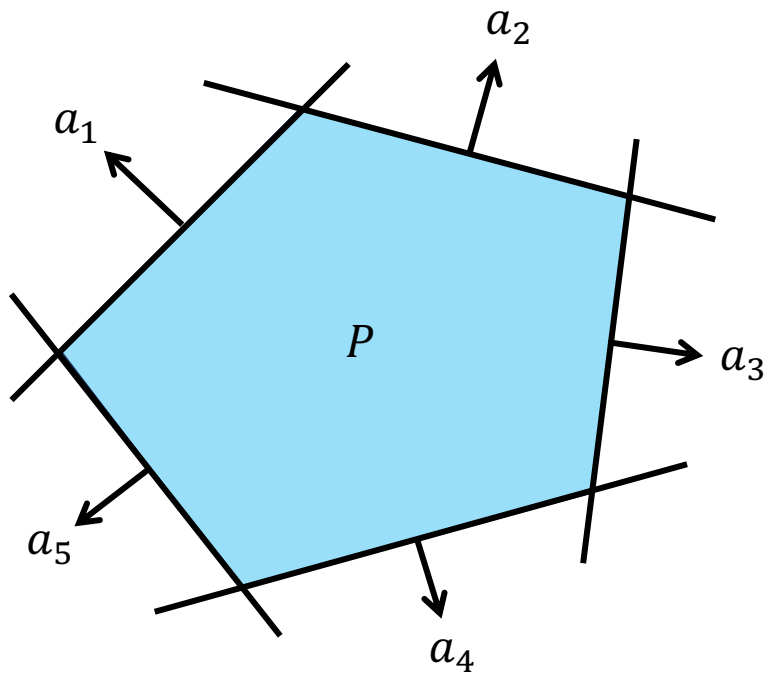


Common Convex Sets (cont.)

Polyhedra: Intersection of a **finite** set of halfspaces or hyperplanes

$$P = \{x \mid a_j^\top x \leq b_j, j = 1, \ldots, m, \qquad c_j^\top x = d_j, j = 1, \ldots, p\}$$

- It is defined as the solution set of a finite number of linear equalities and inequalities
- Used in various machine learning techniques like SVM
- ℓ_1 constraints lead to sparse solutions

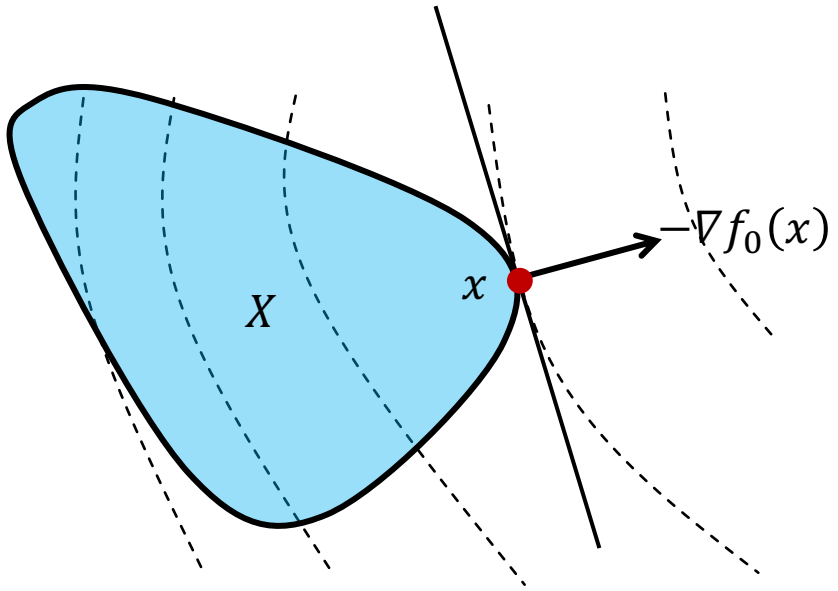


Unconstrained Optimization

First-Order Optimality Condition

Constrained optimization: Given feasible set X

$$x \text{ is optimal} \quad \Leftrightarrow \quad \nabla f_0(x)^\top (y - x) \geq 0, \quad \forall\, y \in X$$



Unconstrained optimization: If $X = \mathbb{R}^n$, then all directions $y = x - \epsilon \nabla f_0(x)$ are feasible

$$x \text{ is optimal} \quad \Leftrightarrow \quad \nabla f_0(x) = 0$$

Constrained boundary optimum: If x is on the boundary of X, not all directions d and so, optimality requires $\nabla f_0(x)^\top d \geq 0$ for all feasible d; therefore,

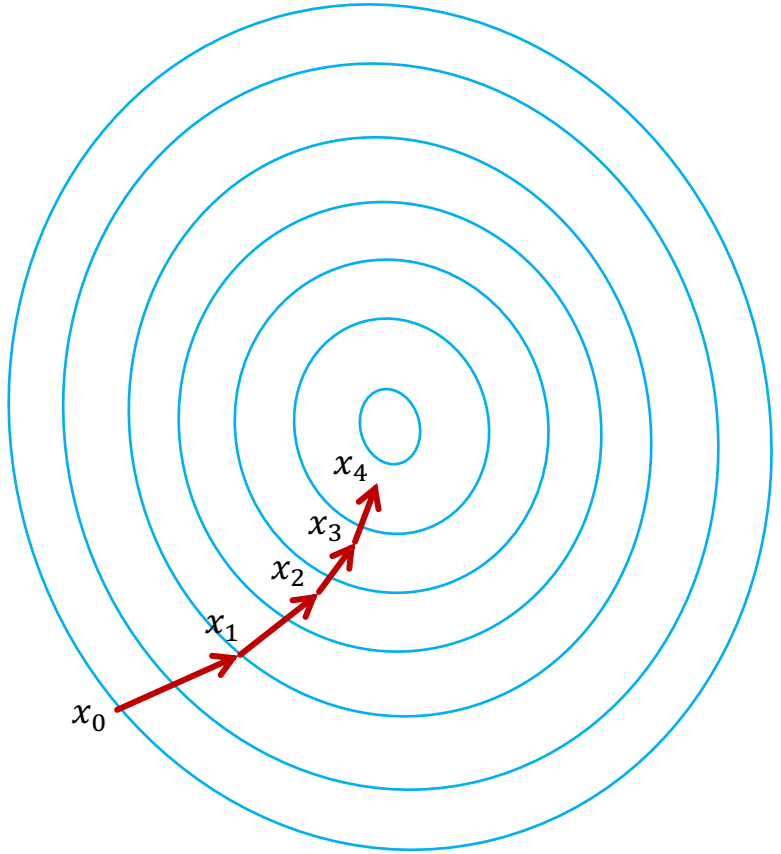
$$-\nabla f_0(x) \;\perp\; \text{tangent space of } X \text{ at } x$$

Gradient Descent

- One way to solve an unconstrained optimization problem is gradient descent (GD)
- Given an initial guess, we iteratively refine the guess by taking the direction of the **negative gradient**
- Think about going down a hill by taking the **steepest direction** at each step
- Update rule:

$$x^{t+1} = x^t - \gamma_t \nabla f_0(x^t)$$

$\gamma_t > 0$ is called the step size or **learning rate**



In ML, GD iteratively improves model parameters to reduce training loss

Gradient Descent (cont.)

How GD works: It operationalizes the condition $\nabla f(x) = 0$

- For an unconstrained problem, a necessary optimality condition is

$$\nabla f_0(x^*) = 0$$

- If gradient descent reaches such this point, then

$$x^{t+1} = x^t - \gamma_t \nabla f_0(x^t) = x^t$$

- In practice, GD rarely reaches this point, so it stops when

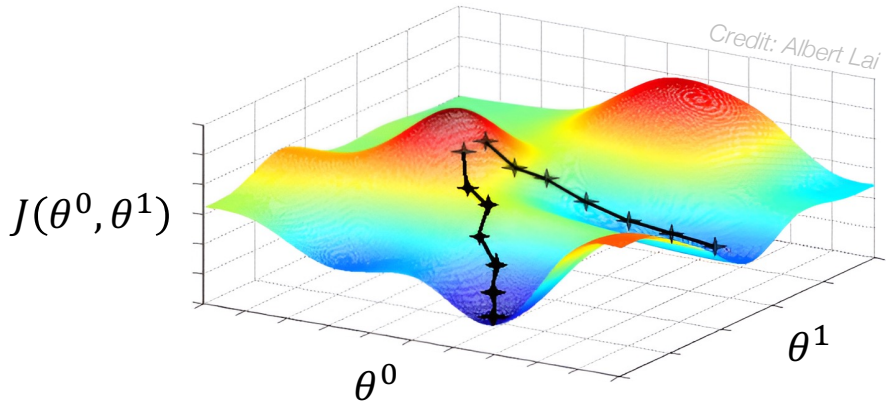
$$\|x^{t+1} - x^t\| < \epsilon$$ ← ϵ: a very mall coefficient

What could go wrong if γ_t is poorly chosen?

Gradient Descent for Linear Regression

Batch gradient descent (or **ascent**) algorithm to minimize MSE:

$$\min_{\theta} L(\theta) \coloneqq \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2$$



Why average all samples here?

Input: data $\{(x^i, y^i)\}_{i=1}^m$, step size γ_t, tolerance ϵ

Initialize: θ^0

Repeat for $t = 1,2,\ldots$

1. Compute residuals

$$r^i \coloneqq y^i - \theta^\top x^i, \qquad \forall i = 1,\ldots,m$$

2. Update parameters:

$$\theta^{t+1} \coloneqq \theta^t + \boxed{\frac{\gamma_t}{m}\sum_{i=1}^{m} r^i x^i} \quad \nearrow -\gamma_t \nabla L(\theta)$$

until $\|\theta^{t+1} - \theta^t\| \leq \epsilon$

Output: θ^{t+1}

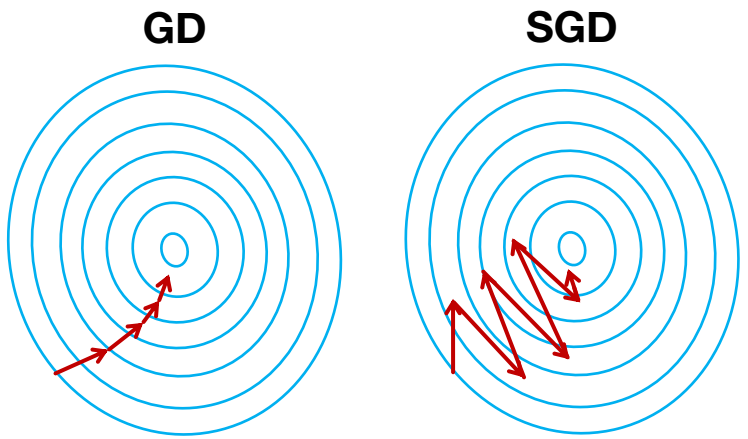
Stochastic Optimization

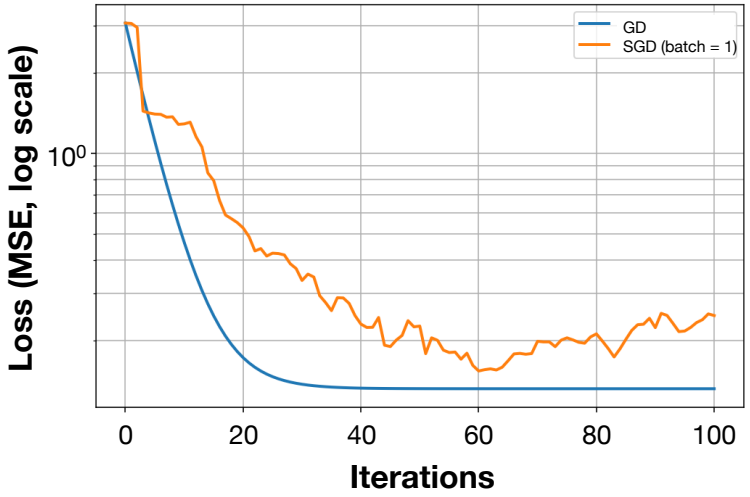
Batch vs Stochastic Gradient

- The algorithm is called **batch gradient descent**
- To compute the gradient at each iteration, we need to sum over all data points in the dataset
- What if we have a huge dataset?
- Note that gradient **decouples**—it consists of sum of evaluations over individual samples:

$$\nabla L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - (\theta^t)^\top x^i\right)x^i$$

SGD trades accuracy for speed and scalability





Stochastic Gradient Descent

- At each iteration, randomly sample a small subset S_t data point (x_i, y_i), $i \in S_t$ (extreme case: one sample in S_t)
- Use gradient estimated using a small subset of data

$$\nabla L(\theta) = \frac{1}{|S_t|} \sum_{i \in S_t} \left(y^i - (\theta^t)^\top x^i\right) x^i$$

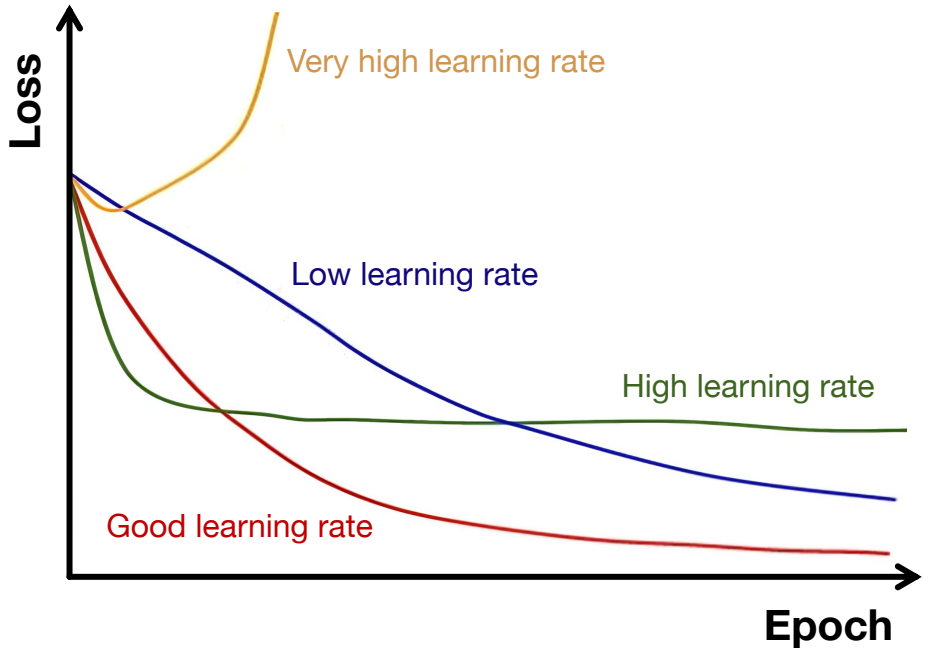
- Each iteration uses a different subset S_t, $t = 1, 2, \ldots$
- Eventually loop through the entire training data, and may loop through the data multiple times

If SGD uses noisy gradients, why doesn't it diverge?

Step Size (Learning Rate)

Step size γ_t (aka **learning rate**) is a positive scalar that controls how far the optimization algorithm moves along the negative gradient direction at each iteration

- If γ_t is too large, the algorithm may diverge; if too small, convergence can be very slow
- Constant step size $\gamma_t = \gamma$
- Diminishing step size $\gamma_t \propto 1/t$
- Constant step length $\gamma_t \propto 1/\|\nabla L(\theta^t)\|$
- Adaptive step-sizes automatically adjust learning rates during training



In practice, adaptive methods (Adam, RMSProp) reduce tuning effort

Stopping Criteria

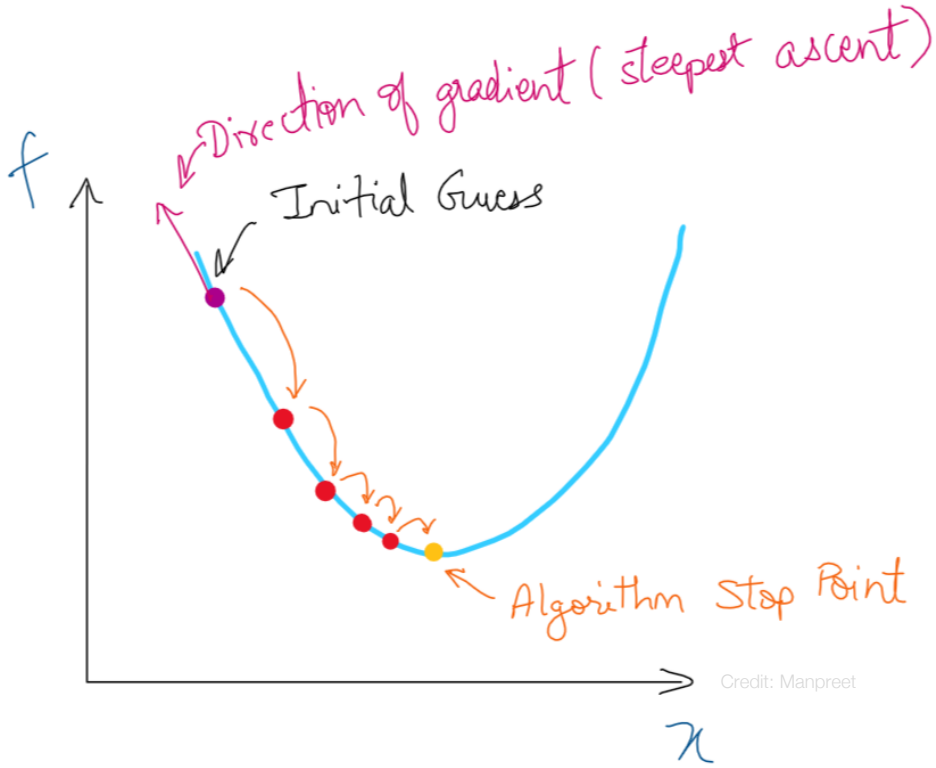
A set of rule that determine when to terminate the optimization algorithm, balancing **computational cost** and **solution accuracy**

- Constant number of iterations
- Stop when loss function change is small*:

$$|L(\theta^t) - L(\theta^{t-1})| < \varepsilon$$

- Stop when parameter change small*:

$$\|\theta^t - \theta^{t-1}\| < \varepsilon$$



In machine learning, stopping is often based on validation loss

* These criteria monitor convergence of the training loss, not generalization performance

Matrix Formulation & Constraints

Matrix-Vector Form: Linear Regression

$$L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2 \xrightarrow{\text{Gadient}} \nabla L(\theta) = -\frac{2}{m}\sum_{i=1}^{m} x^i\left(y^i - \theta^\top x^i\right)$$

Matrix-vector form: $L(\theta) = \frac{1}{m}\|y - X\theta\|_2^2$

$$y = [y^1 \cdots y^m]^\top \qquad X = \begin{bmatrix} (x^1)^\top \\ \vdots \\ (x^m)^\top \end{bmatrix} \in \mathbb{R}^{m\times n}$$

Gradient: $\nabla L(\theta) = -\frac{2}{m}X^\top(y - X\theta)$

Why do we care about matrix form instead of scalar equations?

Handling Constraints

For an **unconstrained** problem, the condition becomes

$$\nabla f_0(x) = 0$$

For **constrained** problems, we need to use the Lagrange multipliers to convert constraints into penalties

$$L(x, \mu, \lambda) = f_0(x) + \underbrace{\sum_{j=1}^{p} \mu_j h_j(x)}_{\text{Equality Constraints}} + \underbrace{\sum_{i=1}^{m} \lambda_i f_i(x)}_{\text{Inequality Constraints}} \qquad \text{s.t.} \quad \lambda_i \geq 0$$

It is a **lower bound** of $f_0(x)$ for all $x \in X$, since $h_j(x)$=0, $f_i(x) \leq 0$ and $\lambda_i \geq 0$ and $L(x, \mu, \lambda) \leq f_0(x)$ for all $x \in X$

Lagrange Dual Function

The dual problem provides **bounds** and alternative **optimization paths**

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda)$$

→ **Definition (Infimum):** Let $S \subseteq R$. The infimum of S, denoted $\inf S$, is the greatest number a such that $a \leq s$, for all $s \in S$

It is the lower bound for the optimal value

$$g(\mu, \lambda) = \inf_x L(x, \mu, \lambda) \leq L(x^*, \mu, \lambda) \leq f_0(x^*)$$

We want to maximize the lower bound to make it tight

$$g(\mu^*, \lambda^*) = \max g(\mu, \lambda)$$

Primal and Dual Problems

Primal problem:

$$\begin{aligned} \text{minimize} \quad & f_0(x) \\ \text{subject to} \quad & f_i(x) \leq 0, \ i = 1, \ldots, m \\ & h_i(x) = 0, \ i = 1, \ldots, p \end{aligned}$$

Dual problem:

$$\begin{aligned} \text{maximize} \quad & g(\mu, \lambda) \\ \text{subject to} \quad & \lambda_i \geq 0, \ i = 1, \ldots, m \end{aligned}$$

Strong duality: For convex problems satisfying regularity conditions:

$$g(\mu^*, \lambda^*) = f_0(x^*)$$

Slater's condition: There exists an x inside the relative interior of the domain X such that $f_i(x) < 0, \ i = 1, \ldots, m$

KKT Conditions

Conditions for an optimal triplet (x^*, μ^*, λ^*):

$$\nabla f_0(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla f_i(x^*) + \sum_{j=1}^{p} \mu_j^* \nabla h_j(x^*) = 0 \quad \leftarrow \text{Stationarity}$$

$$\lambda_i^* f_i(x^*) = 0 \quad \leftarrow \text{Complementary slackness}$$

$$f_i(x^*) \leq 0$$
$$h_j(x^*) = 0 \quad \Big\} \text{Primal feasibility}$$

$$\lambda_i^* \geq 0 \quad \leftarrow \text{Dual feasibility}$$

KKT conditions generalize "gradient = 0" to constrained problems

Key Takeaways

What We Learned This Week

- Machine learning training can be framed as optimization of an objective function over model parameters
- Convex vs. non-convex problems differ fundamentally in guarantees, difficulty, and solution strategies
- Gradient descent optimizes smooth objectives using full-data gradients and has stable convergence
- Stochastic gradient descent uses noisy gradient estimates, enabling scalability to large datasets
- Learning rate, batch size, and stopping criteria critically affect optimization performance
- Matrix-vector formulations enable efficient, scalable implementations
- Constraints and regularization can be handled using Lagrangians, duality, and KKT conditions