Contents

1 Linear Algebra Tools

This chapter introduces inner product to give geometric meaning to vectors and vector spaces, enabling calculations of length, distance, and angles.

Definition (Symmetric Positive Definitive Matrix)**.** *A symmetric matrix $A \in \mathbb{R}^{n\times n}$ that satisfies*

$$\text{for every nonzero vector } x : x^T Ax > 0 \tag{1.1}$$

*is called **positive definite**. If only $\geq$ holds in 1.1, then A is called **positive semidefinite**.*

These properties helps in identifying positive definite matrices without having to check the definition explicitly:

1. The null space of A contains only the null vector;
2. The diagonal elements a_{ii} of A are positive;
3. The eigenvalues of A are real and positive.

1.1 Angles and Orthogonality

The angle ω between vectors x and y is computed as:

$$\cos\omega = \frac{\langle x, y\rangle}{\|x\|_2\|y\|_2}$$

Here, $\langle x, y\rangle$ denotes the inner product between x and y.
This angle indicated the vectors' similarity in orientation.

Definition (Orthogonal vectors)**.** *Two vectors are orthogonal if $\langle x, y\rangle = 0$. If additionally $\|x\| = 1 = \|y\|$, then x and y are orthonormal.*

Definition (Orthogonal matrix)**.** *A square matrix is an orthogonal matrix if and only if its columns are orthonormal so that*

$$AA^T = I = A^T A$$

which implies that

$$A^{-1} = A^T$$

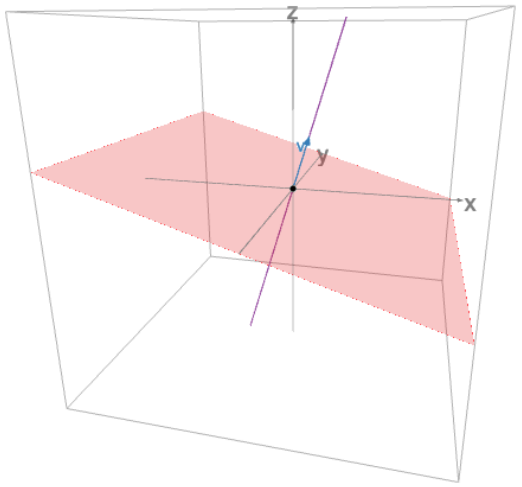
The length of a vector x is not changed when transforming it using an orthogonal matrix A.

$$\|Ax\|_2^2 = \|x\|_2^2$$

Moreover, the angle between any two vectors x, y is also unchanged when transforming both of them using an orthogonal matrix A.

Definition (Orthonormal Basis)**.** *In an n-dimensional vector space V with a basis set $\{b_1, \ldots, b_n\}$, if all the basis vectors are orthogonal to each other, the basis is called as an **orthogonal basis**. Additionally, if the length of each basis vector is 1, the basis is referred to as an **orthonormal basis**.*

We can also have vector spaces that are orthogonal to each other. Given a vector space V of dimension D, let's consider a subspace U of dimension M such that $U \subseteq V$. Then its **orthogonal complement** $U^\perp$ is a $D - M$ dimensional subspace V and contains all vectors in V that are orthogonal to every vector in U.



1.1.1 Orthogonal Projections

Projections are key linear transformations in machine learning and are particularly useful for handling high-dimensional data. Often, only a few dimensions in such data are essential for capturing the most relevant information. By projecting the original high-dimensional data onto a lower dimensional feature space, we can work more efficiently to learn about the dataset and extract significant patterns.

Definition (Projection)**.** *Let V be a vector space and $U \subseteq V$ a subspace of V. A linear mapping $\pi : V \to U$ is called **projection** if it satisfies $\pi^2 = \pi \circ \pi = \pi$.*

Given that linear mappings can be represented by transformation matrices, the above definition extends naturally to *projection matrices* P_π. These matrices exhibit the property that $P_\pi^2 = P_\pi$.
The projection $\pi_U(x)$ of a vector $x \in \mathbb{R}^n$ onto a subspace U is the closest point necessarily in U to x.

2 Matrix Decompositions

2.1 Eigenvalues and Eigenvectors

Eigenanalysis helps us understand linear transformations represented by a matrix A. Eigenvectors x are special vectors that only get scaled, not rotated, when multiplied by A. The scaling factor is the eigenvalue λ, which indicated how much x is stretched or shrunk. λ can also be zero.

Definition (Eigenvalue and Eigenvector)**.** *Let $A \in \mathbb{R}^{n\times n}$ be a square matrix. Then $\lambda \in \mathbb{R}$ is an **eigenvalue** of A and nonzero vector x is the corresponding **eigenvector** of A if*

$$Ax = \lambda x \tag{2.1}$$

*We call 2.1 the **eigenvalue equation**.*

The following statements are equivalent:

- λ is an eigenvalue of $A \in \mathbb{R}^{n\times n}$.
- A nonzero vector x exists such that $Ax = \lambda x$ or, equivalently, $(A - \lambda I_n)x = 0$ for $x \neq 0$.
- Then $A - \lambda I$ is a **singular matrix** and its determinant is **zero**.

Each eigenvector x has one unique eigenvalue λ, but each λ can have multiple eigenvectors.

Definition (Eigenspace and Eigenspectrum)**.** *For $A \in \mathbb{R}^{n\times n}$, the set of all eigenvectors of A associated with an eigenvalue λ spans a subspace of $\mathbb{R}^n$, which is called the **eigenspace** of A with respect to λ and is denoted by E_λ. The set of all eigenvalues of A is called the **eigenspectrum** of A.*

Definition. *Let λ_i be an eigenvalue of a square matrix A. Then the **geometric multiplicity** of λ_i is the number of linearly independent eigenvectors associated with λ_i. In other words, it is the dimensionality of the eigenspace spanned by the eigenvectors associated with λ_i.*

Theorem. *The eigenvectors $x_1, \ldots, x_n$ of a matrix $A \in \mathbb{R}^{n\times n}$ with n distinct eigenvalues $\lambda_1, \ldots, \lambda_n$ are linearly independent.*

This theorem states that eigenvectors of a matrix with n distinct eigenvalues form a basis of $\mathbb{R}^n$.

3 Vector calculus

Firstly, we'll explore partial derivatives and gradients, focusing on functions that take a vector as input and produce a single real number as output. These functions are formally represented as $f : \mathbb{R}^n \to \mathbb{R}$.
Subsequently, we will extend these ideas to functions that not only take a vector as input but also produce a vector as output. These functions can be written as $f : \mathbb{R}^n \to \mathbb{R}^m$.

3.1 Gradients of Real-Valued Functions

When we deal with a function that depends on multiple variables, such as $f(x) = f(x_1, x_2)$, we use the **gradient** to represent its derivative. The gradient is a vector composed of **partial derivates** of the function. To compute each partial derivates, we differentiate the function with respect to one variable while keeping all other variables constant.

$$\nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{1\times n} \tag{3.1}$$

where n is the number of variables.

Basic Rules of Partial Differentiation

Product rule:
$$\frac{\partial}{\partial x}(f(x)g(x)) = \frac{\partial f}{\partial x}g(x) + f(x)\frac{\partial g}{\partial x}$$

Sum rule:
$$\frac{\partial}{\partial x}(f(x) + g(x)) = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial x}$$

Chain rule:
$$\frac{\partial}{\partial x}(g \circ f)(x) = \frac{\partial}{\partial x}\left(g(f(x))\right) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial x}$$

In the context of the chain rule, consider f as implicitly a composition $f \circ g$.
If a function $f(x_1, x_2)$ is a function of x_1 and x_2, where $x_1(t)$ and $x_2(t)$ are themselves functions of a single variable t, the chain rule yields the partial derivates

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial t}{\partial x_2}\frac{\partial x_2}{\partial t}$$

Example

Consider $f(x_1, x_2) = x_1^2 + 2x_2$, where $x_1 = \sin t$ and $x_2 = \cos t$, then

$$\text{with} \quad \frac{\partial f}{\partial x_1} = 2x_1, \quad \frac{\partial f}{\partial x_2} = 2$$

$$\begin{aligned} \frac{\mathrm{d}f}{\mathrm{d}t} &= 2\sin t\frac{\partial \sin t}{\partial t} + 2\frac{\partial \cos t}{\partial t} \\ &= 2\sin t\cos t - 2\sin t \end{aligned}$$

If a function $f(x_1, x_2)$ is a function of x_1 and x_2, where $x_1(s, t)$ and $x_2(s, t)$ are themselves functions of two variables s and t, the chain rule yields the partial derivates

$$\frac{\mathrm{d}f}{\mathrm{d}(s,t)} = \begin{bmatrix} \frac{\partial f}{\partial s} & \frac{\partial f}{\partial t} \end{bmatrix}$$

where

$$\begin{aligned} \frac{\partial f}{\partial s} &= \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s} \\ \frac{\partial f}{\partial t} &= \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \end{aligned}$$

Another way to obtain these two partial derivatives is to represent the previous formula as a row vector containing the partial derivatives of f with respect to x_1 and x_2. This row vector is then multiplied by a matrix composed of the partial derivatives of x_1 and x_2 with respect to s and t. When you perform this multiplication, you get the exact same result as above.

$$\begin{bmatrix} \frac{\partial f}{\partial s} & \frac{\partial f}{\partial t} \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial s} & \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial s} & \frac{\partial x_2}{\partial t} \end{bmatrix}$$

Example

Given the following functions:
$g : \mathbb{R}^2 \to \mathbb{R}^2 \quad g(s,t) = (\sin(t)s, \cos(s)t)$
$f : \mathbb{R}^2 \to \mathbb{R} \quad f(x_1, x_2) = x_1^2 + 2x_2$
$f \circ g : \mathbb{R}^2 \to \mathbb{R}$
Compute $\nabla_{(s,t)}(f \circ g)$ and evaluate $\nabla_{(s,t)}(f \circ g)(0,0)$.

$$= \begin{bmatrix} 2s\sin(t) & 2 \end{bmatrix} \begin{bmatrix} \sin(t) & s\cos(t) \\ -t\sin(s) & \cos(s) \end{bmatrix}$$
$$= \begin{bmatrix} 2s\sin^2(t) - 2t\sin(s) \\ 2s^2\sin(t)\cos(t) + 2\cos t \end{bmatrix} = (0, 2)$$

3.2 Gradients of Vector-Valued Functions

We can express a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$ as a column vector of m real-valued functions $f_i : \mathbb{R}^n \to \mathbb{R}$. Given an input vector $x = [x_1, \ldots, x_n]^T \in \mathbb{R}^n$, the output is defined as:

$$f(x) = \begin{bmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{bmatrix} \in \mathbb{R}^m$$

Definition (Jacobian)**.** *By contrast, in Equation 3.1, each partial derivative $\frac{\partial f}{\partial x_i}$ is a column vector.*

$$J = \nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$
$$J(i,j) = \frac{\partial f_i}{\partial x_j}$$

*The collection of all first-order partial derivatives of a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$ is called the **Jacobian**. The Jacobian J is an $m \times n$ matrix.*

Example

$$f : \mathbb{R}^2 \to \mathbb{R}^3, \quad f : (x_1, x_2) = \begin{pmatrix} x_1 + x_2 \\ 2x_1^2 - x_2 \\ -x_1 x_2 \end{pmatrix}$$
$$J(f) : \mathbb{R}^2 \to \mathbb{R}^{3\times 2}, \quad J(i,j) = \begin{bmatrix} 1 & 1 \\ 4x_1 & -1 \\ -x_2 & -x_1 \end{bmatrix}, \quad J(1,1) = \begin{bmatrix} 1 & 1 \\ 4 & -1 \\ -1 & -1 \end{bmatrix}$$

Example

Let us consider the linear model

$$y = \Phi\theta$$

where $\theta \in \mathbb{R}^D$ is a parameter vector, $\Phi \in \mathbb{R}^{N\times D}$ are input features, and $y \in \mathbb{R}^N$ are the corresponding observations. We define the functions

$$e : \mathbb{R}^D \to \mathbb{R}^N, \quad e(\theta) = y - \Phi\theta$$
$$L : \mathbb{R}^N \to \mathbb{R}, \quad L(e) = \|e\|_2^2, \quad L(\theta) = \|y - \Phi\theta\|_2^2$$

This is called a **least-squares loss** function.
We want to find $\frac{\partial L}{\partial \theta}$, which is derivative of the loss function with respect to the parameters θ. This will allow us to find the optimal θ that minimizes the loss function $L(\theta)$.
The chain rule allows us to compute the gradient as

$$\frac{\partial L}{\partial e} = \frac{\partial L}{\partial e}\frac{\partial e}{\partial \theta}$$

We know that $\|e\|_2^2 = e^T e$ and so

$$\frac{\partial L}{\partial e} = 2e^T \in \mathbb{R}^{1\times N}$$

Furthermore, we obtain

$$\frac{\partial e}{\partial \theta} = -\Phi \in \mathbb{R}^{N\times D}$$

such that our desired derivative is

$$\nabla L_\theta = -2e^T\Phi = -2\underbrace{(y^T - \theta^T\Phi^T)}_{1\times N}\underbrace{\Phi}_{N\times D} \in \mathbb{R}^{1\times D}$$

3.3 Backpropagation and Automatic Differentiation

In machine learning, finding optimal model parameters often involves performing gradient descent. This requires computing the gradient of a learning objective with respect to the model's parameters. Calculating the gradient explicitly can be impractical due to the complexity and length of the resulting derivative equations. To address this, the **backpropagation** algorithm was introduced in 1962 as an efficient way to compute these gradients, particularly for neural networks.

In neural networks, the output y is computed through a multi-layered function composition $y = (f_K \circ f_{K-1} \circ \cdots f_1)(x)$. Here, x are the inputs (e.g., images), y are the observations (e.g., class labels). Each functions $f_i, i = 1, \ldots, K$, has its own parameters. Specifically, in the i^{th} layer, the function is given $f_i(x_{i-1}) = \sigma(A_{i-1} + b_{i-1})$, where x_{i-1} is the output from layer $i-1$ and σ is an activation function.

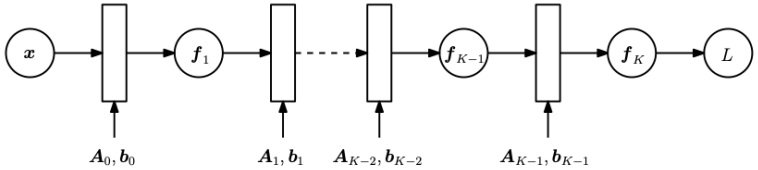


Figure 5.2 Forward pass in a multi-layer neural network to compute the loss L as a function of the inputs $\boldsymbol{x}$ and the parameters $\boldsymbol{A}_i,\ \boldsymbol{b}_i$.

In order to train a neural network, we aim to minimize a loss function L with respect to all parameters A_j, b_j for $j = 0, \ldots, K-1$. Specifically, we're interested in optimizing these parameters to minimize the squared loss given by

$$L(\theta) = \|y - f_K(\theta, x)\|^2$$

where $\theta = \{A_0, b_0, \ldots, A_{K-1}, b_{K-1}\}$.

To minimize $L(\theta)$ we need to compute its gradients of L to the parameter set θ. This involes calculating the partial derivatives of L with respect to the parameters $\theta_j = \{A_j, b_j\}$ for each layer $j = 0, \ldots, K-1$. The chain rule allows us to determine the partial derivatives as

$$\begin{aligned}
\frac{\partial L}{\partial \theta_{K-1}} &= \frac{\partial L}{\partial f_K}\frac{\partial f_K}{\partial \theta_{K-1}} \\
\frac{\partial L}{\partial \theta_{K-2}} &= \frac{\partial L}{\partial f_K}\boxed{\frac{\partial f_K}{\partial f_{K-1}}\frac{\partial f_{K-1}}{\partial \theta_{K-2}}} \\
\frac{\partial L}{\partial \theta_{K-3}} &= \frac{\partial L}{\partial f_K}\frac{\partial f_K}{\partial f_{K-1}}\boxed{\frac{\partial f_{K-1}}{\partial f_{K-2}}\frac{\partial f_{K-2}}{\partial \theta_{K-3}}} \\
\frac{\partial L}{\partial \theta_i} &= \frac{\partial L}{\partial f_K}\frac{\partial f_K}{\partial f_{K-1}}\cdots\boxed{\frac{\partial f_{i+2}}{\partial f_{i+1}}\frac{\partial f_{i+1}}{\partial \theta_i}}
\end{aligned}$$

The red terms are partial derivatives of the output of a layer with respect to its inputs, whereas the blue terms are partial derivatives of the output of a layer with respect to its parameters.

The key insight of backpropagation is to reuse previously computed derivatives to avoid redundant calculations. When we've computed the partial derivatives $\frac{\partial L}{\partial \theta_{i+1}}$, we can reuse them to efficiently calculate the partial derivatives $\frac{\partial L}{\partial \theta_i}$.

It turns out that backpropagation is a special case of a set of techniques known as **automatic differentiation**. Automatic differentiation numerically evaluate the exact (up to machine precision) gradient of a function by working with intermediate variables and applying the chain rule.

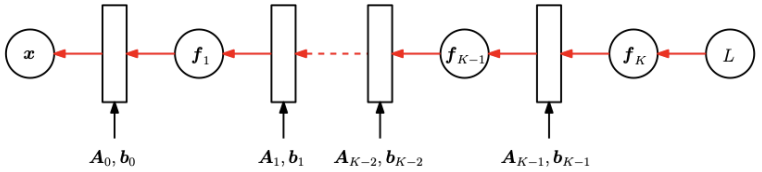


Figure 5.2 Backward pass in a multi-layer neural network to compute the gradients of the loss function.

Example

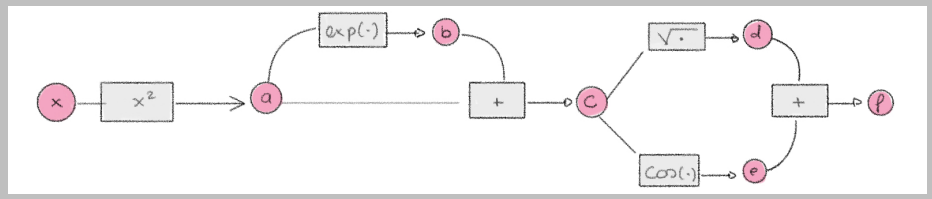
Consider the real-valued function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2))$$

Another way to attach this would be to just define some *intermediate variables*. Say

$$\begin{aligned}
a &= x^2 \\
b &= \exp(a) \\
c &= a + b \\
d &= \sqrt{c} \\
e &= \cos(c) \\
f &= d + e
\end{aligned}$$

The set of equations that include intermediate variables can be thought of as a computational graph



By looking at the computation graph, we can compute $\frac{\partial f}{\partial x}$ by working backward from the end of the graph and obtain the derivative of each variable, making the use of the derivatives of the children of that variable

$$\begin{aligned}
\frac{\partial f}{\partial d} &= \frac{\partial f}{\partial e} = 1 \\
\frac{\partial f}{\partial c} &= \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} + \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} \\
\frac{\partial f}{\partial b} &= \frac{\partial f}{\partial c}\frac{\partial c}{\partial b} \\
\frac{\partial f}{\partial a} &= \frac{\partial f}{\partial b}\frac{\partial b}{\partial a} + \frac{\partial f}{\partial c}\frac{\partial c}{\partial a} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial a}\frac{\partial a}{\partial x}
\end{aligned}$$

We observe that the computation required for calculating the derivative is of similar complexity as the computation of the function itself (forward pass).

Automatic differentiation is a formalization of last Example. Let $x_1, \ldots, x_d$ be the input variables to the function, $x_{d+1}, \ldots, x_{D-1}$ be the intermediate variables, and x_D the output variable. Then the computation graph can be expressed as follows:

$$\text{For } i = d+1, \ldots, D: \quad x_i = g_i(x_{Pa}(x_i)) \tag{3.2}$$

where the $g_i(\cdot)$ are elementary functions and $x_{Pa}(x_i)$ are the parent nodes of the variable x_i in the graph.
Recall that by definition $f = x_D$ and hence

$$\frac{\partial f}{\partial x_D} = 1$$

For other variables x_i, we apply the chain rule

$$\frac{\partial f}{\partial x_i} = \sum_{x_j : x_i \in Pa(x_j)} \frac{\partial f}{\partial x_j}\frac{\partial x_j}{\partial x_i} = \sum_{x_j : x_i \in Pa(x_j)} \frac{\partial f}{\partial x_j}\frac{\partial g_j}{\partial x_i} \tag{3.3}$$

where $Pa(x_j)$ is the set of parent nodes of x_j in the computation graph. Equation 3.2 is the forward pass, whereas 3.3 is the backward pass.
The automatic differentiation approach works whenever we have a function that can be expressed as a computation graph, where the elementary functions are differentiable.

4 Continuous Optimization

Training a machine learning essentially involves identifying a good set of parameters. What constitutes "good" is defined by the objective function. Optimization algorithms are employed to locate the best possible value of this function. Typically, the aim is to minimize the objective function, implying that the best value is the minimum one.

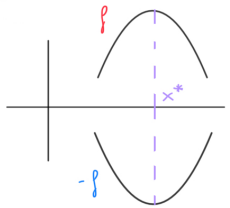


Figure 1: $\arg\max_{x\in\mathbb{R}^n} f(x) = \arg\min_{x\in\mathbb{R}^n} -f(x)$

We will assume in this chapter that our objective function $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable, hence we have access to a gradient to help us find the optimal value. Intuitively, finding the best value is like finding the valleys of the objective function, and the gradients point us uphill. The idea is to move downhill (opposite to the gradient) and hope to find the deepest point.

4.1 Conditions for the existence of the minimum

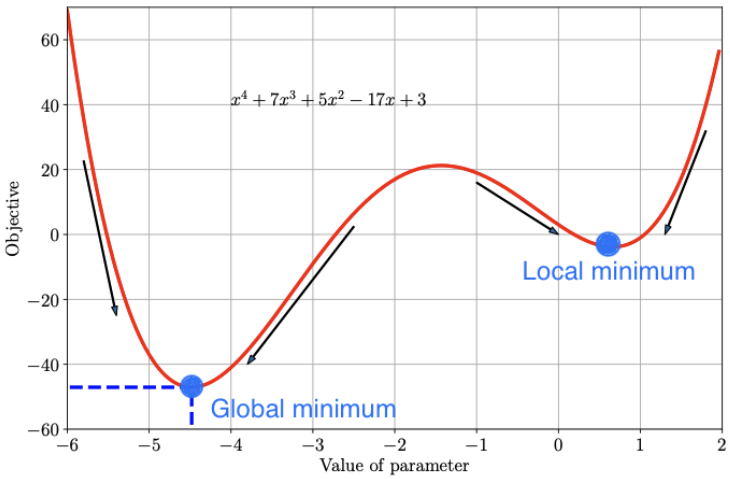
Definition. *f is differentiable if the partial derivates $\frac{\partial f}{\partial x_i}, i = 1, \dots, n$ exist and are continuous.*

Definition. *$x^* \in \mathbb{R}^n$ is a (strict) **local minimum** of f if there exists $\epsilon > 0$ such that:*

$$f(x^*)(<) \leq f(x) \quad \forall x : \|x - x^*\| < \epsilon$$

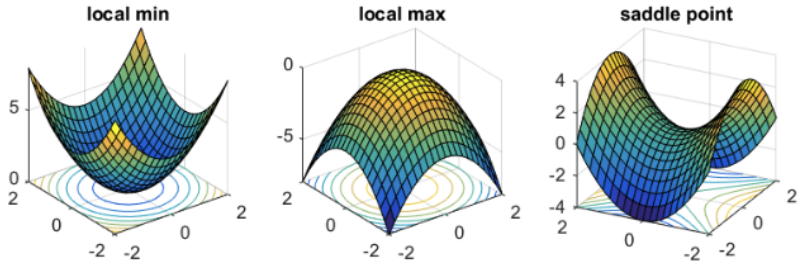
Definition. *$x^* \in \mathbb{R}^n$ is a (strict) **global minimum** of f if*

$$f(x^*)(<) \leq f(x) \quad \forall x \in \mathbb{R}^N$$



Definition (First order conditions)**.** *If x^* is a minimum point of f, then $\nabla f(x^*) = 0$. Furthermore, if $\nabla f(x^*) = 0$ for $x^* \in \mathbb{R}^n$, then x^* can be either a (local) minimum, a (local) maximum or a saddle point of $f(x)$.*

Consequently, we want to find a point $x^* \in \mathbb{R}^n$ such that $\nabla f(x^*) = 0$. Those points are stationary points for f.



Definition (Second order conditions)**.** *if f is twice differentiable and if $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ (the hessian of f) is positive definitive then x^* is a strict local minimum for f.*

4.2 Algorithm to compute the minimum

Iterative methods. Given an initial vector $x_0 \in \mathbb{R}^n$, it is possible to approximate a solution to a given optimization problem by applying iterative methods. In particular, by using these methods, one can compute x_{k+1} as follows:

$$x_{k+1} = g(x_k)$$

until convergence. In this case g is an arbitrary function. Using these methods, $x_k \to x^*$ for $k \to \infty$, where x^* is a stationary point.

Descent methods are iterative methods in which one can compute x_{k+1} as follows:

$$x_{k+1} = x_k + \alpha_k p_k$$

where $p_k \in \mathbb{R}^n$ and $\alpha_k \in \mathbb{R}$.

Definition. *p_k is called a **descent direction** for f in x if there exists $\alpha_k > 0$ such that:*

$$f(x_k + \alpha_k p_k) < f(x_k)$$

In this case:

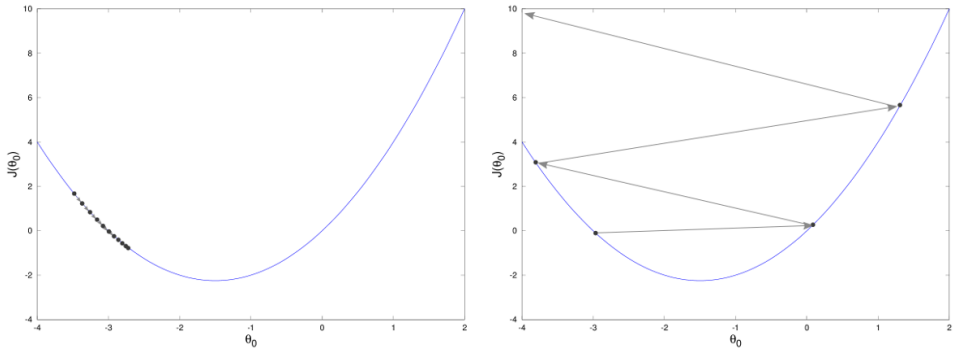
$$p_k^T \nabla f(x_k) < 0 \quad \text{if } p \neq 0$$

In other words, descent direction is a direction that along that line decreases the function.

and α_k is a positive parameter called **step size** that measures the step along the direction p_k.
The direction p_k corresponds in the **gradient descent method** to $-\nabla f(x_k)$, thus

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

The selection of α_k is crucial task for ensuring convergence to the minimum of a function. A step size that is too small can lead to excessively slow convergence, potentially never reaching the minimum, while a step size that is too large may cause bouncing around the minimum without ever converging to it.



If α_k is chosen with the **backtracking procedure** (Armijo rule) then the algorithm converges to a stationary point of f. The idea is to start from an initial value for α_k, and then reducing it as $\alpha_k = \phi \alpha_k$ with $\phi < 1$ until the following condition is met:

$$f(x_k - \alpha_k \nabla f(x_k)) \leq f(x_k) - \sigma \alpha_k \|\nabla f(x_k)\|^2$$

where σ is typically 0.25 and lies in the range $(0, 0.5)$. The typical value of ϕ is also 0.5.
Since we cannot run infinite iterations (there exists a truncation error), a **stopping criteria** is needed:

- We can use the property of x^*, where $\nabla f(x^*) = 0$, to test whether the approximation x_k is close to the solution within a specified tolerance. The criteria can be:
  - **Absolute criterion**: $\|\nabla f(x_k)\| < \tau_A$
  - **Relative criterion**: $\frac{\|\nabla f(x_k)\|}{\|\nabla f(x_0)\|} < \tau_R$
- We can set a maximum number, k^*, of iterations.
- Additionally, as an heuristic, we stop when the norm of the gradient starts to flatten.

```
input: f, x_0
while stopping criteria holds:
     p_k = - grad(f(x_k))
     a_k = backtrack_procedure
     x_k = x_k + a_k * p_k
     k = k + 1
 output: x_k
```

Initialization. The initial point x_0 influences the local minimum that is found. It is usually chosen randomly within the range of $[-1, 1]$ or $[0, 1]$. Moreover, if $f(x)$ is convex, then every stationary point is a global minimum of $f(x)$ and the choice of x_0 isn't important. Otherwise when $f(x)$ isn't convex, we have to choose an initial point as closest as possible to the *right* stationary point.

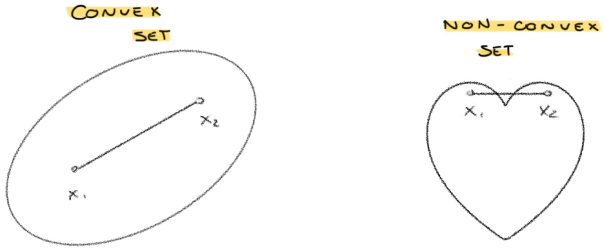
The algorithm introduced doesn't always work well because of the following reasons:

- If the objective function has flat areas or potholes on its loss surface, the procedure might be too slow or lead to a poor solution. Techniques such momentum, that inherit the rate of descent from previous steps, are often able to navigate through local potholes and flat regions. The idea is akin a stone rolling down a hill, gathering speed as it rolls down.
- If the components of the gradient have very different magnitudes, this causes problems for gradient-descent methods.
- If the objective function has a steep region in its loss surface, the descent direction within this area changes quickly. This rapid change increase the likelihood of the divergence.

- The objective function may present non-differentiable points, which can create problems in calculating the gradient.

4.3 Convex functions

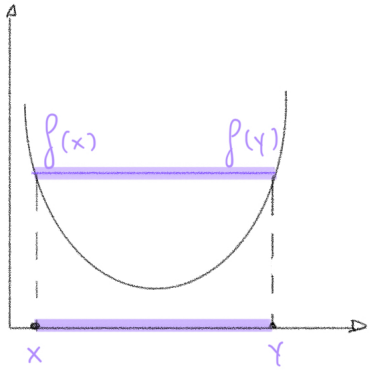
A convex set is a set where, for any two points within the set, the line segment connecting these two points entirely lies within the set.



Definition. *Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$, where Ω is a convex set. The function f is (strictly) **convex** if, $\forall x, y \in \Omega$ and $\forall \theta : 0 \leq \theta \leq 1$, the following inequality holds:*

$$f(\theta x + (1-\theta)y)(<) \leq \theta f(x) + (1-\theta)f(y)$$

In other words, the function of a point lying on the segment connecting x and y is below the segment connecting $f(x)$ and $f(y)$.



4.3.1 Quadratic functions

An example of a strictly convex function is the quadratic function, which take the following form:

$$f(x) = \frac{1}{2}x^T Bx + c^T x + (w)$$

with $b, c \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$ symmetric positive definitive.
A typical quadratic function is the least square:

$$\|Ax - b\|^2$$

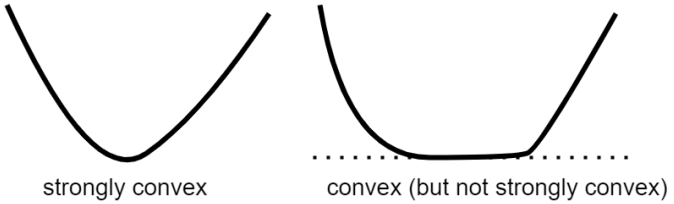
Proof.

$$\begin{aligned}
\frac{1}{2}\|Ax-b\|^2 &= \frac{1}{2}(Ax-b)^T(Ax-b) \\
&= \frac{1}{2}(x^TA^T - b^T)(Ax-b) \\
&= \frac{1}{2}(x^TA^TAx - b^TAx - x^TA^Tb + b^Tb) \\
&= \frac{1}{2}x^T \underbrace{A^TA}_{B} x \underbrace{-b^TA}_{c^T} x + \frac{1}{2}b^Tb
\end{aligned}$$

which is exactly the same as the above form. ■

4.3.2 Properties

1. If f is convex, any point of local minimum is also a global minimum.
2. While a convex function can have multiple local minima, a strictly convex function has only one local minimum, which is also a global minimum.



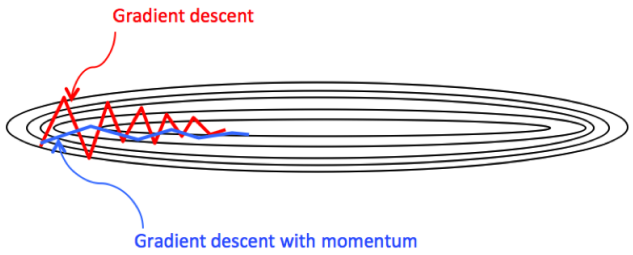
3. If f is convex and differentiable any stationary point is a global minimum for f.

4.4 Variants of gradient descent algorithm

- Gradient descent with **momentum** method improves the convergence of the gradient descent method by memorizing and utilizing, at each step, what happened in the previous iteration. In particular:

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k) + \beta \Delta x_k$$

where $\beta \in [0, 1]$ and $\Delta x_k = x_k - x_{k-1}$ is the update obtained at iteration k. This update smooths the gradient updates and, thus, reduces the oscillations. This approach is analogous to a heavy ball in motion, where the momentum term represents the ball's resistance to change directions.



- In machine learning, we typically train models by finding the optimal vector of parameters, denoted as θ, that minimize a loss function $L(\theta)$. We can see this loss functions as the aggregate of individual losses L_n incurred by each of the N data points in the training set. Thus, the loss function is expressed as:

$$L(\theta) = \sum_{n=1}^{N} L_n(\theta)$$

The gradient of such loss function is then computed as follows:

$$\nabla(\theta) = \sum_{n=1}^{N} \nabla L_n(\theta_k)$$

In gradient descent, the optimization is performed by using the full training set and by updating the vectors of parameters according to:

$$\theta_{k+1} = \theta_k - \alpha_k \sum_{n=1}^{N} (\nabla L_n(\theta_k))$$

Evaluating the sum gradient may require expensive evaluations of the gradients from all individual functions L_n. If we consider the term $\sum_{n=1}^{N}(\nabla L_N(\theta_k))$, we can reduce the amount of the computation by taking a sum over a smaller set of L_n.

  - *batch* $\rightarrow$ all L_n functions;
  - *mini-batch* $\rightarrow$ randomly choose a subset of L_n functions. This can be a single L_n or more. Large mini-batches lead to more stable convergence, but the calculations will be more expensive. Small mini-batches are quick to estimate, and the noise in gradient estimation might help to escape from some bad local optima.

The technique is used by **stochastic gradient descent**. It requires more iterations to converge, but with a small enough α_k, it almost surely converges to a local minimum. Why use it? If there are constraints, such as memory limitations.

Moreover, with stochastic gradient descent, we speak about **epoch** and not iterations. An epoch refers to the iterations necessary to "see" all the data.

$$\nabla L(\theta) = \nabla L_{n_1}(\theta) \quad i = 1,\ n_1 \in \{1 \dots N\}$$

$$\nabla L(\theta) = \nabla L_{n_2}(\theta) \quad i = 1,\ n_2 \in \{1 \dots N\} \setminus \{n_1\}$$

The mini-batches do not repeat themselves before the entire epoch has been completed.

5 Probability and statistics