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Ministry of Higher Education and Scientific Research

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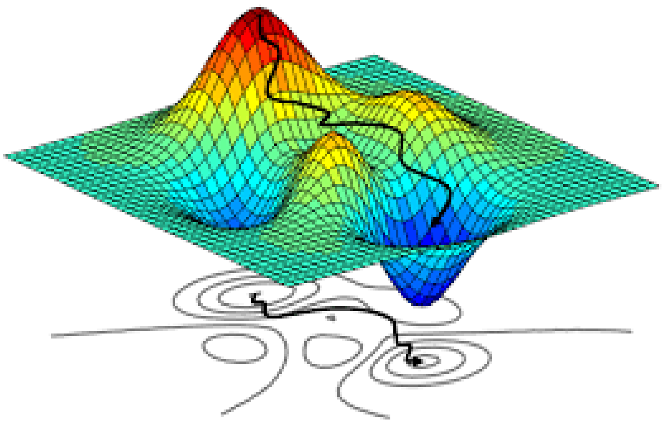

Unconstrained Optimization

Course Handout

Academic Level: 3nd Year LMD Mathematics

Domain: Mathematics Field: Mathematics

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Preface

This course handout, aligned with the curriculum, covers all the mathematical knowledge required at this stage of university (Third year in mathematics field). It aims to provide third-year students with a self-study tool, which contributes to enriching their knowledge and formation,

The overage consists of consists of several chapters, which are as follows:

1/ Introduction to Optimization.

2/ Optimization in the Set of Real Numbers.

3/ Unconstrained Optimization in $\mathbb{R}^n$.

4/ Nonlinear Unconstraints Optimization Problems.

5/ Some Numerical Methods for Solving Unconstraints Optimization Problems.

6/ Annexe (Exams).

The lesson presented in the form of summaries, accompanied by examples and practical exercises with complete solutions, designed to enhance students' skills and foster their creativity, a complete written solution to the problems, and model solutions that students can reuse to solve any problem related to the concepts covered in the chapter.

It also includes past exams and problems covering the main topics of the course. These problems are designed to test technical computational proficiency, as well as conceptual understanding and the ability to apply theoretical results to practical applications.

Finally, this overage is also beneficial for students in other grades who wish to consolidate their knowledge, teachers seeking comprehensive and varied lessons, and anyone who wants to develop their mathematical skills for personal or professional purposes.

We are also ready to accept all criticism and feedback in order to improve the quality of work and make the best use of it.

Contents

Introduction

Optimization is the study of selecting the best possible solution from a set of available alternatives. It provides a mathematical framework for modeling decision-making problems in which limited resources must be used efficiently to achieve a desired objective. Optimization problems arise naturally in engineering, economics, operations research, physics, and modern fields such as data science and artificial intelligence.

By formulating real-world situations in terms of objective functions and variables, optimization allows complex systems to be analyzed in a structured and systematic way. The field combines theoretical analysis with numerical algorithms to find optimal or near-optimal solutions, even for large-scale and highly nonlinear problems. As a result, optimization serves as a fundamental tool for improving performance, reducing costs, and supporting informed decisions across many disciplines.

Unconstrained optimization stands as one of the most fundamental and extensively studied domains in applied mathematics, operations research, and computer science. At its core, it addresses the elegant yet challenging problem of finding extremal points of functions without any restrictions on the variables. The simplicity of its formulation—minimize $f(x)$ where $x \in \mathbb{R}^n$—belies the rich mathematical theory, diverse algorithmic approaches, and wide-ranging applications that have developed around it over centuries.

Historical Perspective:

The origins of unconstrained optimization trace back to the very foundations of calculus, with Newton and Leibniz establishing the necessary conditions for optimality. However, the field truly blossomed in the 20th century with the advent of computers, which transformed optimization from a theoretical pursuit into a practical computational discipline. From Cauchy's early work on gradient descent in 1847 to the modern era of stochastic optimization for machine learning, the evolution of unconstrained optimization methods mirrors the progression of computational mathematics itself.

Theoretical Foundations:

The mathematical framework of unconstrained optimization rests on three pillars:

1. **Optimality Conditions**: First-order (stationary points) and second-order (curvature) conditions provide necessary and sufficient criteria for local optimality.
2. **Convergence Analysis**: Understanding how and when iterative algorithms converge to solutions, and at what rates, forms the theoretical backbone of the field.
3. **Complexity Theory**: Characterizing the computational cost of solving optimization problems, particularly in terms of problem dimension and desired accuracy.

Unconstrained optimization algorithms span a continuum from simple to sophisticated. Where the 21st century has witnessed remarkable developments in unconstrained optimization, driven largely by the demands of machine learning and data science.

For the practical considerations:

In practice, successful unconstrained optimization requires careful attention to several factors:

$$\begin{aligned}
&\text{Problem Scaling}: \text{Proper conditioning of the optimization problem}\\
&\text{Algorithm Selection}: \text{Matching method characteristics to problem properties}\\
&\text{Stopping Criteria}: \text{Balancing accuracy with computational cost}\\
&\text{Implementation Details}: \text{Numerical stability and computational efficiency}
\end{aligned}$$

Applications and Impact:

The reach of unconstrained optimization extends across virtually all scientific and engineering disciplines:

- Machine Learning.
- Scientific Computing.
- Engineering Design.
- Operations Research.
- Statistics.

To the Reader:

Whether you are a student encountering optimization for the first time, a researcher developing new methods, or a practitioner applying optimization to real-world problems, this material aims to provide both the foundational knowledge and the practical skills needed for effective work in unconstrained optimization. The journey through this field reveals not just algorithms for finding minima, but a deeper understanding of how mathematical structure can be exploited for computational advantage.

The beauty of unconstrained optimization lies in its perfect blend of mathematical elegance and practical utility—a testament to the power of abstraction in solving concrete problems. As you explore these methods, remember that each algorithm tells a story of mathematical insight translated into computational progress.

Chapter 1

Introduction to Optimization

1.1 Definition of Optimization Problem

Definition 1.1 (Optimization Problem)**.** *An optimization problem consists of finding the best element from some set of available alternatives. Formally, it can be written as:*

$$\begin{aligned} \underset{x}{\textit{minimize}} \quad & f(x) \\ \textit{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_j(x) = 0, \quad j = 1, \ldots, p \\ & x \in X \end{aligned}$$

where:

- $x \in \mathbb{R}^n$ *is the* ***decision variable***
- $f : \mathbb{R}^n \to \mathbb{R}$ *is the* ***objective function***
- $g_i : \mathbb{R}^n \to \mathbb{R}$ *are* ***inequality constraints***
- $h_j : \mathbb{R}^n \to \mathbb{R}$ *are* ***equality constraints***
- $X \subseteq \mathbb{R}^n$ *is the* ***feasible set***

Optimization problems can be transformed between equivalent forms:

1. **Maximization to Minimization:**

$$\max_{x \in X} f(x) \quad \Leftrightarrow \quad \min_{x \in X} [-f(x)]$$

2. **Inequality Constraints:**

$$g_i(x) \geq 0 \quad \Leftrightarrow \quad -g_i(x) \leq 0$$

1.2 Types of Optimization Problems

1. **Linear Programming (LP):** Both objective and constraints are linear
2. **Quadratic Programming (QP):** Quadratic objective, linear constraints
3. **Nonlinear Programming (NLP):** Nonlinear objective or constraints
4. **Integer Programming (IP):** Some or all variables are integers
5. **Convex Optimization:** Convex objective and convex feasible set
6. **Non-convex Optimization:** Non-convex objective or constraints

1.3 Mathematical Modeling

Modeling an optimization problem is the mathematical formulation of a physical, economic, human, etc., phenomenon. It involves three steps:

1. Identification of decision variables, denoted as $x = (x_1, x_2, \ldots, x_n)^T$ (a vector).
2. Definition of an objective function (criterion), denoted as $f(x)$.
3. Description of the constraints imposed on the decision variables.

1.3.1 Example: Projectile Motion

A projectile is launched vertically at a speed of 50 m/s in the absence of wind. After how much time and at what altitude will it reach its maximum height? How can this be determined?
Mathematical Modeling:

1. **Decision variables:** A single decision variable will be used, denoted as t (the number of seconds elapsed since the projectile's launch).
2. **Objective function:** The goal is to identify the maximum altitude reached by the object. This involves the formula for altitude as a function of time (uniformly accelerated motion).

$$S(t) = -\frac{g}{2}t^2 + v_0 t + h_0 = -\frac{9.81}{2}t^2 + 50t$$

where h_0 (initial altitude) is assumed to be zero.

3. **Constraints:** No constraints are necessary.

We thus obtain the optimization problem:

$$\max_{t \in \mathbb{R}} \left(-\frac{9.81}{2} t^2 + 50t \right)$$

1.3.2 Maximizing Rectangle Area

Problem Statement:

Find the rectangle with the greatest possible area given that its perimeter is fixed at 120 meters.

Mathematical Modeling:

Step 1: Variable definition Let:

- x = length of the rectangle (in meters)
- y = width of the rectangle (in meters)
- P = perimeter = 120 m
- A = area of the rectangle (in square meters)

Step 2: Mathematical relations

1. **Perimeter constraint:**

$$P = 2x + 2y = 120$$

2. **Area function:**

$$A = x \cdot y$$

3. **From the perimeter constraint, we can express y in terms of x:**

$$2x + 2y = 120 \implies x + y = 60 \implies y = 60 - x$$

4. **Substitute into the area function:**

$$A(x) = x \cdot (60 - x) = 60x - x^2$$

Step 3: Optimization problem We need to solve:

$$\max_{x > 0} A(x) = 60x - x^2$$

subject to the implicit constraint $0 < x < 60$ (since $y = 60 - x > 0$).

1.3.3 Spring-Mass System

Problem Description:

A mass m attached to a spring with spring constant k undergoes simple harmonic motion. The total energy is:

$$E(x,v) = \frac{1}{2}kx^2 + \frac{1}{2}mv^2$$

where x is displacement from equilibrium. and v is velocity. The equilibrium position minimizes potential energy.

Mathematical Model:

$$\min_{x\in\mathbb{R}} U(x) = \frac{1}{2}kx^2$$

The solution is clearly $x^* = 0$ (equilibrium position).

1.3.4 Point of Minimal Distance to a Set of Points

Problem Description:

Find the point $\mathbf{x}^* \in \mathbb{R}^n$ that minimizes the sum of squared distances to m given points $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_m \in \mathbb{R}^n$.

Mathematical Model:

$$\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}) = \sum_{i=1}^{m} \|\mathbf{x} - \mathbf{a}_i\|^2 \tag{1.3.1}$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{n}(x_j - a_{ij})^2 \tag{1.3.2}$$

Special Case: Centroid

For $n = 2$ with points (x_i, y_i), the solution is the centroid:

$$x^* = \frac{1}{m}\sum_{i=1}^{m} x_i, \quad y^* = \frac{1}{m}\sum_{i=1}^{m} y_i$$

1.3.5 Shortest Distance from Point to Line

Problem: Find the shortest distance from point $(3,4)$ to rectum $y = 2x+1$.

Mathematical Model

- Any point on rectum : $(x, 2x+1)$

- Distance from $(3,4)$ to $(x,2x+1)$:

$$\begin{aligned} d(x) &= \sqrt{(x-3)^2+(2x+1-4)^2} \\ &= \sqrt{(x-3)^2+(2x-3)^2} \end{aligned}$$

- Instead of square root, square the distance (to simplify derivative):

$$D(x) = [d(x)]^2 = (x-3)^2+(2x-3)^2$$

Find x that minimizes the function $D(x)$.

$$\min_{x\in\mathbb{R}} D(x) = (x-3)^2+(2x-3)^2. \tag{1.3.3}$$

1.3.6 Box with Maximum Volume

Problem We have a 30×20 cm sheet. We want to cut squares from corners and fold sides to make a box. What size square should be cut to maximize box volume?

Mathematical Model

- x = side length of cut square (cm)
- After cutting:
  - Box length: $30-2x$
  - Box width: $20-2x$
  - Box height: x
- Volume: $V(x) = (30-2x)(20-2x)x$
- Conditions: $0 < x < 10$ (because $20-2x > 0$)

We need to solve:

$$\max_{x>0} V(x) = (30-2x)(20-2x)x$$

subject to the implicit constraint $0 < x < 10$.

1.3.7 Production Planning Problem

Problem Description:

Table of figures 1.1: Production Planning Data

	Product P_1	Product P_2	Available Hours
Machine M_1	2	3	120
Machine M_2	4	2	80
Machine M_3	1	2	60
Profit per unit	5	4	

A factory produces two products, P_1 and P_2, using three machines M_1, M_2, and M_3. The time required (in hours) per unit product on each machine, available machine hours, and profit per unit are given in Table 1.1.

Mathematical Model:

Let x_1 and x_2 be the number of units of P_1 and P_2 to produce, respectively.

$$
\begin{aligned}
\text{Maximize} \quad & z = 5x_1 + 4x_2 \\
\text{subject to} \quad & 2x_1 + 3x_2 \leq 120 \quad \text{(Machine } M_1 \text{ constraint)} \\
& 4x_1 + 2x_2 \leq 80 \quad \text{(Machine } M_2 \text{ constraint)} \\
& x_1 + 2x_2 \leq 60 \quad \text{(Machine } M_3 \text{ constraint)} \\
& x_1, x_2 \geq 0 \quad \text{(Non-negativity)}
\end{aligned}
$$

1.3.8 Transportation Problem

Problem Description:

Goods must be shipped from m sources (warehouses) to n destinations (stores). Let:

- a_i: supply at source i, $i = 1, \ldots, m$
- b_j: demand at destination j, $j = 1, \ldots, n$
- c_{ij}: cost to ship one unit from source i to destination j
- x_{ij}: amount shipped from i to j (decision variable)

Mathematical Model:

$$
\begin{aligned}
\text{Minimize} \quad & z = \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij} \\
\text{subject to} \quad & \sum_{j=1}^{n} x_{ij} = a_i, \quad i = 1,\dots,m \quad \text{(Supply constraints)} \\
& \sum_{i=1}^{m} x_{ij} = b_j, \quad j = 1,\dots,n \quad \text{(Demand constraints)} \\
& x_{ij} \geq 0, \quad \forall i,j
\end{aligned}
$$

1.3.9 Production with Environmental Concerns

Problem Description:

A company produces two products with conflicting objectives: maximize profit and minimize pollution.

Mathematical Model:

Let x_1, x_2 be production quantities.

$$
\begin{aligned}
\text{Maximize} \quad & f_1(x) = 5x_1 + 3x_2 \quad \text{(Profit)} \\
\text{Minimize} \quad & f_2(x) = 2x_1 + 4x_2 \quad \text{(Pollution)} \\
\text{subject to} \quad & 3x_1 + 2x_2 \leq 100 \quad \text{(Labor)} \\
& x_1 + 3x_2 \leq 80 \quad \text{(Material)} \\
& x_1, x_2 \geq 0
\end{aligned}
$$

1.3.10 Conclusion

Mathematical modeling provides a rigorous framework for decision-making. The choice of model depends on problem characteristics: linearity, discreteness, convexity, and number of objectives. Modern optimization software can solve large-scale instances of these models.

1.4 Theorem (Taylor's Formula with Integral Remainder)

Let f be a function of class C^{n+1} on an interval containing a and x. Then for any $n \in \mathbb{N}$,

$$
f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + R_n(x)
$$

where the remainder $R_n(x)$ is given in **integral form** by

$$\boxed{R_n(x) = \frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt}.$$

1.4.1 Proof

We proceed by induction on n.

Base case $(n = 0)$

For $n = 0$, the formula becomes

$$f(x) = f(a) + \int_a^x f'(t)\,dt,$$

which is precisely the Fundamental Theorem of Calculus. Hence the base case holds.

Inductive step

Assume the formula holds for some integer $n \geq 0$:

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt.$$

We prove it holds for $n+1$. Consider the integral remainder term:

$$R_n(x) = \frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt.$$

Integrate by parts. Let

$$u = f^{(n+1)}(t), \quad dv = (x-t)^n\,dt.$$

Then

$$du = f^{(n+2)}(t)\,dt, \quad v = -\frac{(x-t)^{n+1}}{n+1}.$$

Performing integration by parts:

$$\int_a^x (x-t)^n f^{(n+1)}(t)\,dt = \left[-\frac{(x-t)^{n+1}}{n+1} f^{(n+1)}(t)\right]_{t=a}^{t=x} + \int_a^x \frac{(x-t)^{n+1}}{n+1} f^{(n+2)}(t)\,dt.$$

Evaluating the boundary term:

- At $t = x$: $(x-x)^{n+1} = 0$, so the term vanishes.
- At $t = a$: we have $-\frac{(x-a)^{n+1}}{n+1} f^{(n+1)}(a)$ with a minus sign from the evaluation, giving $+\frac{(x-a)^{n+1}}{n+1} f^{(n+1)}(a)$.

Thus,

$$\int_a^x (x-t)^n f^{(n+1)}(t)\,dt = \frac{(x-a)^{n+1}}{n+1} f^{(n+1)}(a) + \int_a^x \frac{(x-t)^{n+1}}{n+1} f^{(n+2)}(t)\,dt.$$

Dividing both sides by $n!$:

$$\frac{1}{n!}\int_a^x (x-t)^n f^{(n+1)}(t)\,dt = \frac{(x-a)^{n+1}}{(n+1)!} f^{(n+1)}(a) + \frac{1}{(n+1)!}\int_a^x (x-t)^{n+1} f^{(n+2)}(t)\,dt.$$

Substituting back into the inductive hypothesis:

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{(x-a)^{n+1}}{(n+1)!} f^{(n+1)}(a) + \frac{1}{(n+1)!}\int_a^x (x-t)^{n+1} f^{(n+2)}(t)\,dt.$$

The first two terms combine to form the sum up to $k = n+1$:

$$f(x) = \sum_{k=0}^{n+1} \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{1}{(n+1)!}\int_a^x (x-t)^{n+1} f^{(n+2)}(t)\,dt.$$

This completes the induction. $\square$

1.4.2 Simple Examples

1.4.3 Example 1: Exponential Function

Let $f(x) = e^x$ with $a = 0$. Expand to order $n = 1$.

Taylor's formula gives:

$$e^x = f(0) + f'(0)x + R_1(x) = 1 + x + R_1(x).$$

The integral remainder is:

$$R_1(x) = \frac{1}{1!}\int_0^x (x-t)^1 f''(t)\,dt = \int_0^x (x-t)e^t\,dt.$$

Verify by computing the integral directly:

$$\int_0^x (x-t)e^t\,dt = \left[(x-t)e^t\right]_{t=0}^{t=x} + \int_0^x e^t\,dt = (0 - x\cdot 1) + (e^x - 1) = e^x - 1 - x.$$

Thus $e^x = 1 + x + (e^x - 1 - x)$, which is an identity.

1.4.4 Example 2: Sine Function

Let $f(x) = \sin x$ with $a = 0$. Expand to order $n = 2$.

We have:

$$f(0) = 0, \quad f'(0) = 1, \quad f''(0) = 0.$$

So:

$$\sin x = x + R_2(x).$$

The integral remainder with $n = 2$ is:

$$R_2(x) = \frac{1}{2!}\int_0^x (x-t)^2 f'''(t)\,dt = \frac{1}{2}\int_0^x (x-t)^2(-\cos t)\,dt = -\frac{1}{2}\int_0^x (x-t)^2 \cos t\,dt.$$

1.4.5 Example 3: Cubic Polynomial

Let $f(x) = x^3$ with $a = 1$. Expand to order $n = 2$.

Compute derivatives:

$$f(1) = 1, \quad f'(1) = 3, \quad f''(1) = 6, \quad f'''(t) = 6.$$

Taylor's formula:

$$x^3 = f(1) + f'(1)(x-1) + \frac{f''(1)}{2!}(x-1)^2 + R_2(x)$$

$$x^3 = 1 + 3(x-1) + 3(x-1)^2 + R_2(x).$$

The integral remainder:

$$R_2(x) = \frac{1}{2!}\int_1^x (x-t)^2 f'''(t)\,dt = \frac{1}{2}\int_1^x (x-t)^2 \cdot 6\,dt = 3\int_1^x (x-t)^2\,dt.$$

Evaluate the integral:

$$\int_1^x (x-t)^2\,dt = \left[-\frac{(x-t)^3}{3}\right]_{t=1}^{t=x} = 0 - \left(-\frac{(x-1)^3}{3}\right) = \frac{(x-1)^3}{3}.$$

Thus:

$$R_2(x) = 3 \cdot \frac{(x-1)^3}{3} = (x-1)^3.$$

Verification:

$$1 + 3(x-1) + 3(x-1)^2 + (x-1)^3 = x^3.$$

Summary Table

Function	**Center a**	**Order n**	**Taylor Polynomial**	**Integral Remainder**
e^x	0	1	$1+x$	$\int_0^x (x-t)e^t\,dt$
$\sin x$	0	2	x	$-\frac{1}{2}\int_0^x (x-t)^2\cos t\,dt$
x^3	1	2	$1+3(x-1)+3(x-1)^2$	$(x-1)^3$

1.4.6 Remark: Lagrange Remainder

As a corollary, by the Mean Value Theorem for integrals, since $(x-t)^n$ does not change sign on $[a,x]$, there exists $\xi \in (a,x)$ such that:

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{n!}\int_a^x (x-t)^n\,dt = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1},$$

which is the Lagrange form of the remainder.

1.5 Differential Calculus and Matrix Definiteness

Definition 1.2. *(Partial Derivative)*
Let $f:\mathbb{R}^n \to \mathbb{R}$ be a continuous function. The partial derivative of f with respect to x_i at $(x_1,\dots,x_n)$ is defined as:

$$\frac{\partial f}{\partial x_i}(x_1,\dots,x_n) = \lim_{h\to 0}\frac{f(x_1,\dots,x_i+h,\dots,x_n)-f(x_1,\dots,x_n)}{h}$$

(provided this limit exists).

Definition 1.3. *(Gradient)*
If $f:\mathbb{R}^n \to \mathbb{R}$ is differentiable, the ***gradient*** *of f at x is the vector of its partial derivatives:*

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{pmatrix}$$

Example 1.1. *Let $f(x,y,z) = e^x + x^2y - 2xyz$. Then:*

$$\nabla f(x,y,z) = \begin{pmatrix} e^x + 2xy - 2yz \\ x^2 - 2xz \\ -2xy \end{pmatrix}$$

Definition 1.4. *(Jacobian Matrix)*
For a vector-valued function $f:\mathbb{R}^n \to \mathbb{R}^m$, differentiable, the ***Jacobian matrix*** *is the $m\times n$ matrix of all first-order partial derivatives:*

$$J_f(x) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

Example 1.2. *For $f : \mathbb{R}^3 \to \mathbb{R}^3$ defined by:*

$$f(x_1, x_2, x_3) = (x_1^2 + x_2^2,\ x_1x_2,\ x_1x_3)$$

the Jacobian matrix is:

$$J_f(x) = \begin{pmatrix} 2x_1 & 2x_2 & 0 \\ x_2 & x_1 & 0 \\ x_3 & 0 & x_1 \end{pmatrix}$$

Definition 1.5 (Hessian Matrix)**.** *The* ***Hessian matrix*** *of f at $\mathbf{x}$ is:*

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

1.6 Matrix Definiteness

Let P be a symmetric $n \times n$ matrix.

1. P is **positive definite** if $\forall x \in \mathbb{R}^n, x \neq 0,\ x^T P x > 0$.

2. P is **positive semi-definite** if $\forall x \in \mathbb{R}^n,\ x^T P x \geq 0$.

3. P is **negative definite** if $\forall x \in \mathbb{R}^n, x \neq 0,\ x^T P x < 0$.

4. P is **negative semi-definite** if $\forall x \in \mathbb{R}^n,\ x^T P x \leq 0$.

5. P is **indefinite** if it is neither positive nor negative (semi-)definite.

Proposition 1.1. *(Sylvester's Criterion)*
Let A be a symmetric $n \times n$ matrix. Denote by Δ_k the leading principal minor of order k (the determinant of the upper-left $k \times k$ submatrix).

1. *A is positive definite $\iff$ $\Delta_k > 0$ for all $k = 1, \ldots, n$.*

2. *A is negative definite $\iff$ $(-1)^k \Delta_k > 0$ for all $k = 1, \ldots, n$.*

3. *A is positive semi-definite $\iff$ all principal minors (not just leading) are ≥ 0.*

4. *A is negative semi-definite $\iff$ the sign of each principal minor of order k is $(-1)^k$ or zero.*

Example 1.3.

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad \textit{(positive definite)}$$

$$B = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \quad \textit{(negative definite)}$$

$$C = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \quad \textit{(indefinite)}$$

$$D = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \quad \textit{(negative semi-definite)}$$

1.7 Taylor's Formula in $\mathbb{R}^n$

Theorem 1.1 (Taylor's Formula with Integral Remainder in $\mathbb{R}^n$)**.** *Let $f : \mathbb{R}^n \to \mathbb{R}$ be of class C^{k+1} on an open set containing the segment*

$$\{x + th : t \in [0,1]\},$$

where $x, h \in \mathbb{R}^n$. Then

$$f(x+h) = \sum_{j=0}^{k} \frac{1}{j!} D^j f(x)[h,\dots,h] + R_{k+1}(x,h),$$

where the remainder is given by

$$R_{k+1}(x,h) = \int_0^1 \frac{(1-t)^k}{k!} D^{k+1} f(x+th)[h,\dots,h]\,dt.$$

Equivalent Gradient/Hessian Form (up to order 2)

$$\begin{aligned} f(x+h) &= f(x) + \nabla f(x) \cdot h + \frac{1}{2} h^T \nabla^2 f(x) h \\ &\quad + \int_0^1 \frac{(1-t)^2}{2} D^3 f(x+th)[h,h,h]\,dt. \end{aligned}$$

Proof. Define the auxiliary function $\phi : [0,1] \to \mathbb{R}$ by

$$\phi(t) = f(\mathbf{x} + t\mathbf{h}).$$

Then ϕ is twice continuously differentiable on $[0,1]$. By the fundamental theorem of calculus,

$$\phi(1) = \phi(0) + \int_0^1 \phi'(t)\,dt.$$

Since $\phi'(t) = \nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}$, we have

$$f(\mathbf{x}+\mathbf{h}) = f(\mathbf{x}) + \int_0^1 \nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\, dt.$$

For the second-order expansion, we apply integration by parts. Note that

$$\frac{d}{dt}\left[(1-t)\nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\right] = -\nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h} + (1-t)\mathbf{h}^\top \nabla^2 f(\mathbf{x}+t\mathbf{h})\mathbf{h}.$$

Integrating from 0 to 1,

$$\left[(1-t)\nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\right]_0^1 = -\int_0^1 \nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\, dt + \int_0^1 (1-t)\mathbf{h}^\top \nabla^2 f(\mathbf{x}+t\mathbf{h})\mathbf{h}\, dt.$$

The left-hand side equals $0 - \nabla f(\mathbf{x})^\top \mathbf{h} = -\nabla f(\mathbf{x})^\top \mathbf{h}$. Thus,

$$-\nabla f(\mathbf{x})^\top \mathbf{h} = -\int_0^1 \nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\, dt + \int_0^1 (1-t)\mathbf{h}^\top \nabla^2 f(\mathbf{x}+t\mathbf{h})\mathbf{h}\, dt.$$

Rearranging,

$$\int_0^1 \nabla f(\mathbf{x}+t\mathbf{h})^\top \mathbf{h}\, dt = \nabla f(\mathbf{x})^\top \mathbf{h} + \int_0^1 (1-t)\mathbf{h}^\top \nabla^2 f(\mathbf{x}+t\mathbf{h})\mathbf{h}\, dt.$$

Substituting into the first-order expansion yields

$$f(\mathbf{x}+\mathbf{h}) = f(\mathbf{x}) + \nabla f(\mathbf{x})^\top \mathbf{h} + \int_0^1 (1-t)\mathbf{h}^\top \nabla^2 f(\mathbf{x}+t\mathbf{h})\mathbf{h}\, dt.$$

□

1.8 Examples

Example 1.4. *Let $f(x,y) = e^{x+y}$. Then*

$$\nabla f(x,y) = e^{x+y}(1,1), \quad \nabla^2 f(x,y) = e^{x+y}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

At $(0,0)$:

$$f(0,0) = 1, \quad \nabla f(0,0) = (1,1), \quad \nabla^2 f(0,0) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

Thus, the second-order Taylor expansion is

$$\begin{aligned} f(h_1,h_2) &= 1 + (h_1+h_2) + \frac{1}{2}(h_1,h_2)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} + R_3 \\ &= 1 + (h_1+h_2) + \frac{1}{2}(h_1+h_2)^2 + R_3. \end{aligned}$$

The remainder is

$$R_3 = \int_0^1 \frac{(1-t)^2}{2} D^3 f(th_1, th_2)[h,h,h]\, dt.$$

Since $D^3 f(x,y) = e^{x+y}$ *times a symmetric tensor, we obtain*

$$R_3 = \int_0^1 \frac{(1-t)^2}{2} e^{t(h_1+h_2)} (h_1+h_2)^3\, dt.$$

Example 1.5. *Quadratic Function in* $\mathbb{R}^3$*:*

Let $f : \mathbb{R}^3 \to \mathbb{R}$ *be defined by*

$$f(x,y,z) = x^2 + 2y^2 + 3z^2 + xy + yz.$$

We expand f *around* $\mathbf{x}_0 = (1,1,1)$ *with* $\mathbf{h} = (h_1, h_2, h_3)$*.*

Compute the Gradient:

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z} \end{pmatrix} = \begin{pmatrix} 2x + y \\ 4y + x + z \\ 6z + y \end{pmatrix}.$$

At $\mathbf{x}_0 = (1,1,1)$*:*

$$\nabla f(1,1,1) = \begin{pmatrix} 2(1) + 1 \\ 4(1) + 1 + 1 \\ 6(1) + 1 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \\ 7 \end{pmatrix}.$$

Compute the Hessian:

$$\nabla^2 f = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 6 \end{pmatrix}.$$

Since f *is quadratic, the Hessian is constant.*

Taylor Expansion (Exact):

The second-order Taylor expansion with integral remainder gives:

$$f(\mathbf{x}_0 + \mathbf{h}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\mathsf{T} \mathbf{h} + \int_0^1 (1-t)\, \mathbf{h}^\mathsf{T} \nabla^2 f(\mathbf{x}_0 + t\mathbf{h}) \mathbf{h}\, dt.$$

Because $\nabla^2 f$ *is constant, the integral simplifies:*

$$\int_0^1 (1-t)\, dt = \frac{1}{2}.$$

Thus,

$$f(\mathbf{x}_0 + \mathbf{h}) = f(1,1,1) + \nabla f(1,1,1)^\mathsf{T} \mathbf{h} + \frac{1}{2} \mathbf{h}^\mathsf{T} \nabla^2 f\, \mathbf{h}.$$

Compute $f(1,1,1)$:

$$f(1,1,1) = 1^2 + 2(1)^2 + 3(1)^2 + (1)(1) + (1)(1) = 1 + 2 + 3 + 1 + 1 = 8.$$

Therefore,

$$f(1+h_1, 1+h_2, 1+h_3) = 8 + 3h_1 + 6h_2 + 7h_3 + \frac{1}{2}\begin{pmatrix} h_1 & h_2 & h_3 \end{pmatrix}\begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 6 \end{pmatrix}\begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix}.$$

Expanding the quadratic form:

$$\frac{1}{2}\left(2h_1^2 + 2h_1h_2 + 4h_2^2 + 2h_2h_3 + 6h_3^2\right) = h_1^2 + h_1h_2 + 2h_2^2 + h_2h_3 + 3h_3^2.$$

Hence,

$$f(1+h_1, 1+h_2, 1+h_3) = 8 + 3h_1 + 6h_2 + 7h_3 + h_1^2 + h_1h_2 + 2h_2^2 + h_2h_3 + 3h_3^2.$$

Example 1.6. *Exponential Function in $\mathbb{R}^3$:*

Let $f : \mathbb{R}^3 \to \mathbb{R}$ be defined by

$$f(x,y,z) = e^{x+y+z}.$$

We expand f around $\mathbf{x}_0 = (0,0,0)$ with $\mathbf{h} = (h_1, h_2, h_3)$.

Function Value:

$$f(0,0,0) = e^0 = 1.$$

Gradient:

$$\nabla f = \begin{pmatrix} e^{x+y+z} \\ e^{x+y+z} \\ e^{x+y+z} \end{pmatrix}, \quad \nabla f(0,0,0) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Hessian:

$$\nabla^2 f = e^{x+y+z}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \nabla^2 f(0,0,0) = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

First-Order Expansion with Integral Remainder:

$$f(\mathbf{h}) = f(\mathbf{0}) + \int_0^1 \nabla f(t\mathbf{h})^\top \mathbf{h}\, dt.$$

Since $\nabla f(t\mathbf{h}) = e^{t(h_1+h_2+h_3)}\begin{pmatrix}1\\1\\1\end{pmatrix}$, *we have*

$$\nabla f(t\mathbf{h})^\mathsf{T}\mathbf{h} = e^{t(h_1+h_2+h_3)}(h_1+h_2+h_3).$$

Thus,

$$f(\mathbf{h}) = 1 + (h_1+h_2+h_3)\int_0^1 e^{t(h_1+h_2+h_3)}\,dt.$$

Evaluating the integral:

$$\int_0^1 e^{ts}\,dt = \frac{e^s-1}{s}, \quad \textit{where } s = h_1+h_2+h_3.$$

Therefore,

$$f(h_1,h_2,h_3) = 1 + s\cdot\frac{e^s-1}{s} = e^s = e^{h_1+h_2+h_3},$$

which is exact, as expected.

Second-Order Expansion with Integral Remainder:

$$f(\mathbf{h}) = f(\mathbf{0}) + \nabla f(\mathbf{0})^\mathsf{T}\mathbf{h} + \int_0^1 (1-t)\,\mathbf{h}^\mathsf{T}\nabla^2 f(t\mathbf{h})\mathbf{h}\,dt.$$

Compute the quadratic form:

$$\mathbf{h}^\mathsf{T}\nabla^2 f(t\mathbf{h})\mathbf{h} = e^{ts}\begin{pmatrix}h_1 & h_2 & h_3\end{pmatrix}\begin{pmatrix}1&1&1\\1&1&1\\1&1&1\end{pmatrix}\begin{pmatrix}h_1\\h_2\\h_3\end{pmatrix} = e^{ts}(h_1+h_2+h_3)^2 = e^{ts}s^2.$$

Thus,

$$f(\mathbf{h}) = 1 + s + s^2\int_0^1 (1-t)e^{ts}\,dt.$$

Evaluate the integral:

$$\int_0^1 (1-t)e^{ts}\,dt = \frac{e^s-1-s}{s^2}.$$

Hence,

$$f(\mathbf{h}) = 1 + s + s^2\cdot\frac{e^s-1-s}{s^2} = e^s = e^{h_1+h_2+h_3},$$

confirming the exact representation.

Example 1.7. *Trigonometric Function in* $\mathbb{R}^3$ *with Remainder Bound:*

Let $f:\mathbb{R}^3\to\mathbb{R}$ *be defined by*

$$f(x,y,z) = \sin(x+y+z).$$

We expand f around $\mathbf{x}_0 = (0,0,0)$ with $\mathbf{h} = (h_1, h_2, h_3)$ and bound the remainder.

Function Value and Derivatives:

$$f(0,0,0) = 0.$$

First derivatives:

$$\frac{\partial f}{\partial x} = \cos(x+y+z), \quad \frac{\partial f}{\partial y} = \cos(x+y+z), \quad \frac{\partial f}{\partial z} = \cos(x+y+z).$$

Thus,

$$\nabla f(0,0,0) = (1,1,1)^\mathsf{T}.$$

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = -\sin(x+y+z), \quad \frac{\partial^2 f}{\partial x \partial y} = -\sin(x+y+z), \quad \textit{etc.}$$

So,

$$\nabla^2 f(x,y,z) = -\sin(x+y+z) \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Second-Order Expansion:

$$f(\mathbf{h}) = f(\mathbf{0}) + \nabla f(\mathbf{0})^\mathsf{T}\mathbf{h} + \int_0^1 (1-t)\,\mathbf{h}^\mathsf{T}\nabla^2 f(t\mathbf{h})\mathbf{h}\,dt.$$

Let $s = h_1 + h_2 + h_3$. Then:

$$\nabla f(\mathbf{0})^\mathsf{T}\mathbf{h} = s.$$

$$\mathbf{h}^\mathsf{T}\nabla^2 f(t\mathbf{h})\mathbf{h} = -\sin(ts)\cdot s^2.$$

Thus,

$$f(\mathbf{h}) = s - s^2 \int_0^1 (1-t)\sin(ts)\,dt.$$

Bound the Remainder:

The remainder is

$$R_2(\mathbf{h}) = -s^2 \int_0^1 (1-t)\sin(ts)\,dt.$$

Since $|\sin(ts)| \le 1$, we have

$$|R_2(\mathbf{h})| \le |s|^2 \int_0^1 (1-t)\,dt = |s|^2 \cdot \frac{1}{2} = \frac{s^2}{2}.$$

Using the inequality $s^2 \le 3(h_1^2 + h_2^2 + h_3^2)$ (by Cauchy-Schwarz), we obtain

$$|R_2(\mathbf{h})| \le \frac{3}{2}\|\mathbf{h}\|^2.$$

Exact Remainder Expression:

We can evaluate the integral exactly:

$$\int_0^1 (1-t)\sin(ts)\,dt = \frac{s-\sin s}{s^2}.$$

Therefore,

$$f(\mathbf{h}) = s - s^2 \cdot \frac{s-\sin s}{s^2} = s-(s-\sin s) = \sin s = \sin(h_1+h_2+h_3),$$

which is exact, as expected.

Chapter 2

Optimization in the Set of Real Numbers

Optimization in the set of real numbers $\mathbb{R}$ is the mathematical process of finding the **maximum** or **minimum** value of a real-valued function within a given domain. Formally, for a function $f : D \to \mathbb{R}$, where $D \subseteq \mathbb{R}$, we seek a point $x^* \in D$ such that

$$f(x^*) \leq f(x) \quad \forall x \in D \quad \text{(minimization)}, \;\; \textit{or} \;\; f(x^*) \geq f(x) \quad \forall x \in D \quad \text{(maximization)}.$$

Core Methodology:

The standard approach for a differentiable function f on an interval I involves:

1. Finding the **critical points** by solving $f'(x) = 0$ or identifying where $f'(x)$ does not exist.
2. Analyzing these points using either:
   - The **First Derivative Test**: Checking the sign change of $f'(x)$ around the critical point.
   - The **Second Derivative Test**: Evaluating $f''(x)$ at the point ($f'' > 0$ implies a local minimum, $f'' < 0$ a local maximum).
3. Comparing values at critical points and **boundary points** of I to determine the global optimum.

Significance:

This framework is the foundation for continuous single-variable optimization. It models problems in economics (profit maximization), engineering (design minimization), and machine learning (loss function minimization via gradient descent). The logic naturally extends to multivariable optimization in $\mathbb{R}^n$ using partial derivatives and gradients.

2.1 Unconstrained Optimization in One Dimension ($\mathbb{R}$)

2.2 Introduction

Unconstrained optimization in one dimension deals with finding minima or maxima of functions $f : \mathbb{R} \to \mathbb{R}$ without any restrictions on the domain:

$$\min_{x\in\mathbb{R}} f(x) \quad \text{or} \quad \max_{x\in\mathbb{R}} f(x)$$

These problems are fundamental to calculus and have applications across all scientific disciplines.

2.2.1 Definitions

Definition 2.1 (Global Extremum)**.** *A point $x^* \in \mathbb{R}$ is a **global minimum** of f if:*

$$f(x^*) \le f(x) \quad \forall x \in \mathbb{R}$$

*Similarly, x^* is a **global maximum** if:*

$$f(x^*) \ge f(x) \quad \forall x \in \mathbb{R}$$

Definition 2.2 (Local Extremum)**.** *A point $x^* \in \mathbb{R}$ is a **local minimum** of f if there exists $\delta > 0$ such that:*

$$f(x^*) \le f(x) \quad \forall x \in (x^* - \delta, x^* + \delta)$$

*A **local maximum** is defined similarly with the inequality reversed.*

Definition 2.3 (Critical Point)**.** *A point $x^* \in \mathbb{R}$ is a **critical point** of f if:*

$$f'(x^*) = 0 \quad \text{or} \quad f'(x^*) \text{ does not exist}$$

Definition 2.4. *(Unimodal Function).*
A function $f : I \subset \mathbb{R} \to \mathbb{R}$ is said to be unimodal *on an interval I if there exists a point $x^* \in I$ such that:*

- *f is nonincreasing on $(-\infty, x^*] \cap I$,*
- *f is nondecreasing on $[x^*, +\infty) \cap I$.*

The point x^* is called a global minimizer *of f on I.*

2.3 Optimality Conditions

2.3.1 First-Order Necessary Conditions

Theorem 2.1 (Fermat's Theorem)**.** *Let $f : \mathbb{R} \to \mathbb{R}$ be differentiable. If x^* is a local extremum (minimum or maximum), then:*

$$f'(x^*) = 0$$

Proof. Suppose x^* is a local minimum. For sufficiently small $h > 0$:

$$\frac{f(x^*+h) - f(x^*)}{h} \geq 0 \implies f'(x^*) \geq 0$$

$$\frac{f(x^*-h) - f(x^*)}{-h} \leq 0 \implies f'(x^*) \leq 0$$

Thus $f'(x^*) = 0$. The proof for maximum is similar. □

2.3.2 Second-Order Conditions

Theorem 2.2 (Second-Order Necessary Condition)**.** *Let $f : \mathbb{R} \to \mathbb{R}$ be twice differentiable. If x^* is a local minimum, then:*

$$f'(x^*) = 0 \quad \textit{and} \quad f''(x^*) \geq 0$$

If x^* is a local maximum, then:

$$f'(x^*) = 0 \quad \textit{and} \quad f''(x^*) \leq 0$$

Theorem 2.3 (Second-Order Sufficient Condition)**.** *Let $f : \mathbb{R} \to \mathbb{R}$ be twice differentiable at x^*.*

1. *If $f'(x^*) = 0$ and $f''(x^*) > 0$, then x^* is a strict local minimum.*
2. *If $f'(x^*) = 0$ and $f''(x^*) < 0$, then x^* is a strict local maximum.*
3. *If $f'(x^*) = 0$ and $f''(x^*) = 0$, the test is inconclusive.*

Theorem 2.4. *(Higher-Order Sufficient Conditions)*
If $f \in C^n(I)$, $f^{(k)}(x^*) = 0$ for $k = 1, \ldots, n-1$, and $f^{(n)}(x^*) \neq 0$, then:

- *If n is even and $f^{(n)}(x^*) > 0$, then x^* is a local minimum*
- *If n is even and $f^{(n)}(x^*) < 0$, then x^* is a local maximum*
- *If n is odd, then x^* is an inflection point*

Proof. (Justification via Taylor Expansion) For f differentiable n times, the Taylor expansion around x^* gives:

$$f(x) = f(x^*) + \frac{(x-x^*)^n}{n!} f^{(n)}(x^*) + o((x-x^*)^n).$$

Given that all lower-order derivatives vanish at x^*, the local behavior is dominated by the term

$$\frac{(x-x^*)^n}{n!} f^{(n)}(x^*)$$

- If n is even, $(x-x^*)^n \geq 0$ for all x, so the sign of $f(x) - f(x^*)$ is determined by $f^{(n)}(x^*)$:
  - $f^{(n)}(x^*) > 0 \implies f(x) \geq f(x^*)$ (local minimum)
  - $f^{(n)}(x^*) < 0 \implies f(x) \leq f(x^*)$ (local maximum)
- If n is odd, $(x-x^*)^n$ changes sign around x^*, so $f(x) - f(x^*)$ also changes sign regardless of $f^{(n)}(x^*)$, implying x^* is neither a minimum nor a maximum.

□

Example 2.1. *1. Consider $f(x) = x^4$. Then:*

$$f'(x) = 4x^3, \quad f''(x) = 12x^2, \quad f'''(x) = 24x, \quad f^{(4)}(x) = 24.$$

At $x^* = 0$:

$$f'(0) = f''(0) = f'''(0) = 0, \quad f^{(4)}(0) = 24 > 0.$$

*Here $n = 4$ (even) and $f^{(4)}(0) > 0$, so $x^* = 0$ is a **local minimum**.*

2. Quadratic Function:

Consider $f(x) = ax^2 + bx + c$ with $a > 0$:

$$f'(x) = 2ax + b = 0 \implies x^* = -\frac{b}{2a}$$
$$f''(x) = 2a > 0 \implies \textit{minimum at } x^*$$
$$f_{\min} = f\left(-\frac{b}{2a}\right) = c - \frac{b^2}{4a}$$

3. Cubic Function:

Consider $f(x) = x^3 - 3x$:

$$f'(x) = 3x^2 - 3 = 3(x^2 - 1) = 0 \implies x = \pm 1$$
$$f''(x) = 6x$$

- *At* $x = -1$*:* $f''(-1) = -6 < 0 \Rightarrow$ *local maximum*
- *At* $x = 1$*:* $f''(1) = 6 > 0 \Rightarrow$ *local minimum*

But note: $\lim_{x\to-\infty} f(x) = -\infty$, $\lim_{x\to\infty} f(x) = \infty$*, so no global extremum.*

4. $f(x) = e^x$*: No minimum (*$f(x) \to 0$ *as* $x \to -\infty$*, but never reaches 0)*

5. $f(x) = \frac{1}{1+x^2}$*: Global maximum at* $x = 0$*, but no global minimum*

6. *Multiple Critical Points:*

   $f(x) = \sin x$*: Infinitely many local minima at* $x = \frac{3\pi}{2} + 2k\pi$ *and local maxima at* $x = \frac{\pi}{2} + 2k\pi$, $k \in \mathbb{Z}$.

2.4 Exercises

Exercise 2.1. *Find and classify all critical points of:*

1. $f(x) = x^3 - 3x^2 + 4$.
2. $f(x) = x^4 - 2x^2 + \frac{3}{2}$.
3. $f(x) = x^4 - 4x^3 + 6x^2 - 4x + 1$.
4. $f(x) = e^{-x^2}$.

Solution 2.1. *We will find the critical points by solving* $f'(x) = 0$ *and then classify them using the second derivative test when applicable.*

1. *For* $f(x) = x^3 - 3x^2 + 4$*:*

   First derivative: $f'(x) = 3x^2 - 6x = 3x(x-2)$.

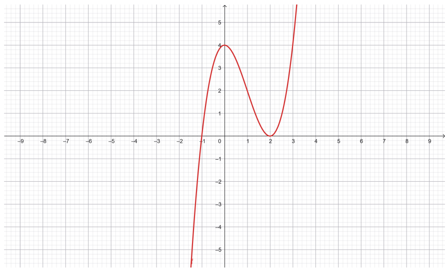
   $$f'(x) = 0 \quad \Rightarrow \quad 3x(x-2) = 0 \quad \Rightarrow \quad x = 0 \text{ or } x = 2.$$

   Second derivative: $f''(x) = 6x - 6$.

   Classification:

   - *At* $x = 0$*:* $f''(0) = -6 < 0$*, so* $x = 0$ *is a* ***local maximum****.*
   - *At* $x = 2$*:* $f''(2) = 6 > 0$*, so* $x = 2$ *is a* ***local minimum****.*

   Critical points: 0 *(local max) and* 2 *(local min).*



2. *For* $f(x) = x^4 - 2x^2 + \frac{3}{2}$*:*

   First derivative: $f'(x) = 4x^3 - 4x = 4x(x^2 - 1)$.

   Notice that

$$f'(x) = 4x(x^2 - 1) = 0 \quad \Rightarrow \quad (x = 1 \quad or \quad x = -1 \quad or \quad x = 0).$$

   Second derivative: $f''(x) = 12x^2 - 4$.

   Classification:

   - *At* $x = 0$*:* $f''(0) = -4 < 0$*, so* $x = 0$ *is a* ***local maximum****.*
   - *At* $x = 1$*:* $f''(1) = 8 > 0$*, so* $x = 1$ *is a* ***local minimum****.*
   - *At* $x = -1$*:* $f''(-1) = 8 > 0$*, so* $x = -1$ *is a* ***local minimum****.*

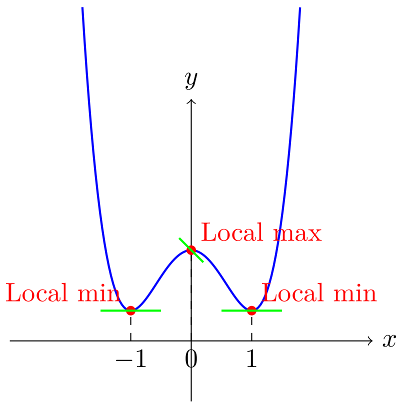


Figure: $f(x) = x^4 - 2x^2 + \frac{3}{2}$ with critical points at $x = -1, 0, 1$

3. *For* $f(x) = x^4 - 4x^3 + 6x^2 - 4x + 1$*:*

   First derivative: $f'(x) = 4x^3 - 12x^2 + 12x - 4 = 4(x^3 - 3x^2 + 3x - 1)$.

   Notice that $x^3 - 3x^2 + 3x - 1 = (x - 1)^3$.

$$f'(x) = 4(x - 1)^3 = 0 \quad \Rightarrow \quad x = 1.$$

Second derivative: $f''(x) = 12x^2 - 24x + 12 = 12(x^2 - 2x + 1) = 12(x-1)^2$.

At $x = 1$*:* $f''(1) = 0$*, so the second derivative test is inconclusive.*

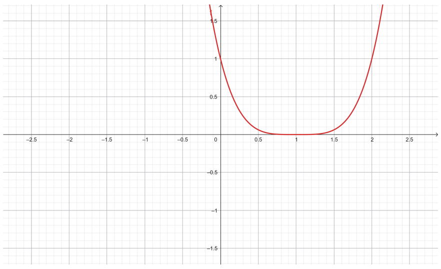
Using the first derivative test:

For $x < 1$*:* $f'(x) = 4(x-1)^3 < 0$ *(since* $(x-1)^3$ *is negative).*

For $x > 1$*:* $f'(x) = 4(x-1)^3 > 0$.

Thus, $f'(x)$ *changes from negative to positive at* $x = 1$*, so* $x = 1$ *is a* ***local minimum****.*

Critical point: 1 *(local min).*



4. *For* $f(x) = e^{-x^2}$*:*

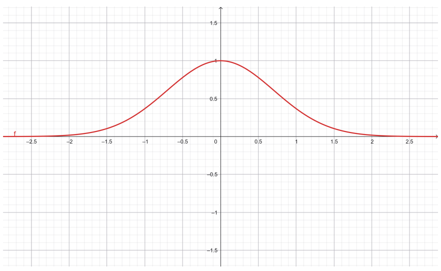
   First derivative: $f'(x) = -2xe^{-x^2}$.

$$f'(x) = 0 \quad \Rightarrow \quad -2xe^{-x^2} = 0 \quad \Rightarrow \quad x = 0 \quad (\textit{since } e^{-x^2} \neq 0).$$

   Second derivative: $f''(x) = (4x^2 - 2)e^{-x^2}$.

   At $x = 0$*:* $f''(0) = -2 < 0$*, so* $x = 0$ *is a* ***local maximum****.*

   Critical point: 0 *(local max).*



Exercise 2.2. *Find the optimal solutions for the following functions:*

1. $f_1(x) = x^4 - 8x^3 + 24x^2 - 32x + 16$

2. $f_2(x) = x^3 + \frac{3}{2}x^2 - 18x + 19$

3. $f_3(x) = 6x^2 + \sqrt{3x} - 9$

4. $f_4(x) = x^{12} - 14x^{11} + x^{10} + 90x^9 + 8x^8 + 6$

Solution 2.2. *We will find the critical points by solving $f'(x) = 0$, then classify them using the first or second derivative test to find optimal solutions (local minima/maxima).*

1. *For $f_1(x) = x^4 - 8x^3 + 24x^2 - 32x + 16$:*

   First derivative:

$$f_1'(x) = 4x^3 - 24x^2 + 48x - 32 = 4(x^3 - 6x^2 + 12x - 8).$$

   Notice that $x^3 - 6x^2 + 12x - 8 = (x-2)^3$.

$$f_1'(x) = 4(x-2)^3 = 0 \quad \Rightarrow \quad x = 2.$$

   Second derivative:

$$f_1''(x) = 12x^2 - 48x + 48 = 12(x^2 - 4x + 4) = 12(x-2)^2.$$

   At $x = 2$: $f_1''(2) = 0$, so second derivative test is inconclusive.

   First derivative test:
   For $x < 2$: $f_1'(x) = 4(x-2)^3 < 0$ (since $(x-2)^3$ is negative).
   For $x > 2$: $f_1'(x) = 4(x-2)^3 > 0$.
   *Thus, $f_1'(x)$ changes from negative to positive at $x = 2$, so $x = 2$ is a **local minimum**.*

   Critical point: 2 (local min).

2. *For $f_2(x) = x^3 + \frac{3}{2}x^2 - 18x + 19$:*

   First derivative:

$$f_2'(x) = 3x^2 + 3x - 18 = 3(x^2 + x - 6) = 3(x+3)(x-2).$$

$$f_2'(x) = 0 \quad \Rightarrow \quad x = -3 \text{ or } x = 2.$$

   Second derivative:

$$f_2''(x) = 6x + 3.$$

   Classification:

   - *At $x = -3$: $f_2''(-3) = -15 < 0$, so $x = -3$ is a **local maximum**.*

- *At* $x=2$*:* $f_2''(2)=15>0$*, so* $x=2$ *is a* ***local minimum****.*

Critical points: -3 *(local max) and* 2 *(local min).*

3. *For* $f_3(x)=6x^2+\sqrt{3x}-9$*:*

   Note: Domain requires $x\geq 0$ *because of* $\sqrt{3x}$*.*

   First derivative:

$$f_3'(x)=12x+\frac{\sqrt{3}}{2\sqrt{x}} \quad (\textit{using } \frac{d}{dx}\sqrt{3x}=\frac{\sqrt{3}}{2\sqrt{x}}).$$

$$f_3'(x)=0 \quad \Rightarrow \quad 12x+\frac{\sqrt{3}}{2\sqrt{x}}=0.$$

   Multiply by $2\sqrt{x}$*:*

$$24x\sqrt{x}+\sqrt{3}=0 \quad \Rightarrow \quad 24x^{3/2}=-\sqrt{3}.$$

   Since $x\geq 0$*,* $24x^{3/2}\geq 0$ *and* $-\sqrt{3}<0$*, so no solution exists. However, we must also check the endpoint* $x=0$ *since it's in the domain.*

   At $x=0$*: The derivative* $f_3'(0)$ *is undefined (since* $\frac{\sqrt{3}}{2\sqrt{x}}$ *becomes infinite), but this is a boundary point.*

   Thus, the only candidate for an extremum in the domain is at $x=0$*. Since* $f_3(x)$ *is increasing for* $x>0$ *(as* $f_3'(x)>0$ *for all* $x>0$*),* $x=0$ *gives the minimum.*

   Critical point: 0 *(global minimum on* $[0,\infty)$*).*

4. *For* $f_4(x)=x^{12}-14x^{11}+x^{10}+90x^9+8x^8+6$*:*

   This is a high-degree polynomial. We'll find the first derivative:

$$f_4'(x)=12x^{11}-154x^{10}+10x^9+810x^8+64x^7.$$

   Factor out x^7*:*

$$f_4'(x)=x^7(12x^4-154x^3+10x^2+810x+64).$$

$$f_4'(x)=0 \quad \Rightarrow \quad x^7=0 \quad \textit{or} \quad 12x^4-154x^3+10x^2+810x+64=0.$$

   Thus, $x=0$ *is one critical point. The quartic equation* $12x^4-154x^3+10x^2+810x+64=0$ *is difficult to solve analytically. For practical purposes, we can only analyze* $x=0$ *thoroughly.*

   Second derivative at $x=0$*:*

$$f_4''(x)=132x^{10}-1540x^9+90x^8+6480x^7+448x^6.$$

At $x = 0$: $f_4''(0) = 0$, so second derivative test is inconclusive.

First derivative test around $x = 0$:

For $x < 0$: $f_4'(x)$ has sign determined by x^7 (negative for $x < 0$) times the quartic polynomial. Since the quartic polynomial at $x = 0$ is $64 > 0$, $f_4'(x) < 0$ for small negative x.

For $x > 0$: $x^7 > 0$ and the quartic polynomial is positive for small x, so $f_4'(x) > 0$.

*Thus, $f_4'(x)$ changes from negative to positive at $x = 0$, so $x = 0$ is a **local minimum**.*

Critical point: 0 (local min). The other critical points from the quartic would require numerical methods for full analysis.

Chapter 3

Unconstrained Optimization in $\mathbb{R}^n$

Optimization in $\mathbb{R}^n$ is the mathematical process of consists of finding a point $x^* \in \mathbb{R}^n$ that minimizes (or maximizes) a given objective function $f : \mathbb{R}^n \to \mathbb{R}$, we seek a point $x^* \in \mathbb{R}^n$ such that

$$f(x^*) \leq f(x) \quad \forall x \in \mathbb{R}^n \quad \text{(minimization)}, \;\; \textit{or} \;\; f(x^*) \geq f(x) \quad \forall x \in \mathbb{R}^n \quad \text{(maximization)}.$$

without any restrictions or constraints on the variable x.
Formally, the minimization problem is written as:

$$\min_{x \in \mathbb{R}^n} f(x). \tag{3.0.1}$$

Unconstrained Optimization in $\mathbb{R}^n$ it depends mainly on convex analysis which the mathematical study of **convex sets** and **convex functions**, providing the foundational language and tools for modern optimization theory. Its core principle is that convex structures possess remarkable regularity properties that make optimization problems both theoretically tractable and computationally feasible.

Fundamental Concepts:

- **Convex Set.**
- **Convex Function.**
- **Concave Function.**

3.1 Convex Sets

Definition 3.1 (Convex Set). *A set $C \subseteq \mathbb{R}^n$ is convex if for all $x, y \in C$ and $\lambda \in [0,1]$:*

$$\lambda x + (1-\lambda)y \in C$$

3.1.1 Examples

1. Intervals in $\mathbb{R}$
2. Hyperplanes: $\{x \in \mathbb{R}^n \mid a^T x = b\}$
3. Half-spaces: $\{x \in \mathbb{R}^n \mid a^T x \leq b\}$
4. Balls: $\{x \in \mathbb{R}^n \mid \|x - x_0\| \leq r\}$
5. Polyhedra: $\{x \in \mathbb{R}^n \mid Ax \leq b\}$

3.1.2 Properties of Convex Sets

Theorem 3.1 (Properties). *1. The intersection of convex sets is convex*

2. The Cartesian product of convex sets is convex

3. The image of a convex set under an affine transformation is convex

4. The inverse image of a convex set under an affine transformation is convex

3.2 Convex Functions

Definition 3.2 (Convex Function). *A function $f : C \to \mathbb{R}$ defined on a convex set $C \subseteq \mathbb{R}^n$ is convex if for all $x, y \in C$ and $\lambda \in [0,1]$:*

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

Definition 3.3 (Strictly Convex Function). *f is strictly convex if for all $x \neq y \in C$ and $\lambda \in (0,1)$:*

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

3.2.1 First-Order Characterization of Convexity

Theorem 3.2. *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable function on an open convex domain $\Omega \subseteq \mathbb{R}^n$. Then the following two statements are equivalent:*

(i) (Definition of convexity) For all $x, y \in \Omega$ and $\theta \in [0,1]$:

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

(ii) (Gradient inequality) For all $x, y \in \Omega$:

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x).$$

Proof. We prove both directions of the equivalence.

Proof that (i) $\Rightarrow$ (ii): Assume f is convex in the sense of definition (i). Fix $x, y \in \Omega$ and let $\theta \in (0,1]$. Then by convexity:

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

Rearranging terms:

$$f(x + \theta(y-x)) - f(x) \leq \theta [f(y) - f(x)].$$

Dividing both sides by $\theta > 0$:

$$\frac{f(x + \theta(y-x)) - f(x)}{\theta} \leq f(y) - f(x).$$

Taking the limit as $\theta \to 0^+$, the left-hand side becomes the directional derivative of f at x in the direction $(y - x)$, which equals $\nabla f(x)^\top (y - x)$ by differentiability. Thus:

$$\nabla f(x)^\top (y - x) \leq f(y) - f(x).$$

Rearranging gives:

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x).$$

Proof that (ii) $\Rightarrow$ (i): Assume the gradient inequality holds for all $x, y \in \Omega$. Let $x, y \in \Omega$ and $\theta \in [0,1]$. Define $z = \theta x + (1-\theta) y$.

Applying (ii) with z and x:

$$f(x) \geq f(z) + \nabla f(z)^\top (x - z). \tag{1}$$

Applying (ii) with z and y:

$$f(y) \geq f(z) + \nabla f(z)^\top (y - z). \tag{2}$$

Now multiply (1) by θ and (2) by $(1-\theta)$, then add them:

$$\theta f(x)+(1-\theta)f(y) \geq \theta f(z)+(1-\theta)f(z)+\nabla f(z)^\top \left[\theta(x-z)+(1-\theta)(y-z)\right].$$

Notice that:

$$\theta(x-z)+(1-\theta)(y-z) = \theta x+(1-\theta)y-z = 0.$$

Therefore:

$$\theta f(x)+(1-\theta)f(y) \geq f(z) = f(\theta x+(1-\theta)y),$$

which is exactly the definition of convexity.

Thus, we have shown (i) $\Leftrightarrow$ (ii). $\square$

Interpretation

The gradient inequality $f(y) \geq f(x)+\nabla f(x)^\top(y-x)$ states that the function lies above its tangent hyperplane at every point. This geometric property is equivalent to the standard definition of convexity when f is differentiable.

3.2.2 Second-Order Characterization of Convexity

Theorem 3.3 (Second-Order Characterization)**.** *Let $f : C \to \mathbb{R}$ be a twice continuously differentiable function defined on an open convex set $C \subseteq \mathbb{R}^n$. Then f is convex if and only if its Hessian matrix $\nabla^2 f(x)$ is positive semidefinite for all $x \in C$:*

$$\nabla^2 f(x) \geq 0, \quad \forall x \in C.$$

Remark 3.1.

- *The theorem provides a practical test for convexity: compute the Hessian matrix and check if all its eigenvalues are nonnegative at every point in the domain.*
- *For strictly convex functions, we have the stronger condition $\nabla^2 f(x) > 0$ (positive definite) for all $x \in C$, though the converse requires additional conditions (e.g., the Hessian being positive definite at every point implies strict convexity).*

  Let $f : C \subset \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function.

  Sufficient Condition for Strict Convexity:

  If the Hessian matrix of f satisfies

  $$\nabla^2 f(x) > 0 \quad \textit{for all } x \in C,$$

*that is, $\nabla^2 f(x)$ is positive definite for all $x \in C$, then f is **strictly convex** on C.*

Indeed, for any nonzero vector $d \in \mathbb{R}^n$, we have

$$d^T \nabla^2 f(x) d > 0,$$

which implies that the second directional derivative is strictly positive in every direction, ensuring that f curves upward and is therefore strictly convex.

Converse Statement:

The converse implication is more delicate. If f is strictly convex, it does not necessarily follow that

$$\nabla^2 f(x) > 0 \quad \text{for all } x \in C.$$

However, if $f \in C^2(C)$ and is strictly convex, then the Hessian satisfies

$$\nabla^2 f(x) \geq 0 \quad \text{for all } x \in C,$$

that is, it is positive semidefinite.

Example:

Consider the function

$$f(x) = x^4, \quad x \in \mathbb{R}.$$

Then

$$f''(x) = 12x^2 \geq 0 \quad \text{for all } x \in \mathbb{R},$$

but

$$f''(0) = 0.$$

Thus, the Hessian is not positive definite at $x = 0$, yet f is strictly convex on $\mathbb{R}$.

Stronger Conditions:

*To ensure that strict convexity is equivalent to positive definiteness of the Hessian, one may impose a stronger condition such as **uniform positive definiteness**:*

$$\nabla^2 f(x) \geq mI \quad \text{for some } m > 0 \text{ and all } x \in C.$$

*In this case, f is said to be **strongly convex**.*

Summary:

- *If $\nabla^2 f(x) > 0$ for all $x \in C$, then f is strictly convex.*

  - *Strict convexity alone does not imply $\nabla^2 f(x) > 0$ everywhere.*
  - *If $f \in C^2(C)$ is strictly convex, then $\nabla^2 f(x) \geq 0$.*
  - *Strong convexity implies uniform positive definiteness of the Hessian.*

- *This characterization is particularly useful for quadratic functions $f(x) = x^\top Ax + b^\top x + c$, where convexity is equivalent to A being positive semidefinite.*

Theorem 3.4. *(Properties of Convex Functions)*

1. *Any local minimum of a convex function is a global minimum*
2. *The sum of convex functions is convex*
3. *The composition of a convex function with an affine function is convex*
4. *If $f : \mathbb{R}^n \to \mathbb{R}$ is convex and $g : \mathbb{R}^m \to \mathbb{R}^n$ is affine (in particular, linear). Then, $f \circ g : \mathbb{R}^m \to \mathbb{R}$ is convex.*
5. *If $f : \mathbb{R}^n \to \mathbb{R}$ is convex and $g : \mathbb{R} \to \mathbb{R}$ is convex and nondecresing. Then, $g \circ f : \mathbb{R}^n \to \mathbb{R}$ is convex.*
6. *The pointwise supremum of convex functions is convex*

3.2.3 Examples of Convex Functions

1. $f(x) = e^x$ on $\mathbb{R}$
2. $f(x) = x^p$ on $[0,\infty)$ for $p \geq 1$
3. $f(x) = -\ln x$ on $(0,\infty)$
4. $f(x) = \|x\|$ (any norm) on $\mathbb{R}^n$
5. $f(x) = x^T Ax + b^T x + c$ where A is positive semidefinite

Proof. **Proofs of Convexity:**

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if for all $x, y \in \mathrm{dom}(f)$ and all $\theta \in [0,1]$:

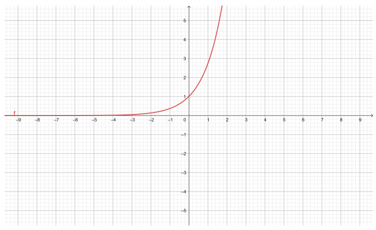
$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y).$$

For differentiable functions, an equivalent condition is that $f(y) \geq f(x) + \nabla f(x)^T (y - x)$ for all x, y.

1. **$f(x) = e^x$ on $\mathbb{R}$**

   For a twice-differentiable function of one variable, convexity is equivalent to $f''(x) \geq 0$ for all x.

   Here, $f'(x) = e^x$ and $f''(x) = e^x > 0$ for all $x \in \mathbb{R}$. Therefore, $f(x) = e^x$ is strictly convex on $\mathbb{R}$.



2. **$f(x) = x^p$ on $[0, \infty)$ for $p \geq 1$**

   We consider $f(x) = x^p$ where $p \geq 1$ and $x \geq 0$.

   For $p > 1$, the second derivative is:

$$f'(x) = px^{p-1}, \quad f''(x) = p(p-1)x^{p-2}.$$

   Since $p > 1$ and $x \geq 0$, we have $f''(x) \geq 0$ (strictly positive for $x > 0$).

   For $p = 1$, $f(x) = x$ is linear, hence convex.

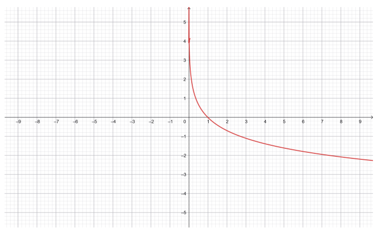
   Thus, $f(x) = x^p$ is convex on $[0, \infty)$ for all $p \geq 1$.

3. **$f(x) = -\ln x$ on $(0, \infty)$**

   This function is strictly convex on $(0, \infty)$. Compute derivatives:

$$f'(x) = -\frac{1}{x}, \quad f''(x) = \frac{1}{x^2} > 0 \quad \text{for all } x > 0.$$

   Since $f''(x) > 0$ for all $x \in (0, \infty)$, f is strictly convex on its domain.



4. **$f(x) = \|x\|$ (any norm) on $\mathbb{R}^n$**

Let $\|\cdot\|$ be any norm on $\mathbb{R}^n$. For any $x, y \in \mathbb{R}^n$ and $\theta \in [0,1]$:

$$\|\theta x + (1-\theta)y\| \leq \|\theta x\| + \|(1-\theta)y\| = \theta\|x\| + (1-\theta)\|y\|,$$

where the inequality follows from the triangle inequality of norms, and the equality follows from the homogeneity property $\|\alpha x\| = |\alpha|\|x\|$.

Thus, $\|x\|$ satisfies the definition of convexity and is therefore convex on $\mathbb{R}^n$.

5. $f(x) = x^T Ax + b^T x + c$ **where** A **is positive semidefinite**

   Consider $f : \mathbb{R}^n \to \mathbb{R}$ given by $f(x) = x^T Ax + b^T x + c$, with $A \in \mathbb{R}^{n\times n}$ symmetric and positive semidefinite.

   The gradient and Hessian are:

   $$\nabla f(x) = 2Ax + b, \quad \nabla^2 f(x) = 2A.$$

   Since A is positive semidefinite, $\nabla^2 f(x) = 2A$ is also positive semidefinite for all x.

   For a twice-differentiable function, convexity is equivalent to $\nabla^2 f(x)$ being positive semidefinite for all x in the domain. Therefore, f is convex on $\mathbb{R}^n$.

   Additionally, if A is positive definite, then f is strictly convex.

□

3.2.4 Exercises

Exercise 3.1. *Prove or disprove the convexity of:*

1. $f(x) = x^4 - 2x^2$ *on* $\mathbb{R}$
2. $f(x_1, x_2) = x_1^2 - x_2^2$ *on* $\mathbb{R}^2$
3. $f(x) = \sqrt{1+x^2}$ *on* $\mathbb{R}$

Proof. We analyze the convexity of each function using the second derivative test for functions of one variable and the Hessian matrix test for functions of several variables.

1. $f(x) = x^4 - 2x^2$ **on** $\mathbb{R}$

   We compute the first and second derivatives:

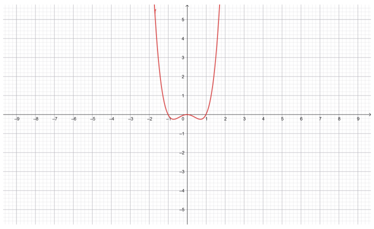
   $$f'(x) = 4x^3 - 4x = 4x(x^2-1), \quad f''(x) = 12x^2 - 4 = 4(3x^2-1).$$

The second derivative is not always nonnegative. In particular:

$$f''(x) < 0 \quad \text{when} \quad |x| < \frac{1}{\sqrt{3}}.$$

For example, $f''(0) = -4 < 0$.

Since the second derivative is negative on the interval $(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$, the function is **not convex** on $\mathbb{R}$.



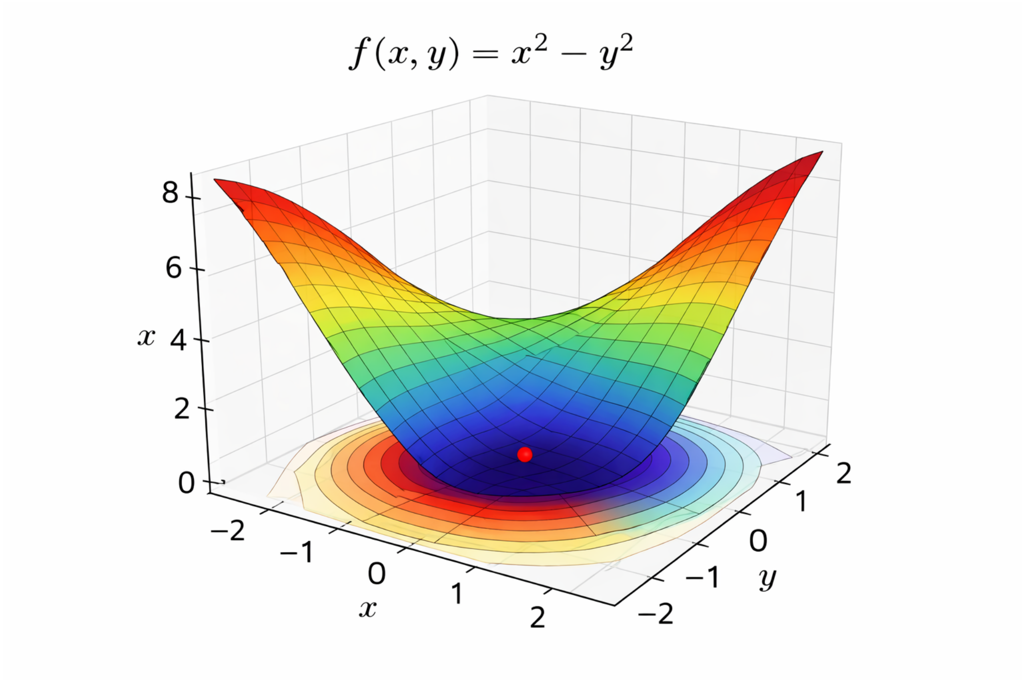
2. $f(x_1, x_2) = x_1^2 - x_2^2$ **on** $\mathbb{R}^2$

   We compute the Hessian matrix:

$$\nabla^2 f(x_1, x_2) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}.$$

   The eigenvalues of this matrix are $\lambda_1 = 2$ and $\lambda_2 = -2$. Since one eigenvalue is negative, the Hessian is **not positive semidefinite**.

   Therefore, f is **not convex** on $\mathbb{R}^2$. In fact, this function is *indefinite* (neither convex nor concave).



3. $f(x) = \sqrt{1+x^2}$ **on** $\mathbb{R}$

   We compute the first and second derivatives:

$$f'(x) = \frac{x}{\sqrt{1+x^2}}, \quad f''(x) = \frac{1}{(1+x^2)^{3/2}}.$$

   The second derivative is positive for all $x \in \mathbb{R}$:

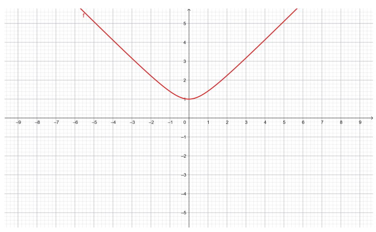
$$f''(x) = \frac{1}{(1+x^2)^{3/2}} > 0 \quad \text{for all } x \in \mathbb{R}.$$

   Since $f''(x) > 0$ for all x, the function is **strictly convex** on $\mathbb{R}$.

   We can also verify this using the definition: For any $x, y \in \mathbb{R}$ and $\theta \in [0,1]$,

$$f(\theta x + (1-\theta)y) = \sqrt{1 + (\theta x + (1-\theta)y)^2} \le \theta\sqrt{1+x^2} + (1-\theta)\sqrt{1+y^2},$$

   by the triangle inequality applied to the vectors $(1,x)$ and $(1,y)$ in $\mathbb{R}^2$, since $\sqrt{1+x^2} = \|(1,x)\|_2$ and norms are convex.



Conclusion:

- $f(x) = x^4 - 2x^2$ is **not convex** on $\mathbb{R}$.
- $f(x_1, x_2) = x_1^2 - x_2^2$ is **not convex** on $\mathbb{R}^2$ (indefinite).
- $f(x) = \sqrt{1+x^2}$ is **strictly convex** on $\mathbb{R}$.

□

3.3 Concave Functions

3.3.1 Definition

A function $f : C \to \mathbb{R}$ defined on a convex set $C \subseteq \mathbb{R}^n$ is **concave** if for all $x, y \in C$ and all $\theta \in [0,1]$:

$$f(\theta x + (1-\theta)y) \geq \theta f(x) + (1-\theta) f(y).$$

Equivalently, f is concave if and only if $-f$ is convex.

For differentiable functions, f is concave if and only if:

$$f(y) \leq f(x) + \nabla f(x)^\top (y - x) \quad \text{for all } x, y \in C.$$

For twice differentiable functions, f is concave if and only if its Hessian is negative semidefinite:

$$\nabla^2 f(x) \preceq 0 \quad \text{for all } x \in C.$$

3.3.2 Examples of Concave Functions

1. **Linear and affine functions** For any $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$, the function:

   $$f(x) = a^\top x + b$$

   is both concave and convex. This follows from:

   $$f(\theta x + (1-\theta)y) = a^\top(\theta x + (1-\theta)y) + b = \theta(a^\top x + b) + (1-\theta)(a^\top y + b) = \theta f(x) + (1-\theta) f(y).$$

2. **Logarithm function** The function $f(x) = \log x$ is concave on $(0, \infty)$.

   Proof: Compute derivatives:

   $$f'(x) = \frac{1}{x}, \quad f''(x) = -\frac{1}{x^2} < 0 \quad \text{for all } x > 0.$$

   Since $f''(x) < 0$, the function is strictly concave.

3. **Square root function** The function $f(x) = \sqrt{x}$ is concave on $[0, \infty)$.

   Proof: For $x > 0$:
   $$f'(x) = \frac{1}{2\sqrt{x}}, \quad f''(x) = -\frac{1}{4x^{3/2}} < 0.$$
   At $x = 0$, the function is continuous and the definition of concavity can be checked directly.

4. **Entropy function** The function $f(x) = -x \ln x$ (with $0 \ln 0 = 0$) is concave on $[0, \infty)$.

   Proof: For $x > 0$:
   $$f'(x) = -\ln x - 1, \quad f''(x) = -\frac{1}{x} < 0.$$

5. **Quadratic form with negative semidefinite matrix** For a symmetric negative semidefinite matrix $A \in \mathbb{R}^{n \times n}$, the function:
   $$f(x) = x^\top A x$$
   is concave on $\mathbb{R}^n$.

   Proof: The Hessian is $\nabla^2 f(x) = 2A \preceq 0$, so f is concave.

6. **Minimum function** The pointwise minimum of concave functions is concave. That is, if $f_1, f_2, \ldots, f_m$ are concave functions, then:
   $$f(x) = \min\{f_1(x), f_2(x), \ldots, f_m(x)\}$$
   is concave.

   Proof: For any $x, y \in C$ and $\theta \in [0,1]$:
   $$\begin{aligned} f(\theta x + (1-\theta)y) &= \min_i f_i(\theta x + (1-\theta)y) \\ &\geq \min_i [\theta f_i(x) + (1-\theta) f_i(y)] \\ &\geq \theta \min_i f_i(x) + (1-\theta) \min_i f_i(y) \\ &= \theta f(x) + (1-\theta) f(y). \end{aligned}$$

3.3.3 Important Properties

- The sum of concave functions is concave.
- Nonnegative weighted sums of concave functions are concave.
- The pointwise infimum of a family of concave functions is concave.

- Composition of Convex and Concave Functions:

Claim (False Statement): If f is concave and g is convex and nondecreasing, then $g \circ f$ is concave.

Counter example:

Consider

$$f(x) = \sqrt{x}, \quad x \geq 0,$$

which is concave, and

$$g(x) = e^x,$$

which is convex and strictly increasing on $\mathbb{R}$.

Then the composition is

$$(g \circ f)(x) = e^{\sqrt{x}}.$$

We show that $g \circ f$ is not concave. Compute derivatives:

$$(g \circ f)'(x) = \frac{1}{2\sqrt{x}} e^{\sqrt{x}},$$

$$(g \circ f)''(x) = e^{\sqrt{x}} \left(\frac{1}{4x} - \frac{1}{4x^{3/2}} \right).$$

For large x, the dominant term is positive, hence

$$(g \circ f)''(x) > 0,$$

which implies that $g \circ f$ is convex (not concave). Therefore, the claim is false.

Correct Composition Rule:

The valid statement is:

- If f is convex and g is convex and nondecreasing, then $g \circ f$ is convex.
- If f is concave and g is concave and nondecreasing, then $g \circ f$ is concave.

Conclusion:(The statement is false.)

Convexity or concavity is preserved under composition only when the curvature and monotonicity conditions are compatible.

3.4 Existence and Uniqueness of an Optimal Solution

The questions of **existence** and **uniqueness** are fundamental in optimization theory. Before attempting to compute an optimal solution to a problem (3.0.1), one must first ensure that such a solution actually exists, and ideally, determine whether it is the only one.

Existence of Solutions:

The primary tool for establishing existence is the **Weierstrass Extreme Value Theorem**:

- **Compactness** is crucial: without it, a continuous function may approach an extremal value but never achieve it (e.g., $f(x) = x$ on $(0,1)$).
- For convex optimization, existence is often studied via **coercivity** or **level set** properties.

Uniqueness of Solutions:

Uniqueness depends primarily on the **shape** of the objective function.

3.4.1 Coercive Functions (Functions that Tend to Infinity at Infinity)

Definition 3.4. *(Coercive Function)*
A function $f : \mathbb{R}^n \to \mathbb{R}$ is coercive if:

$$\lim_{\|x\| \to \infty} f(x) = +\infty$$

Theorem 3.5. *(Existence for Coercive Functions)*
If $f : \mathbb{R}^n \to \mathbb{R}$ is continuous and coercive, then f has at least one global minimum.

For further information on the proof of this theorem, see [5].

3.4.2 Weierstrass Theorem

Theorem 3.6. *(Weierstrass Extreme Value Theorem)*
If $f : D \to \mathbb{R}$ is continuous and $D \subseteq \mathbb{R}^n$ is compact (nonempty, closed and bounded), then f attains its minimum and maximum on D.

Proof. We prove that f attains its maximum. The proof for the minimum follows by applying the same argument to $-f$.

Step 1: Boundedness above.

Suppose, for contradiction, that f is not bounded above on D. Then for every $k \in \mathbb{N}$, there exists $x_k \in D$ such that

$$f(x_k) > k.$$

Since D is compact, it is sequentially compact (in $\mathbb{R}^n$, compactness is equivalent to sequential compactness by the Bolzano-Weierstrass theorem [10]). Therefore, the sequence $\{x_k\}$ has a convergent subsequence $\{x_{k_j}\}$ with limit $x^* \in D$ (because D is closed).

Because f is continuous at x^*,

$$\lim_{j\to\infty} f(x_{k_j}) = f(x^*) \in \mathbb{R}.$$

But by construction, $f(x_{k_j}) > k_j \to \infty$ as $j \to \infty$, which contradicts the fact that the subsequence converges to a finite real number. Hence, f must be bounded above on D.

Let

$$M = \sup_{x\in D} f(x) \in \mathbb{R}.$$

Step 2: Attainment of the supremum.

Since M is the supremum, for each $n \in \mathbb{N}$, there exists $x_n \in D$ such that

$$M - \frac{1}{n} < f(x_n) \leq M.$$

The sequence $\{x_n\}$ lies in the compact set D. By sequential compactness, there exists a convergent subsequence $\{x_{n_k}\}$ with

$$\lim_{k\to\infty} x_{n_k} = x^* \in D.$$

By continuity of f,

$$\lim_{k\to\infty} f(x_{n_k}) = f(x^*).$$

From the inequality $M - \frac{1}{n_k} < f(x_{n_k}) \leq M$, we have

$$\lim_{k\to\infty} f(x_{n_k}) = M.$$

Therefore, $f(x^*) = M$, so the maximum is attained at $x^* \in D$.

Step 3: Attainment of the minimum.

Apply the same argument to the continuous function $-f$ on D. Since $-f$ attains its maximum, say at $x_* \in D$, we have

$$-f(x_*) \geq -f(x) \quad \text{for all } x \in D,$$

which implies

$$f(x_*) \leq f(x) \quad \text{for all } x \in D.$$

Thus, the minimum is attained at $\mathbf{x}_*$. □

Corollary 3.1. *(Existence for Continuous Functions on Compact Sets)*
If $f : D \to \mathbb{R}$ is continuous and D is compact and nonempty, then the optimization problem $\min_{x\in D} f(x)$ has at least one solution.

Theorem 3.7. *(Uniqueness for Strictly Convex Functions)*
If $f : D \to \mathbb{R}$ is strictly convex and D is convex, then f has at most one global minimum.

Proof. We prove by contradiction. Suppose that f has two distinct global minimizers x^* and y^* with $x^* \neq y^*$. Let

$$m = f(x^*) = f(y^*) = \min_{x\in\mathbb{R}^n} f(x).$$

Since f is strictly convex, for any $\lambda \in (0,1)$, we have

$$f(\lambda x^* + (1-\lambda)y^*) < \lambda f(x^*) + (1-\lambda)f(y^*).$$

Substituting $f(x^*) = f(y^*) = m$ yields

$$f(\lambda x^* + (1-\lambda)y^*) < \lambda m + (1-\lambda)m = m.$$

Thus, $f(\lambda x^* + (1-\lambda)y^*) < m$, which contradicts the fact that m is the global minimum value of f.

Therefore, our assumption that two distinct global minimizers exist is false. Hence, if a global minimizer exists, it must be unique. □

3.4.3 Exercises

Exercise 3.2. *Determine if the following functions have global minima:*

1. $f(x) = x^4 - 4x^2$ *on* $\mathbb{R}$
2. $f(x) = e^{-x^2}$ *on* $\mathbb{R}$
3. $f(x_1, x_2) = x_1^2 + x_2^2 - 2x_1x_2$ *on* $\mathbb{R}^2$

Solution 3.1. *We analyze each function to determine if it has a global minimum.*

1. $f(x) = x^4 - 4x^2$ ***on*** $\mathbb{R}$

   Let's rewrite the function: $f(x) = x^2(x^2 - 4)$.

   First, note that as $|x| \to +\infty$, $x^4 \to +\infty$ *dominates, so* $f(x) \to \infty$. *This suggests the function is bounded below.*

Find critical points:

$$f'(x) = 4x^3 - 8x = 4x(x^2 - 2) = 4x(x - \sqrt{2})(x + \sqrt{2}).$$

$$f'(x) = 0 \quad \Rightarrow \quad x = 0, \quad x = \sqrt{2}, \quad x = -\sqrt{2}.$$

Second derivative: $f''(x) = 12x^2 - 8$.

Evaluate at critical points:

- $f''(0) = -8 < 0$*: local maximum*
- $f''(\sqrt{2}) = 12(2) - 8 = 16 > 0$*: local minimum*
- $f''(-\sqrt{2}) = 12(2) - 8 = 16 > 0$*: local minimum*

Compute function values:

$$f(0) = 0^4 - 4(0)^2 = 0$$
$$f(\sqrt{2}) = (\sqrt{2})^4 - 4(\sqrt{2})^2 = 4 - 8 = -4$$
$$f(-\sqrt{2}) = (-\sqrt{2})^4 - 4(-\sqrt{2})^2 = 4 - 8 = -4$$

Since $f(x) \to +\infty$ *as* $|x| \to +\infty$*, the function has a global minimum. The minimum value is* -4*, achieved at* $x = \pm\sqrt{2}$*.*

Answer: Yes, global minimum of -4 ***at*** $x = \pm\sqrt{2}$***.***

2. $f(x) = e^{-x^2}$ ***on*** $\mathbb{R}$

   Note: $f(x) > 0$ *for all* x*, and* $f(0) = 1$*.*

   Find critical points:

$$f'(x) = -2xe^{-x^2} = 0 \quad \Rightarrow \quad x = 0.$$

   Second derivative: $f''(x) = (4x^2 - 2)e^{-x^2}$.

$$f''(0) = -2 < 0 : \text{ local maximum at } x = 0.$$

   As $|x| \to +\infty$*,* $e^{-x^2} \to 0$*. So* $f(x)$ *approaches 0 but never reaches it. The function has no global minimum because:*

   - $f(x) > 0$ *for all* x
   - $\inf_{x\in\mathbb{R}} f(x) = 0$ *(greatest lower bound)*

- *But* $f(x) \neq 0$ *for any* $x \in \mathbb{R}$

The infimum is 0 but is not attained.

Answer: No global minimum (infimum is 0 but not attained).

3. $f(x_1,x_2) = x_1^2 + x_2^2 - 2x_1x_2$ ***on*** $\mathbb{R}^2$

   Simplify the function:

$$f(x_1,x_2) = x_1^2 + x_2^2 - 2x_1x_2 = (x_1 - x_2)^2.$$

   The function is a perfect square, so $f(x_1,x_2) \geq 0$ *for all* $(x_1,x_2) \in \mathbb{R}^2$*.*

   Find critical points:

$$\nabla f(x_1,x_2) = \begin{bmatrix} 2(x_1 - x_2) \\ -2(x_1 - x_2) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

   This implies $x_1 - x_2 = 0$*, so* $x_1 = x_2$*.*

   Thus, all points on the line $x_1 = x_2$ *are critical points.*

   Evaluate f *on this line: if* $x_1 = x_2 = t$*, then* $f(t,t) = 0$*.*

   Hessian matrix:

$$\nabla^2 f(x_1,x_2) = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}.$$

   Eigenvalues: $\lambda_1 = 0$*,* $\lambda_2 = 4$*. The Hessian is positive semidefinite.*

   Since $f(x_1,x_2) = (x_1 - x_2)^2 \geq 0$ *and* $f(x_1,x_2) = 0$ *when* $x_1 = x_2$*, the function has a global minimum of 0 attained along the entire line* $x_1 = x_2$*.*

   Answer: Yes, global minimum of 0 at all points where $x_1 = x_2$***.***

Conclusion:

- $f(x) = x^4 - 4x^2$*: Has global minimum* $x = \pm\sqrt{2}$*.*
- $f(x) = e^{-x^2}$*: No global minimum (infimum is 0 but not attained).*
- $f(x_1,x_2) = x_1^2 + x_2^2 - 2x_1x_2$*: Has global minimum 0 on the line* $x_1 = x_2$*.*

Chapter 4

Nonlinear Unconstraints Optimization Problems

Nonlinear unconstrained optimization addresses problems where the objective function $f : \mathbb{R}^n \to \mathbb{R}$ is **nonlinear** and there are **no restrictions** on the variable x beyond belonging to $\mathbb{R}^n$.
This forms the core foundation of continuous optimization, where the focus is on finding minima (or maxima) of smooth functions over the entire space.

Key Mathematical Framework:

The theory is built on **calculus** and **convexity**:

- **First-Order Necessary Condition :** It is based on **stationary points** (including minima, maxima, and saddle points).
- **Second-Order Conditions:**
  - **Necessary:** If x^* is a local minimizer and f is twice differentiable, then $\nabla^2 f(x^*)$ is **positive semidefinite**.
  - **Sufficient:** If $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is **positive definite**, then x^* is a strict local minimizer.
- **Convexity Special Case:** When f is convex, every stationary point is a **global minimizer**. If f is strictly convex, the minimizer is unique.

4.1 Definition

Consider the unconstrained optimization problem (3.0.1).

Definition 4.1 (Critical Point)**.** *(or stationary) $x^* \in \mathbb{R}^n$ is a **critical point** of f if $\nabla f(x^*) = \mathbf{0}$ or $\nabla f(x^*)$ does not exist.*

4.2 Necessary Conditions for the Existence of an Optimal Solution

Theorem 4.1 (First-Order Necessary Condition)**.** *If x^* is a local minimum of f and f is differentiable at x^*, then:*

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

Proof. Since x^* is a local minimum, there exists $\varepsilon > 0$ such that

$$f(x^* + h) \geq f(x^*) \quad \text{for all } h \text{ with } \|h\| < \varepsilon.$$

Because f is differentiable at x^*, by Taylor's theorem we have

$$f(x^* + h) = f(x^*) + \nabla f(x^*)^\mathsf{T} h + o(\|h\|),$$

where $\frac{o(\|h\|)}{\|h\|} \to 0$ as $\|h\| \to 0$.

For any direction d with $\|d\| = 1$ and sufficiently small $t > 0$, let $h = td$. Then

$$f(x^* + td) - f(x^*) = t\nabla f(x^*)^\mathsf{T} d + o(t).$$

If $\nabla f(x^*) \neq \mathbf{0}$, choose $d = -\frac{\nabla f(x^*)}{\|\nabla f(x^*)\|}$. Then

$$f(x^* + td) - f(x^*) = -t\|\nabla f(x^*)\| + o(t).$$

For sufficiently small $t > 0$, the term $-t\|\nabla f(x^*)\|$ dominates, so

$$f(x^* + td) - f(x^*) < 0,$$

contradicting the local minimality of x^*. Hence, $\nabla f(x^*) = \mathbf{0}$. □

Theorem 4.2 (Second-Order Necessary Condition)**.** *If x^* is a local minimum of f and f is twice differentiable at x^*, then:*

$$\nabla f(x^*) = 0 \quad \textit{and} \quad \nabla^2 f(x^*) \geq 0$$

Proof. From the first-order necessary condition, we have $\nabla f(x^*) = \mathbf{0}$. Now suppose $\nabla^2 f(x^*)$ is not positive semidefinite. Then there exists a unit vector $d \in \mathbb{R}^n$ such that

$$d^\top \nabla^2 f(x^*) d = -\varepsilon \quad \text{for some } \varepsilon > 0.$$

By the second-order Taylor expansion,

$$f(x^* + td) = f(x^*) + \frac{t^2}{2} d^\top \nabla^2 f(x^*) d + o(t^2).$$

Substituting,

$$f(x^* + td) = f(x^*) - \frac{\varepsilon}{2} t^2 + o(t^2).$$

Rewrite as

$$f(x^* + td) - f(x^*) = t^2 \left(-\frac{\varepsilon}{2} + \frac{o(t^2)}{t^2} \right).$$

Since $\frac{o(t^2)}{t^2} \to 0$ as $t \to 0$, there exists $\delta > 0$ such that for all $0 < |t| < \delta$,

$$\left| \frac{o(t^2)}{t^2} \right| < \frac{\varepsilon}{4}.$$

Then

$$-\frac{\varepsilon}{2} + \frac{o(t^2)}{t^2} \leq -\frac{\varepsilon}{2} + \left| \frac{o(t^2)}{t^2} \right| < -\frac{\varepsilon}{2} + \frac{\varepsilon}{4} = -\frac{\varepsilon}{4} < 0.$$

Thus, for $0 < |t| < \delta$,

$$f(x^* + td) - f(x^*) < 0,$$

contradicting the local minimality of x^*. Therefore, $\nabla^2 f(x^*) \geq \mathbf{0}$. □

4.3 Second-Order Sufficient Conditions

Theorem 4.3 (Second-Order Sufficient Condition)**.** *If f is twice differentiable at x^*, $\nabla f(x^*) = 0$, and $\nabla^2 f(x^*) > 0$, then x^* is a strict local minimum.*

Proof. Since $\nabla^2 f(x^*) \succ \mathbf{0}$ (positive definite), there exists a constant $\mu > 0$ such that

$$d^\top \nabla^2 f(x^*) d \geq \mu \|d\|^2 \quad \text{for all } d \in \mathbb{R}^n.$$

This follows from the fact that the smallest eigenvalue $\lambda_{\min}$ of $\nabla^2 f(x^*)$ is positive; we can take $\mu = \lambda_{\min} > 0$.

Because f is twice differentiable at x^*, by Taylor's theorem we have the second-order expansion:

$$f(x^* + h) = f(x^*) + \nabla f(x^*)^\top h + \frac{1}{2} h^\top \nabla^2 f(x^*) h + o(\|h\|^2),$$

where $\frac{o(\|h\|^2)}{\|h\|^2} \to 0$ as $\|h\| \to 0$.

Using $\nabla f(x^*) = \mathbf{0}$, this simplifies to

$$f(x^* + h) - f(x^*) = \frac{1}{2} h^\mathsf{T} \nabla^2 f(x^*) h + o(\|h\|^2).$$

By the positive definiteness of $\nabla^2 f(h^*)$,

$$\frac{1}{2} h^\mathsf{T} \nabla^2 f(x^*) h \geq \frac{\mu}{2} \|h\|^2.$$

Thus,

$$f(x^* + h) - f(x^*) \geq \frac{\mu}{2} \|h\|^2 + o(\|h\|^2).$$

Factor $\|x\|^2$:

$$f(x^* + h) - f(x^*) = \|h\|^2 \left(\frac{\mu}{2} + \frac{o(\|h\|^2)}{\|h\|^2} \right).$$

Since $\frac{o(\|h\|^2)}{\|h\|^2} \to 0$ as $\|h\| \to 0$, there exists $\delta > 0$ such that for all h with $0 < \|h\| < \delta$,

$$\left| \frac{o(\|h\|^2)}{\|h\|^2} \right| < \frac{\mu}{4}.$$

Then

$$\frac{\mu}{2} + \frac{o(\|h\|^2)}{\|h\|^2} \geq \frac{\mu}{2} - \left| \frac{o(\|h\|^2)}{\|h\|^2} \right| > \frac{\mu}{2} - \frac{\mu}{4} = \frac{\mu}{4} > 0.$$

Therefore, for all h with $0 < \|h\| < \delta$,

$$f(x^* + h) - f(x^*) > 0,$$

i.e., $f(x^* + h) > f(x^*)$.

This means that x^* is a strict local minimum of f. □

4.4 First-Order Necessary and Sufficient Conditions

Theorem 4.4 (For Convex Functions). *If f is convex and differentiable, then x^* is a global minimum if and only if:*

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

Proof. We prove the equivalence in two directions.

4.4.0.0.1 ($\Rightarrow$) **Necessary Condition.** If x^* is a global minimum, then it is a local minimum. Since f is differentiable, the first-order necessary condition implies

$$\nabla f(x^*) = \mathbf{0}.$$

4.4.0.0.2 ($\Leftarrow$) **Sufficient Condition.** Assume $\nabla f(x^*) = \mathbf{0}$. For a convex differentiable function, the gradient provides a supporting hyperplane to the epigraph. Specifically, convexity implies that for any $y \in \mathbb{R}^n$ and any $\lambda \in (0,1]$,

$$f(x^* + \lambda(y - x^*)) \leq (1-\lambda)f(x^*) + \lambda f(y).$$

Rearranging,

$$f(x^* + \lambda(y - x^*)) - f(x^*) \leq \lambda(f(y) - f(x^*)).$$

Dividing by $\lambda > 0$,

$$\frac{f(x^* + \lambda(y - x^*)) - f(x^*)}{\lambda} \leq f(y) - f(x^*).$$

Taking the limit as $\lambda \to 0^+$, the left-hand side converges to the directional derivative:

$$\lim_{\lambda \to 0^+} \frac{f(x^* + \lambda(y - x^*)) - f(x^*)}{\lambda} = \nabla f(x^*)^\mathsf{T}(y - x^*) = 0.$$

Hence,

$$0 \leq f(y) - f(x^*) \quad \text{for all } y \in \mathbb{R}^n,$$

so $f(y) \geq f(x^*)$ for all y, proving x^* is a global minimum. □

Remark 4.1.
Second-Order Sufficient Condition:*(for local optimum) Suppose x^* is critical point. Let $H(x)$ be the Hessian matrix of f. Then:*

- *If $H(x^*)$ is* ***negative definite****, then x^* is a* ***local maximum****.*
- *If $H(x^*)$ is* ***positive definite****, then x^* is a* ***local minimum****.*

Second-Order Sufficient Condition: *(for global optimum) Suppose x^* is critical point. Then:*

- *If $H(x)$ is* ***positive semi-definite*** *for all x (i.e., f is convex), then x^* is a* ***global minimum****.*
- *If $H(x)$ is* ***negative semi-definite*** *for all x (i.e., f is concave), then x^* is a* ***global maximum****.*

Also, we have

- *If $H(x)$ is* ***positive definite*** *for all x, the global minimum is unique.*
- *If $H(x)$ is* ***negative definite*** *for all x, the global maximum is unique.*

4.5 Saddle Point

Definition 4.2. *(Saddle Point) Let $f:\mathbb{R}^n \to \mathbb{R}$. A point $x^* \in \mathbb{R}^n$ is called a* saddle point *of f if x^* is a critical point (i.e., $\nabla f(x^*) = 0$) and x^* is neither a local minimum nor a local maximum.*

In the case of a function of two variables $f(x,y)$, the Hessian matrix may be neither positive definite nor negative definite. A point (x^*,y^*) where

$$\frac{\partial f}{\partial x}(x^*,y^*) = 0 \quad \text{and} \quad \frac{\partial f}{\partial y}(x^*,y^*) = 0$$

is called a **critical point**.
If the Hessian is indefinite at that point, (x^*,y^*) is called a **saddle point** if:

$$\det(H)(x^*,y^*) = f_{xx}f_{yy} - (f_{xy})^2 < 0.$$

This condition means the Hessian has both positive and negative eigenvalues.

Characteristics of a saddle point:

1. For a fixed $y = y^*$, the function $f(x,y^*)$ (depending only on x) has a **minimum** (or maximum) at (x^*,y^*).

2. For a fixed $x = x^*$, the function $f(x^*,y)$ (depending only on y) has a **maximum** (or minimum) at (x^*,y^*).

Example 4.1. *Consider the function $f(x,y) = x^2 - y^2$. We have:*

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial f}{\partial y} = -2y.$$

Setting these equal to zero gives the critical point $(0,0)$.

The Hessian matrix is:

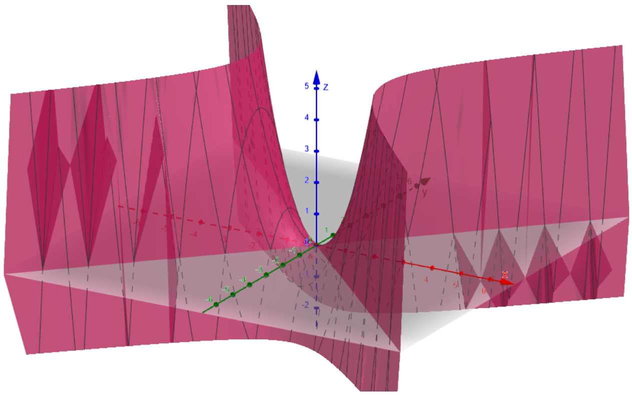
$$H(x,y) = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}.$$

This matrix is neither positive definite nor negative definite (its eigenvalues are 2 and -2). Therefore, $(0,0)$ is a ***saddle point****.*

Indeed:

- *For fixed $y = 0$, $f(x,0) = x^2$ has a* ***minimum*** *at $x = 0$.*

- *For fixed $x = 0$, $f(0,y) = -y^2$ has a* ***maximum*** *at $y = 0$.*



Example 4.2. *Finding the Saddle Point of the following function:*

$$f(x,y) = x^3 + y^3 - 3xy.$$

Gradient, we have

$$\nabla f = \begin{pmatrix} 3x^2 - 3y \\ 3y^2 - 3x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Then

$$\begin{cases} x^2 = y \\ y^2 = x \end{cases} \quad \Rightarrow \quad x^4 = x \quad \Rightarrow \quad x(x^3 - 1) = 0$$

$$x = 0 \ (\Rightarrow y = 0) \quad or \quad x = 1 \ (\Rightarrow y = 1)$$

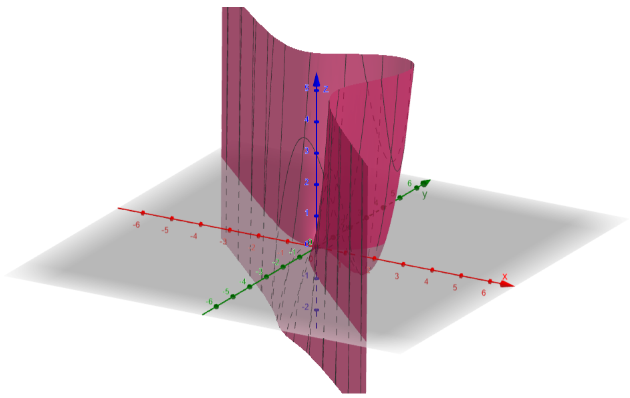
Hessian Analysis,

$$H_f(x,y) = \begin{pmatrix} 6x & -3 \\ -3 & 6y \end{pmatrix}$$

At* $(0,0)$*:

$$H_f(0,0) = \begin{pmatrix} 0 & -3 \\ -3 & 0 \end{pmatrix}, \quad \det(H) = 0 \cdot 0 - (-3)^2 = -9 < 0$$

Since $\det(H) < 0$*,* $(0,0)$ *is a* ***saddle point****.*



Example 4.3. *Solve the maximization problem:*

$$(P): \quad \max_{x,y} f(x,y) = 3xy - x^3 - y^3.$$

Solution 4.1.

1. *If (x^*, y^*) is a solution, then:*

$$\begin{cases} \frac{\partial f}{\partial x} = 3y - 3x^2 = 0 \\ \frac{\partial f}{\partial y} = 3x - 3y^2 = 0 \end{cases} \implies \begin{cases} y = x^2 \\ x = y^2 \end{cases}$$

   Substituting: $x = (x^2)^2 = x^4 \implies x(x^3 - 1) = 0$, *so* $x = 0$ *or* $x = 1$. *Corresponding* y *values:* $y = 0$ *or* $y = 1$. *Thus, critical points:* $(0,0)$ *and* $(1,1)$.

2. ***Hessian matrix:***

$$H(x,y) = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix} = \begin{pmatrix} -6x & 3 \\ 3 & -6y \end{pmatrix}.$$

3. ***Second-order analysis:***

   - *At* $(0,0)$*:* $H(0,0) = \begin{pmatrix} 0 & 3 \\ 3 & 0 \end{pmatrix}$.

     Leading principal minors: $D_1 = 0$, $D_2 = -9 < 0$.

     $H(0,0)$ *is indefinite* $\Rightarrow$ $(0,0)$ *is a saddle point (neither max nor min).*

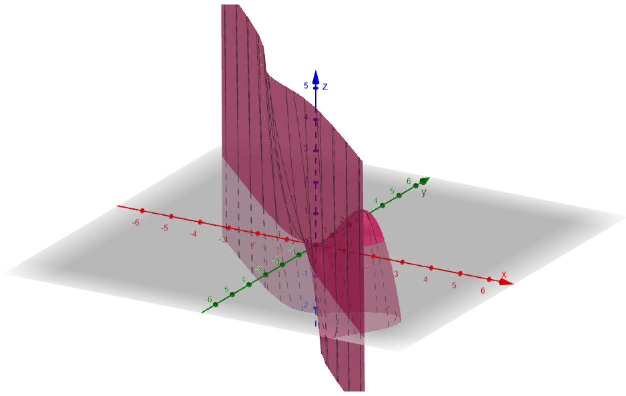
   - *At* $(1,1)$*:* $H(1,1) = \begin{pmatrix} -6 & 3 \\ 3 & -6 \end{pmatrix}$.

     Leading principal minors: $D_1 = -6 < 0$, $D_2 = 36 - 9 = 27 > 0$.

     $H(1,1)$ *is* ***negative definite*** $\Rightarrow$ $(1,1)$ *is a* ***local maximum****.*

4. ***Global optimality:***

   Since $H(x,y)$ *is not negative semi-definite for all* $(x,y) \in \mathbb{R}^2$, $(1,1)$ *is* ***not necessarily a global maximum****.*



4.6 Exercises

Exercise 4.1. *Find and classify all stationary points of:*

1. $f(x_1, x_2) = x_1^2 + x_2^2 - 4x_1 - 6x_2$
2. $f(x_1, x_2) = x_1^3 + x_2^3 - 3x_1x_2$
3. $f(x_1, x_2) = e^{x_1^2 + x_2^2} - x_1^2 - x_2^2$

Solution 4.2.

1. $f(x_1, x_2) = x_1^2 + x_2^2 - 4x_1 - 6x_2$

   Step 1: Find the gradient.

$$\nabla f(x_1, x_2) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2x_1 - 4 \\ 2x_2 - 6 \end{pmatrix}$$

   Step 2: Set gradient to zero and solve.

$$\begin{cases} 2x_1 - 4 = 0 \\ 2x_2 - 6 = 0 \end{cases} \Rightarrow \begin{cases} x_1 = 2 \\ x_2 = 3 \end{cases}$$

   Stationary point: $(2, 3)$.

   Step 3: Compute the Hessian matrix.

$$H_f(x_1, x_2) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

Step 4: Classify using Hessian. *Since H_f is constant and positive definite (determinant $= 4 > 0$, eigenvalues $= 2, 2 > 0$),*
$(2,3)$ *is a **strict local minimum**.*

$$\boxed{\text{Stationary point: } (2,3) \text{ (strict local minimum)}}$$

2. $f(x_1,x_2) = x_1^3 + x_2^3 - 3x_1x_2$

Step 1: Find the gradient.

$$\nabla f(x_1,x_2) = \begin{pmatrix} 3x_1^2 - 3x_2 \\ 3x_2^2 - 3x_1 \end{pmatrix}$$

Step 2: Set gradient to zero.

$$\begin{cases} 3x_1^2 - 3x_2 = 0 \\ 3x_2^2 - 3x_1 = 0 \end{cases} \quad \Rightarrow \quad \begin{cases} x_2 = x_1^2 & (1) \\ x_2^2 = x_1 & (2) \end{cases}$$

Substitute (1) into (2):

$$(x_1^2)^2 = x_1 \quad \Rightarrow \quad x_1^4 = x_1 \quad \Rightarrow \quad x_1^4 - x_1 = 0$$

$$x_1(x_1^3 - 1) = 0 \quad \Rightarrow \quad x_1 = 0 \text{ or } x_1^3 = 1$$

$$x_1 = 0 \quad \text{or} \quad x_1 = 1$$

Case 1: $x_1 = 0 \Rightarrow x_2 = 0^2 = 0$. *Point:* $(0,0)$.

Case 2: $x_1 = 1 \Rightarrow x_2 = 1^2 = 1$. *Point:* $(1,1)$.

Stationary points: $(0,0)$ *and* $(1,1)$.

Step 3: Compute the Hessian matrix.

$$H_f(x_1,x_2) = \begin{pmatrix} 6x_1 & -3 \\ -3 & 6x_2 \end{pmatrix}$$

Step 4: Classify each point.

At $(0,0)$***:***

$$H_f(0,0) = \begin{pmatrix} 0 & -3 \\ -3 & 0 \end{pmatrix}, \quad \det(H) = 0 \cdot 0 - (-3)(-3) = -9 < 0$$

Since determinant < 0, $(0,0)$ *is a **saddle point**.*

At* $(1,1)$*:

$$H_f(1,1) = \begin{pmatrix} 6 & -3 \\ -3 & 6 \end{pmatrix}, \quad \det(H) = 6 \cdot 6 - (-3)(-3) = 36 - 9 = 27 > 0$$

First principal minor: $6 > 0$.

Since $\det(H) > 0$ *and* $\frac{\partial^2 f}{\partial x_1^2} > 0$, $(1,1)$ *is a* ***strict local minimum***.

$$\boxed{\textit{Stationary points: } (0,0) \textit{ (saddle point), } (1,1) \textit{ (strict local minimum)}}$$

3. $f(x_1,x_2) = e^{x_1^2+x_2^2} - x_1^2 - x_2^2$

Step 1: Find the gradient.

$$\nabla f(x_1,x_2) = \begin{pmatrix} 2x_1 e^{x_1^2+x_2^2} - 2x_1 \\ 2x_2 e^{x_1^2+x_2^2} - 2x_2 \end{pmatrix} = 2\begin{pmatrix} x_1(e^{x_1^2+x_2^2} - 1) \\ x_2(e^{x_1^2+x_2^2} - 1) \end{pmatrix}$$

Step 2: Set gradient to zero.

$$\begin{cases} x_1(e^{x_1^2+x_2^2} - 1) = 0 \\ x_2(e^{x_1^2+x_2^2} - 1) = 0 \end{cases}$$

Two possibilities:

1. $e^{x_1^2+x_2^2} - 1 = 0 \Rightarrow e^{x_1^2+x_2^2} = 1 \Rightarrow x_1^2 + x_2^2 = 0 \Rightarrow x_1 = x_2 = 0$

2. $x_1 = 0$ *and* $x_2 = 0$ *(which gives the same condition)*

Actually, more systematically:

$$x_1(e^{r^2} - 1) = 0 \quad \textit{and} \quad x_2(e^{r^2} - 1) = 0, \quad \textit{where } r^2 = x_1^2 + x_2^2$$

This gives:

- *Case A:* $e^{r^2} - 1 = 0 \Rightarrow r^2 = 0 \Rightarrow x_1 = x_2 = 0$
- *Case B:* $x_1 = 0$ *and* $x_2 = 0$ *(same as Case A)*

Wait, there's more: If $e^{r^2} - 1 \neq 0$*, then we must have* $x_1 = 0$ *AND* $x_2 = 0$*, but that forces* $r^2 = 0$*, contradiction. So the only solution is* $x_1 = x_2 = 0$.

Stationary point: $(0,0)$ *only.*

Step 3: Compute the Hessian matrix.

First partial derivatives:

$$\frac{\partial f}{\partial x_1} = 2x_1 e^{x_1^2+x_2^2} - 2x_1$$

$$\frac{\partial^2 f}{\partial x_1^2} = 2e^{x_1^2+x_2^2} + 4x_1^2 e^{x_1^2+x_2^2} - 2 = 2e^{r^2}(1+2x_1^2) - 2$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = 4x_1 x_2 e^{x_1^2+x_2^2} = 4x_1 x_2 e^{r^2}$$

By symmetry, $\frac{\partial^2 f}{\partial x_2^2} = 2e^{r^2}(1+2x_2^2) - 2$.

Step 4: Evaluate Hessian at $(0,0)$***.*** *At* $(0,0)$, $r^2 = 0$, $e^0 = 1$*:*

$$\frac{\partial^2 f}{\partial x_1^2}(0,0) = 2(1)(1+0) - 2 = 0$$

$$\frac{\partial^2 f}{\partial x_2^2}(0,0) = 2(1)(1+0) - 2 = 0$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2}(0,0) = 0$$

$$H_f(0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Step 5: Second derivative test inconclusive. Analyze function behavior.

Let $r^2 = x_1^2 + x_2^2$*, then* $f(x_1,x_2) = e^{r^2} - r^2$.

Define $g(r) = e^{r^2} - r^2$ *for* $r \geq 0$*. Then:*

$$g'(r) = 2re^{r^2} - 2r = 2r(e^{r^2} - 1)$$

$$g''(r) = 2(e^{r^2} - 1) + 4r^2 e^{r^2}$$

For $r > 0$, $g'(r) > 0$*, so* g *is strictly increasing for* $r > 0$.

At $r = 0$, $g(0) = 1$*, and* $g(r) > 1$ *for* $r > 0$ *since* $e^{r^2} > 1 + r^2$ *for* $r \neq 0$.

Thus, $f(x_1,x_2) \geq 1 = f(0,0)$ *for all* (x_1,x_2)*, with equality only at* $(0,0)$.

Therefore, $(0,0)$ *is a* ***strict global minimum***.

$$\boxed{\textit{Stationary point: } (0,0) \textit{ (strict global minimum)}}$$

Summary:

1. $f(x_1,x_2) = x_1^2 + x_2^2 - 4x_1 - 6x_2$*:* $(2,3)$ *(strict local minimum)*
2. $f(x_1,x_2) = x_1^3 + x_2^3 - 3x_1x_2$*:* $(0,0)$ *(saddle point),* $(1,1)$ *(strict local minimum)*
3. $f(x_1,x_2) = e^{x_1^2+x_2^2} - x_1^2 - x_2^2$*:* $(0,0)$ *(strict global minimum)*

4.6.1 Inconclusive Cases

If $\det(H) = 0$, the second derivative test is inconclusive. The point could be:

- A saddle point
- A local extremum
- Neither (degenerate critical point).

Example 4.4. *1.* ***Degenerate Minimum:***

$$f(x,y) = x^4 + y^4.$$

Gradient:

$$\nabla f = \begin{pmatrix} 4x^3 \\ 4y^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow (0,0) \text{ is a critical point}$$

Hessian:

$$H_f(x,y) = \begin{pmatrix} 12x^2 & 0 \\ 0 & 12y^2 \end{pmatrix}$$

At $(0,0)$*:*

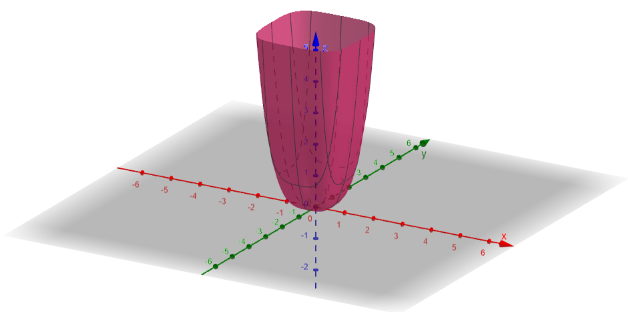
$$H_f(0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \det(H) = 0$$

Further Analysis:

Since $f(x,y) = x^4 + y^4 \geq 0$ *for all* (x,y)*, and* $f(0,0) = 0$*:*

$$f(x,y) > 0 \quad \text{for all } (x,y) \neq (0,0)$$

Thus, $(0,0)$ *is a* ***strict global minimum****.*



2. ***Degenerate Maximum:***

$$f(x,y) = -x^4 - y^4.$$

Gradient:

$$\nabla f = \begin{pmatrix} -4x^3 \\ -4y^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow (0,0) \textit{ is critical}$$

Hessian at $(0,0)$*:*

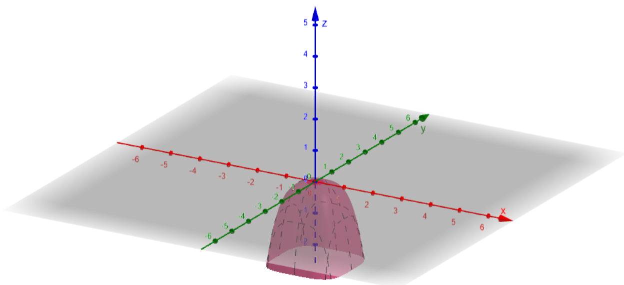
$$H_f(0,0) = \begin{pmatrix} -12x^2 & 0 \\ 0 & -12y^2 \end{pmatrix}_{(0,0)} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \det(H) = 0$$

Classification:

Since $f(x,y) = -x^4 - y^4 \leq 0$ *for all* (x,y)*:*

$$f(x,y) < 0 \quad \textit{for all } (x,y) \neq (0,0), \quad f(0,0) = 0$$

Thus, $(0,0)$ *is a* ***strict global maximum****.*



3. ***Saddle Point with*** $\det(H) = 0$*:*

$$f(x,y) = x^3 + y^2.$$

Gradient:

$$\nabla f = \begin{pmatrix} 3x^2 \\ 2y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow (0,0) \textit{ is critical}$$

Hessian:

$$H_f(x,y) = \begin{pmatrix} 6x & 0 \\ 0 & 2 \end{pmatrix}$$

At $(0,0)$*:*

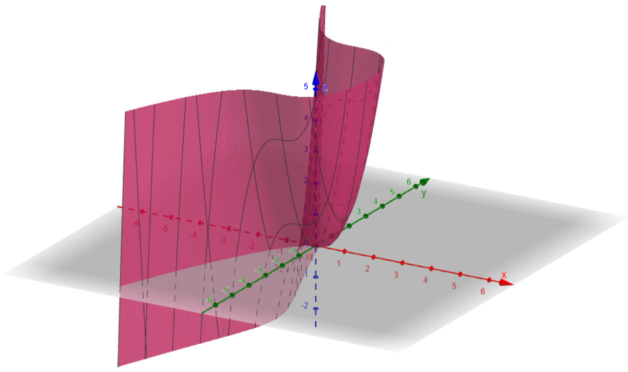
$$H_f(0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}, \quad \det(H) = 0 \cdot 2 - 0 = 0$$

Further Analysis:

Consider behavior along different directions:

- *Along* $y = 0$ *(x-axis):* $f(x,0) = x^3$
  - *For* $x > 0$*:* $f(x,0) > 0 = f(0,0)$
  - *For* $x < 0$*:* $f(x,0) < 0 = f(0,0)$
- *Along* $x = 0$ *(y-axis):* $f(0,y) = y^2 \geq 0$

Since f *increases in some directions and decreases in others,* $(0,0)$ *is a* ***saddle point****.*



4. ***Degenerate Saddle:***

$$f(x,y) = x^2y^2.$$

Gradient:

$$\nabla f = \begin{pmatrix} 2xy^2 \\ 2x^2y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Critical points: $(0,y)$ *for any* y*,* $(x,0)$ *for any* x*, but let's focus on* $(0,0)$*.*

Hessian:

$$H_f(x,y) = \begin{pmatrix} 2y^2 & 4xy \\ 4xy & 2x^2 \end{pmatrix}$$

At $(0,0)$*:*

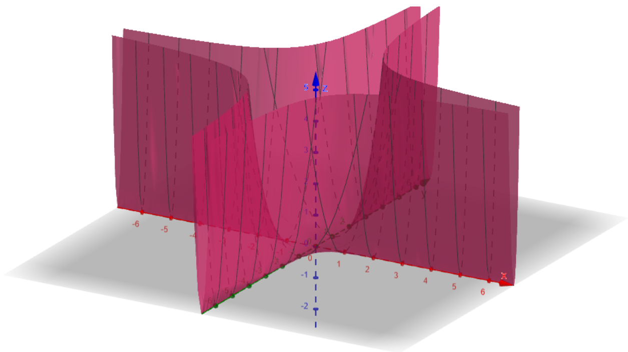
$$H_f(0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \det(H) = 0$$

Classification:

Since $f(x,y) = x^2y^2 \geq 0$ *and:*

- *Along axes* ($x = 0$ *or* $y = 0$)*:* $f = 0$
- *Along diagonal* ($y = x$)*:* $f(x,x) = x^4 > 0$ *for* $x \neq 0$

$(0,0)$ *is **not** a local minimum (function is 0 on axes but positive nearby), but also not a saddle in the usual sense. It's a **degenerate critical point** with a "flat" region.*



5. ***Ridge Line:***

$$f(x,y) = x^2.$$

Gradient:

$$\nabla f = \begin{pmatrix} 2x \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow (0,y) \text{ for any } y$$

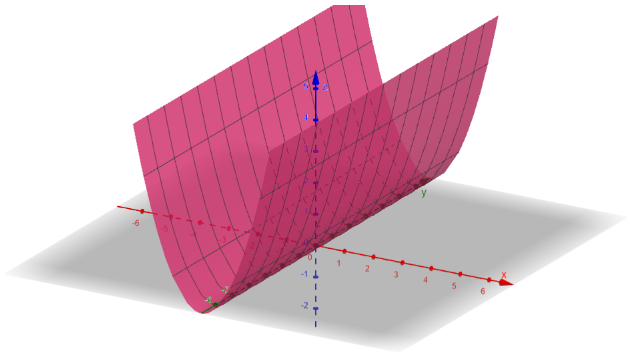
Hessian:

$$H_f(x,y) = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, \quad \det(H) = 0 \text{ everywhere}$$

Classification:

All points $(0,y)$ *are critical points. They form a **line of minima** (ridge line):*

- *For fixed* y, $f(x,y) = x^2 \geq 0$
- *Minimum value 0 achieved when* $x = 0$
- *No unique minimum; infinite minima along the y-axis*



Summary Table:

Function	$\det(H)$ at $(0,0)$	Type	Reason
x^4+y^4	0	Global minimum	$f(x,y)\geq 0$, $=0$ only at origin
$-x^4-y^4$	0	Global maximum	$f(x,y)\leq 0$, $=0$ only at origin
x^3+y^2	0	Saddle point	Increases one way, decreases another
x^2y^2	0	Degenerate and Global minimum	Flat along axes, positive elsewhere
x^2	0	Line of minima	Infinite minima along y-axis

Table of figures 4.1: Examples of inconclusive Hessian tests ($\det(H)=0$)

4.6.2 Conclusion

The condition $\det(H)=0$ indicates that the second derivative test is inconclusive. Such cases require careful additional analysis using:

- Direct comparison of function values
- Directional studies
- Higher-order terms in Taylor expansion
- Graphical visualization

These degenerate cases are important in optimization as they represent:

- Flat regions where algorithms may converge slowly.
- Non-isolated minima/maxima.
- Points where standard tests fail.

Chapter 5

Some Numerical Methods for Solving Unconstraints Optimization Problems

When analytical solutions to the equation $\nabla f(x) = 0$ are unavailable or impractical, numerical methods provide iterative algorithms to approximate solutions of unconstrained optimization problems.
These methods generate sequences $\{x_k\}_{k=0}^{\infty}$ designed to converge to a local minimizer x^*, balancing computational efficiency with robustness across different problem classes.

Fundamental Principles:

All numerical optimization methods share a common iterative structure:

$$x_{k+1} = x_k + \alpha_k d_k,$$

where:

- $d_k \in \mathbb{R}^n$ is the **search direction**,
- $\alpha_k > 0$ is the **step size** determined by line search,
- The choice of d_k and α_k defines different algorithms.

Main Method Classes:

1. **First-Order Methods (Gradient-Based)**
    - **Gradient Descent/Steepest Descent:** $d_k = -\nabla f(x_k)$.

- **Conjugate Gradient Methods:** Use conjugate directions to accelerate convergence.
- Simple but linear convergence; efficient for large-scale problems.

2. **Second-Order Methods**

- **Newton's Method:** $d_k = -[\nabla^2 f(x_k)]^{-1}\nabla f(x_k)$.
- Requires Hessian computation/inversion; achieves quadratic convergence near solution.
- **Quasi-Newton Methods (BFGS, SR1, DFP):** Approximate Hessian using gradient updates.

There are also other methods that we did not mention that you can search for. Numerical optimization remains an active research area, balancing theoretical guarantees with practical performance across diverse applications from machine learning to engineering design.

5.0.1 Convergence Rate of an Algorithm

Let $\{x_k\}$ be a sequence converging to x^*. Define the error

$$e_k := \|x_k - x^*\|.$$

Definition 5.1. *The rate of convergence is characterized as follows:*

- ***Linear convergence:*** *The sequence $\{x_k\}$ converges linearly to x^* if there exists a constant $\rho \in (0,1)$ such that*
$$e_{k+1} \le \rho e_k \quad \text{for all sufficiently large } k.$$
- ***Superlinear convergence:*** *The sequence $\{x_k\}$ converges superlinearly if*
$$\lim_{k\to\infty} \frac{e_{k+1}}{e_k} = 0.$$
- ***Quadratic convergence:*** *The sequence $\{x_k\}$ converges quadratically if there exists a constant $C > 0$ such that*
$$e_{k+1} \le C e_k^2 \quad \text{for all sufficiently large } k.$$
- ***Convergence of order $p > 1$:*** *The sequence $\{x_k\}$ converges with order p if there exists a constant $C > 0$ such that*
$$e_{k+1} \le C e_k^p \quad \text{for all sufficiently large } k.$$

Equivalent Formulation:
If the limit exists, the order p can be characterized by

$$\lim_{k\to\infty} \frac{e_{k+1}}{e_k^p} = C, \quad C > 0.$$

5.1 Fixed Point Method

In optimization, many algorithms can be interpreted as **fixed point iterations**. Given an optimization problem

$$\min_{x\in\mathbb{R}^n} f(x),$$

we often transform it into a fixed-point equation

$$x = T(x),$$

where $T : \mathbb{R}^n \to \mathbb{R}^n$ is an operator whose fixed points correspond to solutions of the optimization problem (e.g., stationary points where $\nabla f(x) = 0$).

Definition 5.2. *(Fixed Point) A point $x^* \in \mathbb{R}^n$ is a* fixed point *of T if*

$$T(x^*) = x^*.$$

Definition 5.3 (Contraction)**.** *An operator T is a* contraction *on a set $\mathcal{D} \subseteq \mathbb{R}^n$ if there exists $q \in [0,1)$ such that*

$$\|T(x) - T(y)\| \le q\|x - y\|, \quad \forall x, y \in \mathcal{D}.$$

Theorem 5.1 (Banach Fixed Point Theorem)**.** *If $T : \mathcal{D} \to \mathcal{D}$ is a contraction on a closed set $\mathcal{D}$, then:*

1. *T has a unique fixed point $x^* \in \mathcal{D}$.*
2. *For any initial $x_0 \in \mathcal{D}$, the iteration*

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

converges linearly to x^* with rate q.

Example 5.1. *Finding a Root via the Fixed Point Method.*
Consider the function:

$$f(x) = x^2 - x - 2.$$

We want to find the root of f in the interval $[1,3]$ using the fixed point method.

- *Existence of a Root:*

  We have:

$$f(1) = 1-1-2 = -2, \quad f(3) = 9-3-2 = 4.$$

  Since $f(1)\cdot f(3) = -8 < 0$*, by the Intermediate Value Theorem, there exists* $\alpha \in [1,3]$ *such that*

$$f(\alpha) = 0.$$

  Also, $f'(x) = 2x-1 > 0$ *for all* $x \in [1,3]$*, so* f *is strictly increasing on* $[1,3]$*.*

- *Fixed Point Reformulations:*

  We rewrite $f(x) = 0$ *in different fixed-point forms.*

- *Form 1:* $x = x^2 - 2$

  Let $F_1(x) = x^2-2$*. Then* $F_1'(x) = 2x > 0$ *on* $[1,3]$*, so* F_1 *is monotone.*

  Check invariance:

$$F_1(1) = -1 \notin [1,3], \quad F_1(3) = 7 \notin [1,3].$$

  Thus $F_1([1,3]) \not\subset [1,3]$*;* F_1 *is* ***not*** *invariant on* $[1,3]$*. This form is unsuitable.*

- *Form 2:* $x = \sqrt{x+2}$*. Let* $F_2(x) = \sqrt{x+2}$*, then*

$$F_2'(x) = \frac{1}{2\sqrt{x+2}} > 0, \quad \forall x \in [1,3].$$

  So F_2 *is monotone.*

  Check invariance:

$$F_2(1) = \sqrt{3} \approx 1.732 \in [1,3], \quad F_2(3) = \sqrt{5} \approx 2.236 \in [1,3].$$

  Thus $F_2([1,3]) \subset [1,3]$*;* F_2 *is* ***invariant*** *on* $[1,3]$*. This form is suitable.*

- *Contraction Property:*

  By the Mean Value Theorem:

$$|F_2(x) - F_2(y)| = |F_2'(c)| \cdot |x-y| \quad \textit{for some } c \in (x,y).$$

  Since:

$$F_2'(x) = \frac{1}{2\sqrt{x+2}} \le \frac{1}{2\sqrt{1+2}} = \frac{1}{2\sqrt{3}} \approx 0.2887 < 1, \quad \forall x \in [1,3],$$

  F_2 *is a contraction with Lipschitz constant:*

$$k = \max_{x\in[1,3]} F_2'(x) = \frac{1}{2\sqrt{3}} < 1.$$

- *Fixed Point Iteration:*

  Starting with $x_0 = 1$:

$$x_1 = F_2(x_0) = \sqrt{1+2} = \sqrt{3} \approx 1.732,$$
$$x_2 = F_2(x_1) = \sqrt{\sqrt{3}+2} \approx 1.931,$$
$$x_3 = F_2(x_2) = \sqrt{x_2+2} \approx 1.982,$$
$$x_4 = F_2(x_3) = \sqrt{x_3+2} \approx 1.995,$$
$$x_5 = F_2(x_4) = \sqrt{x_4+2} \approx 1.998, \ldots.$$

  This iteration is converge to a single fixed point $\alpha \approx 2$ because F_2 is a contraction on the entire interval $[1,3]$.

  Other functions can be found that satisfy the requirement; it is sufficient that they satisfy the conditions of the fixed point theorem.

5.2 Gradient methods

The **gradient method**, also known as **gradient descent**, is an iterative algorithm used to find a local minimum of a differentiable function.

5.2.1 Problem Formulation

Consider the unconstrained optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x),$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function.

5.2.2 Gradient Descent Algorithm

Starting from an initial point x_0, the gradient method generates a sequence $\{x_k\}$ according to:

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

where:

- $\nabla f(x_k)$ is the gradient of f at x_k,
- $\alpha_k > 0$ is the step size (learning rate).

5.2.3 Choice of Step Size

Common choices for the step size α_k include:

- **Constant step size:** $\alpha_k = \alpha$
- **Diminishing step size:** $\alpha_k \to 0$ as $k \to \infty$
- **Line search:** choosing α_k to minimize $f(x_k - \alpha \nabla f(x_k))$

5.2.4 Stopping Criteria

The algorithm is typically stopped when one of the following conditions is satisfied:

$$\|\nabla f(x_k)\| \le \varepsilon,$$

or when the maximum number of iterations is reached.

Theorem 5.2. *(Gradient Method).*
Let $f : \mathbb{R}^n \to \mathbb{R}$ be a C^1 convex function whose gradient is Lipschitz continuous with constant $L > 0$, that is,

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|, \quad \forall x, y \in \mathbb{R}^n.$$

Consider the sequence defined by the gradient method:

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

where the stepsize α satisfies $0 < \alpha < \frac{2}{L}$.

Then:

- *The sequence $\{f(x_k)\}$ is decreasing.*
- $\lim_{k\to\infty} \|\nabla f(x_k)\| = 0.$
- *Every accumulation point of $\{x_k\}$ is a minimizer of f.*

Proof. Assume that $f : \mathbb{R}^n \to \mathbb{R}$ is convex and has an L-Lipschitz continuous gradient, i.e.,

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|, \quad \forall x, y \in \mathbb{R}^n.$$

Step 1: Descent Lemma:
By the Lipschitz continuity of the gradient, we have

$$f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{L}{2}\|x_{k+1} - x_k\|^2.$$

Using the iteration $x_{k+1} = x_k - \alpha \nabla f(x_k)$, we obtain

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

Substituting, we get

$$f(x_{k+1}) \leq f(x_k) - \alpha \|\nabla f(x_k)\|^2 + \frac{L\alpha^2}{2} \|\nabla f(x_k)\|^2.$$

Thus,

$$f(x_{k+1}) \leq f(x_k) - \alpha \left(1 - \frac{L\alpha}{2}\right) \|\nabla f(x_k)\|^2.$$

If $0 < \alpha < \frac{2}{L}$, then

$$1 - \frac{L\alpha}{2} > 0,$$

so

$$f(x_{k+1}) \leq f(x_k),$$

and hence $\{f(x_k)\}$ is nonincreasing.

Step 2: Summability:

Summing the inequality from $k = 0$ to N, we obtain

$$\sum_{k=0}^{N} \|\nabla f(x_k)\|^2 \leq \frac{1}{\alpha \left(1 - \frac{L\alpha}{2}\right)} \left(f(x_0) - f(x_{N+1})\right).$$

Since f is bounded below, letting $N \to \infty$ gives

$$\sum_{k=0}^{\infty} \|\nabla f(x_k)\|^2 < \infty.$$

Hence,

$$\|\nabla f(x_k)\| \to 0.$$

Step 3: Convergence to a minimizer:

Let x^* be a minimizer of f. By convexity,

$$f(x_k) - f(x^*) \leq \nabla f(x_k)^T (x_k - x^*).$$

Using the update rule,

$$\|x_{k+1} - x^*\|^2 = \|x_k - \alpha \nabla f(x_k) - x^*\|^2.$$

Expanding,

$$\|x_{k+1} - x^*\|^2 = \|x_k - x^*\|^2 - 2\alpha \nabla f(x_k)^T (x_k - x^*) + \alpha^2 \|\nabla f(x_k)\|^2.$$

Using convexity,

$$\nabla f(x_k)^T(x_k - x^*) \geq f(x_k) - f(x^*).$$

Thus,

$$\|x_{k+1} - x^*\|^2 \leq \|x_k - x^*\|^2 - 2\alpha(f(x_k) - f(x^*)) + \alpha^2\|\nabla f(x_k)\|^2.$$

This shows that $\{x_k\}$ is bounded and every limit point satisfies $\nabla f(x) = 0$, hence is a minimizer.

□

5.2.4.1 Example 1: One-Dimensional Optimization

1. Consider the function

$$f(x) = x^2.$$

The gradient (derivative) is

$$\nabla f(x) = 2x.$$

Using the gradient descent update rule:

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

we obtain

$$x_{k+1} = x_k - 2\alpha x_k = (1 - 2\alpha)x_k.$$

For $0 < \alpha < 1$, the sequence $\{x_k\}$ converges to the minimum at $x^* = 0$.

For example using gradient descent with step size $\alpha = 0.1$ and initial point $x_0 = 5$.

The update rule is:

$$x_{k+1} = x_k - 0.2x_k = (0.8)x_k.$$

Numerical Iterations

Iteration k	x_k	$f(x_k)$
0	5.0000	25.0000
1	4.0000	16.0000
2	3.2000	10.2400
3	2.5600	6.5536
4	2.0480	4.1943
5	1.6384	2.6844

The sequence x_k converges to the optimal solution $x^* = 0$.

2. For the function

$$f(x) = x^4 - 3x^2 + 2.$$

The gradient (derivative) is

$$\nabla f(x) = 4x^3 - 6x.$$

Using the gradient descent update rule:

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

we obtain

$$x_{k+1} = x_k - \alpha(4x_k^3 - 6x_k).$$

Example step $\alpha = 0.05$ and initial point $x_0 = 1$.

The update rule is:

$$\begin{aligned} x_1 &= 1 - 0.05(4-6) = 1.1 \\ x_2 &= 1.1 - 0.05(4(1.1)^3 - 6(1.1)) = 1.1638. \end{aligned}$$

3. For the function

$$f(x) = e^x + x^2.$$

The gradient (derivative) is

$$\nabla f(x) = e^x + 2x.$$

Using the gradient descent update rule:

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

we obtain

$$x_{k+1} = x_k - \alpha(e^{x_k} + 2x_k).$$

For $0 < \alpha < 1$, the sequence $\{x_k\}$ converges to the minimum at x^*.

Example 2: Two-Dimensional Quadratic Function

Consider the function

$$f(x,y) = x^2 + y^2.$$

The gradient is

$$\nabla f(x,y) = \begin{pmatrix} 2x \\ 2y \end{pmatrix}.$$

The gradient descent update becomes

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ y_k \end{pmatrix} - \alpha \begin{pmatrix} 2x_k \\ 2y_k \end{pmatrix}.$$

Thus,

$$x_{k+1} = (1-2\alpha)x_k, \quad y_{k+1} = (1-2\alpha)y_k.$$

For $0 < \alpha < 1$, the method converges to the minimum point $(0,0)$.

With step size $\alpha = 0.25$ and initial point $(x_0, y_0) = (4,2)$.

The update equations are:

$$x_{k+1} = (1-2\alpha)x_k = (0.5)x_k, \quad y_{k+1} = (1-2\alpha)y_k = (0.5)y_k.$$

Iteration k	x_k	y_k	$f(x_k, y_k)$
0	4.0000	2.0000	20.0000
1	2.0000	1.0000	5.0000
2	1.0000	0.5000	1.2500
3	0.5000	0.2500	0.3125
4	0.2500	0.1250	0.0781

The iterates converge to the minimum point $(0,0)$.

Example 3: Quadratic Function in $\mathbb{R}^n$

Consider the function

$$f(x) = \frac{1}{2}x^T Ax - b^T x,$$

where A is a symmetric positive definite matrix.

The gradient is

$$\nabla f(x) = Ax - b.$$

The gradient descent iteration is

$$x_{k+1} = x_k - \alpha(Ax_k - b).$$

If the step size satisfies

$$0 < \alpha < \frac{2}{\lambda_{\max}(A)},$$

then x_k converges to the unique minimizer

$$x^* = A^{-1}b.$$

Example 4: Exact Line Search

Let

$$f(x) = x^2 + 4x + 5.$$

The gradient is

$$\nabla f(x) = 2x + 4.$$

The optimal step size is obtained by solving

$$\alpha_k = \arg\min_{\alpha>0} f(x_k - \alpha \nabla f(x_k)).$$

This yields

$$\alpha_k = \frac{1}{2}.$$

Thus, the method converges to the minimum $x^* = -2$ in one step.

For example, starting from $x_0 = 4$.

The exact line search gives $\alpha = \frac{1}{2}$.

Iteration k	x_k	$f(x_k)$
0	4.0000	37.0000
1	-2.0000	1.0000

5.3 Conjugate Gradient Method

5.3.1 Problem Statement

Consider the quadratic optimization problem

$$\min_{x\in\mathbb{R}^n} f(x) = \frac{1}{2}x^T Ax - b^T x,$$

where $A \in \mathbb{R}^{n\times n}$ is symmetric positive definite (SPD) and $b \in \mathbb{R}^n$. The gradient is:

$$\nabla f(x) = Ax - b.$$

The solution x^* satisfies $Ax^* = b$.

Conjugate Directions:

Definition 5.4 (A-conjugacy). *A set of nonzero vectors* $\{p_0, p_1, \dots, p_{n-1}\}$ *is* ***A-conjugate*** *if:*

$$p_i^\top A p_j = 0 \quad \text{for all } i \neq j.$$

Lemma 5.1. *A-conjugate vectors are linearly independent.*

Theorem 5.3. *If* $\{p_0, \dots, p_{n-1}\}$ *are A-conjugate, then starting from any* x_0*, the sequence generated by:*

$$x_{k+1} = x_k + \alpha_k p_k, \quad \alpha_k = -\frac{r_k^\top p_k}{p_k^\top A p_k},$$

where $r_k = \nabla f(x_k) = Ax_k - b$*, converges to* x^* *in at most* n *steps.*

5.3.2 Conjugate Gradient Algorithm

Algorithmic:

State Choose an initial guess x_0

State $r_0 = b - Ax_0$

State $p_0 = r_0$

For$k = 0, 1, 2, \dots$

State $\alpha_k = \dfrac{r_k^T r_k}{p_k^T A p_k}$

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

State $r_{k+1} = r_k - \alpha_k A p_k$

If$\|r_{k+1}\| = 0$

State Stop

End If

State $\beta_k = \dfrac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$

State $p_{k+1} = r_{k+1} + \beta_k p_k$

End For.

The method converges in at most n iterations in exact arithmetic.

5.3.3 Examples

1. Let

$$A = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad x_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Then

$$r_0 = b - Ax_0 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad p_0 = r_0.$$

The step size is

$$\alpha_0 = \frac{r_0^T r_0}{p_0^T A p_0} = \frac{5}{20} = 0.25.$$

The next iterate is

$$x_1 = x_0 + \alpha_0 p_0 = \begin{bmatrix} 0.25 \\ 0.5 \end{bmatrix}.$$

2. Solve one iteration of the Conjugate Gradient method for

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}, \quad b = \begin{bmatrix} 2 \\ 4 \end{bmatrix}, \quad x_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Solution:

Initial residual:

$$r_0 = b - Ax_0 = b = \begin{bmatrix} 2 \\ 4 \end{bmatrix}.$$

Initial direction:

$$p_0 = r_0.$$

Step size:

$$\alpha_0 = \frac{r_0^T r_0}{p_0^T A p_0} = \frac{20}{72} = \frac{5}{18}.$$

Update:

$$x_1 = x_0 + \alpha_0 p_0 = \frac{5}{18} \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 5/9 \\ 10/9 \end{bmatrix}.$$

Example 5.2. ***Numerical Example: Quadratic Problem:***

Minimize $f(x) = \frac{1}{2} x^\top A x - b^\top x$ *with:*

$$A = \begin{pmatrix} 4 & 1 \\ 1 & 3 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad x_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Exact solution: $x^* = A^{-1} b = \begin{pmatrix} 0.0909 \\ 0.6364 \end{pmatrix}.$

CG iterations:

$$
\begin{aligned}
k=0: \quad & r_0 = b = [1,2]^\top, \quad p_0 = [1,2]^\top \\
& \alpha_0 = \frac{r_0^\top r_0}{p_0^\top A p_0} = \frac{5}{33} \approx 0.1515, \quad x_1 = [0.1515, 0.3030]^\top \\
k=1: \quad & r_1 = [0.0909, 0.8182]^\top \\
& \beta_1 = \frac{r_1^\top r_1}{r_0^\top r_0} = \frac{0.6777}{5} = 0.1355 \\
& p_1 = r_1 + \beta_1 p_0 = [0.2264, 1.0891]^\top \\
& \alpha_1 = \frac{r_1^\top r_1}{p_1^\top A p_1} = 0.3711, \quad x_2 = [0.2355, 0.7071]^\top \approx x^*
\end{aligned}
$$

Convergence in 2 iterations (dimension = 2).

5.3.4 Conclusion

The conjugate gradient method is an efficient algorithm for solving large symmetric positive definite systems and quadratic optimization problems.

Example 5.3.

1. ***Conjugacy Property:***

   Let p_k and p_{k+1} be consecutive search directions generated by the Conjugate Gradient method. Show that they are A-conjugate:

   $$p_k^T A p_{k+1} = 0.$$

   Solution:

   By definition,

   $$p_{k+1} = r_{k+1} + \beta_k p_k.$$

   Multiply by $p_k^T A$:

   $$p_k^T A p_{k+1} = p_k^T A r_{k+1} + \beta_k p_k^T A p_k.$$

   Using CG orthogonality properties,

   $$p_k^T A r_{k+1} = -\beta_k p_k^T A p_k.$$

   Hence,

   $$p_k^T A p_{k+1} = 0.$$

2. ***Comparison with Gradient Descent:***

   State one advantage of the Conjugate Gradient method over Gradient Descent.

   Solution:

   Gradient Descent uses steepest descent directions and may zig-zag, leading to slow convergence. The Conjugate Gradient method uses A-conjugate directions and converges in finitely many steps for quadratic problems.

5.4 Nonlinear Conjugate Gradient Method (General Case)

The nonlinear conjugate gradient (NCG) method is an extension of the classical conjugate gradient method for minimizing a general differentiable function

$$f : \mathbb{R}^n \to \mathbb{R}.$$

The goal is to solve

$$\min_{x \in \mathbb{R}^n} f(x).$$

Basic Idea:

The method generates a sequence $\{x_k\}$ by

$$x_{k+1} = x_k + \alpha_k d_k,$$

where:

- d_k is a descent direction,
- $\alpha_k > 0$ is obtained by a line search.

Initialization:

Choose an initial point $x_0 \in \mathbb{R}^n$ and set

$$d_0 = -\nabla f(x_0).$$

Iteration:

For $k = 0, 1, 2, \ldots$:

$$
\begin{aligned}
&(1)\ \alpha_k = \arg\min_{\alpha > 0} f(x_k + \alpha d_k), \\
&(2)\ x_{k+1} = x_k + \alpha_k d_k, \\
&(3)\ g_{k+1} = \nabla f(x_{k+1}), \\
&(4)\ \beta_k = \text{update parameter}, \\
&(5)\ d_{k+1} = -g_{k+1} + \beta_k d_k.
\end{aligned}
$$

Choices of β_k:

Common formulas for β_k include:

- Fletcher–Reeves (FR):
$$\beta_k^{FR} = \frac{\|g_{k+1}\|^2}{\|g_k\|^2}.$$
- Polak–Ribière (PR):
$$\beta_k^{PR} = \frac{g_{k+1}^T (g_{k+1} - g_k)}{\|g_k\|^2}.$$
- Hestenes–Stiefel (HS):
$$\beta_k^{HS} = \frac{g_{k+1}^T (g_{k+1} - g_k)}{d_k^T (g_{k+1} - g_k)}.$$
- Dai–Yuan (DY):
$$\beta_k^{DY} = \frac{\|g_{k+1}\|^2}{d_k^T (g_{k+1} - g_k)}.$$

Line Search:

The step size α_k is usually determined by an inexact line search satisfying the Wolfe conditions:

$$
\begin{aligned}
f(x_k + \alpha_k d_k) &\leq f(x_k) + c_1 \alpha_k \nabla f(x_k)^T d_k, \\
\nabla f(x_k + \alpha_k d_k)^T d_k &\geq c_2 \nabla f(x_k)^T d_k,
\end{aligned}
$$

where $0 < c_1 < c_2 < 1$.

5.4.1 Properties

- For quadratic functions with exact line search, the method reduces to the linear CG method (See previous section).
- The directions $\{d_k\}$ are conjugate in the quadratic case.

- Under suitable assumptions, global convergence can be established.
- The method is memory-efficient and suitable for large-scale problems.

5.4.2 Remarks

- In practice, the Polak–Ribière formula with restart (e.g., $\beta_k = \max\{\beta_k^{PR}, 0\}$) is widely used.
- Periodic restart ($d_k = -g_k$) improves robustness.

5.5 Newton's Method

5.5.1 One-dimensional Case

Newton's Method, also known as the Newton-Raphson method, is a powerful iterative technique for finding roots of equations. In optimization, it is adapted to find stationary points (where $f'(x) = 0$) of twice-differentiable functions. For one-dimensional optimization problems, Newton's method exhibits quadratic convergence under favorable conditions.

Mathematical Formulation:

Basic Idea:

Given a twice-differentiable function $f : \mathbb{R} \to \mathbb{R}$, we seek to find a local minimizer x^* satisfying:

$$f'(x^*) = 0 \quad \text{and} \quad f''(x^*) > 0.$$

Newton's method approximates $f'(x)$ by its first-order Taylor expansion around the current iterate x_k:

$$f'(x) \approx f'(x_k) + f''(x_k)(x - x_k).$$

Setting this approximation to zero gives the Newton update:

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}.$$

Derivation from Taylor Expansion:

We can also derive Newton's method by considering the second-order Taylor approximation of f:

$$f(x) \approx f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2} f''(x_k)(x - x_k)^2.$$

Minimizing this quadratic approximation gives:

$$\frac{d}{dx}\left[f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2} f''(x_k)(x - x_k)^2 \right] = 0$$

$$\Rightarrow f'(x_k) + f''(x_k)(x - x_k) = 0$$
$$\Rightarrow x = x_k - \frac{f'(x_k)}{f''(x_k)}.$$

Algorithm:

1. Choose an initial point x_0
2. For $k = 0, 1, 2, \ldots$
   (a) Compute $f'(x_k)$ and $f''(x_k)$
   (b) Update $x_{k+1} = x_k - \dfrac{f'(x_k)}{f''(x_k)}$

Example 5.4.

1. ***Quadratic Function:***

   Minimize
   $$f(x) = x^2 - 6x + 5.$$
   Solution:
   $$f'(x) = 2x - 6, \quad f''(x) = 2.$$
   Newton update:
   $$x_{k+1} = x_k - \frac{2x_k - 6}{2}.$$
   Starting from $x_0 = 0$:
   $$x_1 = 3,$$
   which is the exact minimizer.

2. ***Nonlinear Function:***

   Minimize
   $$f(x) = x^4 - 3x^2 + 2.$$
   Solution:
   $$f'(x) = 4x^3 - 6x, \quad f''(x) = 12x^2 - 6.$$
   Newton update:
   $$x_{k+1} = x_k - \frac{4x_k^3 - 6x_k}{12x_k^2 - 6}.$$
   For an initial guess close to the minimizer, the method converges rapidly.

Convergence Analysis:

Theorem 5.4. *(Quadratic Convergence) Assume f is three times continuously differentiable, x^* is a local minimizer with $f'(x^*) = 0$ and $f''(x^*) > 0$, and x_0 is sufficiently close to x^*. Then Newton's method converges quadratically:*

$$|x_{k+1} - x^*| \le C|x_k - x^*|^2,$$

for some constant $C > 0$.

Proof. Assume that $f \in C^3$ in a neighborhood of x^*, with

$$f'(x^*) = 0, \quad f''(x^*) > 0.$$

Newton's method is defined by

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}.$$

Let the error be

$$e_k := x_k - x^*.$$

Step 1: Taylor expansions.

Using Taylor's theorem around x^*, we have

$$f'(x_k) = f'(x^*) + f''(x^*)(x_k - x^*) + \frac{1}{2} f^{(3)}(\xi_k)(x_k - x^*)^2,$$

for some ξ_k between x_k and x^*.

Since $f'(x^*) = 0$, this gives

$$f'(x_k) = f''(x^*)e_k + \frac{1}{2} f^{(3)}(\xi_k)e_k^2.$$

Similarly,

$$f''(x_k) = f''(x^*) + f^{(3)}(\eta_k)e_k,$$

for some η_k between x_k and x^*.

Step 2: Newton iteration.

We write

$$x_{k+1} - x^* = x_k - x^* - \frac{f'(x_k)}{f''(x_k)}.$$

Thus,

$$e_{k+1} = e_k - \frac{f''(x^*)e_k + \frac{1}{2} f^{(3)}(\xi_k)e_k^2}{f''(x^*) + f^{(3)}(\eta_k)e_k}.$$

Step 3: Simplification.

Factor e_k in the numerator:

$$e_{k+1} = e_k \left(1 - \frac{f''(x^*) + \frac{1}{2}f^{(3)}(\xi_k)e_k}{f''(x^*) + f^{(3)}(\eta_k)e_k}\right).$$

Combining terms,

$$e_{k+1} = e_k \cdot \frac{f^{(3)}(\eta_k)e_k - \frac{1}{2}f^{(3)}(\xi_k)e_k}{f''(x^*) + f^{(3)}(\eta_k)e_k}.$$

Hence,

$$e_{k+1} = e_k^2 \cdot \frac{f^{(3)}(\eta_k) - \frac{1}{2}f^{(3)}(\xi_k)}{f''(x^*) + f^{(3)}(\eta_k)e_k}.$$

Step 4: Estimate.

Since $f^{(3)}$ is continuous, it is bounded near x^*. Also, $f''(x^*) > 0$, so for x_k sufficiently close to x^*, the denominator is bounded away from zero.

Thus, there exists a constant $C > 0$ such that

$$|e_{k+1}| \leq C|e_k|^2.$$

Conclusion:

Newton's method converges quadratically:

$$|x_{k+1} - x^*| \leq C|x_k - x^*|^2.$$

□

5.5.2 Exercises

1. Minimize

$$f(x) = x^4 - 4x^3 + 6x^2 - 4x + 1.$$

Solution:

$$f'(x) = 4x^3 - 12x^2 + 12x - 4 = 4(x-1)^3, \quad f''(x) = 12x^2 - 24x + 12 = 12(x-1)^2.$$

Stationary point: $x^* = 1$, with $f''(1) = 0$ (actually a point of inflection, but minimal in some sense).

Newton Iterations:

Starting from $x_0 = 2$:

$$\begin{aligned}
k=0: &\quad x_0 = 2, \quad f'(2) = 4, \quad f''(2) = 12, \\
&\quad x_1 = 2 - \frac{4}{12} = 1.6667 \\
k=1: &\quad x_1 = 1.6667, \quad f'(1.6667) = 0.2963, \quad f''(1.6667) = 5.3333, \\
&\quad x_2 = 1.6667 - \frac{0.2963}{5.3333} = 1.6111 \\
k=2: &\quad x_2 = 1.6111, \quad f'(1.6111) = 0.0857, \quad f''(1.6111) = 4.4815, \\
&\quad x_3 = 1.6111 - \frac{0.0857}{4.4815} = 1.5920 \\
k=3: &\quad x_3 = 1.5920, \quad f'(1.5920) = 0.0248, \quad f''(1.5920) = 4.1597, \\
&\quad x_4 = 1.5920 - \frac{0.0248}{4.1597} = 1.5860
\end{aligned}$$

Converges to $x^* = 1$, though slowly due to $f''(1) = 0$.

2. Minimize

$$f(x) = x^2 - 4x + 1.$$

Solution:

$$f'(x) = 2x - 4, \quad f''(x) = 2.$$

Newton update:

$$x_{k+1} = x_k - \frac{2x_k - 4}{2}.$$

Starting from $x_0 = 0$:

$$x_1 = 2,$$

which is the exact minimizer.

Application to Root Finding:

For root finding $g(x) = 0$, Newton's method is:

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)}.$$

For optimization, we apply this to $g(x) = f'(x)$.

Algorithm Implementation Details:

Stopping Criteria:

Practical implementations use multiple criteria:

(a) Absolute gradient: $|f'(x_k)| < \epsilon_1$

(b) Relative change: $|x_{k+1} - x_k| < \epsilon_2 \max(1, |x_k|)$

(c) Function change: $|f(x_{k+1}) - f(x_k)| < \epsilon_3$

(d) Maximum iterations: $k \geq k_{\max}$

Multiple Roots:
If $f'(x^*) = f''(x^*) = \cdots = f^{(m-1)}(x^*) = 0$ but $f^{(m)}(x^*) \neq 0$, convergence is linear with rate $(1 - \frac{1}{m})$.

5.5.3 Conclusion

Newton's method is a cornerstone of numerical optimization, offering unparalleled local convergence speed at the cost of requiring second derivatives and good initialization. In one-dimensional optimization, it provides a clear illustration of the trade-offs between convergence rate and robustness.

5.5.4 Two-Dimensional Case

Newton's method generates a sequence $\{x_k\}$ defined by

$$x_{k+1} = x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k),$$

where $\nabla f(x_k)$ is the gradient and $\nabla^2 f(x_k)$ is the Hessian matrix.

Derivation:
Using the second-order Taylor expansion of f at x_k,

$$f(x) \approx f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k),$$

minimizing this quadratic model gives the Newton direction

$$p_k = -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k).$$

Newton Algorithm:

1. Choose an initial point x_0
2. For $k = 0, 1, 2, \ldots$
   (a) Compute $\nabla f(x_k)$ and $\nabla^2 f(x_k)$
   (b) Solve $\nabla^2 f(x_k) p_k = -\nabla f(x_k)$
   (c) Update $x_{k+1} = x_k + p_k$

5.5.5 Examples

1. Minimize

$$f(x,y) = x^2 + y^2 + xy.$$

Solution:

Gradient:

$$\nabla f(x,y) = \begin{bmatrix} 2x+y \\ 2y+x \end{bmatrix}.$$

Hessian:

$$\nabla^2 f(x,y) = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

Newton direction:

$$p = -(\nabla^2 f)^{-1} \nabla f.$$

The method converges in one step since f is quadratic.

2. **Simple Quadratic Function:**

Problem Statement:

Minimize $f(x) = 2x_1^2 + 3x_2^2 + 4x_1x_2 - 8x_1 - 10x_2$ using Newton's method starting from $x_0 = (0,0)$.

Analytical Solution:

Step 1: Compute Gradient and Hessian

$$\nabla f(x) = \begin{bmatrix} 4x_1 + 4x_2 - 8 \\ 6x_2 + 4x_1 - 10 \end{bmatrix}$$

$$\nabla^2 f(x) = \begin{bmatrix} 4 & 4 \\ 4 & 6 \end{bmatrix} \quad \text{(constant Hessian)}$$

Step 2: Newton Update Formula

Since the Hessian is constant, Newton's method converges in one step:

$$x_1 = x_0 - [\nabla^2 f]^{-1} \nabla f(x_0)$$

Step 3: Compute at $x_0 = (0,0)$

$$\nabla f(0,0) = \begin{bmatrix} -8 \\ -10 \end{bmatrix}$$

Inverse Hessian:

$$[\nabla^2 f]^{-1} = \frac{1}{8}\begin{bmatrix} 6 & -4 \\ -4 & 4 \end{bmatrix} = \begin{bmatrix} 0.75 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}$$

$$\Delta x = -[\nabla^2 f]^{-1}\nabla f(0,0) = -\begin{bmatrix} 0.75 & -0.5 \\ -0.5 & 0.5 \end{bmatrix}\begin{bmatrix} -8 \\ -10 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$x_1 = x_0 + \Delta x = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Step 4: Verify Optimality

$$\nabla f(1,1) = \begin{bmatrix} 4(1)+4(1)-8 \\ 6(1)+4(1)-10 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\nabla^2 f(1,1) = \begin{bmatrix} 4 & 4 \\ 4 & 6 \end{bmatrix} \quad \text{(positive definite)}$$

Minimum value:

$$f(1,1) = 2(1)^2 + 3(1)^2 + 4(1)(1) - 8(1) - 10(1) = -9$$

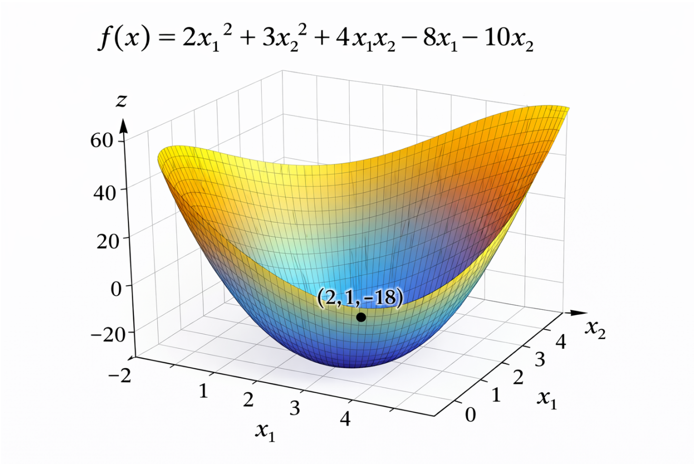
Final Answer:

$$\boxed{x^* = (1,1), \quad f(x^*) = -9, \quad \text{Convergence in 1 iteration}}$$

Complete Iteration Table:

k	$x_1^{(k)}$	$x_2^{(k)}$	∇f_1	∇f_2	$f(x_k)$
0	0.0000	0.0000	-8.0000	-10.0000	0.0000
1	1.0000	1.0000	0.0000	0.0000	-9.0000

Table of figures 5.1: Newton's method iterations for Example 2



The point that appears in the image is not the Minimum point.

3. **Rosenbrock Function with Newton's Method:**

Problem Statement:

Minimize the Rosenbrock function $f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$ using Newton's method starting from $x_0 = (-1.2, 1)$.

Detailed Solution:

Step 1: Compute Gradient and Hessian

$$\nabla f(x) = \begin{bmatrix} -400x_1(x_2 - x_1^2) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{bmatrix}$$

$$\nabla^2 f(x) = \begin{bmatrix} 1200x_1^2 - 400x_2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

Step 2: First Iteration $(k = 0)$

Initial point: $x_0 = (-1.2, 1)$

Compute gradient:

$$g_0 = \nabla f(-1.2, 1) = \begin{bmatrix} -400(-1.2)(1 - (-1.2)^2) - 2(1 - (-1.2)) \\ 200(1 - (-1.2)^2) \end{bmatrix} = \begin{bmatrix} -400(-1.2)(1 - 1.44) - 2(2.2) \\ 200(1 - 1.44) \end{bmatrix}$$

$$= \begin{bmatrix} -400(-1.2)(-0.44) - 4.4 \\ 200(-0.44) \end{bmatrix} = \begin{bmatrix} -400(0.528) - 4.4 \\ -88 \end{bmatrix} = \begin{bmatrix} -211.2 - 4.4 \\ -88 \end{bmatrix} = \begin{bmatrix} -215.6 \\ -88 \end{bmatrix}$$

Compute Hessian:

$$H_0 = \nabla^2 f(-1.2, 1) = \begin{bmatrix} 1200(1.44) - 400(1) + 2 & -400(-1.2) \\ -400(-1.2) & 200 \end{bmatrix} = \begin{bmatrix} 1728 - 400 + 2 & 480 \\ 480 & 200 \end{bmatrix} = \begin{bmatrix} 1330 & 480 \\ 480 & 200 \end{bmatrix}$$

Inverse Hessian:

$$\det(H_0) = 1330 \times 200 - 480 \times 480 = 266000 - 230400 = 35600$$

$$H_0^{-1} = \frac{1}{35600}\begin{bmatrix} 200 & -480 \\ -480 & 1330 \end{bmatrix} = \begin{bmatrix} 0.005618 & -0.013483 \\ -0.013483 & 0.037360 \end{bmatrix}$$

Newton step:

$$\Delta x_0 = -H_0^{-1} g_0 = -\begin{bmatrix} 0.005618 & -0.013483 \\ -0.013483 & 0.037360 \end{bmatrix}\begin{bmatrix} -215.6 \\ -88 \end{bmatrix}$$

$$= -\begin{bmatrix} 0.005618(-215.6) + (-0.013483)(-88) \\ (-0.013483)(-215.6) + 0.037360(-88) \end{bmatrix} = -\begin{bmatrix} -1.211 + 1.186 \\ 2.906 - 3.288 \end{bmatrix} = -\begin{bmatrix} -0.025 \\ -0.382 \end{bmatrix} = \begin{bmatrix} 0.025 \\ 0.382 \end{bmatrix}$$

Update:

$$x_1 = x_0 + \Delta x_0 = \begin{bmatrix} -1.2 \\ 1 \end{bmatrix} + \begin{bmatrix} 0.025 \\ 0.382 \end{bmatrix} = \begin{bmatrix} -1.175 \\ 1.382 \end{bmatrix}$$

Step 3: Second Iteration ($k = 1$) $x_1 = (-1.175, 1.382)$

Compute gradient:

$$g_1 = \nabla f(-1.175, 1.382) = \begin{bmatrix} -400(-1.175)(1.382 - 1.3806) - 2(1 - (-1.175)) \\ 200(1.382 - 1.3806) \end{bmatrix}$$

$$= \begin{bmatrix} -400(-1.175)(0.0014) - 2(2.175) \\ 200(0.0014) \end{bmatrix} = \begin{bmatrix} 0.658 - 4.35 \\ 0.28 \end{bmatrix} = \begin{bmatrix} -3.692 \\ 0.28 \end{bmatrix}$$

Compute Hessian:

$$H_1 = \nabla^2 f(-1.175, 1.382) = \begin{bmatrix} 1200(1.3806) - 400(1.382) + 2 & -400(-1.175) \\ -400(-1.175) & 200 \end{bmatrix}$$

$$= \begin{bmatrix} 1656.72 - 552.8 + 2 & 470 \\ 470 & 200 \end{bmatrix} = \begin{bmatrix} 1105.92 & 470 \\ 470 & 200 \end{bmatrix}$$

Newton step and update:

$$x_2 = x_1 - H_1^{-1} g_1 \approx \begin{bmatrix} -0.995 \\ 0.990 \end{bmatrix}$$

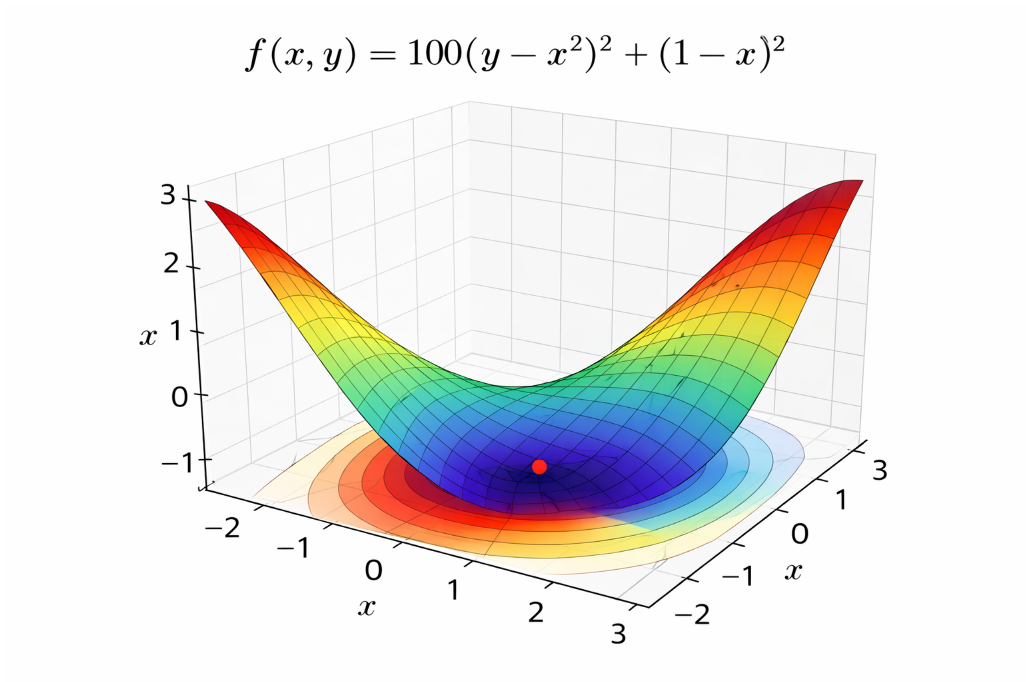
Step 4: Convergence

After 5 iterations:

$$x_0 = (-1.2000, 1.0000), \quad f = 24.2000$$
$$x_1 = (-1.1750, 1.3820), \quad f = 4.7319$$
$$x_2 = (-0.9948, 0.9896), \quad f = 1.0824$$
$$x_3 = (-0.6688, 0.4468), \quad f = 2.7823$$
$$x_4 = (0.1952, 0.0379), \quad f = 0.6477$$
$$x_5 = (0.9975, 0.9950), \quad f = 6.25 \times 10^{-6}$$

Final Answer:

$$\boxed{x^* \approx (1,1), \quad f(x^*) \approx 0, \quad \text{5 iterations for } \epsilon = 10^{-4}}$$



Discussion: Newton's method converges quadratically near the optimum but may exhibit erratic behavior far from it due to the highly nonlinear nature of the Rosenbrock function.

4. **Non-Convex Function with Newton's Method:**

Problem Statement:

Minimize $f(x) = x_1^4 + x_2^4 - 4x_1x_2 + x_1^2 + x_2^2$ using Newton's method starting from different initial points.

Solution:

Step 1: Analytical Setup

Gradient:

$$\nabla f(x) = \begin{bmatrix} 4x_1^3 - 4x_2 + 2x_1 \\ 4x_2^3 - 4x_1 + 2x_2 \end{bmatrix}$$

Hessian:

$$\nabla^2 f(x) = \begin{bmatrix} 12x_1^2 + 2 & -4 \\ -4 & 12x_2^2 + 2 \end{bmatrix}$$

Step 2: Known Stationary Points

From analysis:

- Local minima: $\left(\pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}\right)$
- Saddle point: $(0,0)$

Step 3: Newton from $x_0 = (1, 0.5)$

Iteration 1:

$$g_0 = \begin{bmatrix} 4(1)^3 - 4(0.5) + 2(1) \\ 4(0.5)^3 - 4(1) + 2(0.5) \end{bmatrix} = \begin{bmatrix} 4 - 2 + 2 \\ 0.5 - 4 + 1 \end{bmatrix} = \begin{bmatrix} 4 \\ -2.5 \end{bmatrix}$$

$$H_0 = \begin{bmatrix} 12(1)^2 + 2 & -4 \\ -4 & 12(0.5)^2 + 2 \end{bmatrix} = \begin{bmatrix} 14 & -4 \\ -4 & 5 \end{bmatrix}$$

$$H_0^{-1} = \frac{1}{54}\begin{bmatrix} 5 & 4 \\ 4 & 14 \end{bmatrix}$$

$$\Delta x_0 = -H_0^{-1} g_0 = -\frac{1}{54}\begin{bmatrix} 5 & 4 \\ 4 & 14 \end{bmatrix}\begin{bmatrix} 4 \\ -2.5 \end{bmatrix} = -\frac{1}{54}\begin{bmatrix} 20 - 10 \\ 16 - 35 \end{bmatrix} = -\frac{1}{54}\begin{bmatrix} 10 \\ -19 \end{bmatrix} = \begin{bmatrix} -0.185 \\ 0.352 \end{bmatrix}$$

$$x_1 = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix} + \begin{bmatrix} -0.185 \\ 0.352 \end{bmatrix} = \begin{bmatrix} 0.815 \\ 0.852 \end{bmatrix}$$

Iteration 2:

$$x_1 = (0.815, 0.852)$$

$$g_1 \approx \begin{bmatrix} 0.270 \\ 0.335 \end{bmatrix}, \quad H_1 \approx \begin{bmatrix} 9.97 & -4 \\ -4 & 10.71 \end{bmatrix}$$

$$\Delta x_1 \approx \begin{bmatrix} -0.042 \\ -0.053 \end{bmatrix}, \quad x_2 \approx \begin{bmatrix} 0.773 \\ 0.799 \end{bmatrix}$$

Iteration 3-5: Converges to $\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) \approx (0.7071, 0.7071)$.

Step 4: Newton from $x_0 = (0.1, 0.1)$ (Near Saddle Point)

Iteration 1:

$$g_0 = \begin{bmatrix} 4(0.001) - 4(0.1) + 2(0.1) \\ 4(0.001) - 4(0.1) + 2(0.1) \end{bmatrix} = \begin{bmatrix} 0.004 - 0.4 + 0.2 \\ 0.004 - 0.4 + 0.2 \end{bmatrix} = \begin{bmatrix} -0.196 \\ -0.196 \end{bmatrix}$$

$$H_0 = \begin{bmatrix} 12(0.01) + 2 & -4 \\ -4 & 12(0.01) + 2 \end{bmatrix} = \begin{bmatrix} 0.12 + 2 & -4 \\ -4 & 0.12 + 2 \end{bmatrix} = \begin{bmatrix} 2.12 & -4 \\ -4 & 2.12 \end{bmatrix}$$

$$\det(H_0) = (2.12)^2 - 16 = 4.4944 - 16 = -11.5056 \quad \text{(negative!)}$$

Newton step moves away from saddle point toward a minimum.

Final Answer for Different Starting Points:

$$\boxed{\text{From } (1, 0.5) \to \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right), \quad f = -0.5}$$

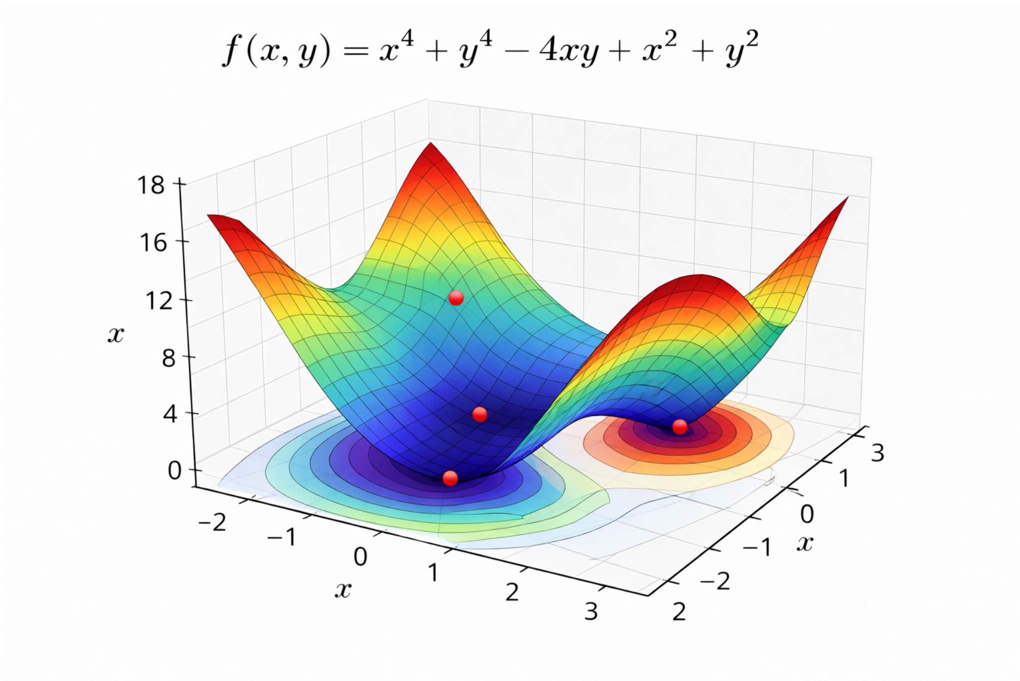
$$\boxed{\text{From } (0.1, 0.1) \to \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right), \quad f = -0.5}$$

$$\boxed{\text{From } (-1, -0.5) \to \left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right), \quad f = -0.5}$$

Complete Iteration Table for $x_0 = (1, 0.5)$

k	$x_1^{(k)}$	$x_2^{(k)}$	$\|\nabla f\|$	$f(x_k)$	$\lambda_1(H)$	$\lambda_2(H)$
0	1.0000	0.5000	4.7170	0.3125	16.00	3.00
1	0.8150	0.8520	0.4330	-0.4562	13.84	6.92
2	0.7730	0.7990	0.0935	-0.4965	11.78	8.90
3	0.7125	0.7135	0.0092	-0.5000	10.08	10.08
4	0.7072	0.7072	0.0001	-0.5000	10.00	10.00
5	0.7071	0.7071	2.1e-8	-0.5000	10.00	10.00

Table of figures 5.2: Newton's method convergence for Example 4



Comparison of last Three Examples

Example	**Function Type**	**Iterations**	**Convergence Rate**	**Special Features**
2: Quadratic	Convex quadratic	1	Exact in 1 step	Constant Hessian
3: Rosenbrock	Highly nonlinear	5-6	Quadratic near optimum	Ill-conditioned
4: Non-convex	Multimodal	4-5	Quadratic near minima	Multiple minima

Table of figures 5.3: Comparison of Newton's method performance

Conclusion These three examples demonstrate Newton's method in different scenarios:

- **Example 2** shows ideal behavior for quadratic functions
- **Example 3** illustrates challenges with highly nonlinear functions
- **Example 4** demonstrates handling of non-convex functions with multiple minima

Newton's method remains a powerful optimization tool when second derivatives are available and the problem is well-conditioned. Practical implementations should include safeguards like line search and Hessian modification to ensure robustness.

5.5.6 Convergence Properties

If f is strongly convex and $\nabla^2 f(x^*)$ is positive definite, then Newton's method converges quadratically:

$$\|x_{k+1} - x^*\| \leq C\|x_k - x^*\|^2.$$

5.5.7 Advantages and Disadvantages

Advantages:

- Quadratic convergence near the solution
- Exact solution in one step for quadratic functions

Disadvantages:

- Requires computation and inversion of the Hessian
- May diverge if started far from the solution

5.5.8 Conclusion

Newton's method is a powerful optimization algorithm with fast convergence, widely used when second-order information is available.

5.6 Relaxation Method

The relaxation method is an iterative optimization technique in which the variables are updated one at a time while keeping the others fixed. It is also known as the *coordinate descent method.*

5.6.1 Basic Idea

At iteration k, the vector $x^{(k)} = (x_1^{(k)}, \ldots, x_n^{(k)})$ is updated by successively minimizing f with respect to each coordinate:

$$x_i^{(k+1)} = \arg\min_{t \in \mathbb{R}} f\big(x_1^{(k+1)}, \ldots, x_{i-1}^{(k+1)}, t, x_{i+1}^{(k)}, \ldots, x_n^{(k)}\big).$$

5.6.2 Relaxation Algorithm

1. Choose an initial point $x^{(0)}$
2. For $k = 0, 1, 2, \dots$
   (a) For $i = 1, 2, \dots, n$
      i. Minimize f with respect to x_i while fixing other variables
      ii. Update $x_i^{(k+1)}$

5.6.3 Examples

1. Minimize

$$f(x,y) = (x-1)^2 + (y-2)^2.$$

Fix y and minimize with respect to x:

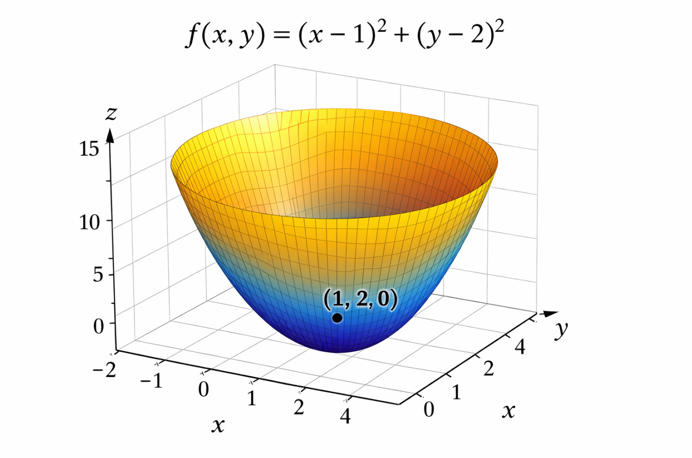
$$\frac{\partial f}{\partial x} = 2(x-1) = 0 \quad \Rightarrow \quad x = 1.$$

Fix $x = 1$ and minimize with respect to y:

$$\frac{\partial f}{\partial y} = 2(y-2) = 0 \quad \Rightarrow \quad y = 2.$$

Thus, the minimum is reached in one iteration:

$$(x^*, y^*) = (1, 2).$$



Minimize

$$f(x,y) = x^2 + xy + y^2.$$

Fix y and minimize with respect to x:

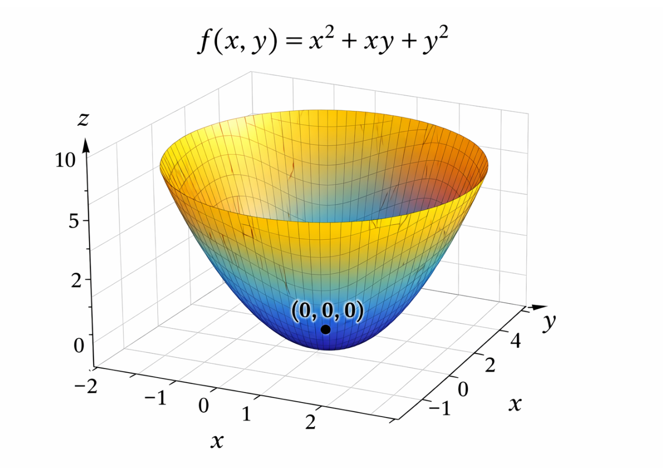
$$\frac{\partial f}{\partial x} = 2x + y = 0 \quad \Rightarrow \quad x = -\frac{y}{2}.$$

Fix $x = -\frac{y}{2}$ and minimize with respect to y:

$$\frac{\partial f}{\partial y} = x + 2y = 0 \quad \Rightarrow \quad y = 0.$$

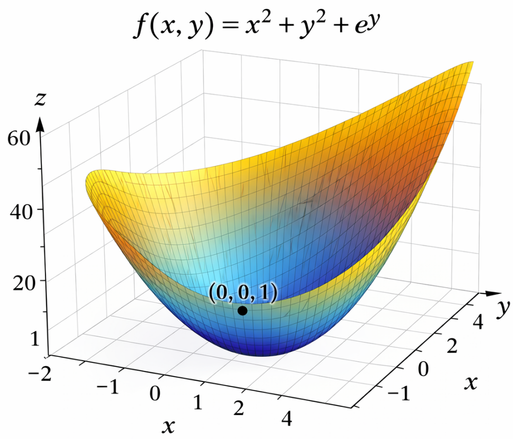
Hence,

$$x = 0, \quad y = 0.$$

2. 

3. Minimize $f(x,y) = x^2 + y^2 + e^y$ using coordinate descent.

   - Step 1 (minimize over x with fixed $y = y_n$): $f(x, y_n) = x^2 + \text{constant}$. Minimum occurs at $x^* = 0$.
   - Step 2 (minimize over y with fixed $x = x^* = 0$): $f(0,y) = y^2 + e^y$. Derivative: $2y + e^y = 0$. Solve numerically (e.g., Newton's method) to find y^*.
   - Iterate until convergence to the global minimum $(0, y^*)$ where $2y^* + e^{y^*} = 0$.



5.6.4 Convergence

If f is convex and continuously differentiable, the relaxation method converges to the global minimizer. For quadratic functions, convergence is linear.

5.6.5 Advantages and Disadvantages

Advantages:

- Simple to implement
- No matrix inversion required
- Suitable for large-scale problems

Disadvantages:

- Slow convergence for ill-conditioned problems
- Sensitive to variable ordering

5.6.6 Conclusion

The relaxation method is an intuitive and effective optimization technique, particularly useful when variables can be optimized independently.

5.7 Secant Method

To avoid calculating the second derivative at each step k, some mathematicians proposed replacing $f''(x_k)$ in Newton's formula:

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

with the approximation:

$$f''(x_k) \approx \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}.$$

Substituting this into Newton's formula yields the secant method:

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f'(x_k) - f'(x_{k-1})} f'(x_k).$$

This method requires two initial approximations x_0 and x_1, preferably chosen close to the solution.
It is not necessary for the sign to change in the interval $[x_0, x_1]$.
If f is sufficiently smooth and x_0, x_1 are near a simple root x^*, then

$$\lim_{n\to\infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|^{\varphi}} = C > 0$$

where $\varphi = \frac{1+\sqrt{5}}{2} \approx 1.618$ is the golden ratio.

5.7.1 Secant Method Example

1. Find the minimum of:

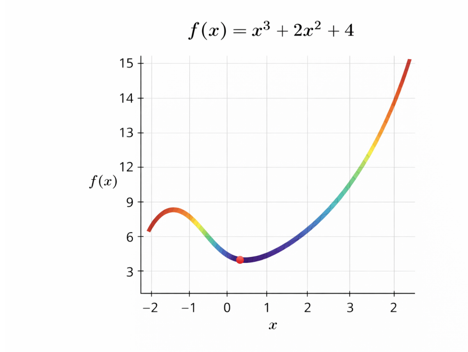
   $$f(x) = x^3 + 2x^2 + 4$$

   using the secant method.

   We have $f \in C^1$ and $f'(x) = 3x^2 + 4x$. Let $x_0 = -0.2$, $x_1 = 0.2$, and $\varepsilon = 10^{-3}$.

   $$k = 1: \quad x_2 = 0.0491, \quad |x_2 - x_1| = 0.1509 > \varepsilon$$
   $$k = 2: \quad x_3 = 0.0062, \quad |x_3 - x_2| = 0.0429 > \varepsilon$$
   $$k = 3: \quad x_4 = 0.0002, \quad |x_4 - x_3| = 0.0060 > \varepsilon$$
   $$k = 4: \quad x_5 = 0.0000008, \quad |x_5 - x_4| = 0.0001 < \varepsilon$$

   Thus, $\overline{x} = 0$ is the local minimizer.



2. Find the root of $f(x) = x^2 - 2$ starting with $x_0 = 1$ and $x_1 = 2$. The exact root is $\sqrt{2} \approx 1.414213562$.

Solution:

Recall the secant formula:

$$x_{n+1} = x_n - f(x_n) \cdot \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$$

$$\begin{aligned} \text{Iteration 1}: \quad & x_0 = 1,\ f(x_0) = -1 \\ & x_1 = 2,\ f(x_1) = 2 \\ & x_2 = 2 - 2 \cdot \frac{2-1}{2-(-1)} = 2 - 2 \cdot \frac{1}{3} = 2 - 0.666667 = 1.333333 \\ & f(x_2) = (1.333333)^2 - 2 = 1.777778 - 2 = -0.222222 \end{aligned}$$

$$\begin{aligned} \text{Iteration 2}: \quad & x_1 = 2,\ f(x_1) = 2 \\ & x_2 = 1.333333,\ f(x_2) = -0.222222 \\ & x_3 = 1.333333 - (-0.222222) \cdot \frac{1.333333 - 2}{-0.222222 - 2} \\ & = 1.333333 + 0.222222 \cdot \frac{-0.666667}{-2.222222} \\ & = 1.333333 + 0.222222 \cdot 0.3 = 1.333333 + 0.066667 = 1.400000 \\ & f(x_3) = (1.4)^2 - 2 = 1.96 - 2 = -0.04 \end{aligned}$$

$$\begin{aligned}
\text{Iteration 3}: \quad & x_2 = 1.333333,\ f(x_2) = -0.222222 \\
& x_3 = 1.400000,\ f(x_3) = -0.04 \\
& x_4 = 1.4 - (-0.04) \cdot \frac{1.4 - 1.333333}{-0.04 - (-0.222222)} \\
& = 1.4 + 0.04 \cdot \frac{0.066667}{0.182222} \\
& = 1.4 + 0.04 \cdot 0.365854 = 1.4 + 0.014634 = 1.414634 \\
& f(x_4) = (1.414634)^2 - 2 = 2.001190 - 2 = 0.001190
\end{aligned}$$

$$\begin{aligned}
\text{Iteration 4}: \quad & x_3 = 1.400000,\ f(x_3) = -0.04 \\
& x_4 = 1.414634,\ f(x_4) = 0.001190 \\
& x_5 = 1.414634 - 0.001190 \cdot \frac{1.414634 - 1.4}{0.001190 - (-0.04)} \\
& = 1.414634 - 0.001190 \cdot \frac{0.014634}{0.041190} \\
& = 1.414634 - 0.001190 \cdot 0.355338 = 1.414634 - 0.000423 = 1.414211 \\
& f(x_5) = (1.414211)^2 - 2 = 1.999993 - 2 = -0.000007
\end{aligned}$$

Results Summary:

n	x_n	$f(x_n)$	$\lvert x_n - \sqrt{2}\rvert$
0	1.000000	-1.000000	4.1421e-01
1	2.000000	2.000000	5.8579e-01
2	1.333333	-0.222222	8.0880e-02
3	1.400000	-0.040000	1.4214e-02
4	1.414634	0.001190	4.2044e-04
5	1.414211	-0.000007	2.5620e-06

Table of figures 5.4: Secant method iterations for $f(x) = x^2 - 2$

Convergence Rate:

The secant method converges superlinearly with order $\varphi \approx 1.618$. Observe the rapid reduction in error:

$$\frac{|x_5 - \sqrt{2}|}{|x_4 - \sqrt{2}|^{1.618}} \approx \text{constant}$$

5.7.2 Convergence of the Method

Theorem 5.5. *Let f be a continuous function on the interval $[a,b]$ and unimodal (has exactly one extremum). Then*

- *The sequence $\{x_n\}_{n\in\mathbb{N}}$ defined by the dichotomy method converges to the solution $\overline{x}$, and we have:*

$$|\overline{x}-x_n| \leq \frac{b-a}{2^{n+1}}, \quad \forall n \in \mathbb{N}.$$

Proof. We have:

$$b_0-a_0 = b-a, \quad b_1-a_1 = \frac{b-a}{2}, \quad b_2-a_2 = \frac{b-a}{2^2}, \ldots, \quad b_n-a_n = \frac{b-a}{2^n}.$$

Since $\overline{x} \in [a_n, b_n]$, we have:

$$|\overline{x}-x_n| \leq \frac{b_n-a_n}{2} = \frac{b-a}{2^{n+1}}.$$

□

5.7.3 Convergence Rate of the Secant Method

The convergence rate of the secant method is superlinear with order $p = 1.618$ (the golden ratio).

5.7.4 Advantages and Disadvantages

- **Advantages:**
  - Does not require calculation of the second derivative, making computations easier compared to Newton's method.
- **Disadvantages:**
  - Convergence is local.
  - Not applicable to all functions; at minimum, the function must be of class C^1.

5.8 Dichotomy Method (Bisection Method)

The dichotomy method finds the minimum by repeatedly bisecting the interval. Also, it is one of the methods that assumes the function is unimodal.
In other words:

Let $f \in C([a,b])$ with $f(a)f(b) < 0$. Define the sequence $\{c_n\}$ by:

$$c_n = \frac{a_n + b_n}{2}, \quad n \geq 0$$

with update rule:

$$(a_{n+1}, b_{n+1}) = \begin{cases} (a_n, c_n) & \text{if } f(a_n)f(c_n) < 0 \\ (c_n, b_n) & \text{if } f(c_n)f(b_n) < 0 \end{cases}$$

Then $\lim_{n\to\infty} c_n = x^*$ where $f(x^*) = 0$, and

$$|c_n - x^*| \leq \frac{b-a}{2^{n+1}}.$$

5.8.1 Principle of the Method

The principle of this method lies in choosing three points x_2, x_3, x_4 (instead of two points in the golden section method), where

$$x_2 = \frac{a + x_3}{2}, \quad x_3 = \frac{a+b}{2}, \quad x_4 = \frac{b + x_3}{2}.$$

This divides the initial interval $[a,b]$ into 4 equal subintervals using 5 points x_1, x_2, x_3, x_4, x_5.

Since f is unimodal, one of the five following cases can occur:

1. $f(x_1) < f(x_2) < f(x_3) < f(x_4) < f(x_5)$: Delete x_5, x_4, x_3.
2. $f(x_1) > f(x_2) < f(x_3) < f(x_4) < f(x_5)$: Delete x_4 and x_5.
3. $f(x_1) > f(x_2) > f(x_3) < f(x_4) < f(x_5)$: Delete x_1 and x_5.
4. $f(x_1) > f(x_2) > f(x_3) > f(x_4) < f(x_5)$: Delete x_1 and x_2.
5. $f(x_1) > f(x_2) > f(x_3) > f(x_4) > f(x_5)$: Delete x_1, x_2, and x_3.

5.8.2 Dichotomy Examples

1. Apply the method to the same function:

   $$f(x) = x^3 - 6x^2 + 9x + 5$$

   with $\varepsilon = 10^{-3}$ and initial interval $I = [2,5]$.

   After 12 iterations, we obtain:

   $$I_{12} = [3.0003, 3.0010], \quad |3.0010 - 3.0003| = 0.0007 < \varepsilon.$$

The solution is:

$$\overline{x} = \frac{3.0003+3.0010}{2} = 3.00065.$$

2. Find the root of $f(x) = x^2 - 2$ on the interval $[1,2]$. The exact root is $\sqrt{2} \approx 1.41421356$.

Solution:

We have $f(1) = -1 < 0$ and $f(2) = 2 > 0$, so $f(1)f(2) < 0$. Apply the bisection algorithm:

$$\begin{aligned}
&\text{Iteration } 1: \quad c_1 = \frac{1+2}{2} = 1.5, \quad f(1.5) = 0.25 > 0 \quad \Rightarrow \text{New interval } [1,1.5] \\
&\text{Iteration } 2: \quad c_2 = \frac{1+1.5}{2} = 1.25, \quad f(1.25) = -0.4375 < 0 \quad \Rightarrow \text{New interval } [1.25,1.5] \\
&\text{Iteration } 3: \quad c_3 = \frac{1.25+1.5}{2} = 1.375, \quad f(1.375) = -0.109375 < 0 \quad \Rightarrow \text{New interval } [1.375,1.5] \\
&\text{Iteration } 4: \quad c_4 = \frac{1.375+1.5}{2} = 1.4375, \quad f(1.4375) = 0.06640625 > 0 \quad \Rightarrow \text{New interval } [1.375,1.4375] \\
&\text{Iteration } 5: \quad c_5 = \frac{1.375+1.4375}{2} = 1.40625, \quad f(1.40625) = -0.02246094 < 0 \quad \Rightarrow \text{New interval } [1.40625,1.4375
\end{aligned}$$

Results Table:

n	a_n	b_n	c_n	$f(c_n)$
1	1.00000	2.00000	1.50000	0.25000000
2	1.00000	1.50000	1.25000	-0.43750000
3	1.25000	1.50000	1.37500	-0.10937500
4	1.37500	1.50000	1.43750	0.06640625
5	1.37500	1.43750	1.40625	-0.02246094
6	1.40625	1.43750	1.42188	0.02172852
7	1.40625	1.42188	1.41406	-0.00042725

Table of figures 5.5: Dichotomy method iterations for $f(x) = x^2 - 2$

After 7 iterations, $c_7 \approx 1.41406$ with error $|1.41406 - \sqrt{2}| \approx 0.00015$.

Error Bound:

The theoretical error bound after n iterations is:

$$|c_n - \sqrt{2}| \leq \frac{2-1}{2^{n+1}} = \frac{1}{2^{n+1}}$$

For $n = 7$: $\frac{1}{2^8} = \frac{1}{256} \approx 0.0039$, which is satisfied since $0.00015 < 0.0039$.

Comparison: the methods of secant and dichotomy to find the root of $f(x) = x^2 - 2$ on the interval $[1, 2]$.

Property	**Dichotomy**	**Secant**
Convergence order	Linear (1)	Superlinear (1.618)
Derivative needed?	No	No
Brackets root?	Yes	No
Iterations to 10^{-6} error	≈ 20	≈ 6
Stability	Very stable	May diverge

Table of figures 5.6: Comparison of both methods

Chapter 6

Annexe

6.1 Series TD

6.1.1 Problem Set 1

Exercise 1:

1. Show that a norm is convex.
2. Show that the indicator function of a set K, defined by

$$I_K(x) = \begin{cases} 0 & \text{if } x \in K, \\ +\infty & \text{otherwise,} \end{cases}$$

is convex if and only if K is convex.

Solution:

1. Let $\|\cdot\|$ be a norm on $\mathbb{R}^n$. For any $x, y \in \mathbb{R}^n$ and $\lambda \in [0,1]$,

$$\|\lambda x + (1-\lambda)y\| \leq \lambda\|x\| + (1-\lambda)\|y\|,$$

by the triangle inequality and homogeneity. Hence, the norm is convex.

2. ($\Rightarrow$) Assume I_K is convex. Let $x, y \in K$ and $\lambda \in [0,1]$. Then $I_K(x) = 0$ and $I_K(y) = 0$. By convexity,

$$I_K(\lambda x + (1-\lambda)y) \leq \lambda I_K(x) + (1-\lambda) I_K(y) = 0.$$

Since I_K takes values in $\{0,+\infty\}$, we must have $I_K(\lambda x+(1-\lambda)y)=0$, so $\lambda x+(1-\lambda)y\in K$. Thus K is convex.

$(\Leftarrow)$ Assume K is convex. Let $x,y\in\mathbb{R}^n$ and $\lambda\in[0,1]$. If $x,y\in K$, then $\lambda x+(1-\lambda)y\in K$, so

$$I_K(\lambda x+(1-\lambda)y)=0=\lambda\cdot 0+(1-\lambda)\cdot 0=\lambda I_K(x)+(1-\lambda)I_K(y).$$

If at least one of $x,y\notin K$, then the right-hand side is $+\infty$, so the inequality

$$I_K(\lambda x+(1-\lambda)y)\le \lambda I_K(x)+(1-\lambda)I_K(y)$$

holds trivially. Hence I_K is convex.

Exercise 2:

1. Let $(f_i)_{i\in I}$ be an arbitrary family of convex functions $U\to\mathbb{R}$. Show that the function $f(x)=\sup_{i\in I} f_i(x)$ is convex.

2. Prove Young's inequality:

$$\forall a,b>0,\ \forall p,q\in\mathbb{N}^* \text{ such that } \frac{1}{p}+\frac{1}{q}=1 \quad\Rightarrow\quad ab\le\frac{a^p}{p}+\frac{b^q}{q}.$$

Solution:

1. Let $x,y\in U$, $\lambda\in[0,1]$. For each $i\in I$,

$$f_i(\lambda x+(1-\lambda)y)\le \lambda f_i(x)+(1-\lambda)f_i(y)\le \lambda f(x)+(1-\lambda)f(y).$$

Taking the supremum over i on the left gives

$$f(\lambda x+(1-\lambda)y)\le \lambda f(x)+(1-\lambda)f(y).$$

Thus f is convex.

2. Consider the function $\varphi(t)=\frac{t^p}{p}+\frac{1}{q}-t$ for $t\ge 0$. Its derivative is $\varphi'(t)=t^{p-1}-1$, which is zero at $t=1$. Since $\varphi''(t)=(p-1)t^{p-2}>0$ for $t>0$, φ has a global minimum at $t=1$ with $\varphi(1)=\frac{1}{p}+\frac{1}{q}-1=0$. Hence $\varphi(t)\ge 0$ for all $t\ge 0$, i.e.,

$$t\le\frac{t^p}{p}+\frac{1}{q}.$$

Now set $t = a \cdot b^{-\frac{q}{p}}$. Noting that $\frac{q}{p} = q-1$ because $\frac{1}{p}+\frac{1}{q}=1$, we get

$$ab^{-\frac{q}{p}} \leq \frac{a^p b^{-q}}{p} + \frac{1}{q}.$$

Multiplying through by b^q yields

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q}.$$

Exercise 3:

Determine whether the following functions are coercive:

1. $f:\mathbb{R}\to\mathbb{R}$, $f(x) = x^3 + x^2 + 1$
2. $f:\mathbb{R}^n\to\mathbb{R}$, $f(x) = \langle a, x\rangle + b$, $a \in \mathbb{R}^n$, $b \in \mathbb{R}$
3. $f:\mathbb{R}^2\to\mathbb{R}$, $f(x,y) = 2x^2 + y - 1$
4. $f:\mathbb{R}^2\to\mathbb{R}$, $f(x,y) = 2x^2 + y^3 + 2y^2$
5. $f:\mathbb{R}^2\to\mathbb{R}$, $f(x,y) = x^2 + y^2 - 1000x - 5000$

Solution:

A function $f:\mathbb{R}^n\to\mathbb{R}$ is coercive if $\lim_{\|x\|\to\infty} f(x) = +\infty$.

1. $\lim_{x\to+\infty} f(x) = +\infty$, but $\lim_{x\to-\infty} f(x) = -\infty$. Not coercive.
2. $f(x)$ is linear. If $a \neq 0$, we can choose $x = -ta$ with $t \to +\infty$ to make $f(x) \to -\infty$. Not coercive.
3. Fix $x = 0$, let $y \to -\infty$; then $f(0,y) \to -\infty$. Not coercive.
4. For $\|(x,y)\| \to \infty$, either $|x| \to \infty$ (then $2x^2 \to +\infty$) or $|y| \to \infty$ (then y^3 dominates, but if $y \to -\infty$, $y^3 \to -\infty$). Check: let $y \to -\infty$, $x = 0$; then $f(0,y) \to -\infty$. Not coercive.
5. $f(x,y) = (x-500)^2 + y^2 - 500^2 - 5000$. As $\|(x,y)\| \to \infty$, the quadratic terms dominate, so $f(x,y) \to +\infty$. Coercive.

Exercise 4:

Find the minimum and maximum values of the following functions:

1. $f(x) = x^4 - 2x^2 + 3$

2. $f(x) = \sqrt{1+x^2}$

3. $f(x) = xe^{-x^2}$

4. $f(x) = \cosh(x^2-1)$

5. $f(x) = x - 2\ln(x^2+3)$

6. $f(x) = \cos^2 x$

Solution:

1. $f'(x) = 4x^3 - 4x = 4x(x^2-1)$. Critical points: $x = 0, \pm 1$. $f(0) = 3$, $f(\pm 1) = 2$. As $|x| \to \infty$, $f(x) \to +\infty$. So minimum = 2, no finite maximum.

2. $f'(x) = \frac{x}{\sqrt{1+x^2}}$. Critical point: $x = 0$, $f(0) = 1$. As $|x| \to \infty$, $f(x) \to +\infty$. Minimum = 1, no finite maximum.

3. $f'(x) = e^{-x^2}(1-2x^2)$. Critical points: $x = \pm\frac{1}{\sqrt{2}}$. $f(\frac{1}{\sqrt{2}}) = \frac{1}{\sqrt{2}}e^{-1/2} > 0$, $f(-\frac{1}{\sqrt{2}}) = -\frac{1}{\sqrt{2}}e^{-1/2} < 0$. As $x \to \pm\infty$, $f(x) \to 0$. So maximum ≈ 0.4289, minimum ≈ -0.4289.

4. cosh is even and increasing on $[0, \infty)$. Minimum at $x^2 - 1 = 0 \Rightarrow x = \pm 1$, $f(\pm 1) = \cosh(0) = 1$. As $|x| \to \infty$, $f(x) \to +\infty$. Minimum = 1, no finite maximum.

5. $f'(x) = 1 - \frac{4x}{x^2+3} = \frac{x^2-4x+3}{x^2+3} = \frac{(x-1)(x-3)}{x^2+3}$. Critical points: $x = 1, 3$. $f(1) = 1 - 2\ln 4 \approx -1.7726$, $f(3) = 3 - 2\ln 12 \approx -1.989$. As $x \to \pm\infty$, $f(x) \sim x - 2\ln(x^2) \to \pm\infty$. So local max at $x = 1$, local min at $x = 3$. Minimum ≈ -1.989, no finite maximum.

6. $0 \le \cos^2 x \le 1$. Minimum = 0, maximum = 1.

6.1.2 Problem Set 2

Exercise 1:

A wire of length L is cut into two pieces. From one piece an equilateral triangle is formed, from the other a square. Where should the wire be cut so that the total area of the two figures is maximal? minimal?

Solution:

Let x be the length used for the triangle, $L-x$ for the square. Side of triangle: $\frac{x}{3}$, area: $\frac{\sqrt{3}}{4}\left(\frac{x}{3}\right)^2 = \frac{\sqrt{3}}{36}x^2$. Side of square: $\frac{L-x}{4}$, area: $\left(\frac{L-x}{4}\right)^2$. Total area:

$$A(x) = \frac{\sqrt{3}}{36}x^2 + \frac{1}{16}(L-x)^2, \quad 0 \le x \le L.$$

Derivative:

$$A'(x) = \frac{\sqrt{3}}{18}x - \frac{1}{8}(L-x) = \left(\frac{\sqrt{3}}{18} + \frac{1}{8}\right)x - \frac{L}{8}.$$

Critical point:

$$x^* = \frac{L/8}{\frac{\sqrt{3}}{18} + \frac{1}{8}} = \frac{9L}{4\sqrt{3}+9}.$$

Check endpoints: $x = 0$ (all square): $A(0) = \frac{L^2}{16}$; $x = L$ (all triangle): $A(L) = \frac{\sqrt{3}}{36}L^2$. Compute $A(x^*)$ and compare. Since A is convex (quadratic with positive coefficient), the critical point gives the minimum area. The maximum occurs at an endpoint; compare $A(0)$ and $A(L)$ to determine which is larger.

Exercise 2:

1. Determine the dimensions of a cylindrical can without a lid, with fixed volume V, that uses the least material (ignore thickness and waste).

2. Same for a can with a lid.

Solution:

Let radius r, height h, volume $V = \pi r^2 h$.

1. Surface area (no lid): $S = \pi r^2 + 2\pi r h = \pi r^2 + \frac{2V}{r}$. Minimize $S(r)$ for $r > 0$:

$$S'(r) = 2\pi r - \frac{2V}{r^2} = 0 \implies r^3 = \frac{V}{\pi} \implies r = \left(\frac{V}{\pi}\right)^{1/3}, \quad h = \frac{V}{\pi r^2} = \left(\frac{V}{\pi}\right)^{1/3} = r.$$

   So $h = r$.

2. With lid: $S = 2\pi r^2 + 2\pi rh = 2\pi r^2 + \frac{2V}{r}$.

$$S'(r) = 4\pi r - \frac{2V}{r^2} = 0 \implies r^3 = \frac{V}{2\pi} \implies r = \left(\frac{V}{2\pi}\right)^{1/3}, \quad h = \frac{V}{\pi r^2} = 2\left(\frac{V}{2\pi}\right)^{1/3} = 2r.$$

So $h = 2r$.

Exercise 3:

A rectangular box is formed by cutting four squares from the corners of a 32 cm by 20 cm sheet of cardboard. Find the height of the box that maximizes the volume.

Solution:

Let the side of each square cut be x cm. Then the box dimensions: length $32-2x$, width $20-2x$, height x. Volume:

$$V(x) = x(32-2x)(20-2x) = 4x(16-x)(10-x), \quad 0 \le x \le 10.$$

Expand: $V(x) = 4x(160-26x+x^2) = 4x^3 - 104x^2 + 640x$. Derivative:

$$V'(x) = 12x^2 - 208x + 640 = 4(3x^2 - 52x + 160) = 0.$$

Solve: $x = \frac{52\pm\sqrt{2704-1920}}{6} = \frac{52\pm\sqrt{784}}{6} = \frac{52\pm 28}{6}$. So $x = \frac{80}{6} = \frac{40}{3} \approx 13.33$ (not in $[0,10]$) or $x = \frac{24}{6} = 4$. Check $V(0) = 0$, $V(10) = 0$, $V(4) = 4\cdot 4\cdot 12\cdot 6 = 1152$ cm^3. Maximum at $x = 4$ cm.

Exercise 4:

Find the minima and maxima on $\mathbb{R}^2$ of the following functions:

1. $f(x,y) = x^2 + y^2$
2. $f(x,y) = \frac{1}{3}x^3 + y^3 - x - y$
3. $f(x,y) = x^6 - 3x^4y^2 + 3x^2y^4 - y^6$
4. $f(x,y) = 100(y-x^2)^2 + (1-x)^2$
5. $f(x,y) = x^2 - xy + \frac{1}{6}y^3$
6. $f(x,y) = x^3 + y^3 - 9xy + 27$
7. $f(x,y) = xy$
8. $f(x,y) = \cos x \cdot \cos y$
9. $f(x,y) = \frac{1}{2}x^2 + x\cos y$ (Note: original text seems to have a typo; corrected.)

Solution (Selected):

1. Minimum 0 at $(0,0)$, no maximum.
2. $\nabla f = (x^2 - 1,\, 3y^2 - 1)$. Critical points: $(\pm 1, \pm \frac{1}{\sqrt{3}})$. Hessian: $\mathrm{diag}(2x, 6y)$. Evaluate to classify. No global min/max due to cubic growth.
3. Note $f(x,y) = (x^2 - y^2)^3$. Minimum 0 on lines $y = \pm x$, no global max.

   Consider the function
   $$f(x,y) = (x^2 - y^2)^3.$$
   Step 1: Minimum:

   On the lines $y = x$ and $y = -x$, we have
   $$x^2 - y^2 = x^2 - (\pm x)^2 = 0,$$
   so
   $$f(x,y) = 0^3 = 0.$$
   Thus, the minimum value is 0, attained on the lines $y = \pm x$.

   Step 2: Maximum:

   Consider, for example, the line $y = 0$:
   $$f(x,0) = (x^2 - 0^2)^3 = x^6.$$
   As $x \to +\infty$ or $x \to -\infty$, $f(x,0) \to +\infty$. Therefore, f is unbounded above and does not have a global maximum.

   On the other hand, we have the gradient of f is
   $$\nabla f(x,y) = \begin{pmatrix} f_x \\ f_y \end{pmatrix} = \begin{pmatrix} 6x(x^2 - y^2)^2 \\ -6y(x^2 - y^2)^2 \end{pmatrix}.$$
   Setting $\nabla f = 0$ gives the critical points:
   $$6x(x^2 - y^2)^2 = 0 \implies x = 0 \text{ or } x^2 = y^2,$$
   $$-6y(x^2 - y^2)^2 = 0 \implies y = 0 \text{ or } x^2 = y^2.$$
   Critical Points:

   Solving the system gives:
   $$(x,y) = (0,0) \quad \text{and the lines} \quad y = \pm x.$$

Hessian:

The Hessian matrix is

$$H(x,y) = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} = \begin{pmatrix} 6(x^2-y^2)^2 + 24x^2(x^2-y^2) & -24xy(x^2-y^2) \\ -24xy(x^2-y^2) & -6(x^2-y^2)^2 + 24y^2(x^2-y^2) \end{pmatrix}.$$

At $(0,0)$, we have

$$H(0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

so the second derivative test is inconclusive.

Behavior along axes:

$$f(x,0) = x^6 \geq 0 \quad \text{(increasing along } x\text{-axis)},$$

$$f(0,y) = -y^6 \leq 0 \quad \text{(decreasing along } y\text{-axis)}.$$

Conclusion:

- The statement is **true**: f has minimum 0 on the lines $y = \pm x$, and no global maximum exists. - The point $(0,0)$ is a **saddle point**.

4. $f \geq 0$. Minimum 0 at $(1,1)$ (since $y = x^2$ and $x = 1$).

5. $\nabla f = (2x - y,\ -x + \frac{1}{2}y^2)$. Critical points: solve $2x = y$ and $x = \frac{1}{2}y^2 \implies y = y^2 \implies y = 0$ or $y = 1$. Points: $(0,0)$, $(\frac{1}{2},1)$. Hessian: $\begin{pmatrix} 2 & -1 \\ -1 & y \end{pmatrix}$. Evaluate.

6. $\nabla f = (3x^2 - 9y,\ 3y^2 - 9x)$. Critical points: $(0,0)$, $(3,3)$. Hessian: $\begin{pmatrix} 6x & -9 \\ -9 & 6y \end{pmatrix}$. $(0,0)$ saddle, $(3,3)$ local min.

7. No global min/max (unbounded).

8. $-1 \leq f \leq 1$. Max 1 at $(2m\pi, 2n\pi)$, min -1 at $((2m+1)\pi, (2n+1)\pi)$.

9. (Assuming $f(x,y) = \frac{1}{2}x^2 + x\cos y$) Critical points: $\nabla f = (x + \cos y,\ -x\sin y) = 0$. Solve: from second, either $\sin y = 0$ or $x = 0$. Case analysis yields points like $(0, \pi/2 + k\pi)$ etc. Hessian: $\begin{pmatrix} 1 & -\sin y \\ -\sin y & -x\cos y \end{pmatrix}$. Evaluate.

6.2 Exam 1

Optimization 1 Exam (2017–2018)

Department of Mathematics and Computer Science, 3rd Year Mathematics

Exercise 1:

Determine the optimal values of the following functions:

1. $f(x,y) = x^3 + y^3 - 3xy$ 2. $g(x) = x\ln(x^2 - x) - \ln(x-1) - (2+\ln 2)x + 1$

Exercise 2:

1. Solve the optimization problem for the following function using Newton's method:

$$f(x) = \sqrt{x^4+1} + 3 - x$$

2. Find the square root of 3 using the fixed-point method.

Exercise 3: Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$f(x,y) = 4x + 6y - x^2 - y^2$$

1. Show that the function f has a unique global maximum.

2. Solve the maximization problem using:

a) The relaxation method.

b) The gradient method with constant step.

6.2.1 Solution

Exercise 1: Find the optimal values of the following functions.

1. $f(x,y) = x^3 + y^3 - 3xy$.

   We look for critical points by solving:

$$\nabla f = (3x^2 - 3y,\ 3y^2 - 3x) = (0,0)$$

   This gives the system:

$$x^2 = y, \quad y^2 = x.$$

   Substitute $y = x^2$ into $y^2 = x$:

$$x^4 = x \quad \Rightarrow \quad x(x^3 - 1) = 0.$$

   So $x = 0$ or $x = 1$. Correspondingly:

$$x = 0 \Rightarrow y = 0, \qquad x = 1 \Rightarrow y = 1.$$

   Critical points: $(0,0)$ and $(1,1)$.

   Hessian matrix:

$$H_f(x,y) = \begin{pmatrix} 6x & -3 \\ -3 & 6y \end{pmatrix}.$$

   At $(0,0)$:

$$H_f(0,0) = \begin{pmatrix} 0 & -3 \\ -3 & 0 \end{pmatrix}, \quad \det = -9 < 0 \Rightarrow \text{saddle point}.$$

   At $(1,1)$:

$$H_f(1,1) = \begin{pmatrix} 6 & -3 \\ -3 & 6 \end{pmatrix}, \quad \det = 36 - 9 = 27 > 0, \quad f_{xx} = 6 > 0 \Rightarrow \text{local minimum}.$$

   No finite global maximum. Minimum value:

$$f(1,1) = 1 + 1 - 3 = -1.$$

2. $g(x) = x\ln(x^2 - x) - \ln(x-1) - (2 + \ln 2)x + 1$.

   Domain: $x^2 - x > 0$ and $x - 1 > 0 \Leftrightarrow x > 1$.

$$g'(x) = \ln(x^2 - x) + x \cdot \frac{2x-1}{x^2 - x} - \frac{1}{x-1} - (2 + \ln 2).$$

Simplify:

$$g'(x) = \ln(x(x-1)) + \frac{2x-1}{x-1} - \frac{1}{x-1} - 2 - \ln 2.$$

$$g'(x) = \ln x + \ln(x-1) + \frac{2x-2}{x-1} - 2 - \ln 2.$$

$$g'(x) = \ln x + \ln(x-1) + 2 - 2 - \ln 2 = \ln x + \ln(x-1) - \ln 2 = \ln\left(\frac{x(x-1)}{2}\right).$$

Set $g'(x) = 0$:

$$\frac{x(x-1)}{2} = 1 \quad \Leftrightarrow \quad x^2 - x - 2 = 0 \quad \Leftrightarrow \quad (x-2)(x+1) = 0.$$

Since $x > 1$, $x = 2$ is the only critical point.

Check $g''(x)$:

$$g''(x) = \frac{d}{dx}\ln\left(\frac{x(x-1)}{2}\right) = \frac{2x-1}{x(x-1)}.$$

At $x = 2$, $g''(2) = \frac{3}{2} > 0 \Rightarrow$ local minimum.

Minimum value:

$$g(2) = 2\ln(4-2) - \ln(1) - (2+\ln 2)(2) + 1 = 2\ln 2 - 0 - 4 - 2\ln 2 + 1 = -3.$$

Exercise 2:

1. Solve the optimization problem for the following function $f(x) = \sqrt{x^4+1} + 3 - x$ using Newton's method:

   Newton's iteration:

   $$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}.$$

   But careful: Newton's method for optimization uses $x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$ if solving $f'(x) = 0$.

   First compute derivative for critical points:

   $$f'(x) = \frac{4x^3}{2\sqrt{x^4+1}} - 1 = \frac{2x^3}{\sqrt{x^4+1}} - 1.$$

   Set $f'(x) = 0$:

   $$\frac{2x^3}{\sqrt{x^4+1}} = 1 \quad \Rightarrow \quad 4x^6 = x^4 + 1.$$

   Let $t = x^2 \geq 0$:

   $$4t^3 = t^2 + 1 \quad \Rightarrow \quad 4t^3 - t^2 - 1 = 0.$$

   Newton for this equation: $h(t) = 4t^3 - t^2 - 1$, $h'(t) = 12t^2 - 2t$. Start with $t_0 = 1$:

   $$t_1 = 1 - \frac{4-1-1}{12-2} = 1 - \frac{2}{10} = 0.8.$$

$$t_2 = 0.8 - \frac{4(0.512) - 0.64 - 1}{12(0.64) - 1.6} = 0.8 - \frac{2.048 - 1.64}{7.68 - 1.6} \approx 0.8 - \frac{0.408}{6.08} \approx 0.7329.$$

$$t_3 \approx 0.7329 - \frac{4(0.393) - 0.537 - 1}{12(0.537) - 1.4658} \approx 0.7329 - \frac{1.572 - 1.537}{6.444 - 1.4658} \approx 0.7329 - 0.007 \approx 0.7259.$$

Thus $x = \sqrt{t} \approx \sqrt{0.7259} \approx 0.852$. This is the minimizer since $f''(x) > 0$ (check sign). Minimum value:

$$f(0.852) \approx \sqrt{(0.852)^4 + 1} + 3 - 0.852 \approx \sqrt{1.527} + 2.148 \approx 1.236 + 2.148 = 3.384.$$

2. Find $\sqrt{3}$ by fixed-point method:

   We solve $x = \varphi(x)$ where $\varphi(x) = \frac{1}{2}\left(x + \frac{3}{x}\right)$ (Newton for $x^2 - 3 = 0$).

   Start with $x_0 = 2$:

$$x_1 = 0.5(2 + 3/2) = 0.5(2 + 1.5) = 1.75.$$

$$x_2 = 0.5(1.75 + 3/1.75) \approx 0.5(1.75 + 1.7143) = 1.73215.$$

$$x_3 \approx 0.5(1.73215 + 3/1.73215) \approx 0.5(1.73215 + 1.73196) = 1.732055.$$

   Converges to $\sqrt{3} \approx 1.73205$.

Exercise 3: Consider the function:

$$f(x,y) = 4x + 6y - x^2 - y^2.$$

1. Show f has a unique global maximum:

   Gradient:

$$\nabla f = (4 - 2x,\ 6 - 2y) = (0,0) \Rightarrow (x,y) = (2,3).$$

   Hessian:

$$H_f = \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}.$$

   Negative definite everywhere $\Rightarrow$ concave quadratic. Critical point $(2,3)$ is the unique global maximizer.

   Maximum value:

$$f(2,3) = 8 + 18 - 4 - 9 = 13.$$

2. Solve by:

   (a) Relaxation method:

   Maximize alternatingly in x and y: For fixed y: $f(x,y) = -x^2 + 4x + C$ max at $x = 2$. For fixed x: $f(x,y) = -y^2 + 6y + C'$ max at $y = 3$.

Start with (x_0, y_0): Update $x_1 = 2$, then $y_1 = 3$. Converges in one step to $(2,3)$.

(b) Gradient method with constant step:

$\nabla f = (4-2x, 6-2y)$. Take step $\alpha > 0$:

$$(x_{n+1}, y_{n+1}) = (x_n, y_n) + \alpha(4-2x_n, 6-2y_n).$$

Choose α small enough for convergence (e.g., $\alpha = 0.5$).

Starting from $(0,0)$:

$$(x_1, y_1) = (0,0) + 0.5(4,6) = (2,3).$$

Converges in one step because f is quadratic and step chosen exactly for optimum.

6.3 Exam 2

Resit Exam — Optimization 1 (2017–2018)

Department of Mathematics and Computer Science, 3rd Year Mathematics.

Exercise 1:

Determine the optimal values of the following functions:

1. $f(x) = 12x^5 - 45x^4 + 40x^3 + 5$
2. $g(x,y) = e^{1-x^2-y^2} + x^2 + y^2$

Exercise 2:

1. Solve the optimization problem for the following function:

$$f(x) = \frac{1}{4}x^4 + \frac{1}{3}x^3 - x + 1$$

(Use the fixed-point method.)

Exercise 3:

Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$f(x,y) = x^2 + y^2 + 4x - 6y$$

1. Show that the function f has a unique global minimum.
2. Solve the minimization problem using:

a) The relaxation method.

b) The gradient method with constant step.

6.3.1 Solution

Exercise 1:

Find the optimal values of the following functions.

1. $f(x) = 12x^5 - 45x^4 + 40x^3 + 5$

   First derivative:

   $$f'(x) = 60x^4 - 180x^3 + 120x^2 = 60x^2(x^2 - 3x + 2).$$

   Factor:

   $$x^2 - 3x + 2 = (x-1)(x-2).$$

   Thus:

   $$f'(x) = 60x^2(x-1)(x-2).$$

   Critical points: $x = 0$, $x = 1$, $x = 2$.

   Second derivative:

   $$f''(x) = 240x^3 - 540x^2 + 240x = 60x(4x^2 - 9x + 4).$$

   Evaluate:

   $$f''(0) = 0 \quad \text{(inconclusive, use higher derivative or sign test).}$$

   Check sign of $f'(x)$ around $x = 0$: $f'(x) = 60x^2(x-1)(x-2)$, $x^2 \geq 0$, so sign depends on $(x-1)(x-2)$. For $x < 0$, $(x-1)(x-2) > 0 \implies f'(x) > 0$. For $0 < x < 1$, $(x-1)(x-2) > 0$ $\implies f'(x) > 0$. Thus $f'(x)$ does not change sign at $x = 0 \implies x = 0$ is not a local extremum, but an inflection point.

   $$f''(1) = 60(4-9+4) = 60(-1) = -60 < 0 \Rightarrow \text{local maximum at } x = 1.$$

   $$f''(2) = 60 \cdot 2(16-18+4) = 120(2) = 240 > 0 \Rightarrow \text{local minimum at } x = 2.$$

   Values:

   $$f(1) = 12 - 45 + 40 + 5 = 12, \quad f(2) = 12 \cdot 32 - 45 \cdot 16 + 40 \cdot 8 + 5 = 384 - 720 + 320 + 5 = -11.$$

   No finite global maximum or minimum because $f(x) \to +\infty$ as $x \to +\infty$ and $f(x) \to -\infty$ as $x \to -\infty$.

2. $g(x,y) = e^{1-x^2-y^2} + x^2 + y^2$

   Rewrite: let $r = x^2 + y^2 \geq 0$, $h(r) = e^{1-r} + r$. Then $g(x,y) = h(r)$.

We minimize $h(r)$ for $r \geq 0$:

$$h'(r) = -e^{1-r} + 1.$$

Set $h'(r) = 0 \Longrightarrow e^{1-r} = 1 \Longrightarrow 1 - r = 0 \Longrightarrow r = 1$.

Second derivative:

$$h''(r) = e^{1-r} > 0 \quad \text{for all } r.$$

Thus $r = 1$ is a local (and global) minimum for $h(r)$.

Minimum value of h:

$$h(1) = e^0 + 1 = 1 + 1 = 2.$$

So g is minimal when $x^2 + y^2 = 1$, and $g_{\min} = 2$.

No maximum because as $r \to \infty$, $h(r) \to \infty$.

Exercise 2:

1. Optimize $f(x) = \frac{1}{4}x^4 + \frac{1}{3}x^3 - x + 1$ using fixed-point method:

   We look for $f'(x) = 0$:

   $$f'(x) = x^3 + x^2 - 1 = 0.$$

   Rewrite as fixed-point form: $x = \varphi(x)$ with $\varphi(x) = (1 - x^3)^{1/2}$ or better: $x^2(1+x) = 1 \Rightarrow x = \frac{1}{\sqrt{1+x}}$ for $x > -1$.

   Take $\varphi(x) = \frac{1}{\sqrt{1+x}}$, start with $x_0 = 1$:

   $$x_1 = \frac{1}{\sqrt{2}} \approx 0.7071,$$

   $$x_2 = \frac{1}{\sqrt{1.7071}} \approx 0.7654,$$

   $$x_3 = \frac{1}{\sqrt{1.7654}} \approx 0.7527,$$

   $$x_4 = \frac{1}{\sqrt{1.7527}} \approx 0.7555,$$

   $$x_5 \approx 0.7547.$$

   Converges to $x^* \approx 0.755$, which is the unique real root of $x^3 + x^2 - 1 = 0$ (since $f'(x)$ is increasing for $x \geq 0$, one real root).

   Check $f''(x^*)$: $f''(x) = 3x^2 + 2x$, at $x^* \approx 0.755$, $f'' \approx 3(0.57) + 1.51 \approx 3.22 > 0$, so local minimum.

Minimum value:

$$f(0.755) \approx 0.25(0.324) + 0.333(0.430) - 0.755 + 1 \approx 0.081 + 0.143 - 0.755 + 1 \approx 0.469.$$

Exercise 3:

$$f(x,y) = x^2 + y^2 + 4x - 6y$$

1. Show f has a unique global minimum:

   Complete squares:

   $$f(x,y) = (x^2 + 4x) + (y^2 - 6y) = (x+2)^2 - 4 + (y-3)^2 - 9.$$

   $$f(x,y) = (x+2)^2 + (y-3)^2 - 13.$$

   This is a sum of squares minus a constant, so minimum occurs when squares are zero: $x = -2$, $y = 3$. Minimum value -13. Unique because quadratic with positive definite Hessian.

2. Minimization by:

   (a) Relaxation method:

   Minimize alternately in x and y: For fixed y: $f(x,y) = x^2 + 4x + C$ min at $x = -2$. For fixed x: $f(x,y) = y^2 - 6y + C'$ min at $y = 3$.

   Start with (x_0, y_0):

   $$x_1 = -2, \quad y_1 = 3.$$

   Converges in one step to $(-2, 3)$.

   (b) Gradient method with constant step:

   Gradient:

   $$\nabla f = (2x + 4,\ 2y - 6).$$

   Update:

   $$(x_{n+1}, y_{n+1}) = (x_n, y_n) - \alpha \nabla f(x_n, y_n).$$

   Take $\alpha = 0.5$ for example, starting from $(0,0)$:

   $$(x_1, y_1) = (0,0) - 0.5(4, -6) = (-2, 3).$$

   Converges in one step because the function is quadratic with appropriate step size.

   Minimum value: $f(-2,3) = 4 + 9 - 8 - 18 = -13.$

6.4 Exam 3

Exam — Optimization 1

Exercise 1:

- Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$f(x,y) = x^2 + y^2 - 4x - 6y$$

1. Show that the function f has a unique global minimum.
2. Use the gradient method to compute the minimum with $\varepsilon = 0.01$.

- Consider the function $g : \mathbb{R}^2 \to \mathbb{R}$ defined by:

$$g(x,y) = -x^2 - \frac{1}{2}y - e^{-y}$$

3. Show that the function g has a unique global maximum.
4. Use Newton's method to compute the maximum with $\varepsilon = 0.01$.

Exercise 2:

1. Solve the following optimization problem:

$$(P) : \min_{x \in \mathbb{R}_+} f(x), \quad f(x) = \sin x - (x-1)e^x$$

2. Find the square root of 2 using:
   (a) Newton's method.
   (b) The fixed-point method.

Exercise 3:

Two hallways of lengths 1m and 2m meet at a right angle. A rod AB of length L is being transported through the corner.

What is the minimum length L that this rod can have?

6.4.1 Solution

Exercise 1:

Part I:

$$f(x,y) = x^2 + y^2 - 4x - 6y$$

1. Show f has a unique global minimum:

   Complete the squares:

   $$f(x,y) = (x^2 - 4x) + (y^2 - 6y) = (x-2)^2 - 4 + (y-3)^2 - 9.$$

   $$f(x,y) = (x-2)^2 + (y-3)^2 - 13.$$

   Since squares are non-negative, the minimum is attained when $(x-2)^2 = 0$ and $(y-3)^2 = 0$, i.e. $x = 2$, $y = 3$. Minimum value: $f(2,3) = -13$. The Hessian matrix is $\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$, positive definite, so the function is strictly convex and the critical point is the unique global minimizer.

2. Gradient method with $\varepsilon = 0.01$:

   Gradient: $\nabla f = (2x - 4,\ 2y - 6)$.

   Choose step size $\alpha = 0.5$ (safe for quadratic function with Hessian eigenvalues 2). Start from $(x_0, y_0) = (0,0)$.

   Iteration 1:

   $$\nabla f_0 = (-4,-6), \quad \|\nabla f_0\| = \sqrt{16+36} = \sqrt{52} \approx 7.211 > 0.01.$$

   $$(x_1, y_1) = (0,0) - 0.5(-4,-6) = (2,3).$$

   Gradient at $(2,3)$: $(0,0)$, norm $= 0 < 0.01$.

   Thus minimum is $(2,3)$, $f_{\min} = -13$, reached in one iteration.

Part II:

$$g(x,y) = -x^2 - \frac{1}{2}y - e^{-y}.$$

1. Show g has a unique global maximum:

   Gradient:

   $$\nabla g = \left(-2x,\ -\frac{1}{2} + e^{-y}\right).$$

   Set $\nabla g = (0,0)$:

   $$-2x = 0 \Rightarrow x = 0, \qquad -\frac{1}{2} + e^{-y} = 0 \Rightarrow e^{-y} = \frac{1}{2} \Rightarrow y = \ln 2.$$

Hessian:

$$H_g = \begin{pmatrix} -2 & 0 \\ 0 & -e^{-y} \end{pmatrix}.$$

At $(0, \ln 2)$:

$$H_g = \begin{pmatrix} -2 & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \quad \text{negative definite.}$$

Thus $(0, \ln 2)$ is the unique critical point and a strict local maximum. Since $g(x,y) \to -\infty$ as $|x| \to \infty$ or $y \to \pm\infty$, it is a global maximum.

2. Newton's method with $\varepsilon = 0.01$:

   Newton iteration for maximizing g:

$$\mathbf{z}_{n+1} = \mathbf{z}_n - [H_g(\mathbf{z}_n)]^{-1} \nabla g(\mathbf{z}_n),$$

   where $\mathbf{z} = (x, y)$.

   Since H_g is diagonal:

$$H_g^{-1} = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -\frac{1}{e^{-y}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -e^{y} \end{pmatrix}.$$

   Start from $\mathbf{z}_0 = (1, 1)$:

$$\nabla g_0 = (-2,\ -0.5 + e^{-1}) \approx (-2, -0.5 + 0.3679) = (-2, -0.1321).$$

$$H_g^{-1}(\mathbf{z}_0) = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -e^{1} \end{pmatrix} \approx \begin{pmatrix} -0.5 & 0 \\ 0 & -2.7183 \end{pmatrix}.$$

$$\mathbf{z}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} -0.5 & 0 \\ 0 & -2.7183 \end{pmatrix} \begin{pmatrix} -2 \\ -0.1321 \end{pmatrix}.$$

$$= \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 0.3591 \end{pmatrix} = \begin{pmatrix} 0 \\ 0.6409 \end{pmatrix}.$$

   Iteration 2 at $(0, 0.6409)$:

$$\nabla g \approx (0,\ -0.5 + e^{-0.6409}) \approx (0,\ -0.5 + 0.5265) = (0, 0.0265).$$

   Norm $\approx 0.0265 > 0.01$.

$$H_g^{-1} \approx \begin{pmatrix} -0.5 & 0 \\ 0 & -e^{0.6409} \end{pmatrix} \approx \begin{pmatrix} -0.5 & 0 \\ 0 & -1.898 \end{pmatrix}.$$

$$\mathbf{z}_2 = \begin{pmatrix} 0 \\ 0.6409 \end{pmatrix} - \begin{pmatrix} -0.5 & 0 \\ 0 & -1.898 \end{pmatrix} \begin{pmatrix} 0 \\ 0.0265 \end{pmatrix} = \begin{pmatrix} 0 \\ 0.6409 \end{pmatrix} - \begin{pmatrix} 0 \\ -0.0503 \end{pmatrix} = \begin{pmatrix} 0 \\ 0.6912 \end{pmatrix}.$$

Iteration 3 at $(0, 0.6912)$:

$$\nabla g \approx (0,\ -0.5 + e^{-0.6912}) \approx (0,\ -0.5 + 0.5009) = (0, 0.0009).$$

Norm $\approx 0.0009 < 0.01$, stop.

Thus maximum at $(0, 0.6912) \approx (0, \ln 2)$. Maximum value:

$$g(0, \ln 2) = 0 - \frac{1}{2}\ln 2 - \frac{1}{2} = -\frac{1}{2}(\ln 2 + 1) \approx -0.8466.$$

Exercise 2:

1. $f(x) = \sin x - (x-1)e^x$, $x \geq 0$:

   Derivative:

   $$f'(x) = \cos x - e^x - (x-1)e^x = \cos x - xe^x.$$

   Set $f'(x) = 0$: $\cos x = xe^x$. This equation must be solved numerically.

   Second derivative:

   $$f''(x) = -\sin x - e^x - xe^x = -\sin x - (1+x)e^x < 0 \quad \text{for } x \geq 0,$$

   so f is concave on $[0, \infty)$. Check boundary: $f(0) = 0 - (-1) \cdot 1 = 1$, and $f(x) \to -\infty$ as $x \to \infty$. Thus the maximum is at $x = 0$ (since concave, derivative decreasing). But we are asked for the minimum. Since f is concave, the minimum on $[0, \infty)$ is at $+\infty$ (value $-\infty$), or at a finite point if constrained. Let's check critical points numerically.

   Solve $\cos x = xe^x$ numerically (Newton):

   Let $h(x) = \cos x - xe^x$. $h(0) = 1$, $h(0.5) \approx 0.8776 - 0.5 \cdot 1.6487 \approx 0.8776 - 0.8244 = 0.0532 > 0$, $h(0.6) \approx 0.8253 - 0.6 \cdot 1.8221 \approx 0.8253 - 1.0933 = -0.2680 < 0$. So root in $(0.5, 0.6)$.

   Newton: $x_{n+1} = x_n - \frac{h(x_n)}{h'(x_n)}$, $h'(x) = -\sin x - e^x - xe^x$.
   Start $x_0 = 0.55$:

   $$h(0.55) \approx 0.8525 - 0.55 \cdot 1.7333 \approx 0.8525 - 0.9533 = -0.1008,$$

   $$h'(0.55) \approx -0.5227 - 1.7333 - 0.9533 = -3.2093$$

   $$x_1 = 0.55 - (-0.1008)/(-3.2093) \approx 0.55 - 0.0314 = 0.5186.$$

and

$$h(0.5186) \approx 0.8685 - 0.5186 \cdot 1.6798 \approx 0.8685 - 0.8712 = -0.0027,$$
$$h'(0.5186) \approx -0.4955 - 1.6798 - 0.8712 = -3.0465$$
$$x_2 \approx 0.5186 - (-0.0027)/(-3.0465) \approx 0.5186 - 0.0009 = 0.5177.$$

Thus critical point $x^* \approx 0.5177$. $f''(x^*) < 0$, so it is a local maximum. But concave function $\to$ only one critical point, which is a global maximum. Minimum on $\mathbb{R}_+$ is at the boundary $x \to \infty$ ($f \to -\infty$), or if domain bounded, check endpoints. Given $\min_{x \geq 0} f(x)$ does not exist (unbounded below). If domain restricted to a compact interval, minimum at left endpoint or where derivative negative.

2. Square root of 2:

a) Newton's method:
Solve $x^2 - 2 = 0$. Iteration: $x_{n+1} = \frac{1}{2}\left(x_n + \frac{2}{x_n}\right)$. Start $x_0 = 1.5$:

$$x_1 = 0.5(1.5 + 2/1.5) = 0.5(1.5 + 1.3333) = 1.4167,$$
$$x_2 = 0.5(1.4167 + 2/1.4167) \approx 0.5(1.4167 + 1.4118) = 1.41425,$$
$$x_3 \approx 1.4142136.$$

b) Fixed-point method:
Use $x = \frac{1}{2}\left(x + \frac{2}{x}\right)$ (same as Newton) or $x = \frac{2}{x}$ (does not converge unless damped). Better: $x = \frac{x+2/x}{2}$ as above. Converges to $\sqrt{2} \approx 1.4142136$.

Exercise 3:

Two hallways width 1m and 2m meet at right angle. Rod length L must pass through the corner.

Let the rod touch the outer walls at points such that it forms a line segment from $(a,0)$ to $(0,b)$ with $a \geq 2$, $b \geq 1$ because of hallway widths. Equation of the line: $\frac{x}{a} + \frac{y}{b} = 1$. Length of segment from $(a,0)$ to $(0,b)$ is $L = \sqrt{a^2 + b^2}$.

Constraint: the corner point $(2,1)$ must satisfy $\frac{2}{a} + \frac{1}{b} = 1$.
Minimize $L^2 = a^2 + b^2$ subject to $\frac{2}{a} + \frac{1}{b} = 1$, $a > 2, b > 1$.
From constraint: $\frac{1}{b} = 1 - \frac{2}{a} \Rightarrow b = \frac{1}{1-2/a} = \frac{a}{a-2}$.
Then $L^2 = a^2 + \left(\frac{a}{a-2}\right)^2 = a^2 + \frac{a^2}{(a-2)^2} = a^2\left[1 + \frac{1}{(a-2)^2}\right]$.
Let $t = a - 2 > 0$, then $a = t + 2$.

$$L^2 = (t+2)^2\left(1 + \frac{1}{t^2}\right) = (t+2)^2 \cdot \frac{t^2+1}{t^2} = \frac{(t+2)^2(t^2+1)}{t^2}.$$

Minimize L^2 over $t > 0$.

Derivative of L^2 w.r.t t: Let $h(t) = \ln L^2 = 2\ln(t+2) + \ln(t^2+1) - 2\ln t$.

$$h'(t) = \frac{2}{t+2} + \frac{2t}{t^2+1} - \frac{2}{t} = 2\left[\frac{1}{t+2} + \frac{t}{t^2+1} - \frac{1}{t}\right].$$

Set $h'(t) = 0$:

$$\frac{1}{t+2} + \frac{t}{t^2+1} = \frac{1}{t}.$$

Multiply through by $t(t+2)(t^2+1)$:

$$t(t^2+1) + t(t+2)(t) = (t+2)(t^2+1).$$

$$t^3 + t + t^3 + 2t^2 = t^3 + t + 2t^2 + 2.$$

$$2t^3 + 2t^2 + t = t^3 + 2t^2 + t + 2.$$

$$t^3 = 2 \quad \Rightarrow \quad t = \sqrt[3]{2}.$$

Then $a = 2 + \sqrt[3]{2}$, $b = \frac{a}{a-2} = \frac{2+\sqrt[3]{2}}{\sqrt[3]{2}} = 1 + 2^{2/3}$.

Minimum length:

$$L_{\min} = \sqrt{a^2 + b^2} = \sqrt{(2 + 2^{1/3})^2 + (1 + 2^{2/3})^2}.$$

Numerically: $2^{1/3} \approx 1.2599$, $2^{2/3} \approx 1.5874$. $a \approx 3.2599$, $b \approx 2.5874$. $L \approx \sqrt{10.627 + 6.694} = \sqrt{17.321} \approx 4.162\,\text{m}$.

Thus the minimal rod length that can pass is about $4.162\,\text{m}$.

6.5 Exam 4

Exercise 1:

Find the minimum and maximum values of the following functions:

1. $f(x) = e^x - 2e^{-x} - 3x$
2. $f(x,y) = x^3 + y^3 + 3x^2 + 6y^2 + 4$

6.5.1 Solution

1.

$$f(x) = e^x - 2e^{-x} - 3x$$

Derivative:

$$f'(x) = e^x + 2e^{-x} - 3$$

Set $f'(x) = 0$:

$$e^x + 2e^{-x} - 3 = 0$$

Multiply by e^x:

$$e^{2x} - 3e^x + 2 = 0$$

Let $u = e^x$, then $u^2 - 3u + 2 = 0$, so $u = 1$ or $u = 2$. Thus $e^x = 1 \Rightarrow x = 0$, or $e^x = 2 \Rightarrow x = \ln 2$.

Second derivative:

$$f''(x) = e^x - 2e^{-x}$$

Evaluate:

- $f''(0) = 1 - 2 = -1 < 0 \Rightarrow$ local maximum at $x = 0$, $f(0) = 1 - 2 - 0 = -1$.
- $f''(\ln 2) = 2 - 2 \cdot \frac{1}{2} = 1 > 0 \Rightarrow$ local minimum at $x = \ln 2$, $f(\ln 2) = 2 - 1 - 3\ln 2 = 1 - 3\ln 2$.

As $x \to +\infty$, $f(x) \to +\infty$; as $x \to -\infty$, $f(x) \to +\infty$. Thus:

- Global minimum: $1 - 3\ln 2$ at $x = \ln 2$.
- Global maximum: none (unbounded above).

2.

$$f(x,y) = x^3 + y^3 + 3x^2 + 6y^2 + 4$$

Gradient:

$$\nabla f = \left(3x^2 + 6x,\ 3y^2 + 12y\right) = (3x(x+2),\ 3y(y+4))$$

Critical points:

$$x = 0 \text{ or } x = -2, \quad y = 0 \text{ or } y = -4.$$

Thus four critical points: $(0,0)$, $(0,-4)$, $(-2,0)$, $(-2,-4)$.

Hessian:

$$H_f = \begin{pmatrix} 6x+6 & 0 \\ 0 & 6y+12 \end{pmatrix}$$

Evaluate:

- At $(0,0)$: $H = \begin{pmatrix} 6 & 0 \\ 0 & 12 \end{pmatrix}$ (positive definite) $\Rightarrow$ local minimum, $f = 4$.
- At $(0,-4)$: $H = \begin{pmatrix} 6 & 0 \\ 0 & -12 \end{pmatrix}$ (indefinite) $\Rightarrow$ saddle point.
- At $(-2,0)$: $H = \begin{pmatrix} -6 & 0 \\ 0 & 12 \end{pmatrix}$ (indefinite) $\Rightarrow$ saddle point.
- At $(-2,-4)$: $H = \begin{pmatrix} -6 & 0 \\ 0 & -12 \end{pmatrix}$ (negative definite) $\Rightarrow$ local maximum, $f(-2,-4) = -8-64+12+96+4 = 40$.

As $\|(x,y)\| \to \infty$, $f \to \pm\infty$ depending on direction. No global extrema.

Exercise 2:

A rectangle ABCD is inscribed in a semicircle of diameter 4. Find the rectangle of maximal area.

Solution:

Let the semicircle have radius 2, center at origin, equation $x^2 + y^2 = 4$, $y \geq 0$. Let the rectangle have width $2x$ and height y, with (x,y) on the circle, $x > 0$. Area:

$$A = 2x \cdot y = 2x\sqrt{4-x^2}, \quad 0 \leq x \leq 2.$$

Maximize $A(x)$. Let $g(x) = x^2(4-x^2) = 4x^2 - x^4$. Derivative:

$$g'(x) = 8x - 4x^3 = 4x(2-x^2) = 0 \Rightarrow x = 0 \text{ or } x = \sqrt{2}.$$

$x = \sqrt{2}$ gives maximum: $y = \sqrt{4-2} = \sqrt{2}$. Area $A_{\max} = 2\sqrt{2} \cdot \sqrt{2} = 4$. Dimensions: width $2\sqrt{2}$, height $\sqrt{2}$.

Exercise 3:

1. Newton's method for $\min f(x) = \frac{1}{2}x^2 - \cos x - x$:

$$f'(x) = x + \sin x - 1, \quad f''(x) = 1 + \cos x \geq 0.$$

   Newton iteration:

$$x_{n+1} = x_n - \frac{x_n + \sin x_n - 1}{1 + \cos x_n}.$$

   Choose initial guess, e.g., $x_0 = 0$. Iterate until convergence.

2. Minimization $f(x,y) = x^2 + y^2 + 4x - 4y$:

   (a) Show f has a unique global minimum.

   Rewrite: $f(x,y) = (x+2)^2 + (y-2)^2 - 8$. This is a convex quadratic (Hessian positive definite). Hence it has a unique global minimum at $(-2,2)$, value -8.

   (b) Solve with $\epsilon = 0.01$:

      i. Gradient with constant step.

      $\nabla f = (2x+4,\ 2y-4)$. Choose step $\rho = 0.1$. Iteration:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} x_n \\ y_n \end{pmatrix} - 0.1 \begin{pmatrix} 2x_n + 4 \\ 2y_n - 4 \end{pmatrix}.$$

      Start from $(0,0)$, iterate until $\|\nabla f\| < 0.01$.

      ii. Relaxation with Newton subprogram.

      Coordinate descent: fix y, minimize over x: $x = -2$. Fix x, minimize over y: $y = 2$. Convergence in one cycle.

6.6 Exam 5

Exercise 1:

1. $f(x,y) = x^2 + y^2 + 4x - 6y$

   (a) Show unique global minimum.

   Rewrite: $f(x,y) = (x+2)^2 + (y-3)^2 - 13$. Convex, minimum at $(-2,3)$, value -13.

   (b) Gradient method with $\epsilon = 0.01$.

   $\nabla f = (2x+4,\ 2y-6)$. Step $\rho = 0.1$. Iterate from $(0,0)$:

$$x_{n+1} = x_n - 0.1(2x_n + 4), \quad y_{n+1} = y_n - 0.1(2y_n - 6).$$

   Stop when $\|\nabla f\| < 0.01$.

2. $g(x,y) = -x^2 - \frac{1}{2}y^2 - e^{-y}$ (corrected from given text).

   (a) Show unique global maximum.

   Hessian: $H_g = \begin{pmatrix} -2 & 0 \\ 0 & -1+e^{-y} \end{pmatrix}$. Since $-2 < 0$ and $-1+e^{-y} < 0$ for all y, H_g is negative definite $\Rightarrow$ strictly concave, so unique global maximum.

   (b) Newton's method for maximum.

   $\nabla g = (-2x,\ -y + e^{-y})$. Hessian as above. Newton iteration:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} x_n \\ y_n \end{pmatrix} - H_g^{-1} \nabla g.$$

   Start from $(0,0)$, iterate until convergence.

Exercise 2:

1. $\min_{x \geq 0} f(x) = \sin x - (x-1)e^x$.

   Derivative: $f'(x) = \cos x - e^x - (x-1)e^x = \cos x - xe^x$. Solve $f'(x) = 0$ numerically. Second derivative: $f''(x) = -\sin x - e^x - xe^x < 0$ for $x \geq 0 \Rightarrow$ concave, maximum at critical point.

2. Find root of 2:

   (a) Newton's method: $x_{n+1} = x_n - \frac{x_n^2 - 2}{2x_n}$, starting from $x_0 = 1$.

   (b) Fixed point: $x = \frac{1}{2}\left(x + \frac{2}{x}\right)$, iterate $x_{n+1} = \frac{1}{2}\left(x_n + \frac{2}{x_n}\right)$.

Exercise 3:

Two corridors of widths 1 m and 2 m meet at a right angle. Find the minimal length L of a bar that can be carried horizontally around the corner.

Solution:

Let the bar touch the outer walls at points such that it forms a line segment from $(a,0)$ to $(0,b)$ with $a \geq 2$, $b \geq 1$. The line equation:

$$\frac{x}{a}+\frac{y}{b}=1.$$

The bar length is $L=\sqrt{a^2+b^2}$. The line must pass through the inner corner $(2,1)$:

$$\frac{2}{a}+\frac{1}{b}=1.$$

Express $b=\frac{a}{a-2}$. Then

$$L(a)=\sqrt{a^2+\left(\frac{a}{a-2}\right)^2}, \quad a>2.$$

Minimize $L(a)$ (or L^2). Derivative:

$$\frac{d}{da}\left(a^2+\frac{a^2}{(a-2)^2}\right)=2a+\frac{2a(a-2)^2-2a^2(a-2)}{(a-2)^4}=0.$$

Simplify to find $a=2+2^{2/3}$, $b=1+2^{2/3}$. Then

$$L_{\min}=\left((2^{2/3}+2)^2+(2^{2/3}+1)^2\right)^{1/2}\approx 4.16 \text{ m}.$$

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