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Non-linear Programming Problems

1.1 Basic Terminology and Notations

Definition 1.1.1 ▸ General Non-linear Programming (NLP) Problems

Define the function $f : \mathbf{R}^n \to \mathbf{R}$. Let $\boldsymbol{x} \in \mathbf{R}^n$ be a vector, then a general NLP problem aims to **optimise** (i.e. maximise or minimise) $f(\boldsymbol{x})$ subject to the constraint $\boldsymbol{x} \in S \subseteq \mathbf{R}^n$, where

- f is known as the **objective function**;
- S is known as the **feasible set**;
- A solution (point) $\boldsymbol{x} \in S$ is known as a **feasible solution (point)**. Otherwise, it is known as an **infeasible solution(point)**.

Remark. Note that to maximise $f(\mathrm{x})$ is equivalent to minimising $-f(\mathrm{x})$, so it suffices to only study minimisation problems.

The word "optimal", however, can be ambiguous due to its qualitative nature. Thus, we shall define what it means to be optimal quantitatively with more rigorous terms.

Definition 1.1.2 ▸ Optimal Solution

Consider a minimisation problem subject to constraint $\boldsymbol{x} \in S \subseteq \boldsymbol{R}^n$ whose objective function is $f(\boldsymbol{x})$. A feasible solution $\boldsymbol{x}^*$ is called an **optimal solution** if $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in S$. We can write

$$\boldsymbol{x}^* = \operatorname*{argmin}_{x \in S} f(\boldsymbol{x}).$$

$f(\boldsymbol{x}^*)$ is then known as the **optimal value**.

Remark. For maximisation problems, we can write

$$\boldsymbol{x}^* = \operatorname*{argmax}_{x \in S} f(\boldsymbol{x})$$

Note that not all optimisation problems have an optimal solution. We shall still expect to encounter problems for which no optimal solution nor value exists.

Definition 1.1.3 ▸ Unboundedness

Consider a minimisation problem subject to constraint $\boldsymbol{x} \in S \subseteq \boldsymbol{R}^n$ whose objective function is $f(\boldsymbol{x})$. The objective value is said to be **unbounded** if for all $K \in \mathbf{R}$, there exists some $\boldsymbol{x} \in S$ such that $f(\boldsymbol{x}) < K$.

1.2 Unconstrained Non-linear Programs

To introduce the notion of an unconstrained NLP, we shall first define the openness of a set.

Definition 1.2.1 ▸ Open Set

Let $S \subseteq \boldsymbol{R}^n$ be a set. S is called **open** if for all $\boldsymbol{x} \in S$ there exists $\epsilon > 0$ such that the ball

$$B(\boldsymbol{x}, \epsilon) := \{\boldsymbol{y} \in \boldsymbol{R}^n : \ \|\boldsymbol{y} - \boldsymbol{x}\| < \epsilon\}$$

is a subset of S.

Definition 1.2.2 ▸ Unconstrained NLP

An **unconstrained** NLP is an NLP whose feasible set $\mathcal{X}$ is an **open** subset of $\mathbf{R}^n$.

1.3 Constrained Non-linear Programs

Similarly, to introduce the notion of a constrained NLP, we shall first define the closed-ness of a set.

Definition 1.3.1 ▸ Closed Set

Let $S \subseteq \boldsymbol{R}^n$ be a non-empty set. S is said to be **closed** if for all convergent sequences $\{\boldsymbol{x}_i\}_{i=1}^{\infty}$ with $\boldsymbol{x}_i \in S$ for $i = 1, 2, \cdots$, the limit $\lim_{i \to \infty} \boldsymbol{x}_i \in S$.

The empty set and Euclidean spaces $\mathbb{R}^n$ are both open and closed.

> *Remark.* Note that a set which is not open may not necessarily be closed. However, a set is open if and only if its complement is closed.

Theorem 1.3.2 ▶ Intersection of Closed Sets

If C_1 and C_2 are both closed, then $C_1 \cap C_2$ is closed.

Proof. The case where $C_1 \cap C_2 = \varnothing$ is trivial. If $C_1 \cap C_2 \neq \varnothing$, let $\{\boldsymbol{x}_i\}_{i=1}^{\infty}$ be an arbitrary convergent sequence in $C_1 \cap C_2$. Since $\{\boldsymbol{x}_i\}_{i=1}^{\infty} \in C_1$ which is closed, we have $\lim_{i\to\infty} \boldsymbol{x}_i \in C_1$. Similarly, $\lim_{i\to\infty} \boldsymbol{x}_i \in C_2$. Therefore, $\lim_{i\to\infty} \boldsymbol{x}_i \in C_1 \cap C_2$.

Therefore, $C_1 \cap C_2$ is closed. □

We then follow up by introducing three important closed sets.

Proposition 1.3.3

Let $g: \mathbb{R}^n \to \mathbb{R}$ be a continuous function, then the sets

$$\begin{aligned} S_1 &= \{\boldsymbol{x} \in \mathbb{R}^n : g(\boldsymbol{x}) \leq 0\}, \\ S_2 &= \{\boldsymbol{x} \in \mathbb{R}^n : g(\boldsymbol{x}) \geq 0\}, \\ S_3 &= \{\boldsymbol{x} \in \mathbb{R}^n : g(\boldsymbol{x}) = 0\} \end{aligned}$$

are closed.

Proof. Consider S_1. Let $\{\boldsymbol{x}_i\}_{i=1}^{\infty}$ be any convergent sequence with $\boldsymbol{x}_i \in S_1$ for $i = 1, 2, \cdots$, then

$$g\left(\lim_{i\to\infty} \boldsymbol{x}_i\right) \leq 0$$

since $\boldsymbol{x}_i \leq 0$. Therefore, $\lim_{i\to\infty} \boldsymbol{x}_i \in S_1$ and so S_1 is closed.
S_2 and S_3 can be proved similarly. □

By Theorem 1.3.2, we know that $S_1 \cup S_2 \cup S_3$ is closed, which motivates the following definition:

Definition 1.3.4 ▶ Constrained NLP

A **constrained** NLP is an NLP whose feasible set

$$S := \left\{\boldsymbol{x} \in \mathbb{R}^n : g_i(\boldsymbol{x}) = 0, i = 1, 2, \cdots, p, h_j(\boldsymbol{x}) \leq 0, j = 1, 2, \cdots, q\right\}$$

is **closed**, where each of the g_i's is known as an equality constraint and each of the h_j's is known as an inequality constraint.

If the feasible set of a constraind NLP is *bounded*, then it will be easy to find an optimal solution.

Definition 1.3.5 ▸ Boundedness

Let $S \subseteq \mathbf{R}^n$. S is said to be **bounded** if there exists some $M \in \mathbb{R}^+$ such that $\|\boldsymbol{x}\| \leq M$ for all $\boldsymbol{x} \in S$.

Note that a closed set may not be bounded and a bounded set may not be closed, so we are motivated to define a *closed and bounded set* rigorously.

Definition 1.3.6 ▸ Compact Set

A set $S \subseteq \mathbf{R}^n$ is **compact** if it is closed and bounded.

It turns out that, on a compact feasible set, the existence of global minimiser is guaranteed!

Theorem 1.3.7 ▸ Weiestrass Theorem

Let f be a continuous function on some non-empty $S \subseteq \mathbf{R}^n$. If S is compact, then f has a global minimiser and a global maximiser.

2 Convex Functions

2.1 Convexity of Sets and Functions

Intuitively, we describe two types of shapes in natural languages: the shapes which, if you choose any of its edges, lies in the same side of that edge, and the shapes which span across both sides from some chosen edge of its.

Graphically, this means that some shapes are "convex" to all directions, where as some other shapes are "concave". We shall define this rigorously as follows:

Definition 2.1.1 ▶ Convex Set

A set $D \subseteq \mathbf{R}^n$ is said to be **convex** if for all $\boldsymbol{x}, \boldsymbol{y} \in D$ and for all $\lambda \in [0, 1]$,

$$\lambda \boldsymbol{x} + (1 - \lambda)\boldsymbol{y} \in D.$$

We can define convexity over functions as follows:

Definition 2.1.2 ▶ Convex Function

A function $f : D \to \mathbf{R}^n$ is said to be **convex** if for all $\boldsymbol{x}, \boldsymbol{y} \in D$ and for all $\lambda \in [0, 1]$,

$$f(\lambda \boldsymbol{x} + (1 - \lambda)\boldsymbol{y}) \leq \lambda f(\boldsymbol{x}) + (1 - \lambda) f(\boldsymbol{y}).$$

Definition 2.1.3 ▶ Concave Function

A function $f : D \to \mathbf{R}^n$ is said to be **concave** if for all $\boldsymbol{x}, \boldsymbol{y} \in D$ and for all $\lambda \in [0, 1]$,

$$f(\lambda \boldsymbol{x} + (1 - \lambda)\boldsymbol{y}) \geq \lambda f(\boldsymbol{x}) + (1 - \lambda) f(\boldsymbol{y}).$$

Remark. A function which is not convex must be concave. However, a function which is convex may not be non-concave (consider $f(x) = x$).

We may derive the following relationship between a convex set and a convex function:

Proposition 2.1.4 ▸ Relations between Convex Sets and Convex Functions

Let $D \subseteq \mathbf{R}^n$ be a convex set and let $f : D \to \mathbf{R}$ be a convex function, then for all $\alpha \in \mathbf{R}$, the set

$$S_\alpha \coloneqq \{\boldsymbol{x} \in D : f(\boldsymbol{x}) \leq \alpha\}$$

is convex.

Proof. Take $\boldsymbol{x}, \boldsymbol{y} \in S_\alpha$, then $f(\boldsymbol{x}) \leq \alpha$ and $f(\boldsymbol{y}) \leq \alpha$. Note that for any $\lambda \in [0, 1]$, we have

$$\begin{aligned} f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) &\leq \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y}) \\ &\leq \lambda\alpha + (1-\lambda)\alpha \\ &= \alpha. \end{aligned}$$

Therefore, $\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y} \in S_\alpha$, and so S_α is convex. □

Next, we introduce the notion of an *epigraph*.

Definition 2.1.5 ▸ Epigraph

Let $f : D \to \mathbf{R}$ be a function over a convex set $D \subseteq \mathbf{R}^n$. The **epigraph** of f is the set $E_f \subseteq \mathbf{R}^{n+1}$ defined by

$$E_f \coloneqq \{(\boldsymbol{x}, \alpha) : \boldsymbol{x} \in D, \alpha \in \mathbf{R}, f(\boldsymbol{x}) \leq \alpha\}.$$

Remark. A trivial result: $D \times \operatorname{range}(f) \subseteq E_f$.

Note that graphically, the epigraph of a function is just the region above the graph of the function.

Proposition 2.1.6 ▸ Convexity of Epigraph

Let $f : D \to \mathbf{R}$ be a function over a convex set $D \subseteq \mathbf{R}^n$. The epigraph E_f is convex if and only if f is convex.

Proof. Suppose E_f is convex. Take any $\boldsymbol{x}, \boldsymbol{y} \in D$, then $(\boldsymbol{x}, f(\boldsymbol{x})), (\boldsymbol{y}, f(\boldsymbol{y})) \in E_f$. Let $\lambda \in [0, 1]$, we have

$$\lambda(\boldsymbol{x}, f(\boldsymbol{x})) + (1-\lambda)(\boldsymbol{y}, f(\boldsymbol{y})) = (\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}, \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y})) \in E_f.$$

Therefore,

$$f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) \le \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y}),$$

and so f is convex.

Suppose conversely that f is convex. For any $\boldsymbol{x}, \boldsymbol{y} \in D$ and any $\alpha, \beta \in \mathbf{R}$ such that $f(\boldsymbol{x}) \le \alpha$ and $f(\boldsymbol{y}) \le \beta$, we have $(\boldsymbol{x}, \alpha), (\boldsymbol{y}, \beta) \in E_f$. For all $\lambda \in [0,1]$, consider

$$\lambda(\boldsymbol{x}, \alpha) + (1-\lambda)(\boldsymbol{y}, \beta) = (\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}, \lambda\alpha + (1-\lambda)\beta).$$

Since f is convex, we have

$$\begin{aligned} f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) &\le \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y}) \\ &\le \lambda\alpha + (1-\lambda)\beta \end{aligned}$$

for all $\lambda \in [0,1]$. Therefore, $(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}, \lambda\alpha + (1-\lambda)\beta) \in E_f$, and so E_f is convex. □

Lastly, we generalise the notion of a *convex combination*.

Proposition 2.1.7 ▸ Generalised Convex Combination

Let $k \in \mathbb{N}^+$ and let $f : S \to \mathbf{R}$ be a convex function on the convex set $S \subseteq \mathbf{R}^n$ and let $\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_k \in S$, then

$$f\left(\sum_{i=1}^{k} \lambda_i \boldsymbol{x}_i\right) \le \sum_{i=1}^{k} \lambda_i f(\boldsymbol{x}_i),$$

where $\sum_{i=1}^{k} \lambda_i = 1$ and $\lambda_i \ge 0$ for $i = 1, 2, \cdots, k$.

Proof. The case where $k = 1$ is trivial.

Suppose that there exists some $n \in \mathbb{N}^+$ such that

$$f\left(\sum_{i=1}^{n} \lambda_i \boldsymbol{x}_i\right) \le \sum_{i=1}^{n} \lambda_i f(\boldsymbol{x}_i),$$

□

2.2 Tangent Plane Characterisation

Recall that for a function $f : \mathbf{R}^n \to \mathbf{R}$, the *gradient vector* of f at $\mathbf{x}$ is given by

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(\boldsymbol{x}) \\ \frac{\partial}{\partial x_2} f(\boldsymbol{x}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(\boldsymbol{x}) \end{bmatrix}.$$

Proposition 2.2.1 ▸ Directional Derivative

Let f be a function over $D \subseteq \mathbf{R}^n$ and let $\boldsymbol{d} \in \mathbf{R}^n$ be non-zero, then the directional derivative of f at $\boldsymbol{x}$ along $\boldsymbol{d}$ is

$$\nabla f(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{d} = \lim_{\lambda \to 0} \frac{f(\boldsymbol{x} + \lambda \boldsymbol{d}) - f(\boldsymbol{x})}{\lambda}.$$

In particular, if $\|\mathbf{d}\| = 1$, then the above gives the rate of change of f in the direction of $\boldsymbol{d}$.

Remark. f increases the fastest along the direction of $\nabla f(\boldsymbol{x})$ and decreases the fastest along the direction of $-\nabla f(\boldsymbol{x})$ for any $\boldsymbol{x} \in \mathbf{R}^n$.

The gradient vector of a function allows us to establish its tangent plane at a given point. Intuitively, we can see that a function is convex if its tangent plane lies below its graph. This can be described rigorously as follows:

Proposition 2.2.2 ▸ Tangent Plane Characterisation of Convex Functions

Let f be a function over an open convex set $S \subseteq \mathbf{R}^n$ with continuous first partial derivatives, then f is convex if and only if

$$f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{x}) \leq f(\boldsymbol{y})$$

for all $\boldsymbol{x}, \boldsymbol{y} \in S$. In particular, f is strictly convex if and only if the above inequality is strict.

Proof. Suppose that f is convex. Let $\boldsymbol{x}, \boldsymbol{y} \in S$ and let $\lambda \in [0, 1]$, then we have

$$f(\boldsymbol{x} + \lambda(\boldsymbol{y} - \boldsymbol{x})) = f(\lambda \boldsymbol{y} + (1 - \lambda)\boldsymbol{x}) \leq \lambda f(\boldsymbol{y}) + (1 - \lambda) f(\boldsymbol{x}).$$

Therefore,
$$\frac{f\left(\boldsymbol{x}+\lambda(\boldsymbol{y}-\boldsymbol{x})\right)-f(\boldsymbol{x})}{\lambda} \leq f(\boldsymbol{y})-f(\boldsymbol{x}).$$
Taking the limit as $\lambda \to 0$ on both sides, we have
$$\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y}-\boldsymbol{x}) = \lim_{\lambda\to 0}\frac{f\left(\boldsymbol{x}+\lambda(\boldsymbol{y}-\boldsymbol{x})\right)-f(\boldsymbol{x})}{\lambda} \leq f(\boldsymbol{y})-f(\boldsymbol{x}),$$
and so
$$f(\boldsymbol{x})+\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y}-\boldsymbol{x}) \leq f(\boldsymbol{y}).$$
Suppose conversely that
$$f(\boldsymbol{x})+\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y}-\boldsymbol{x}) \leq f(\boldsymbol{y}).$$
Take $\boldsymbol{u},\boldsymbol{v}\in S$ and let $\boldsymbol{w}=\lambda\boldsymbol{u}+(1-\lambda)\boldsymbol{v}$ for some $\lambda\in[0,1]$, then
$$\boldsymbol{u}-\boldsymbol{w}=(1-\lambda)(\boldsymbol{u}-\boldsymbol{v}), \qquad \boldsymbol{v}-\boldsymbol{w}=-\lambda(\boldsymbol{u}-\boldsymbol{v}).$$
Therefore, we have
$$\begin{aligned} f(\boldsymbol{w})+\nabla f(\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{u}-\boldsymbol{w}) &\leq f(\boldsymbol{u}),\\ f(\boldsymbol{w})+\nabla f(\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{v}-\boldsymbol{w}) &\leq f(\boldsymbol{v}).\end{aligned}$$
Note that
$$\lambda\left(f(\boldsymbol{w})+\nabla f(\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{u}-\boldsymbol{w})\right)+(1-\lambda)\left(f(\boldsymbol{w})+\nabla f(\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{v}-\boldsymbol{w})\right)=f(\boldsymbol{w}),$$
so we have
$$\begin{aligned} f(\lambda\boldsymbol{u}+(1-\lambda)\boldsymbol{v}) &= f(\boldsymbol{w})\\ &\leq \lambda f(\boldsymbol{u})+(1-\lambda)f(\boldsymbol{v}).\end{aligned}$$
Hence, f is convex.

We can similarly prove that f is strictly convex if $f(\boldsymbol{x})+\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y}-\boldsymbol{x}) < f(\boldsymbol{y})$. Now suppose that f is strictly convex but there exists $\boldsymbol{x},\boldsymbol{y}\in S$ with $\boldsymbol{x}\neq\boldsymbol{y}$ such that
$$f(\boldsymbol{x})+\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y}-\boldsymbol{x}) \geq f(\boldsymbol{y}).$$

Take $\boldsymbol{z} = \frac{1}{2}\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}$. We have

$$\begin{aligned}
\frac{1}{2}f(\boldsymbol{x}) + \frac{1}{2}f(\boldsymbol{y}) > f(\boldsymbol{z}) \\
&\geq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{z} - \boldsymbol{x}) \\
&= f(\boldsymbol{x}) + \frac{1}{2}\nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{x}) \\
&\geq f(\boldsymbol{x}) + \frac{1}{2}(f(\boldsymbol{y}) - f(\boldsymbol{x})) \\
&= \frac{1}{2}f(\boldsymbol{x}) + \frac{1}{2}f(\boldsymbol{y}),
\end{aligned}$$

which is a contradiction. □

Proposition 2.2.2 helps us determine whether a point is the global minimiser of a certain convex function.

Theorem 2.2.3 ▸ Global Minimiser of Convex Functions

Let $f : C \to \mathbf{R}$ be a convex and continuously differentiable function over a convex set $C \subseteq \mathbf{R}^n$. Then $\boldsymbol{x}^* \in C$ is a global minimiser for the minimisation problem

$$\min\{f(\boldsymbol{x}) : \boldsymbol{x} \in C\}$$

if and only if

$$\nabla f(\boldsymbol{x}^*)^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}^*) \geq 0$$

for all $\boldsymbol{x} \in C$.

Proof. Suppose $\nabla f(\boldsymbol{x}^*)^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}^*) \geq 0$. By Proposition 2.2.2, we have

$$\nabla f(\boldsymbol{x}^*)^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}^*) \leq f(\boldsymbol{x}) - f(\boldsymbol{x}^*).$$

This means that $f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$ for all $\boldsymbol{x} \in C$, and so $\boldsymbol{x}^*$ is a global minimiser.

Suppose that $\boldsymbol{x}^*$ is a global minimiser for f but there exists some $\boldsymbol{x}_0 \in C$ such that

$$\nabla f(\boldsymbol{x}^*)^{\mathrm{T}}(\boldsymbol{x}_0 - \boldsymbol{x}^*) < 0.$$

Consider $\boldsymbol{y} = \lambda\boldsymbol{x}_0 + (1-\lambda)\boldsymbol{x}^*$ for $\lambda \in (0,1)$. Notice that $f(\boldsymbol{y}) \geq f(\boldsymbol{x}^*)$, so by using

Proposition 2.2.2 we have

$$\begin{aligned} 0 &\leq f(\boldsymbol{y}) - f(\boldsymbol{x}^*) \\ &\leq -\nabla f(\boldsymbol{y})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{x}^*) \\ &\leq \nabla f(\boldsymbol{y})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{x}^*) \\ &= \lambda \nabla f\left(\lambda \boldsymbol{x}_0 + (1-\lambda)\boldsymbol{x}^*\right)^{\mathrm{T}} (\boldsymbol{x}_0 - \boldsymbol{x}^*) \\ &\leq \nabla f\left(\lambda \boldsymbol{x}_0 + (1-\lambda)\boldsymbol{x}^*\right)^{\mathrm{T}} (\boldsymbol{x}_0 - \boldsymbol{x}^*). \end{aligned}$$

Therefore,

$$\begin{aligned} \lim_{\lambda \to 0^+} \left[\nabla f\left(\lambda \boldsymbol{x}_0 + (1-\lambda)\boldsymbol{x}^*\right)^{\mathrm{T}} (\boldsymbol{x}_0 - \boldsymbol{x}^*)\right] &= \nabla f(\boldsymbol{x}^*)^{\mathrm{T}}(\boldsymbol{x}_0 - \boldsymbol{x}^*) \\ &\geq 0, \end{aligned}$$

which is a contradiction. □

2.3 Hessian Matrices

So far we have learnt how to determine a function's convexity by either Definition 2.1.2 or Proposition 2.2.2. However, there are certain functions which are difficult to manipulate and apply those methods algebraically. Therefore, we introduce another method to determine convexity by *Hessian Matrices*.

Definition 2.3.1 ▸ Hessian Matrix

Let $f : S \to \mathbf{R}$ where $S \subseteq \mathbf{R}^n$ is non-empty and let $\boldsymbol{x}$ be an **interior point** of S. The **Hessian** of f at $\boldsymbol{x}$ is the $n \times n$ matrix

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

Remark. If f has continuous second order derivatives, then $H_f(\boldsymbol{x})$ is symmetric.

To use Hessian Matrices in convexity test, we also need to introduce the following notion of *(semi)definiteness*:

Definition 2.3.2 ▶ (Semi)Definiteness

et $\boldsymbol{A}$ be a real square matrix.

- $\boldsymbol{A}$ is said to be **positive semidefinite** if $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} \geq 0$ for all $\boldsymbol{x} \in \boldsymbol{R}$.
- $\boldsymbol{A}$ is said to be **positive definite** if $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} > 0$ for all $\boldsymbol{x} \in \boldsymbol{R}$.
- $\boldsymbol{A}$ is said to be **negative semidefinite** if $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} \leq 0$ for all $\boldsymbol{x} \in \boldsymbol{R}$.
- $\boldsymbol{A}$ is said to be **negative definite** if $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} < 0$ for all $\boldsymbol{x} \in \boldsymbol{R}$.
- $\boldsymbol{A}$ is said to be **indefinite** if it is neither positive semidefinite nor negative semidefinite.

To determine the definiteness of a matrix, we may use the following eigenvalue tests:

Theorem 2.3.3 ▶ Eigenvalue Test

If $\boldsymbol{A}$ is a symmetric real square matrix, then:

- *$\boldsymbol{A}$ is positive semidefinite if and only if all eigenvalues of $\boldsymbol{A}$ are non-negative.*
- *$\boldsymbol{A}$ is positive definite if and only if all eigenvalues of $\boldsymbol{A}$ are positive.*
- *$\boldsymbol{A}$ is negative semiefinite if and only if all eigenvalues of $\boldsymbol{A}$ are non-positive.*
- *$\boldsymbol{A}$ is negative definite if and only if all eigenvalues of $\boldsymbol{A}$ are negative.*
- *$\boldsymbol{A}$ is indefinite if and only if it has at least one positive eigenvalue and at least one negative eigenvalue.*

Proof. We will only prove that $\boldsymbol{A}$ is positive semidefinite if and only if all eigenvalues of $\boldsymbol{A}$ are non-negative. The rest of the tests can be proven similarly.

Suppose $\boldsymbol{A}$ is positive semidefinite. Let λ be any eigenvalue of $\boldsymbol{A}$ and let $\boldsymbol{x}$ be a corresponding eigenvector, then $\boldsymbol{A}\boldsymbol{x} = \lambda\boldsymbol{x}$. Therefore,

$$\lambda\|\boldsymbol{x}\|^2 = \lambda\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} \geq 0.$$

Since $\|\boldsymbol{x}\|^2 \geq 0$, this implies that $\lambda \geq 0$.

Suppose conversely that all eigenvalues of $\boldsymbol{A}$ are non-negative. Consider the diagonal matrix

$$\boldsymbol{D} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

where λ_i is the i-th eigenvalue of $\boldsymbol{A}$. Then there exists some orthogonal square matrix

$\boldsymbol{Q}$ such that

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^{\mathrm{T}}.$$

Let $\boldsymbol{x} \in \mathbf{R}^n$ be an arbitrary vector, then

$$\begin{aligned}\boldsymbol{x}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x} &= \boldsymbol{x}^{\mathrm{T}}\boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{x} \\ &= \left(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{x}\right)^{\mathrm{T}}\boldsymbol{D}\left(\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{x}\right) \\ &= \sum_{i=1}^{n}\left(\lambda_i\left\|\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{x}\right\|^2\right) \\ &\geq 0.\end{aligned}$$

Therefore, $\boldsymbol{A}$ is positive semidefinite. □

However, eigenvalues can be troublesome to compute. Thus for **small matrices**, we may use the following test with the *principal minors*:

Definition 2.3.4 ▶ Principal Minor

Let $\boldsymbol{A}$ be an $n \times n$ matrix. The k-th **principal minor** Δ_k of $\boldsymbol{A}$ is defined to be the determinant of the kth principal submatrix of $\boldsymbol{A}$, i.e.,

$$\Delta_k = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{vmatrix}$$

Theorem 2.3.5 ▶ Definiteness Test Using Principal Minors

Let $\boldsymbol{A}$ be a symmetric $n \times n$ matrix, then $\boldsymbol{A}$ is positive definite if and only if $\Delta_k > 0$, and negative definite if and only if $(-1)^k\Delta_k > 0$, for all $k = 1, 2, \cdots, n$.

2.3.1 Taylor's Theorem

Note that we have not given the proof to Theorem 2.3.7. Now to prove it, we need to first introduce *Taylor's Theorem*.

Theorem 2.3.6 ▸ Taylor's Theorem

Suppose that $f : S \to \mathbf{R}$ *is a function with continuous second partial derivatives. Consider the set*

$$[\boldsymbol{x}, \boldsymbol{y}] := \{\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y} : \boldsymbol{x}, \boldsymbol{y} \in \mathbf{R}^n, \lambda \in [0,1]\}.$$

If $[\boldsymbol{x}, \boldsymbol{y}]$ *is contained in the interior of* S*, then there exists some* $\boldsymbol{z} \in [\boldsymbol{x}, \boldsymbol{y}]$ *such that*

$$f(\boldsymbol{y}) = f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{x}) + \frac{1}{2}(\boldsymbol{y} - \boldsymbol{x})^{\mathrm{T}} H_f(\boldsymbol{z})(\boldsymbol{y} - \boldsymbol{x}).$$

Now, we are able to apply the following tests:

Theorem 2.3.7 ▸ Convexity Test for Differentiable Functions

Let a function f *have continuous second order derivatives on an open convex set* $D \subseteq \mathbf{R}^n$.

- $H_f(\boldsymbol{x})$ *is positive semidefinite for all* $\boldsymbol{x} \in D \iff f$ *is convex on* D.
- $H_f(\boldsymbol{x})$ *is positive definite for all* $\boldsymbol{x} \in D \implies f$ *is strictly convex on* D.
- $H_f(\boldsymbol{x})$ *is negative semidefinite for all* $\boldsymbol{x} \in D \iff f$ *is concave on* D.
- $H_f(\boldsymbol{x})$ *is negative definite for all* $\boldsymbol{x} \in D \implies f$ *is strictly concave on* D.
- $H_f(\boldsymbol{x})$ *is indefinite for some* $\boldsymbol{x} \in D \implies f$ *is neither convex nor concave on* D.

3

Unconstrained NLPs

3.1 Coercive Functions

Definition 3.1.1 ▸ Coercive Function

A **continuous** function $f : \mathbf{R}^n \to \mathbf{R}$ is said to be **coercive** if

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

More formally, f is coercive if and only if for all $M > 0$, there is some $r > 0$ such that $f(\boldsymbol{x}) > M$ whenever $\|\boldsymbol{x}\| > r$.

Theorem 3.1.2 ▸ Global Minimiser of Coercive Functions

If a function $f : \mathbf{R}^n \to \mathbf{R}$ is coercive, then f has at least one global minimiser.

Proof. Take $M = |f(0)| + 1 > 0$. Since f is coercive, there exists some $r > 0$ such that $f(\boldsymbol{x}) > M > f(0)$ whenever $\|\boldsymbol{x}\| > r$. Consider

$$B(0, r) = \{\boldsymbol{x} \in \mathbf{R}^n : \|\boldsymbol{x}\| \le r\}$$

which is a compact set. So by Weiestrass' Theorem, there exists some $\boldsymbol{x}^* \in B(0, r)$ such that $f(\boldsymbol{x}^*) \le f(\boldsymbol{x}) \le f(0)$ for all $\boldsymbol{x} \in B(0, r)$. Now, this means that for all $\boldsymbol{x} \in \mathbf{R}^n$, we have $(\boldsymbol{x}^*) \le f(\boldsymbol{x})$, which means that $\boldsymbol{x}^*$ is a global minimiser for f. □

Definition 3.1.3 ▸ Stationary (Critical) Point

Let $X \subseteq \mathbf{R}^n$ be an open set and let $f : X \to \mathbf{R}$ be a function. An interior point $\boldsymbol{x}^*$ is called a **stationary point** of f if $\nabla f(\boldsymbol{x}^*) = 0$.

Definition 3.1.4 ▸ Saddle Point

A stationary point $\boldsymbol{x}^*$ of a function f which is neither a local minimisr nor a local maximiser is called a **saddle point**.

Corollary 3.1.5

Let $\boldsymbol{x}^*$ be a stationary point of f. If $H_f(\boldsymbol{x}^*)$ is indefinite, then $\boldsymbol{x}^*$ is a saddle point.

4

Numerical Methods

4.1 Bisection

Recall the *Intermediate Value Theorem*:

Theorem 4.1.1 ▶ Intermediate Value Theorem

Let f be a continuous function on $[a, b]$ with $f(a)f(b) < 0$, then there exists some $r \in (a, b)$ such that $f(r) = 0$.

Code Snippet 4.1.2 ▶ Sample Code in Python

```
def bisection(f: Callable[[float], float],\
    a: float, b: float, t: float, x: float) -> float:
    while (Math.abs(a - b) > t):
        if (f(a) * f(x) < 0):
            b = x;
            x = (b - a) / 2;
    return x;
```

4.2 Newton's Method

4.2.1 Multivariable Case

Let f be a multivariable function with continuous second order partial derivatives. Given $\boldsymbol{x}_0 \in \mathbf{R}^n$, by Taylor expansion there is some quadratic function q such that

$$f(\boldsymbol{x}) \approx q(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^{\mathrm{T}}(\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^{\mathrm{T}} H_f(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0).$$

Assumptions:

- The Hessian $H_f(\boldsymbol{x}^*)$ at the stationary point $\boldsymbol{x}^*$ is non-singular.
- $H_f(\boldsymbol{x})$ is Lipschitz continuous in a neighbourhood of $\boldsymbol{x}^8$.

Proposition 4.2.1 ▶ Convergence of the Newton Method

If $\boldsymbol{x}_0$ is sufficiently close to $\boldsymbol{x}^*$, then the sequence $\{\boldsymbol{x}_k\}$ generated by the Newton Method converges to $\boldsymbol{x}^*$ quadratically, i.e., there exists some $M \in \mathbb{R}$ such that

$$\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\| \leq M\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2.$$

4.2.2 Armijo Line Search

4.3 Goldern Section Method

Definition 4.3.1 ▶ Unimodal Function

A function f is said to be **unimodal** on $[a, b]$ if it has exactly one global minimiser (maximiser) x^* in $[a, b]$ and is strictly decreasing (increasing) on $[a, x^*]$ abd strictly increasing (decreasing) on $[x^*, b]$.

Technique 4.3.2 ▶ Golden Section Method

Let f be a unimodal function. Consider $[a_0, b_0]$ as the initial interval. For each iteration, we consider

$$\lambda_n = b_n - \Phi(b_n - a_n)$$
$$\mu_n = a_n + \Phi(b_n - a_n)$$

where $\Phi = \frac{\sqrt{5}-1}{2}$ is the Golden Ratio constant. Then we update the interval by:

$$[a_{n+1}, b_{n+1}] = \begin{cases} [\lambda_n, b_n], & \text{if } f(\lambda_n) > f(\mu_n) \\ [a_n, \mu_n], & \text{if } f(\lambda_n) < f(\mu_n) \\ [\lambda_n, \mu_n], & \text{if } f(\lambda_n) = f(\mu_n) \end{cases} .$$

The reason why we use Φ to generate the intervals recursively is because that it reduces the number of computations. Consider that $[a_k, b_k] = [\lambda_{k-1}, b_{k-1}]$, then

$$\begin{aligned}
\lambda_k &= b_k - \Phi(b_k - a_k) \\
&= b_{k-1} - \Phi(b_{k-1} - \lambda_{k-1}) \\
&= b_{k-1} - \Phi(b_{k-1} - b_{k-1} + \Phi(b_{k-1} - a_{k-1})) \\
&= b_{k-1} - \Phi^2(b_{k-1} - a_{k-1}) \\
&= b_{k-1} - (1 - \Phi)(b_{k-1} - a_{k-1}) \\
&= a_{k-1} + \Phi(b_{k-1} - a_{k-1}) \\
&= \mu_{k-1}.
\end{aligned}$$

However, note that we have already computed μ_{k-1} in the previous iteration! Therefore, by applying ideas of *dynamic programming*, this eliminates the need to recompute its value. Similarly, we can show that $\mu_k = \lambda_{k-1}$ if $f(\lambda_k) < f(\mu_k)$.

4.4 General Framework of Optimisation Algorithms

Pseudo-code

```
Initialise x with some guess;
while the interval > tolerance, do:
    x -> f(x);
return x;
```

4.5 Steepest Descent

Recall that f decreases most rapidly along the direction of $-\nabla f$. So we can take

$$\hat{\boldsymbol{d}} = -\frac{\nabla f(\boldsymbol{x})}{\|\nabla f(\boldsymbol{x})\|}$$

at any given point $\boldsymbol{x}$, where $-\nabla f(\boldsymbol{x})$ is known as the *steepest descent direction*. Notice that $f(\boldsymbol{x} + \delta\hat{\boldsymbol{d}}) = f(\boldsymbol{x}) - \delta\|\nabla f(\boldsymbol{x})\|$.

Technique 4.5.1 ▶ Steepest Descent Method

Let f be an objective function and $\boldsymbol{x}_0$ be an initial guess. Let $\epsilon > 0$ be the tolerance level.

At the k-th iteration, we evaluate the steepest descent direction

$$\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k).$$

If $\|\boldsymbol{d}_k\| < \epsilon$, $\boldsymbol{x}_k$ is an approximate minimiser. Otherwise, compute

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t_k \boldsymbol{d}_k,$$

where t_k is such that $f(\boldsymbol{x}_k + t_k \boldsymbol{d}_k)$ is minimised and is known as the step size.

With a graphical illustration, one might observe that the approximations obtained via the steepest descent method trace out a "zig-zag" path. This behaviour is rigorously described as follows:

Proposition 4.5.2

If $(\boldsymbol{x}_k)$ be a sequence of approximations for the function $f(\boldsymbol{x})$ using steepest descent method, then

$$(\boldsymbol{x}_{k+2} - \boldsymbol{x}_{k+1})^{\mathrm{T}}(\boldsymbol{x}_{k+1} - \boldsymbol{x}_k) = 0$$

for all $k \in \mathbb{N}$.

4.6 Conjugate Gradient Method

Definition 4.6.1 ▸ Conjugate Vectors

A set of vectors $\{\boldsymbol{p}_0, \boldsymbol{p}_1, \cdots, \boldsymbol{p}_n\}$ is **conjugate** with respect to $\boldsymbol{A}$, where $\boldsymbol{A} \succ 0$, if

$$\boldsymbol{p}_i^{\mathrm{T}} \boldsymbol{A} \boldsymbol{p}_j = 0 \qquad \text{for all } i \neq j.$$

5

Karush-Kuhn-Tucker Condition

Definition 5.0.1 ▸ Active Constraint

An inequality constraint $h_j(\boldsymbol{x}) \leq 0$ is said to be **active** at $\boldsymbol{x}^* \in S$ if $h_j(\boldsymbol{x}^*) = 0$. Otherwise, it is said to be **inactive** or **slack** at $\boldsymbol{x}^*$.

Note that for any equality constraint $g_i(\boldsymbol{x}) = 0$, any $\boldsymbol{x}^* \in S$ is always active.

Definition 5.0.2 ▸ Regular Point

Let $\boldsymbol{x}^* \in S$ and let

$$J(\boldsymbol{x}^*) = \left\{j \in \{1, \cdots, p\} \, : \, h_j(\boldsymbol{x}^*) = 0\right\}$$

be the index set of active ineqaulity constraints at $\boldsymbol{x}^*$. If the set of gradient vectors

$$\{\nabla g_i(\boldsymbol{x}^*)\} \cup \left\{\nabla h_j(\boldsymbol{x}^*) : \, j \in J(\boldsymbol{x}^*)\right\}$$

is linearly independent, then we say that $\boldsymbol{x}^*$ is a **regular point**.

Definition 5.0.3 ▸ KKT First Order Necessary Conditions

Let $\boldsymbol{x}^*$ be a regular point. $\boldsymbol{x}^*$ satisfies the **KKT first order necessary conditions** if there are scalars $\lambda_1, \cdots, \lambda_m$ and $\mu_1, \cdots, \mu_p$ such that

$$\nabla f(\boldsymbol{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\boldsymbol{x}^*) + \sum_{j=1}^{p} \mu_j \nabla h_j(\boldsymbol{x}^*) = \boldsymbol{0},$$

where $\mu_j \geq 0$ for all $j \in J(\boldsymbol{x}^*)$ and $\mu_j = 0$ for all $j \notin J(\boldsymbol{x}^*)$.

Note that the condition for the μ_j's is equivalent to $\mu_j h_j(\boldsymbol{x}^*) = 0$ for all $j \in \mathbb{N}^+$. The reasoning is as follows:

Suppose that h_j is inactive at $\boldsymbol{x}^*$, then we will have $\mu_j = 0$. Otherwise, h_j is active at $\boldsymbol{x}^*$, and so $h_j(\boldsymbol{x}^*) = 0$. Either way, $\mu_j h_j(\boldsymbol{x}^*) = 0$.