Mathematical Analysis 2

Course notes 2022/23

By

Everyone who contributed.

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Preface

This text accompanies the course "Mathematical Analysis 2" taught at the University of Rome Tor Vergata in the department of engineering for the academic year 2022/23. The course was led by Oliver Butterley, in collaboration with Giovanni Canestrari.

The aim of this document is to concisely describe the fundamental details related to the material of the course. They are aptly named as "notes" and are most likely not the comprehensive source of all relevant information. We have easy access to a huge volume of resources and so here we will make connections to whatever is useful, whenever we can.

These notes are merely written text whereas the central part of the course remains the time spent working with the material, be it doing exercises, discussing, doing calculations, etc. This is not text for memorising, this is text that aims to help us practice and become stronger thinkers.

This text is freely[1] available at **github.com/oliver-butterley/ma2**. Everyone is encouraged to contribute improvements to the document during the progress of the course.

Some of the text comes from previous years and from many other sources, some of the text came to be during the course. The current version is the product of many people, in particular everyone who has made suggestions in class and pointed out errors or imprecisions and to everyone who suggested useful additional content.

[1] Free both in the sense of "free speech" and "free beer".

Contents

Introduction

We start by looking at examples which demonstrate some of the motives behind studying analysis in general.

Example (Series)**.** The geometric series $S = 1 + \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \cdots$ can be summed by the following simple trick. Multiplying by 2 we obtain that

$$2S = 2 + 1 + \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \cdots = 2 + S$$

and so $S = 2$. If we try to do the same to the sum $T = 1 + 2 + 4 + 8 + 16 + \cdots$ we get the nonsensical answer

$$2T = 2 + 4 + 8 + 16 + \cdots = T - 1$$

and so $T = -1$. Why should we trust the argument in the first case and not in the second?

Example (Interchanging sums)**.** If we consider any matrix of numbers, for example,

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

we can sum first the rows $6 + 15 + 24 = 45$ or first the columns $12 + 15 + 18 = 45$ to obtain the total sum of all numbers. This is the rule

$$\sum_{j=1}^{m} \sum_{k=1}^{n} a_{jk} = \sum_{k=1}^{n} \sum_{j=1}^{m} a_{jk}.$$

We would like to believe that also $\sum_{j=1}^{\infty} \sum_{k=1}^{\infty} a_{jk} = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} a_{jk}$. However this doesn't work for the following matrix:

$$\begin{pmatrix} 1 & 0 & 0 & \cdots \\ -1 & 1 & 0 & \cdots \\ 0 & -1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

We often want to swap the order of summing (or integrating) and often need to consider infinite sums (or integrals). When can we do this and can't we?

Example (Interchanging integrals)**.** Let's try to integrate $e^{-xy} - xye^{-xy}$ with respect to both x and y. We would like to believe that

$$\int_0^\infty \left[\int_0^1 (e^{-xy} - xye^{-xy})\, dy \right] dx \stackrel{?}{=} \int_0^1 \left[\int_0^\infty (e^{-xy} - xye^{-xy})\, dx \right] dy.$$

Since $\int_0^1 (e^{-xy} - xye^{-xy})\, dy = [ye^{-xy}]_{y=0}^1 = e^{-x}$, the left-hand side is $\int_0^\infty e^{-x}\, dx = [-e^{-x}]_0^\infty = 1$. However, since $\int_0^\infty (e^{-xy} - xye^{-xy})\, dx = [xe^{-xy}]_{x=0}^\infty = 0$, the right-hand side is $\int_0^1 0\, dx = 0$. So how do we know when to trust the interchange of intervals?

Example (interchanging limits)**.** We could easily believe that

$$\lim_{x\to 0} \lim_{y\to 0} \frac{x^2}{x^2 + y^2} \stackrel{?}{=} \lim_{y\to 0} \lim_{x\to 0} \frac{x^2}{x^2 + y^2}.$$

However $\lim_{y\to 0} \frac{x^2}{x^2+y^2} = \frac{x^2}{x^2+0} = 1$ and so the left-hand side is 1 whereas $\lim_{x\to 0} \frac{x^2}{x^2+y^2} = \frac{0}{0+y^2} = 0$ so the right-hand side is 0. What does the graph of this function look like? This example shows that the interchange of limits is untrustworthy. Under what circumstances is it legitimate?

We need to be rigorous in our logic otherwise, as we have seen in these examples, the conclusions can be erroneous and the difficulties are often subtle.

Curves of constant width

The above examples are calculus based but it is worthwhile to consider a real world application of the rigour and reasoning we aspire to. Suppose we are organising the production facilities which manufacture a component that is round (maybe a rocket body, maybe a propellant tube, etc.). As part of the production it is important to have a procedure which guarantees that the fabrication is done to the correct tolerance. The idea proposed is:

> "We measure the width from all angles to confirm that the manufactured component is correct."

This is a two-dimensional problem in the sense we assume that the object is a closed

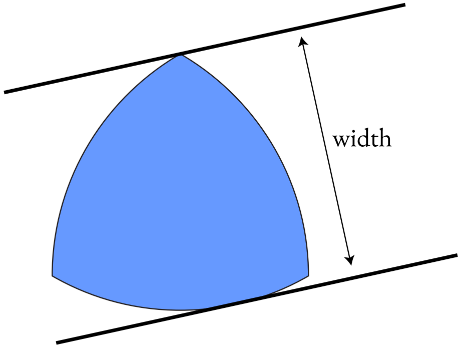


FIGURE 1: The Reuleaux triangle is a curve of constant width.

curve in $\mathbb{R}^2$. For a given angle we define the width of this curve to be the smallest distance between two parallel lines which touch the curve in a single point but never cross it (one each side of the curve). We say that the curve has constant width if this width is equal from every direction. This is just what we would check using calipers on a part and rotating. The following statement is intuitive and true.

Theorem. *A circle has constant width.*

However the converse is not true, indeed the following is true.

Theorem. *There exist constant width curves which are not circles.*

This can be proved by constructing many such curves, for example the Reuleaux triangle. Indeed there are such curves which look similar to regular polygons but still have constant width.

MA2 versus MA1

Much of what we do in this course builds on ideas established in Mathematical Analysis 1. In particular many of the ideas are extended to the higher dimensional setting. See Table 1.

Suggested further reading

- "Analysis 1" by Terence Tao. (Particularly §1.2 "Why Analysis?" and Appendix A "The basics of mathematical logic").

Mathematical Analysis 1	Mathematical Analysis 2
Sequences & series of numbers $a_1, a_2, a_3, \ldots$ $\sum_{n=0}^{\infty} a_n$	Sequences & series of functions $f_1(x), f_2(x), f_3(x), \ldots$ $\sum_{n=0}^{\infty} f_n(x)$
(Functions) $f : \mathbb{R} \to \mathbb{R}$	$f : \mathbb{R}^n \to \mathbb{R}$ (Scalar fields) $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ (Vector fields) $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$ (Paths)
(Derivative) $f'(x) = \frac{df}{dx}(x)$	$\frac{\partial f}{\partial x_j}(x_1, \ldots, x_n)$ (Partial derivatives) ∇f (Gradient) $D_v f$ (Directional derivative) $\boldsymbol{\alpha}'$ (Derivative of path) Df (Jacobian matrix) $\nabla \cdot \mathbf{f}$ (Divergence) $\nabla \times \mathbf{f}$ (Curl)
(Extrema) $\sup_{x\in\mathbb{R}} f(x)$	$\sup_{x\in\mathbb{R}^n} f(x)$ (Extrema) Lagrange multiplier method
Integral $\int_a^b f(x)\, dx$	Multiple integral Line integral Surface integral

Table 1: Ma2 versus MA1

Chapter 1

Sequences & series of functions

Analogously to sequences of numbers we can consider a sequence of functions $f_0(x)$, $f_1(x)$, $f_2(x)$, $f_3(x)$, etc. Often it is convenient to write such a sequence as $\{f_n(x)\}_{n\in\mathbb{N}}$. For example, the following are sequences of functions.

- ▷ $f_1(x) = x^2$, $f_2(x) = x^4$, $f_3(x) = x^6, \ldots$
- ▷ $f_1(x) = e^x$, $f_2(x) = e^{2x}$, $f_3(x) = e^{3x}, \ldots$
- ▷ $f_n(x) = n \exp\left(-\frac{1}{2}n^2x^2\right)$

Note that in the first case we could have instead written $f_n(x) = x^{2n}$ and in the second case we could have written $f_n(x) = e^{nx}$. The natural number n is called the index. Typically the index of the sequence starts from $n = 0$ or $n = 1$ but that's not essential. The index doesn't need to be n, any other letter, or indeed symbol, can be used.

1.1 Convergence & continuity

We start by recalling the notion of convergence for sequences of numbers.

Definition 1.1. A sequence of numbers $a_1, a_2, a_3, \ldots$ is said to *converge* to a if, for each $\epsilon > 0$, exists $N \in \mathbb{N}$ such that $|a_n - a| < \epsilon$ whenever $n \geq N$.

If a sequence $\{a_n\}_n$ converges to a then we write $a_n \to a$ (as $n \to \infty$). For sequences of functions we will need to consider two different notions of convergence. In order to understand this difficulty let us consider the following example.

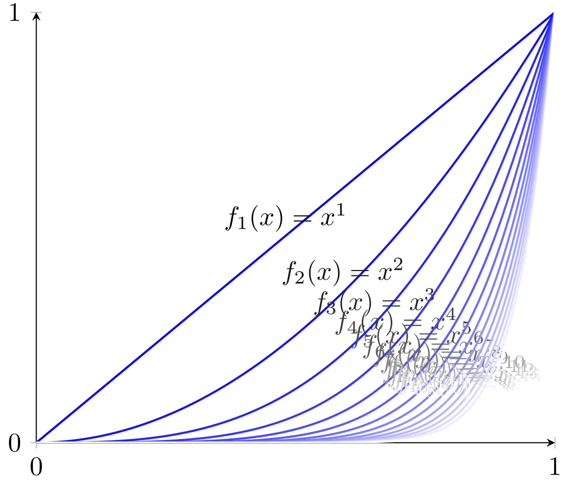


FIGURE 1.1: The sequence of functions $f_n(x) = x^n$.

Example. Consider the sequence $f_n(x) = x^n$ for $x \in (0, 1)$. For each $x \in (0, 1)$ we see that $f_n(x) \to 0$. On the other hand, for each n, $2^{\frac{1}{n}} \in (0, 1)$ and $f_n(2^{\frac{1}{n}}) = \frac{1}{2}$.

Up until now we haven't mentioned the domain of the functions in the sequence but to proceed we need to be make this detail rigorous. We will write that "$\{f_n(x)\}_n$ is a sequence of functions on $D \subset \mathbb{R}$" to mean that there is a fixed $D \subset \mathbb{R}$ and, for each $n \in \mathbb{N}$, f_n is a function with domain D (i.e., $f_n : D \to \mathbb{R}$).

Definition 1.2 (pointwise convergence)**.** Let $D \subset \mathbb{R}$, let $f_n(x)$ be a sequence of functions on D and let $f(x)$ be a function on D. If $f_n(x) \to f(x)$ for each $x \in D$ we say that f_n is *pointwise convergent* to f.

Definition 1.3 (uniform convergence)**.** Let $f_n(x)$ be a sequence of functions on $D \subset \mathbb{R}$ and let $f(x)$ be a function on D. If, for each $\epsilon > 0$, there exists N such that for every $n \geq N$ and every $x \in D$, $|f_n(x) - f(x)| < \epsilon$ then we say that f_n is *uniformly convergent* to f.

Example. Show that $f_n(x) = x^n$ converges uniformly on $(0, \frac{1}{2})$.

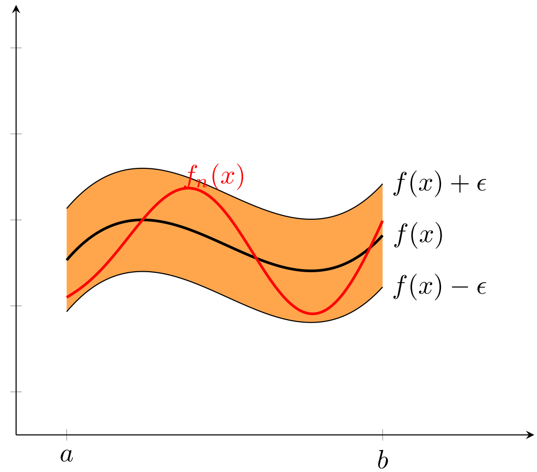


FIGURE 1.2: Uniform convergence (Definition 1.3) requires that f_n is "close" to $f(x)$ in the uniform sense illustrated here.

Solution. We observe that it converges pointwise to the constant function $f(x) = 0$. We also observe that $|f_n(x) - f(x)| \leq \frac{1}{2^n}$ for all $x \in (0, \frac{1}{2})$. This means that, for every $\epsilon > 0$, if we can choose $N = -\log_2(\epsilon)$ then $|f_n(x) - f(x)| \leq \epsilon$ whenever $n \geq N$. □

Definition 1.4. Let $f(x)$ be a functions on $D \subset \mathbb{R}$. We say that f is *continuous* at $p \in D$ if, for each $\epsilon > 0$, there is $\delta > 0$ such that $|f(x) - f(p)| < \epsilon$ whenever $x \in D$, $|x - p| < \delta$. We say that f is *continuous on D* if f is continuous at every $p \in D$.

It is natural to consider a sequence of continuous functions which converge and ask if the function they converge to is continuous. What about the sequence of functions $f_n(x) = \arctan(nx)$?

Theorem 1.5. *Suppose that $f_n \to f$ uniformly on D and that the f_n are continuous on D. Then f is continuous on D.*

Proof. Let $p \in D$. Uniform convergence means that, for each $\epsilon > 0$, there exists N such that for every $n \geq N$ and every $x \in D$, $|f_n(x) - f(x)| < \frac{\epsilon}{3}$. By continuity of

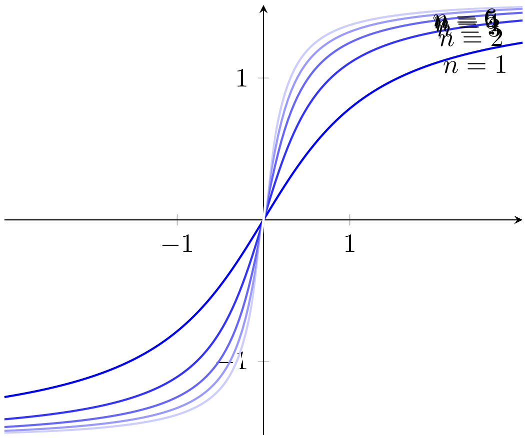


FIGURE 1.3: The sequence of functions $f_n(x) = \arctan(nx)$.

$f_N(x)$ at $x = p$, there is a $\delta > 0$ such that $|f_N(x) - f_N(p)| < \frac{\epsilon}{3}$ whenever $x \in D$, $|x - p| < \delta$. Since

$$|f(x) - f(p)| = |f(x) - f_N(x) + f_N(x) - f_N(p) + f_N(p) - f(p)|$$

this means that, for all $|x - p| < \delta$,

$$\begin{aligned}|f(x) - f(p)| &\leq |f(x) - f_N(x)| + |f_N(x) - f_N(p)| + |f_N(p) - f(p)| \\ &< 3\frac{\epsilon}{3} = \epsilon.\end{aligned}$$

This proves the continuity of f at p. Since $p \in D$ is arbitrary this shows the continuity of f on D. □

Recall that integrals are defined rigorously using the notion of a step functions.

Theorem 1.6. *Suppose that f_n are continuous functions on $[a, b] \subset \mathbb{R}$, uniformly convergent to f. Then*

$$\lim_{n\to\infty} \int_a^b f_n(x)\,dx = \int_a^b f(x)\,dx.$$

Proof. The uniform convergence implies that for each $\epsilon > 0$, there exists N such that for every $n \geq N$ and every $x \in D$, $|f_n(x) - f(x)| < \frac{\epsilon}{b-a}$. This means that

$$\Big|\int_a^b f_n(x)\,dx - \int_a^b f(x)\,dx\Big| \leq \int_a^b |f_n(x) - f(x)|\,dx$$
$$\leq (b-a)\frac{\epsilon}{b-a} = \epsilon.$$

This shows that $\int_a^b f_n(x)\,dx \to \int_a^b f(x)\,dx$. ☐

Series of functions

Recall that, if $\{a_n\}_n$ is a sequence of numbers, then the series $\sum_n a_n$ is the sequence $\{\sum_{k=1}^n a_k\}_n$ of numbers (the partial sums). We say that the series $\sum_n a_n$ is convergent if $\{\sum_{k=1}^n a_k\}_n$ is convergent.

Definition 1.7. Let $\{f_n\}$ be a sequence of functions. We say that the series $\sum_n f_n$

- ▷ is *pointwise convergent* if $\sum_{k=1}^n f_k(x)$ is pointwise convergent,
- ▷ is *uniformly convergent* if $\sum_{k=1}^n f_k(x)$ is uniformly convergent.

Theorem 1.8. *Suppose that the series $\sum_n f_n$ is uniformly convergent to g on D and the f_n are continuous on D. Then g is continuous on D.*

Proof. If the f_k are continuous then the $\sum_{k=1}^n f_k$ are continuous. This means that Theorem 1.5 applies. ☐

Theorem 1.9. *Suppose that the series $\sum_n f_n$ is uniformly convergent to g and the f_n are continuous. Then*

$$\lim_{n\to\infty} \int_a^b \sum_{k=1}^n f_k(x)\,dx = \int_a^b g(x)\,dx.$$

Proof. Again, that the f_k are continuous means that the $\sum_{k=1}^n f_k$ are continuous. This means that Theorem 1.6 applies. ☐

Here and subsequently it is convenient to recall several commons tests which are useful for proving convergence: ratio test, root test, comparison test, alternating series test, integral test for convergence. For series of functions we have the following test for convergence.

Theorem 1.10 (Weierstrass M-test). *Suppose that $\{f_n\}_n$ is a sequence of functions on D, that $\{M_n\}_n$ is a sequence of positive numbers and that $|f_n(x)| \leq M_n$. If $\sum_{n=0}^{\infty} M_n$ is convergent then the series $\sum_{n=0}^{\infty} f_n$ converges absolutely and uniformly on D.*

Proof. By the comparison test $\sum |f_n(x)|$ is convergent for all $x \in D$. I.e., for each x the series $\sum f_n(x)$ is absolutely convergent and so we let $f(x)$ be the limit. We compute

$$\left| f(x) - \sum_{k=1}^{n} f_k(x) \right| = \left| \sum_{k=n+1}^{\infty} f_k(x) \right| \leq \sum_{k=n+1}^{\infty} |f_k(x)| \leq \sum_{k=n+1}^{\infty} M_k.$$

As $\sum_n M_n$ is convergent this last expression tends to 0 as $k \to \infty$. This estimate is independent of x. □

1.2 Power series

Definition 1.11. Let $\{a_n\}_n$ be a series of numbers and let c be a number. The series $\sum_n a_n(x-c)^n$ is called a *power series* (centred at c).

Typically the power series will converge for some x and diverge for other x. We could permit x to be a complex number and the entire work of this section holds verbatim. However, for the present purposes we will assume that $x \in \mathbb{R}$ and that the coefficients $a_n \in \mathbb{R}$ and that $c \in \mathbb{R}$. To simplify formulae we will often work with the case that $c = 0$ since we can always transform a given problem to this special case.

Example. Let $a_n = 2^{-n}$. The power series $\sum_n a_n x^n = \sum_n \frac{x^n}{2^n}$ is convergent when $|x| < 2$ and divergent when $|x| > 2$. To see this we apply the root test and observe that $\lim_{n\to\infty} \left(2^{-n} |x|^n\right)^{\frac{1}{n}} = \frac{|x|}{2}$.

Example. Let $a_n = \frac{1}{n!}$. The power series $\sum_n a_n x^n = \sum_n \frac{x^n}{n!}$ is convergent for all x. To see this we use the ratio test and observe that $\left|\frac{x^{n+1}}{(n+1)!}\right| / \left|\frac{x^n}{n!}\right| = \frac{|x|}{n+1}$ and that $\lim_{n\to\infty} \frac{|x|}{n+1} = 0$ for any x.

Example. A convergent power series defines a function $f(x) = \sum_n a_n x^n$. In the above two examples, are these functions something familiar? *Hint: in the first example, compare $f(x)$ with $xf(x)$, in the second compare $f(x)$ with $f'(x)$.*

1.3 Radius of convergence

A key notion is determining exactly the domain on which a power series converges.

Theorem 1.12 (uniformly convergent power series). *Suppose that $\sum_n a_n x^n$ converges for some $x = x_0 \neq 0$. Let $R < |x_0|$. Then the series is uniformly and absolutely convergent for all x such that $|x| \leq R$.*

Proof. Since $\sum_n a_n x_0^n$ is convergent there exists $M > 0$ such that, for all n, $|a_n x_0^n| \leq M$. Observe that

$$|a_n x^n| = |a_n x_0^n| \left|\frac{x}{x_0}\right|^n \leq M \frac{R^n}{|x_0|^n}.$$

The series $\sum_n M \frac{R^n}{|x_0|^n}$ is a geometric sum and so convergent. Consequently, by the M-test, the series is uniformly and absolutely convergent when $|x| \leq R$. □

Theorem 1.13 (radius of convergence). *Suppose exists $x_1, x_2 \neq 0$ such that $\sum_n a_n x_1^n$ is convergent and $\sum_n a_n x_2^n$ is divergent. Then exists $r > 0$ such that $\sum_n a_n x^n$ is convergent for $|x| < r$ and divergent for $|x| > r$.*

Proof. Let A be the set of real numbers for which $\sum_n a_n x^n$ is convergent and let r be the least upper bound of A. The series $\sum_n a_n x^n$ is convergent whenever $|x| < r$. If $|x| > r$ and $\sum_n a_n x^n$ is convergent then this contradicts the definition of A and so $\sum_n a_n x^n$ is divergent for $|x| > r$. □

In the above paragraphs we worked with the case $c = 0$ but all of these notions hold for the general $c \in \mathbb{R}$. Consequently Theorem 1.13 implies that the series is convergent on an interval $(c - r, c + r) = \{x : |x - c| < r\}$ but divergent when $|x - c| > r$.

The convergence for the sequence for $x = c - r$ and $x = c + r$ must be manually checked and can differ for the left and right end points.

Definition 1.14. This r is the *radius of convergence* of the series $\sum_n a_n(x-c)^n$.

We use the following convention: if $\sum_n a_n x^n$ converges for all $x \in \mathbb{C}$ we say the radius of convergence is ∞; if $\sum_n a_n x^n$ doesn't converge except $x = 0$ we say the radius of convergence is 0. All of the above concerning power series holds verbatim for x a complex number and so "radius" is more meaningful since it truly corresponds to a disk in the complex plane.

1.4 Integrating & differentiating power series

Let $a_n \in \mathbb{R}$, $x \in \mathbb{R}$. If the series $\sum_n a_n x^n$ converges we define the function $f(x) = \sum_{n=0}^{\infty} a_n x^n$. In general exchanging limits with derivatives and integrals is problematic but for power series the situation is good.

Theorem 1.15 (integrating power series)**.** *Suppose that, for $x \in (-r, r)$, the series $f(x) = \sum_{n=0}^{\infty} a_n x^n$ is convergent. Then $f(x)$ is continuous and $\int_0^x f(y)\,dy = \sum_{n=0}^{\infty} \frac{a_n}{n+1} x^{n+1}$.*

Proof. Let $|x| < R < r$. Observe that the series is uniformly convergent for $y \in [-R, R]$. This means that $f(x)$ is continuous and so we can interchange limit and integral,

$$\int_0^x f(y)\,dy = \sum_{n=0}^{\infty} \int_0^x a_n x^n = \sum_{n=0}^{\infty} \frac{a_n}{n+1} x^{n+1}.$$

□

Theorem 1.16 (differentiating power series)**.** *Suppose that, for $x \in (-r, r)$, the series $f(x) = \sum_{n=0}^{\infty} a_n x^n$ is convergent. Then $f(x)$ is differentiable and $f'(x) = \sum_{n=1}^{\infty} n a_n x^{n-1}$, convergent for $x \in (-r, r)$.*

Proof. Let $|x| < R < r$. Observe that

$$\sum_{n=1}^{\infty} n a_n x^{n-1} = \sum_{n=1}^{\infty} a_n R^n \cdot \frac{n}{R} \cdot \frac{x^{n-1}}{R^{n-1}}.$$

Since $\sum_{n=1}^{\infty} a_n R^n$ is absolutely convergent and $\frac{n}{R} \cdot \left(\frac{|x|}{R}\right)^{n-1}$ is bounded we know that $\sum_{n=1}^{\infty} n a_n x^{n-1}$ is absolutely convergent (comparison test). For convenience let $g(x) = \sum_{n=1}^{\infty} n a_n x^{n-1}$ and observe that $\int_0^x g(y)\, dy = \sum_{n=1}^{\infty} a_n x^n = f(x) - a_0$ (by Theorem 1.15). By the fundamental theorem of calculus this concludes the proof. □

Let a, x and the coefficients a_n be real numbers. The series

$$f(x) = \sum_{n=0}^{\infty} a_n (x-a)^n$$

defines a function on the interval $(a-r, a+r)$, where r is the *radius of convergence*. The series is said to *represent* the function f and is called the *power series expansion* of f about a.

Two important questions are: Given the series, what are the properties of f? Given a function f, can it be represented by a power series? Only rather special functions possess power-series expansions however the class of such functions is very useful in practice.

1.5 Uniqueness & Taylor series

In the next paragraphs we develop the idea that, if two power series represent the same function, then they must be the same power series. In this sense we have the uniqueness of power series. The following result is a crucial piece of information about power series and is one major reason why they are useful.

Theorem 1.17 (uniqueness of power series). *Suppose that two power series are convergent and are equal in a neighbourhood of* a *in the sense that, for* $|x-a|<\epsilon$,

$$\sum_n a_n(x-a)^n = \sum_n b_n(x-a)^n = f(x).$$

Then the two series are equal term-by-term, i.e., $a_n = b_n$ *for every* $n \in \mathbb{N}$. *Moreover,*

$$a_n = b_n = \frac{f^{(n)}(a)}{n!}.$$

Proof. The conclusion of Theorem 1.16 can be iterated and implies that $f(x)$ has derivatives of every order and, for $k \in \mathbb{N}$,

$$f^{(k)}(x) = k!a_k + \sum_{n=k+1}^{\infty} n(n-1)\cdots(n-k+1)a_n(x-a)^{n-k}.$$

This means that $f^{(k)}(a) = k!a_k$ because all the terms in the sum vanish. □

Definition 1.18. Suppose that a function $f(x)$ is infinitely differentiable on an open interval about a. The *Taylor's series generated by* f *at* a is (formally)

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n.$$

Observe how the coefficients in the Taylor's series coincide with the formula obtained in the above results. **Question:** Does the Taylor's series converge on the entire interval? In general, no. However we can calculate the radius of convergence of the power series. **Question:** If the Taylor's series converges, is it equal to $f(x)$ on the interval? In general it might not as seen in the following example.

Example. Let $f(x) = e^{-1/x^2}$. If we proceed to calculate the Taylor's series about $x=0$ we obtain:

$$\begin{aligned} f(x) &= \exp(-x^{-2}) & f(0) &= 0 \\ f'(x) &= 2x^{-3}\exp(-x^{-2}) & f'(0) &= 0 \\ f''(x) &= (-6x^{-4}+4x^{-6})\exp(-x^{-2}) & f''(0) &= 0 \\ f'''(x) &= 4(2x^{-9}-9x^{-7}+6x^{-5})\exp(-x^{-2}) & f'''(0) &= 0 \end{aligned}$$

The Taylor's series is consequently $\sum_{n=0}^{\infty} 0 = 0$. It does converge but has nothing to do with the original function.

Example. What is Taylor's series for $f(x) = e^x$? Does differentiating this power series correspond to expectations?

Error term in Taylor's series

We define the error term in the n^{th} approximation given by Taylor's series as

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

Convergence of the Taylor's series to $f(x)$ is implied by $E_n(x) \to 0$ as $n \to \infty$. Using this idea we have the following sufficient condition for convergence of a Taylor's series.

Theorem 1.19. *Assume f is infinitely differentiable on $I = (a-r, a+r)$ and there exists $A > 0$ such that*

$$\left|f^{(n)}(x)\right| \le A^n, \quad \text{for all } n \in \mathbb{N}, x \in I.$$

Then then Taylor's series generated by f at a converges to $f(x)$ for each $x \in I$.

Proof. We will first show, by induction, that

$$E_n(x) = \frac{1}{n!} \int_a^x (x-y)^n f^{(n+1)}(y)\, dy.$$

Since, by definition, $E_0(x) = f(x) - f(a)$, the case $n = 0$ is immediate. We now assume that the statement is true for n and prove it for $n+1$. Observe that

$$E_{n+1}(x) = E_n(x) - \frac{f^{(n+1)}}{(n+1)!}(x-a)^{n+1}$$

and that $(x-a)^{n+1} = (n+1)\int_a^x (x-y)^n\, dy$. Consequently

$$\begin{aligned} E_{n+1}(x) &= \frac{1}{n!} \int_a^x (x-y)^n f^{(n+1)}(y)\, dy - \frac{f^{(n+1)}(a)}{(n+1)!}(x-a)^{n+1} \\ &= \frac{1}{n!} \int_a^x (x-y)^n f^{(n+1)}(y)\, dy - \frac{1}{n!} \int_a^x f^{(n+1)}(a)(x-y)^n\, dy. \end{aligned}$$

Combining the integrals and integrating by parts we obtain the claimed statement for $n+1$. Using the formula for $E_n(x)$ which we have just proved, we estimate

$$|E_n(x)| \leq \frac{1}{n!} \int_a^x |x-y|^n \, A^{n+1} \, dy \leq \frac{1}{n!} r r^n A^{n+1} = rA \frac{(rA)^n}{n!}.$$

Since $\frac{(rA)^n}{n!} \to 0$ as $n \to \infty$ we have shown that $|E_n(x)| \to 0$ as $n \to \infty$. □

1.6 Power series & differential equations

In this section we will use some of the strength of power series in a particular application. This is a method which we can use to solve certain power series. The method is best illustrated with an example. This method of solving differential equations is called the "method of undetermined coefficients".

Task 1.6.1. *Find a function $y(x)$ which satisfies the differential equation*

$$(1-x^2)y''(x) = -2y(x)$$

and satisfies the initial conditions $y(0) = 1$, $y'(0) = 1$.

We start by assuming that there exists a power series solution $y(x) = \sum_{n=0}^{\infty} a_n x^n$ convergent for $x \in (-r, r)$ for some $r > 0$ to be determined later.

1. By Theorem 1.16,

$$y'(x) = \sum_{n=1}^{\infty} n a_n x^{n-1} \quad \text{and} \quad y''(x) = \sum_{n=2}^{\infty} n(n-1) a_n x^{n-2}.$$

2. And so

$$\begin{aligned} -2\sum_{n=0}^{\infty} a_n x^n = (1-x^2)y''(x) &= (1-x^2)\sum_{n=2}^{\infty} n(n-1)a_n x^{n-2} \\ &= \sum_{n=2}^{\infty} n(n-1)a_n x^{n-2} - \sum_{n=2}^{\infty} n(n-1)a_n x^n \\ &= \sum_{n=0}^{\infty} (n+2)(n+1)a_{n+2} x^n - \sum_{n=0}^{\infty} n(n-1)a_n x^n \end{aligned}$$

3. Consequently, by Theorem 1.17, $0 = 2a_n + (n+2)(n+1)a_{n+2} - n(n-1)a_n$ for each $n \in \mathbb{N}_0$;
4. Equivalently $a_{n+2} = \frac{n-2}{n+2}a_n$;
5. Using the initial conditions, $a_0 = y(0) = 1$, $a_1 = y'(0) = 1$;
6. For the even coefficients:
   - ▷ $a_2 = \frac{0-2}{0+2}a_0 = -1$,
   - ▷ $a_4 = \frac{2-2}{2+2}a_2 = 0$,
   - ▷ $a_6 = \frac{4-2}{4+2}a_4 = 0, \ldots$;
7. For the odd coefficients:
   - ▷ $a_3 = \frac{1-2}{1+2}a_1 = -\frac{1}{3}$,
   - ▷ $a_5 = \frac{3-2}{3+2}a_3 = \frac{1}{5}(-\frac{1}{3}), \ldots$
   - ▷ $a_{2n+1} = \frac{1}{(2n+1)(2n-1)}$;
8. Formally we have the series solution

$$y(x) = 1 - x^2 + \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)(2n-1)}, \tag{1.1}$$

9. We see that this series is convergent for $|x| < 1$.

Consequently we have shown that the function defined above (1.1) is well-defined in the interval $(-1, 1)$ and is a solution to the given differential equation.

Chapter 2

Differential calculus in higher dimension

In this part of the course we start to consider higher dimensional space. That is, instead of $\mathbb{R}$ we consider $\mathbb{R}^n$ for $n \in \mathbb{N}$. We will particularly focus on 2D and 3D but everything also holds in any dimension. Going beyond $\mathbb{R}$ we have more options for functions and correspondingly more options for derivatives.

Various different notation is commonly used. Here we will primarily use $(x, y) \in \mathbb{R}^2$, $(x, y, z) \in \mathbb{R}^3$ or, more generally, $\mathbf{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ where $x_1 \in \mathbb{R}, \ldots, x_n \in \mathbb{R}$. For example, $\mathbb{R}^2$ is the plane, $\mathbb{R}^3$ is 3D space.

Definition 2.1 (inner product). $\mathbf{x} \cdot \mathbf{y} = \sum_{k=1}^{n} x_k y_k \in \mathbb{R}$

We recall that the inner product being zero has a geometric meaning, it means that the two vectors are orthogonal. We also recall that the "length" of a vector is given by the norm, defined as follows.

Definition 2.2 (norm). $\|\mathbf{x}\| = \sqrt{\mathbf{x} \cdot \mathbf{x}} = (\sum_{k=1}^{n} x_k^2)^{\frac{1}{2}}$.

For example, in $\mathbb{R}^2$ then $\|(x, y)\| = \sqrt{x^2 + y^2}$. There are various convenient properties for working with norms and inner products, in particular, the Cauchy-Schwarz inequality $|x \cdot y| \leq \|\mathbf{x}\| \, \|\mathbf{y}\|$ and the triangle inequality $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$.

The primary higher-dimensional functions we consider in this course are:

$$\begin{aligned} \text{Scalar fields:} \quad & f : \mathbb{R}^n \to \mathbb{R} \\ \text{Vector fields:} \quad & \mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n \\ \text{Paths:} \quad & \boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n \\ \text{Change of coordinates:} \quad & \mathbf{x} : \mathbb{R}^n \to \mathbb{R}^n \end{aligned}$$

These possibilities all fit into the general pattern of $f : \mathbb{R}^n \to \mathbb{R}^m$ for $n, m \in \mathbb{N}$ but tradition and use of the function gives us different terminology and symbols. Such functions are useful for representing various practical things, for example: gravitational force; temperature in a region; wind velocity; fluid flow; electric field; etc.

2.1 Open sets, closed sets, boundary, continuity

Let $\mathbf{a} \in \mathbb{R}^n$, $r > 0$. The open n-ball of radius r and centre $\mathbf{a}$ is written as

$$B(\mathbf{a}, r) := \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{a}\| < r\}.$$

Definition 2.3 (interior point). Let $S \subset \mathbb{R}^n$. A point $\mathbf{a} \in S$ is said to be an *interior point* if there is $r > 0$ such that $B(\mathbf{a}, r) \subset S$. The set of all interior points of S is denoted $\operatorname{int} S$.

Definition 2.4 (open set). A set $S \subset \mathbb{R}^n$ is said to be *open* if all of its points are interior points, i.e., if $\operatorname{int} S = S$.

For example, open intervals, open disks, open balls, unions of open intervals, etc., are all open sets.

Lemma. *Let $r > 0$, $\mathbf{a} \in \mathbb{R}^n$. The set $B(\mathbf{a}, r) \subset \mathbb{R}^n$ is open.*

Proof. Let $\mathbf{b} \in B(\mathbf{a}, r)$. It suffices to show that $\mathbf{b}$ is an interior point. (1) Let $r_1 = \|\mathbf{b} - \mathbf{a}\| < r$. (2) Let $r_2 = (r - r_1)/2$. (3) We claim that $B(\mathbf{b}, r_2) \subset B(\mathbf{a}, r)$: In order to see this take any $\mathbf{c} \in B(\mathbf{b}, r_2)$ and observe that

$$\|\mathbf{c} - \mathbf{a}\| \le \|\mathbf{c} - \mathbf{b}\| + \|\mathbf{b} - \mathbf{a}\| \le r_2 + r_1 = \frac{r + r_1}{2} < r.$$

Observe that the radius of the ball will be small for points close to the boundary. □

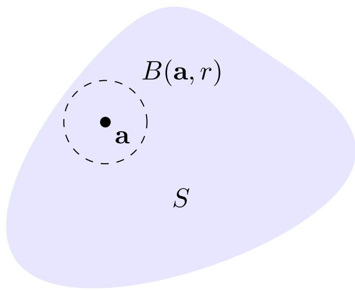


FIGURE 2.1: Interior points are the centre of a ball contained within the set.

Definition 2.5 (Cartesian product). If $A_1 \subset \mathbb{R}$, $A_2 \subset \mathbb{R}$ then the *Cartesian product* is defined as

$$A_1 \times A_2 := \{(x, y) : x \in A_1, y \in A_2\} \subset \mathbb{R}^2.$$

Analogously the Cartesian product can be defined in higher dimensions: If $A_1 \subset \mathbb{R}^m$, $A_2 \subset \mathbb{R}^n$ then the *Cartesian product* $A_1 \times A_2$ is defined as the set of all points $(x_1, \ldots, x_m, y_1, \ldots, y_n) \in \mathbb{R}^{m+n}$ such that $(x_1, \ldots, x_m) \in A_1$ and $(y_1, \ldots, y_n) \in A_2$.

Lemma. *If A_1, A_2 are open subsets of $\mathbb{R}$ then $A_1 \times A_2$ is an open subset of $\mathbb{R}^2$.*

Proof. Let $\mathbf{a} = (a_1, a_2) \in A_1 \times A_2 \subset \mathbb{R}^2$. Since A_1 is open there exists $r_1 > 0$ such that $B(a_1, r_1) \subset A_1$. Similarly for A_2. Let $r = \min\{r_1, r_2\}$. This all means that $B(\mathbf{a}, r) \subset B(a_1, r_1) \times B(a_2, r_2) \subset A_1 \times A_2$. □

Discussing the "interior" of the set naturally suggests the topic of the "boundary" of the set. In the following definitions we develop this idea.

Definition 2.6 (exterior points). Let $S \subset \mathbb{R}^n$. A point $\mathbf{a} \notin S$ is said to be an *exterior point* if there exists $r > 0$ such that $B(\mathbf{a}, r) \cap S = \emptyset$. The set of all exterior points of S is denoted $\operatorname{ext} S$.

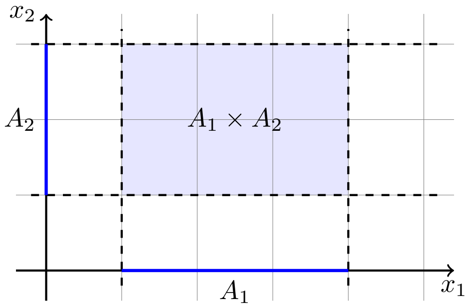


FIGURE 2.2: If A_1, A_2 are intervals then $A_1 \times A_2$ is a rectangle.

Observe that ext S is an open set. We use the notation $S^c = \mathbb{R}^n \setminus S$ and we say that C^c is the *complement* of the set S.

Definition 2.7 (boundary). The set $\mathbb{R}^n \setminus (\text{int } S \cup \text{ext } S)$ is called the boundary of $S \subset \mathbb{R}^n$ and is denoted ∂S.

Definition 2.8 (closed). A set $S \subset \mathbb{R}^n$ is said to be *closed* if $\partial S \subset S$.

Lemma 2.9. *S is open $\iff$ S^c is closed.*

Proof. Observe that $\mathbb{R}^n = \text{int } S \cup \partial S \cup \text{ext } S$ (disjointly). If $\mathbf{x} \in \partial S$ then, for every $r > 0$, $B(\mathbf{x}, r) \cap S \neq \emptyset$ and so $\mathbf{x} \in \partial(S^c)$. Similarly with S and S^c swapped and so $\partial S = \partial(S^c)$. If S is open then int $S = S$ and $S^c = \text{ext } S \cup \partial S = \text{ext } S \cup \partial(S^c)$ and so S^c is closed. If S is not open then there exists $\mathbf{a} \in \partial S \cap S$. Additionally $\mathbf{a} \in \partial(S^c) \cap S$ hence S^c is not closed. $\square$

Limits and continuity

Let $S \subset \mathbb{R}^n$ and $\mathbf{f} : S \to \mathbb{R}^m$. If $\mathbf{a} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$ we write $\lim_{\mathbf{x} \to \mathbf{a}} \mathbf{f}(\mathbf{x}) = \mathbf{b}$ to mean that $\|\mathbf{f}(\mathbf{x}) - \mathbf{b}\| \to 0$ as $\|\mathbf{x} - \mathbf{a}\| \to 0$. Observe how, if $n = m = 1$, this is the familiar notion of continuity for functions on $\mathbb{R}$.

Definition 2.10 (continuous)**.** A function $\mathbf{f}$ is said to be *continuous* at $\mathbf{a}$ if $\mathbf{f}$ is defined at $\mathbf{a}$ and $\lim_{\mathbf{x}\to\mathbf{a}} \mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{a})$. We say $\mathbf{f}$ is continuous on S if $\mathbf{f}$ is continuous at each point of S.

Even functions which look "nice" can fail to be continuous as we can see in the following example.

Example (continuity in higher dimensions)**.** Let f be defined, for $(x, y) \neq (0, 0)$, as

$$f(x, y) = \frac{xy}{x^2 + y^2}$$

and $f(0, 0) = 0$. What is the behaviour of f when approaching $(0, 0)$ along the following lines?

line	value
$\{x = 0\}$	$f(0, t) = 0$
$\{y = 0\}$	$f(t, 0) = 0$
$\{x = y\}$	$f(t, t) = \frac{1}{2}$
$\{x = -y\}$	$f(t, t) = -\frac{1}{2}$.

Theorem 2.11. *Suppose that* $\lim_{\mathbf{x}\to\mathbf{a}} \mathbf{f}(\mathbf{x}) = \mathbf{b}$ *and* $\lim_{\mathbf{x}\to\mathbf{a}} \mathbf{g}(\mathbf{x}) = \mathbf{c}$. *Then*

1. $\lim_{\mathbf{x}\to\mathbf{a}} (\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})) = \mathbf{b} + \mathbf{c}$,
2. $\lim_{\mathbf{x}\to\mathbf{a}} \lambda\mathbf{f}(\mathbf{x}) = \lambda\mathbf{b}$ *for every* $\lambda \in \mathbb{R}$,
3. $\lim_{\mathbf{x}\to\mathbf{a}} \mathbf{f}(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}) = \mathbf{b} \cdot \mathbf{c}$,
4. $\lim_{\mathbf{x}\to\mathbf{a}} \|\mathbf{f}(\mathbf{x})\| = \|\mathbf{b}\|$.

We prove a couple of the parts of the above theorem here, the other parts are left as exercises.

Proof of 3. Observe that $\mathbf{f}(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}) - \mathbf{b} \cdot \mathbf{c} = (\mathbf{f}(\mathbf{x}) - \mathbf{b}) \cdot (\mathbf{g}(\mathbf{x}) - \mathbf{c}) + \mathbf{b} \cdot (\mathbf{g}(\mathbf{x}) - \mathbf{c}) + \mathbf{c} \cdot (\mathbf{f}(\mathbf{x}) - \mathbf{b})$. By the triangle inequality and Cauchy-Schwarz,

$$\begin{aligned} \|\mathbf{f}(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}) - \mathbf{b} \cdot \mathbf{c}\| \leq {} & \|\mathbf{f}(\mathbf{x}) - \mathbf{b}\| \, \|\mathbf{g}(\mathbf{x}) - \mathbf{c}\| \\ & + \|\mathbf{b}\| \, \|\mathbf{g}(\mathbf{x}) - \mathbf{c}\| \\ & + \|\mathbf{c}\| \, \|\mathbf{f}(\mathbf{x}) - \mathbf{b}\| \, . \end{aligned}$$

Since we already know that $\|\mathbf{f}(\mathbf{x}) - \mathbf{b}\| \to 0$ and $\|\mathbf{g}(\mathbf{x}) - \mathbf{c}\| \to 0$ as $\mathbf{x} \to \mathbf{a}$, this implies that $\|\mathbf{f}(\mathbf{x}) \cdot \mathbf{g}(\mathbf{x}) - \mathbf{b} \cdot \mathbf{c}\| \to 0$. □

Proof of 4. Take $\mathbf{f} = \mathbf{g}$ in part (c) implies that $\lim_{\mathbf{x}\to\mathbf{a}} \|\mathbf{f}(\mathbf{x})\|^2 = \|\mathbf{b}\|^2$. ☐

When writing a vector field (or similar functions) it is often convenient to divide the higher-dimensional function into smaller parts. We call these parts the *components of a vector field*. For example $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}))$ in 2D, $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), f_3(\mathbf{x}))$ in 3D, etc.

Theorem 2.12. *Let $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}))$. Then $\mathbf{f}$ is continuous if and only if f_1 and f_2 are continuous.*

Proof. We will independently prove the two implications.

(⇒) Let $\mathbf{e}_1 = (1, 0)$, $\mathbf{e}_2 = (0, 1)$ and observe that $f_k(\mathbf{x}) = \mathbf{f}(\mathbf{x}) \cdot \mathbf{e}_k$. We have already shown that the continuity of two vector fields implies the continuity of the inner product.

(⇐) By definition of the norm $\|\mathbf{f}(\mathbf{x}) - \mathbf{f}(\mathbf{a})\|^2 = \sum_{k=1}^{2} (f_k(\mathbf{x}) - f_k(\mathbf{a}))^2$ and we know $\|f_k(\mathbf{x}) - f_k(\mathbf{a})\| \to 0$ as $\|\mathbf{x} - \mathbf{a}\| \to 0$. ☐

In higher dimensions the analogous statement is true for the vector field $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_m(\mathbf{x}))$ with exactly the same proof. I.e., $\mathbf{f}$ is continuous if and only if each f_k is continuous.

Example (polynomials)**.** A *polynomial* in n variables is a scalar field on $\mathbb{R}^n$ of the form

$$f(x_1, \ldots, x_n) = \sum_{k_1=0}^{j} \cdots \sum_{k_n=0}^{j} c_{k_1,\ldots,k_n} x_1^{k_1} \cdots x_n^{k_n}.$$

E.g., $f(x, y) := x + 2xy - x^2$ is a polynomial in 2 variables. Polynomials are continuous everywhere in $\mathbb{R}^n$. This is because they are the finite sum of products of continuous scalar fields.

Example (rational functions)**.** A *rational function* is a scalar field

$$f(\mathbf{x}) = \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

where $p(\mathbf{x})$ and $q(\mathbf{x})$ are polynomials. A rational function is continuous at every point $\mathbf{x}$ such that $q(\mathbf{x}) \neq 0$.

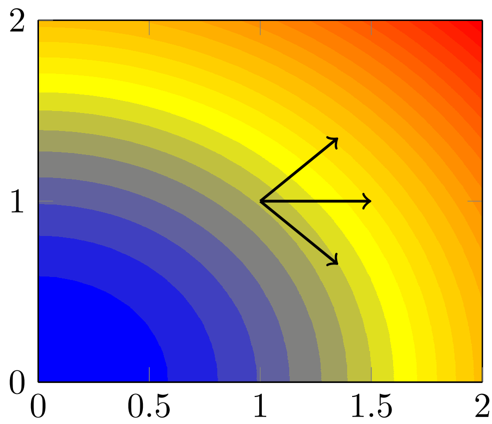


FIGURE 2.3: Plot where colour represents the value of $f(x,y) = x^2 + y^2$. The change in f depends on direction.

As described in the following result, the continuity of functions continues to hold, in an intuitive way, under composition of functions.

Theorem 2.13. *Suppose $S \subset \mathbb{R}^l$, $T \subset \mathbb{R}^m$, $\mathbf{f} : S \to \mathbb{R}^m$, $\mathbf{g} : T \to \mathbb{R}^n$ and that $\mathbf{f}(S) \subset T$ so that*

$$(\mathbf{g} \circ \mathbf{f})(\mathbf{x}) = \mathbf{g}(\mathbf{f}(\mathbf{x}))$$

makes sense. If $\mathbf{f}$ is continuous at $\mathbf{a} \in S$ and $\mathbf{g}$ is continuous at $\mathbf{f}(\mathbf{a})$ then $\mathbf{g} \circ \mathbf{f}$ is continuous at $\mathbf{a}$.

Proof. $\lim_{\mathbf{x} \to \mathbf{a}} \|\mathbf{f}(\mathbf{g}(\mathbf{x})) - \mathbf{f}(\mathbf{g}(\mathbf{a}))\| = \lim_{\mathbf{y} \to \mathbf{g}(\mathbf{a})} \|\mathbf{f}(\mathbf{y}) - \mathbf{f}(\mathbf{g}(\mathbf{a}))\| = 0$ □

Example. We can consider the scalar field $f(x,y) = \sin(x^2 + y) + xy$ as the composition of functions.

2.2 Derivatives of scalar fields

We can imagine, for example in Figure 2.3, that in higher dimensions, the derivative of a scalar field depends on the direction. This motivates the following.

Definition 2.14 (directional derivative)**.** Let $S \subset \mathbb{R}^n$ and $f : S \to \mathbb{R}$. For any $\mathbf{a} \in \operatorname{int} S$ and $\mathbf{v} \in \mathbb{R}^n$, $\|v\| = 1$ the directional derivative of f with respect to $\mathbf{v}$ is defined as

$$D_{\mathbf{v}} f(\mathbf{a}) = \lim_{h \to 0} \frac{1}{h} \left(f(\mathbf{a} + h\mathbf{v}) - f(\mathbf{a}) \right).$$

When h is small we can guarantee that $\mathbf{a} + h\mathbf{v} \in S$ because $\mathbf{a} \in \operatorname{int} S$ so this definition makes sense.

Theorem. *Suppose $S \subset \mathbb{R}^n$, $f : S \to \mathbb{R}$, $\mathbf{a} \in \operatorname{int} S$. Let $g(t) := f(\mathbf{a} + t\mathbf{v})$. If one of the derivatives $g'(t)$ or $D_{\mathbf{v}} f(\mathbf{a})$ exists then the other also exists and*

$$g'(t) = D_{\mathbf{v}} f(\mathbf{a} + t\mathbf{v}).$$

In particular $g'(0) = D_{\mathbf{v}} f(\mathbf{a})$.

Proof. By definition $\frac{1}{h}(g(t+h) - g(h)) = \frac{1}{h}(f(\mathbf{a} + h\mathbf{v}) - f(\mathbf{a}))$. □

The following result is useful for proving later results.

Theorem (mean value)**.** *Assume that $D_{\mathbf{v}}(\mathbf{a} + t\mathbf{v})$ exists for each $t \in [0, 1]$. Then for some $\theta \in (0, 1)$,*

$$f(\mathbf{a} + \mathbf{v}) - f(\mathbf{a}) = D_{\mathbf{v}} f(\mathbf{z}), \quad \textit{where } z = \mathbf{a} + \theta \mathbf{v}.$$

Proof. Apply mean value theorem to $g(t) = f(\mathbf{a} + t\mathbf{v})$. □

The following notation is convenient. For any $k \in \{1, 2, \ldots, n\}$, let $\mathbf{e}_k$ be the n-dimensional unit vector where all entries are zero except the k^{th} position which is equal to 1. I.e., $\mathbf{e}_1 = (1, 0, \ldots, 0)$, $\mathbf{e}_1 = (0, 1, 0, \ldots, 0)$, $\mathbf{e}_1 = (0, \ldots, 0, 1)$.

Definition 2.15 (partial derivatives)**.** We define the *partial derivative* in x_k of $f(x_1, \ldots, x_n)$ at $\mathbf{a}$ as

$$\frac{\partial f}{\partial x_k}(\mathbf{a}) = D_{\mathbf{e}_k} f(\mathbf{a}).$$

Remark. Various symbols used for partial derivatives: $\frac{\partial f}{\partial x_k}(\mathbf{a}) = D_k f(\mathbf{a}) = \partial_k f(\mathbf{a})$. If a function is written $f(x, y)$ we write $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}$ for the partial derivatives. Similarly for higher dimension.

In practice, to compute the partial derivative $\frac{\partial f}{\partial x_k}$, one should consider all other x_j for $j \neq k$ as constants and take the derivative with respect to x_k. In a moment we see this rigorously.

If $f : \mathbb{R} \to \mathbb{R}$ is differentiable, then we know that, when x is close to a,

$$f(x) \approx f(a) + (x-a)f'(a).$$

More precisely, we know that[1] $f(x) = f(a) + (x-a)f'(a) + \epsilon(x-a)$ where $|\epsilon(x-a)| = o(|x-a|)$. This way of seeing differentiability is convenient for the higher dimensional definition of differentiability.

Definition 2.16 (differentiable)**.** Let $S \subset \mathbb{R}^n$ be open, $f : S \to \mathbb{R}$. We say that f is *differentiable* at $\mathbf{a} \in S$ if there exists a linear transformation $df_{\mathbf{a}} : \mathbb{R}^n \to \mathbb{R}$ such that, for $\mathbf{x} \in B(\mathbf{a}, r)$,

$$f(\mathbf{x}) = f(\mathbf{a}) + df_{\mathbf{a}}(\mathbf{x}-\mathbf{a}) + \epsilon(\mathbf{x}-\mathbf{a})$$

where $|\epsilon(\mathbf{x}-\mathbf{a})| = o(\|\mathbf{x}-\mathbf{a}\|)$.

For future convenience we introduce the following notation.

Definition 2.17 (gradient)**.** The *gradient* of the scalar field $f(x, y, z)$ at the point $\mathbf{a}$ is

$$\nabla f(\mathbf{a}) = \begin{pmatrix} \frac{\partial f}{\partial x}(\mathbf{a}) \\ \frac{\partial f}{\partial y}(\mathbf{a}) \\ \frac{\partial f}{\partial z}(\mathbf{a}) \end{pmatrix}.$$

In general, when working in $\mathbb{R}^n$ for some $n \in \mathbb{N}$, the *gradient* of the scalar field $f(x_1, \dots, x_n)$ at the point $\mathbf{a}$ is

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

[1]This is *little-o notation* and here means that $|f(x) - f(a) - (x-a)f'(a)| / |x-a| \to 0$ as $|x-a| \to 0$.

Theorem 2.18. *If f is differentiable at $\mathbf{a}$ then $df_{\mathbf{a}}(\mathbf{v}) = \nabla f(\mathbf{a}) \cdot \mathbf{v}$. This means that, for $\mathbf{x} \in B(\mathbf{a}, r)$,*

$$f(\mathbf{x}) = f(\mathbf{a}) + \nabla f(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) + \epsilon(\mathbf{x} - \mathbf{a})$$

where $|\epsilon(\mathbf{x} - \mathbf{a})| = o(\|\mathbf{x} - \mathbf{a}\|)$. Moreover, for any vector $\mathbf{v}$, $\|v\| = 1$,

$$D_{\mathbf{v}} f(\mathbf{a}) = \nabla f(\mathbf{a}) \cdot \mathbf{v}.$$

Proof. Since f is differentiable there exists a linear transformation $df_{\mathbf{a}} : \mathbb{R}^n \to \mathbb{R}$ such that $f(\mathbf{a} + h\mathbf{v}) = f(\mathbf{a}) + h df_{\mathbf{a}}(\mathbf{v}) + \epsilon(h\mathbf{v})$ and hence

$$\begin{aligned} D_{\mathbf{v}} f(\mathbf{a}) &= \lim_{h \to 0} \frac{1}{h}(f(\mathbf{a} + h\mathbf{v}) - f(\mathbf{a})) \\ &= \lim_{h \to 0} \frac{1}{h}(h\, df_{\mathbf{a}}(\mathbf{v}) + \epsilon(h\mathbf{v})) = df_{\mathbf{a}}(\mathbf{v}). \end{aligned}$$

In particular $df_{\mathbf{a}}(\mathbf{e}_k) = D_{\mathbf{e}_k} f(\mathbf{a})$. □

Theorem. *If f is differentiable at $\mathbf{a}$, then it is continuous at $\mathbf{a}$.*

Proof. Observe that $|f(\mathbf{a} + \mathbf{v}) - f(\mathbf{a})| = |df_{\mathbf{a}}(\mathbf{v}) + \epsilon(\mathbf{v})|$. This means that

$$|f(\mathbf{a} + \mathbf{v}) - f(\mathbf{a})| \leq \|df_{\mathbf{a}}\| \, \|\mathbf{v}\| + |\epsilon(\mathbf{v})|$$

and so this tends to 0 as $\|\mathbf{v}\| \to 0$. □

Theorem 2.19. *Suppose that $f(x_1, \ldots, x_n)$ is a scalar field. If the partial derivatives $\partial_1 f(\mathbf{x}), \ldots, \partial_n f(\mathbf{x})$ exist for all $\mathbf{x} \in B(\mathbf{a}, r)$ and are continuous at $\mathbf{a}$ then f is differentiable at $\mathbf{a}$.*

Proof. For convenience define the vectors

$$\begin{aligned} \mathbf{v} &= (v_1, v_2, \ldots, v_n), \\ \mathbf{u}_k &= (v_1, v_2, \ldots, v_k, 0, \ldots, 0). \end{aligned}$$

Observe that

$$\mathbf{u}_k - \mathbf{u}_{k-1} = v_k \mathbf{e}_k, \quad \mathbf{u}_0 = (0, 0, \ldots, 0), \quad \mathbf{u}_n = \mathbf{v}.$$

Using the mean value theorem we know that there exists $\mathbf{z}_k = \mathbf{u}_{k-1} + \theta_k \mathbf{e}_k$ such that $f(\mathbf{a}+\mathbf{u}_k) - f(\mathbf{a}+\mathbf{u}_{k-1}) = v_k D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{z}_k)$. Consequently

$$\begin{aligned} f(\mathbf{a}+\mathbf{v}) - f(\mathbf{a}) &= \sum_{k=1}^{n} f(\mathbf{a}+\mathbf{u}_k) - f(\mathbf{a}+\mathbf{u}_{k-1}) \\ &= \sum_{k=1}^{n} v_k D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{z}_k) \\ &= \sum_{k=1}^{n} v_k D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{u}_{k-1}) \\ &\quad + \sum_{k=1}^{n} v_k \left(D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{z}_k) - D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{u}_{k-1}) \right) \end{aligned}$$

To conclude, observe that the second sum vanishes as $\|\mathbf{v}\| \to 0$ and that the first sum, $\sum_{k=1}^{n} v_k D_{\mathbf{e}_k} f(\mathbf{a}+\mathbf{u}_{k-1})$, converges to $\mathbf{v} \cdot \nabla f(\mathbf{a})$. □

Chain rule

When we are working in $\mathbb{R}$ we know that, if g and h are differentiable, then $f(t) = g \circ h(t)$ is also differentiable and also $f'(t) = g'(h(t))\, h'(t)$. This is called the *chain rule* and is frequently very useful in calculating derivatives. We now investigate how this extends to higher dimension?

Example. Suppose that $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^3$ describes the position $\boldsymbol{\alpha}(t)$ at time t and that $f : \mathbb{R}^3 \to \mathbb{R}$ describes the temperature $f(\boldsymbol{\alpha})$ at a point $\boldsymbol{\alpha}$ The temperature at time t is equal to $g(t) = f(\boldsymbol{\alpha}(t))$. We want to calculate $g'(t)$ because this is the change in temperature with respect to time.

In situations like the above example it is convenient to consider the derivative of a path $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$. Let $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$ and suppose it has the form $\boldsymbol{\alpha}(t) = (\alpha_1(t), \ldots, \alpha_n(t))$. We define the derivative as

$$\boldsymbol{\alpha}'(t) := \begin{pmatrix} x_1'(t) \\ \vdots \\ x_n'(t) \end{pmatrix}.$$

Here $\boldsymbol{\alpha}'$ is a vector-valued function which represents the "direction of movement".

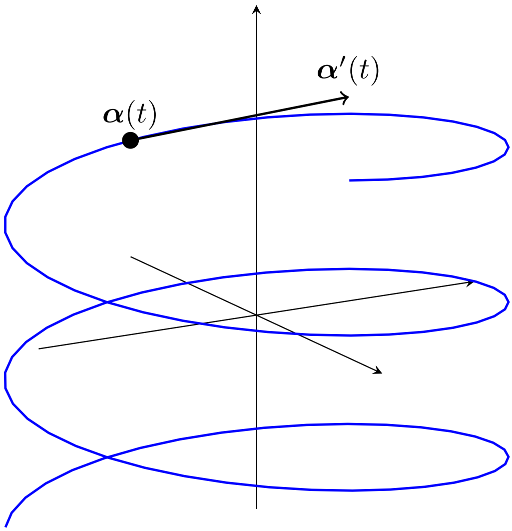


FIGURE 2.4: $\boldsymbol{\alpha}(t) = (\cos t, \sin t, t), t \in \mathbb{R}$.

Theorem. *Let $S \subset \mathbb{R}^n$ be open and $I \subset \mathbb{R}$ an interval. Let $\mathbf{x} : I \to S$ and $f : S \to \mathbb{R}$ and define, for $t \in I$,*

$$g(t) = f(\mathbf{x}(t)).$$

Suppose that $t \in I$ is such that $\mathbf{x}'(t)$ exists and f is differentiable at $\mathbf{x}(t)$. Then $g'(t)$ exists and

$$g'(t) = \nabla f(\mathbf{x}(t)) \cdot \mathbf{x}'(t).$$

Proof. Let $h > 0$ be small,

$$\begin{aligned}\frac{1}{h}[g(t+h) - g(t)] &= \frac{1}{h}[f(\mathbf{x}(t+h) - f(\mathbf{x}(t)))] \\ &= \frac{1}{h}\nabla f(\mathbf{x}(t)) \cdot (\mathbf{x}(t+h) - \mathbf{x}(t)) \\ &\quad + \frac{1}{h}\|\mathbf{x}(t+h) - \mathbf{x}(t)\| E(\mathbf{x}(t), \mathbf{x}(t+h) - \mathbf{x}(t)).\end{aligned}$$

Observe that $\frac{1}{h}(\mathbf{x}(t+h) - \mathbf{x}(t)) \to \mathbf{x}'(t)$ as $h \to 0$. $\square$

Example. A particle moves in a circle and its position at time $t \in [0, 2\pi]$ is given by

$$\mathbf{x}(t) = (\cos t, \sin t).$$

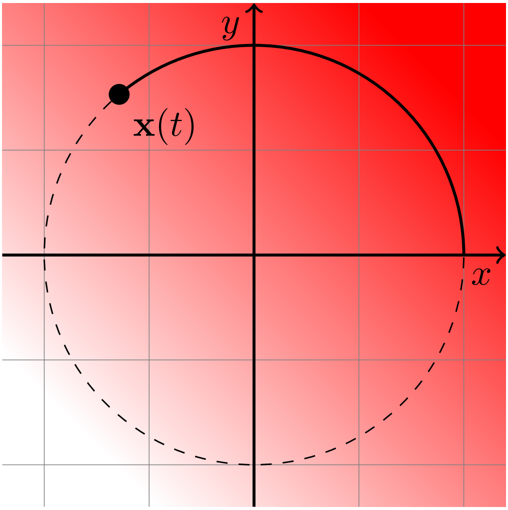


FIGURE 2.5: $\mathbf{x}(t)$ is the position of a particle. Shading represents temperature f.

The temperature at a point $\mathbf{y} = (y_1, y_2)$ is given by the function $f(\mathbf{y}) := y_1 + y_2$, The temperature the particle experiences at time t is given by $g(t) = f(\mathbf{x}(t))$. Temperature change: $g'(t) = \nabla f(\mathbf{x}(t)) \cdot \mathbf{x}'(t) = \left(\begin{smallmatrix}1\\1\end{smallmatrix}\right) \cdot \left(\begin{smallmatrix}-\sin t\\ \cos t\end{smallmatrix}\right) = \cos t - \sin t$.

2.3 Level sets & tangent planes

Let $S \subset \mathbb{R}^2$, $f : S \to \mathbb{R}$. Suppose $c \in \mathbb{R}$ and let

$$L(c) = \{\mathbf{x} \in S : f(\mathbf{x}) = c\}.$$

The set $L(c)$ is called the *level set*. In general this set can be empty or it can be all of S. However the set $L(c)$ is often a curve and this is the case of interest. This is the same notion as that of contour lines on a map. I.e., $\mathbf{x}(t_a) = \mathbf{a}$ for some $t_a \in I$ and

$$f(\mathbf{x}(t)) = c$$

for all $t \in I$. Then

- ▷ $\nabla f(\mathbf{a})$ is normal to the curve at $\mathbf{a}$
- ▷ Tangent line at $\mathbf{a}$ is $\{\mathbf{x} \in \mathbb{R}^2 : \nabla f(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) = 0\}$

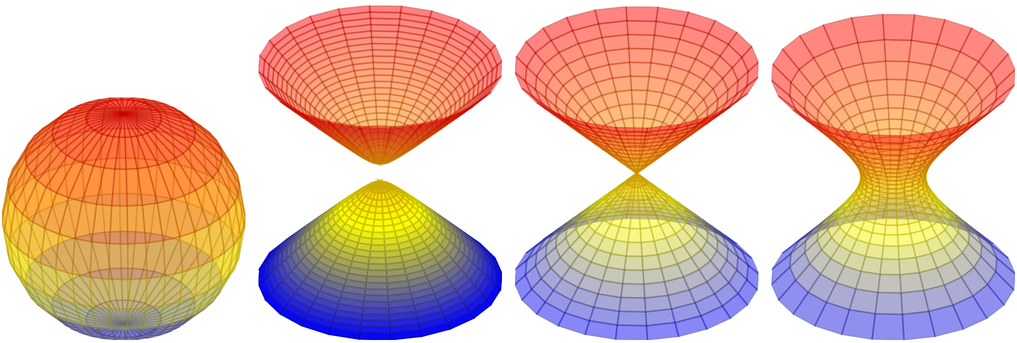
This is because the chain rule implies that $\nabla f(\mathbf{x}(t)) \cdot \mathbf{x}'(t) = 0$.

Example. Let $f(x_1, x_2, x_3) := x_1^2 + x_2^2 + x_3^2$.

- ▷ If $c > 0$ then $L(c)$ is a sphere,
- ▷ $L(0)$ is a single point $(0, 0, 0)$,
- ▷ If $c < 0$ then $L(c)$ is empty.

Example. Let $f(x_1, x_2, x_3) := x_1^2 + x_2^2 - x_3^2$. See Figure 2.6.

- ▷ If $c > 0$ then $L(c)$ is a one-sheeted hyperboloid,
- ▷ $L(0)$ is an infinite cone,
- ▷ If $c < 0$ then $L(c)$ is a two-sheeted hyperboloid.



(A) Sphere (B) 2-sheet hyperboloid (C) Infinite cone (D) 1-sheet hyperboloid

FIGURE 2.6: Various surfaces as level sets.

Let f be a differentiable scalar field on $S \subset \mathbb{R}^3$ and suppose that the level set $L(c) = \{\mathbf{x} \in S : f(\mathbf{x}) = c\}$ defines a surface.

- ▷ The gradient $\nabla f(\mathbf{a})$ is normal to every curve $\boldsymbol{\alpha}(t)$ in the surface which passes through $\mathbf{a}$,
- ▷ The tangent plane at $\mathbf{a}$ is $\{\mathbf{x} \in \mathbb{R}^3 : \nabla f(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) = 0\}$.

Same argument as in $\mathbb{R}^2$ works in $\mathbb{R}^n$.

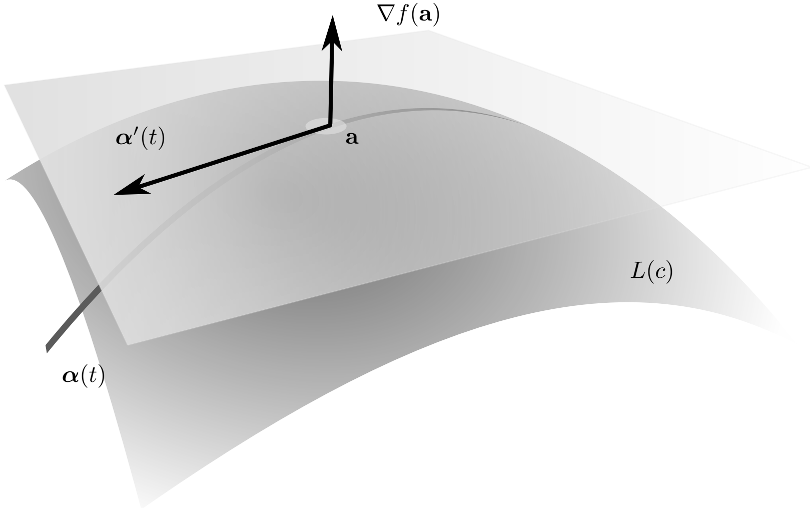


FIGURE 2.7: Tangent plane and normal vector

2.4 Derivatives of vector fields

Essentially everything discussed above for scalar fields extends to vector fields in a predictable way. This is because of the linearity and that we can consider each *component* of the vector field independently.

Definition 2.20 (directional derivative)**.** Let $S \subset \mathbb{R}^n$ and $\mathbf{f} : S \to \mathbb{R}^m$. For any $\mathbf{a} \in \operatorname{int} S$ and $\mathbf{v} \in \mathbb{R}^n$ the derivative of the vector field $\mathbf{f}$ with respect to $\mathbf{v}$ is defined as

$$D_{\mathbf{v}}\mathbf{f}(\mathbf{a}) := \lim_{h \to 0} \frac{1}{h} \left(\mathbf{f}(\mathbf{a} + h\mathbf{v}) - \mathbf{f}(\mathbf{a}) \right).$$

Remark 2.21. If we use the notation $\mathbf{f} = (f_1, \ldots, f_m)$, i.e., we write the function using the "components" where each f_k is a scalar field, then $D_{\mathbf{v}}\mathbf{f} = (D_{\mathbf{v}} f_1, \ldots, D_{\mathbf{v}} f_m)$.

Definition (differentiable)**.** We say that $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ is *differentiable* at $\mathbf{a}$ if there exists a linear transformation $d\mathbf{f}_{\mathbf{a}} : \mathbb{R}^n \to \mathbb{R}^m$ such that, for $\mathbf{x} \in B(\mathbf{a}, r)$,

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{a}) + d\mathbf{f}_{\mathbf{a}}(\mathbf{x} - \mathbf{a}) + \epsilon(\mathbf{x} - \mathbf{a})$$

$|\epsilon(\mathbf{x} - \mathbf{a})| = o(\|\mathbf{x} - \mathbf{a}\|)$.

Theorem 2.22. *If* $\mathbf{f}$ *is differentiable at* $\mathbf{a}$ *then* $\mathbf{f}$ *is continuous at* $\mathbf{a}$ *and* $df_{\mathbf{a}}(\mathbf{v}) = D_{\mathbf{v}}\mathbf{f}(\mathbf{a})$.

Proof. Same as for the case of scalar fields when $f : \mathbb{R}^n \to \mathbb{R}$. □

2.5 Jacobian matrix & the chain rule

The relevant differential for higher-dimensional functions is the Jacobian matrix.

Definition 2.23 (Jacobian matrix)**.** Suppose that $\mathbf{f} : \mathbb{R}^2 \to \mathbb{R}^2$ and use the notation $\mathbf{f}(x, y) = (f_1(x, y), f_2(x, y))$. The *Jacobian matrix* of $\mathbf{f}$ at $\mathbf{a}$ is defined as

$$D\mathbf{f}(\mathbf{a}) = \begin{pmatrix} \frac{\partial f_1}{\partial x}(\mathbf{a}) & \frac{\partial f_1}{\partial y}(\mathbf{a}) \\ \frac{\partial f_2}{\partial x}(\mathbf{a}) & \frac{\partial f_2}{\partial y}(\mathbf{a}) \end{pmatrix}.$$

The *Jacobian matrix* is defined analogously in any dimension. I.e., if $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ the the Jacobian at $\mathbf{a}$ is

$$D\mathbf{f}(\mathbf{a}) = \begin{pmatrix} \partial_1 f_1(\mathbf{a}) & \partial_2 f_1(\mathbf{a}) & \cdots & \partial_n f_1(\mathbf{a}) \\ \partial_1 f_2(\mathbf{a}) & \partial_2 f_2(\mathbf{a}) & \cdots & \partial_n f_2(\mathbf{a}) \\ \vdots & \vdots & & \vdots \\ \partial_1 f_m(\mathbf{a}) & \partial_2 f_m(\mathbf{a}) & \cdots & \partial_n f_m(\mathbf{a}) \end{pmatrix}$$

If we choose a basis then any linear transformation $\mathbb{R}^n \to \mathbb{R}^m$ can be written as a $m \times n$ matrix. We find that $df_{\mathbf{a}}(\mathbf{v}) = D\mathbf{f}(\mathbf{a})\mathbf{v}$.

Let $S \subset \mathbb{R}^n$ and $\mathbf{f} : S \to \mathbb{R}^m$. If f is differentiable at $\mathbf{a} \in S$ then, for all $\mathbf{x} \in B(\mathbf{a}, r) \subset S$,

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{a}) + D\mathbf{f}(\mathbf{a})(\mathbf{x} - \mathbf{a}) + \epsilon(\mathbf{x} - \mathbf{a})$$

where $|\epsilon(\mathbf{x} - \mathbf{a})| = o(\|\mathbf{x} - \mathbf{a}\|)$. This is like a Taylor expansion in higher dimensions.

Here we see that in higher dimensions we have a matrix form of the chain rule.

Theorem 2.24. *Let $S \subset \mathbb{R}^l$, $T \subset \mathbb{R}^m$ be open. Let $\mathbf{f} : S \to T$ and $\mathbf{g} : T \to \mathbb{R}^n$ and define*

$$\mathbf{h} = \mathbf{g} \circ \mathbf{f} : S \to \mathbb{R}^n.$$

Let $\mathbf{a} \in S$. Suppose that $\mathbf{f}$ is differentiable at $\mathbf{a}$ and $\mathbf{g}$ is differentiable at $\mathbf{f}(\mathbf{a})$. Then $\mathbf{h}$ is differentiable at $\mathbf{a}$ and

$$D\mathbf{h}(\mathbf{a}) = D\mathbf{g}(\mathbf{f}(\mathbf{a}))\, D\mathbf{f}(\mathbf{a}).$$

Proof. Let $\mathbf{u} = \mathbf{f}(\mathbf{a}+\mathbf{v}) - \mathbf{f}(\mathbf{a})$. Since $\mathbf{f}$ and $\mathbf{g}$ are differentiable,

$$\begin{aligned}\mathbf{h}(\mathbf{a}+\mathbf{v}) - \mathbf{h}(\mathbf{a}) &= \mathbf{g}(\mathbf{f}(\mathbf{a}+\mathbf{v})) - \mathbf{g}(\mathbf{f}(\mathbf{a})) \\ &= D\mathbf{g}(\mathbf{f}(\mathbf{a}))(\mathbf{f}(\mathbf{a}+\mathbf{v}) - \mathbf{f}(\mathbf{a})) + \boldsymbol{\epsilon}_{\mathbf{g}}(\mathbf{u}) \\ &= D\mathbf{g}(\mathbf{f}(\mathbf{a}))D\mathbf{f}(\mathbf{a})\mathbf{v} + D\mathbf{g}(\mathbf{f}(\mathbf{a}))\boldsymbol{\epsilon}_{\mathbf{f}}(\mathbf{v}) + \boldsymbol{\epsilon}_{\mathbf{g}}(\mathbf{u}).\end{aligned}$$

□

Example (polar coordinates)**.** Here we consider *polar coordinates* and calculate the Jacobian of this transformation. We can write the change of coordinates

$$(r,\theta) \mapsto (r\cos\theta, r\sin\theta)$$

as the function $\mathbf{f}(r,\theta) = (x(r,\theta), y(r,\theta))$ where $\mathbf{f} : (0,\infty) \times [0,2\pi) \to \mathbb{R}^2$. We calculate the Jacobian matrix of this transformation

$$D\mathbf{f}(r,\theta) = \begin{pmatrix} \frac{\partial x}{\partial r}(r,\theta) & \frac{\partial x}{\partial \theta}(r,\theta) \\ \frac{\partial y}{\partial r}(r,\theta) & \frac{\partial y}{\partial \theta}(r,\theta) \end{pmatrix} = \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix}.$$

In particular we see that $\det D\mathbf{f}(r,\theta) = r$, the familiar value used in change of variables with polar coordinated.

Suppose now that we wish to calculate derivatives of $h := g \circ \mathbf{f}$ for some $g : \mathbb{R}^2 \to \mathbb{R}$. Here we take advantage of Theorem 2.24.

$$Dh(r,\theta) = Dg(\mathbf{f}(r,\theta))\, D\mathbf{f}(r,\theta)$$

$$\begin{pmatrix} \frac{\partial h}{\partial r}(r,\theta) & \frac{\partial h}{\partial \theta}(r,\theta) \end{pmatrix} = \begin{pmatrix} \frac{\partial g}{\partial x}(\mathbf{f}(r,\theta)) & \frac{\partial g}{\partial y}(\mathbf{f}(r,\theta)) \end{pmatrix} \begin{pmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{pmatrix}$$

In other words, we have shown that

$$\begin{aligned}\frac{\partial h}{\partial r}(r,\theta) &= \frac{\partial g}{\partial x}(r\cos\theta, r\sin\theta)\cos\theta + \frac{\partial g}{\partial y}(r\cos\theta, r\sin\theta)\sin\theta \\ \frac{\partial h}{\partial \theta}(r,\theta) &= -r\frac{\partial g}{\partial x}(r\cos\theta, r\sin\theta)\sin\theta + r\frac{\partial g}{\partial y}(r\cos\theta, r\sin\theta)\cos\theta.\end{aligned}$$

2.6 Implicit functions & partial derivatives

Just like with derivatives, we can take higher order partial derivatives. For convenience when we want to write $\frac{\partial}{\partial y}\frac{\partial}{\partial x}f(x,y)$, i.e., differentiate first with respect to x and then with respect to y, we write instead $\frac{\partial^2 f}{\partial y \partial x}(x,y)$. The analogous notation is used for higher derivatives and any other choice of coordinates.

We first consider the question of when

$$\frac{\partial^2 f}{\partial y \partial x}(x,y) \overset{?}{=} \frac{\partial^2 f}{\partial x \partial y}(x,y).$$

Example (partial derivative problem)**.** Let $f : \mathbb{R}^2 \to \mathbb{R}$ be defined as $f(0,0) = 0$ and, for $(x,y) \neq (0,0)$,

$$f(x,y) := \frac{xy(x^2-y^2)}{x^2+y^2}.$$

We calculate that $\frac{\partial^2 f}{\partial y \partial x}(0,0) = -1$ but $\frac{\partial^2 f}{\partial x \partial y}(0,0) = 1$.

Theorem 2.25. *Let $f : S \to \mathbb{R}$ be a scalar field such that the partial derivatives $\frac{\partial f}{\partial x}$, $\frac{\partial f}{\partial y}$ and $\frac{\partial^2 f}{\partial y \partial x}$ exist on an open set $S \subset \mathbb{R}^2$ containing $\mathbf{x}$. Further assume that $\frac{\partial^2 f}{\partial y \partial x}$ is continuous on S. Then the derivative $\frac{\partial^2 f}{\partial x \partial y}(\mathbf{x})$ exists and*

$$\frac{\partial^2 f}{\partial x \partial y}(\mathbf{x}) = \frac{\partial^2 f}{\partial y \partial x}(\mathbf{x}).$$

In many cases we can choose to write a given curve/function either in *implicit* or *explicit* form.

Implicit	Explicit
$x^2 - y = 0$	$y(x) = x^2$
$x^2 + y^2 = 1$	$y(x) = \pm\sqrt{1-x^2}$, $\lvert x\rvert \leq 1$
$x^2 - y^2 - 1 = 0$	$y(x) = \pm\sqrt{x^2-1}$, $\lvert x\rvert \geq 1$
$x^2 + y^2 - e^y - 4 = 0$	A mess?
$x^2y^4 - 3 = \sin(xy)$	A huge mess?

Given the above observation, the following method of calculating derivatives is sometimes useful. Suppose that some $f : \mathbb{R}^2 \to \mathbb{R}$ is given and we suppose there exists some $y : \mathbb{R} \to \mathbb{R}$ such that

$$f(x, y(x)) = 0 \quad \text{for all } x.$$

Let $h(x) := f(x, y(x))$ and note that $h'(x) = 0$. Here we are using the idea that $h = f \circ g$ where $g(x) = (x, y(x))$. By the chain rule $h'(x)$ is equal to

$$\begin{pmatrix} \frac{\partial f}{\partial x}(x, y(x)) & \frac{\partial f}{\partial y}(x, y(x)) \end{pmatrix} \begin{pmatrix} 1 \\ y'(x) \end{pmatrix} = 0.$$

Consequently

$$y'(x) = -\frac{\frac{\partial f}{\partial x}(x, y(x))}{\frac{\partial f}{\partial y}(x, y(x))}.$$

Chapter 3

Extrema & other applications

In the previous chapter we introduced various notions of differentials for higher dimensional functions (scalar fields, vector fields, paths, etc.). In this chapter we now explore various applications of these notions and work with some of the implementations, rather than just the objects. Firstly we will consider certain partial differential equations which we now have the tools to solve. Then the majority of the chapter is devoted to searching for extrema (minima / maxima) in various different scenarios. This extends what we already know for functions in $\mathbb{R}$ and we will find that in higher dimensions many more possibilities and subtleties exist.

3.1 Partial differential equations

There are a huge number of different types of partial differential equations (PDEs) and here we consider just two types, *first order linear PDEs* and the *1D wave equation*. We start by consider an example of the first type.

Example. Find all solutions of the PDE, $3\frac{\partial f}{\partial x}(x,y) + 2\frac{\partial f}{\partial y}(x,y) = 0$.

Solution. The given PDE is equivalent to $\left(\begin{smallmatrix}3\\2\end{smallmatrix}\right) \cdot \nabla f(x,y) = 0$. We can also phrase this in terms of the directional derivative, namely

$$D_{\mathbf{v}} f(x,y) = 0 \quad \text{where } \mathbf{v} = \left(\begin{smallmatrix}3\\2\end{smallmatrix}\right).$$

This means that if a function f is a solution to the PDE then it is constant in the direction $\left(\begin{smallmatrix}3\\2\end{smallmatrix}\right)$. This means that all solutions have the form $f(x,y) = g(2x-3y)$ for some $g : \mathbb{R} \to \mathbb{R}$. □

The same idea as used for the above example gives the following general result.

Theorem 3.1. *Let $g : \mathbb{R} \to \mathbb{R}$ be differentiable, $a, b \in \mathbb{R}$, $(a, b) \neq (0, 0)$. If $f(x, y) = g(bx - ay)$ then*

$$a\frac{\partial f}{\partial x}(x,y) + b\frac{\partial f}{\partial y}(x,y) = 0.$$

Conversely, every f which satisfies this equation is of the form $g(bx - ay)$.

Proof. First we prove **(⇒)**. If $f(x, y) = g(bx - ay)$ then, by the chain rule,

$$\partial_x f(x,y) = bg'(bx - ay), \quad \partial_y f(x,y) = -ag'(bx - ay).$$

Consequently $a\partial_x f(x, y) + b\partial_y f(x, y) = abg'(bx - ay) - abg'(bx - ay) = 0$. Now we prove **(⇐)**. It's convenient to work in coordinates which correspond to the lines along which the solutions are constant. Let $\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right) = \left(\begin{smallmatrix} a & b \\ b & -a \end{smallmatrix}\right)\left(\begin{smallmatrix} x \\ y \end{smallmatrix}\right)$. This means that $\left(\begin{smallmatrix} x \\ y \end{smallmatrix}\right) = \frac{-1}{a^2+b^2}\left(\begin{smallmatrix} a & b \\ b & -a \end{smallmatrix}\right)\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right)$. Let $h(u, v) = f(\frac{au+bv}{a^2+b^2}, \frac{bu-av}{a^2+b^2})$. We calculate that

$$\partial_u h(u,v) = \tfrac{1}{a^2+b^2}\left(a\partial_x f + b\partial_y f\right)(au + bv, bu - av) = 0.$$

Namely, $h(u, v)$ is a function of v only and does not depend on u so we take $g(v) = h(u, v)$ and so $f(x, y) = g(bx - ay)$. □

Now we look at another type of PDE. The *1D wave equation* is

$$\frac{\partial^2 f}{\partial x^2}(x,t) = c^2\frac{\partial^2 f}{\partial t^2}(x,t).$$

Here x represents the position along string, t is time and $f(x, t)$ is the displacement of the string from the centre at position x, at time t. The constant c is a fixed parameter depending on the string.

This partial differential equation is derived from the equation of motion $F = ma$ where F is the tension in the string, a is the acceleration from horizontal and m is the mass of a little piece of the string. The equation is valid for small displacement. In this case the *boundary conditions* are natural: Are the ends of the string fixed? Is only one end fixed? At time $t = 0$, is the string already moving?

Theorem 3.2. *Let F be a twice differentiable function and G a differentiable function.*
1. *The function defined as*

$$f(x,t) = \frac{1}{2}(F(x+ct) + F(x-ct)) + \frac{1}{2c}\int_{x-ct}^{x+ct} G(s)\,ds \tag{3.1}$$

satisfies $\frac{\partial^2 f}{\partial x^2}(x,t) = c^2\frac{\partial^2 f}{\partial t^2}(x,t)$, $f(x,0) = F(x)$ *and* $\frac{\partial f}{\partial t}(x,0) = G(x)$.
2. *Conversely, if a solution of*

$$\frac{\partial^2 f}{\partial x^2}(x,t) = c^2\frac{\partial^2 f}{\partial t^2}(x,t)$$

satisfies $\frac{\partial^2 f}{\partial x\partial t} = \frac{\partial^2 f}{\partial t\partial x}$, *then it has the above form* (3.1).

Proof of part 1. Let $f(x,t)$ be as defined (3.1) in the statement of the theorem. We calculate the partial derivatives

$$\begin{aligned}
\tfrac{\partial f}{\partial x}(x,t) &= \tfrac{1}{2}\left(F'(x+ct) + F'(x-ct)\right) \\
&\qquad + \tfrac{1}{2c}\left(G(x+ct) - G(x-ct)\right) \\
\tfrac{\partial^2 f}{\partial x^2}(x,t) &= \tfrac{1}{2}\left(F''(x+ct) + F''(x-ct)\right) \\
&\qquad + \tfrac{1}{2c}\left(G'(x+ct) - G'(x-ct)\right) \\
\tfrac{\partial f}{\partial t}(x,t) &= \tfrac{1}{2}\left(cF'(x+ct) - cF'(x-ct)\right) \\
&\qquad + \tfrac{1}{2}\left(G(x+ct) + G(x-ct)\right) \\
\tfrac{\partial^2 f}{\partial t^2} f(x,t) &= \tfrac{1}{2}\left(c^2F''(x+ct) + c^2F''(x-ct)\right) \\
&\qquad + \tfrac{c}{2}\left(G'(x+ct) + G'(x-ct)\right).
\end{aligned}$$

From this calculation we see that $\frac{\partial^2 f}{\partial x^2}(x,t) = c^2\frac{\partial^2 f}{\partial t^2}(x,t)$. Additionally we have $f(x,0) = F(x)$ and $\frac{\partial f}{\partial t}(x,0) = G(x)$. □

Proof of part 2. Suppose that f satisfies the 1D wave equation; Introduce $u = x+ct$, $v = x-ct$ and observe that $x = \frac{u+v}{2}$, $t = \frac{u-v}{2c}$. Define $g(u,v) = f(\frac{u+v}{2}, \frac{u-v}{2c})$. By the chain rule

$$\begin{aligned}
\tfrac{\partial g}{\partial u}(u,v) &= \tfrac{1}{2}\tfrac{\partial f}{\partial x}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right) + \tfrac{1}{2c}\tfrac{\partial f}{\partial t}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right), \\
\tfrac{\partial^2 g}{\partial v\partial u}(u,v) &= \tfrac{1}{4}\tfrac{\partial^2 f}{\partial x^2}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right) - \tfrac{1}{4c}\tfrac{\partial^2 f}{\partial x\partial t}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right) \\
&\qquad + \tfrac{1}{4c}\tfrac{\partial^2 f}{\partial x\partial t}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right) - \tfrac{1}{4c^2}\tfrac{\partial^2 f}{\partial t^2}\left(\tfrac{u+v}{2}, \tfrac{u-v}{2c}\right) = 0.
\end{aligned}$$

Since the second derivative is zero we know that $\frac{\partial g}{\partial u}$ is constant in v, therefore we can write $\frac{\partial g}{\partial u}(u,v) = \varphi_0(u)$. In turn this means we can write $g(u,v) = \varphi_1(u) + \varphi_2(v)$. I.e., $f(x,t) = \varphi_1(x+ct) + \varphi_2(x-ct)$. Let

$$F(x) = \varphi_1(x) + \varphi_2(x).$$

This means that $F'(x) = \varphi_1'(x) + \varphi_2'(x)$ and $\frac{\partial f}{\partial t}(x,t) = c\varphi_1(x+ct) - c\varphi_2(x-ct)$. Let

$$G(x) = \frac{\partial f}{\partial t}(x,0) = c\varphi_1(x) - c\varphi_2(x).$$

□

Substituting these quantities we show that the required form (3.1) is satisfied.

3.2 Extrema (minima / maxima / saddle)

Let $S \subset \mathbb{R}^n$ be open, $f : S \to \mathbb{R}$ be a scalar field and $\mathbf{a} \in S$.

Definition 3.3 (absolute min/max)**.** If $f(\mathbf{a}) \leq f(\mathbf{x})$ (resp. $f(\mathbf{a}) \geq f(\mathbf{x})$) for all $\mathbf{x} \in S$, then $f(\mathbf{a})$ is said to be the *absolute* minimum (resp. maximum) of f.

Definition 3.4 (relative min/max)**.** If $f(\mathbf{a}) \leq f(\mathbf{x})$ (resp. $f(\mathbf{a}) \geq f(\mathbf{x})$) for all $\mathbf{x} \in B(\mathbf{a}, r)$ for some $r > 0$, then $f(\mathbf{a})$ is said to be a *relative* minimum (resp. maximum) of f.

Collectively we call the these points the *extrema* of the scalar field. In the case of a scalar field defined on $\mathbb{R}^2$ we can visualize the scalar field as a 3D plot like Figure 3.1. Here we see the extrema as the "flat" places. We sometimes use *global* as a synonym of *absolute* and *local* as a synonym of *relative*.

To proceed it is convenient to connect the extrema with the behaviour of the gradient of the scalar field.

Theorem 3.5. *If $f : S \to \mathbb{R}$ is differentiable and has a relative minimum or maximum at $\mathbf{a}$, then $\nabla f(\mathbf{a}) = \mathbf{0}$.*

Proof. Suppose f has a relative minimum at $\mathbf{a}$ (or consider $-f$). For any unit vector $\mathbf{v}$ let $g(u) = f(\mathbf{a} + u\mathbf{v})$. We know that $g : \mathbb{R} \to \mathbb{R}$ has a relative minimum at $u = 0$ so $u'(0) = 0$. This means that the directional derivative $D_{\mathbf{v}} f(\mathbf{a}) = 0$ for every $\mathbf{v}$. Consequently this means that $\nabla f(\mathbf{a}) = \mathbf{0}$. □

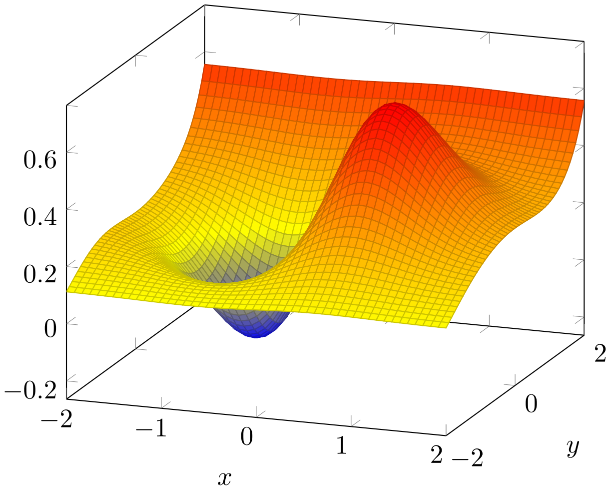


FIGURE 3.1: $f(x,y) := xe^{-(x^2y^2)} + \frac{1}{4}e^{y^{\frac{3}{10}}}$

Observe that here and in the subsequent text, we can always consider the case of $f : \mathbb{R} \to \mathbb{R}$, i.e., the case of $\mathbb{R}^n$ where $n = 1$. Everything still holds and reduces to the arguments and formulae previously developed for functions of one variable.

Definition 3.6 (stationary point)**.** If $\nabla f(\mathbf{a}) = \mathbf{0}$ then $\mathbf{a}$ is called a *stationary point*.

As we see in the example of Figure 3.2, the converse of Theorem 3.5 fails in the sense that a stationary point might not be a minimum or a maximum. The motivates the following.

Definition 3.7 (saddle point)**.** If $\nabla f(\mathbf{a}) = \mathbf{0}$ and $\mathbf{a}$ is neither a minimum nor a maximum then $\mathbf{a}$ is said to be a *saddle point*.

The quintessential saddle has the shape seen in Figure 3.4. However it might be similar to Figure 3.2 or more complicated using the possibilities available in higher dimension.

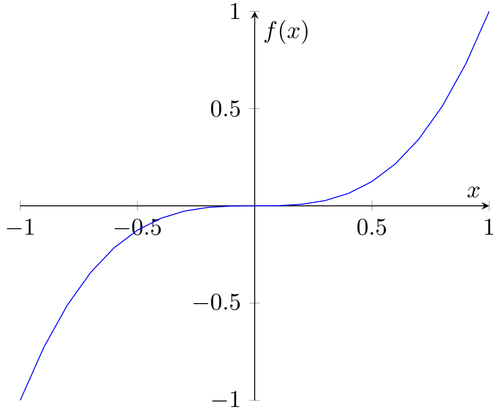


Figure 3.2: $\nabla f(\mathbf{a}) = \mathbf{0}$ doesn't imply a minimum or maximum at $\mathbf{a}$, even in $\mathbb{R}$, as seen with the function $f(x) := x^3$. In higher dimensions even more is possible.

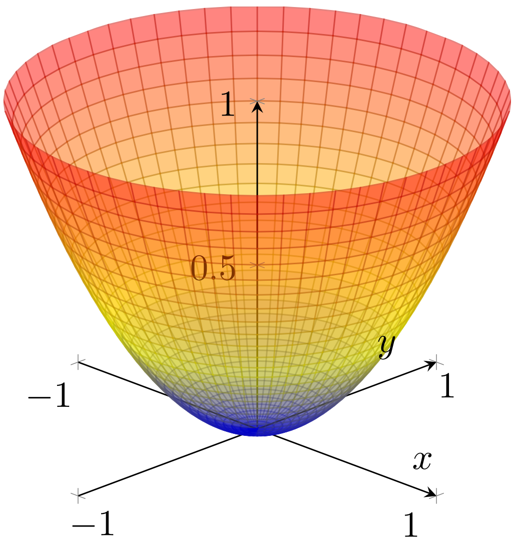


Figure 3.3: If $f(x, y) = x^2 + y^2$ then $\nabla f(x, y) = \binom{2x}{2y}$ and $\nabla f(0, 0) = \binom{0}{0}$. The point $(0, 0)$ is an absolute minimum for f.

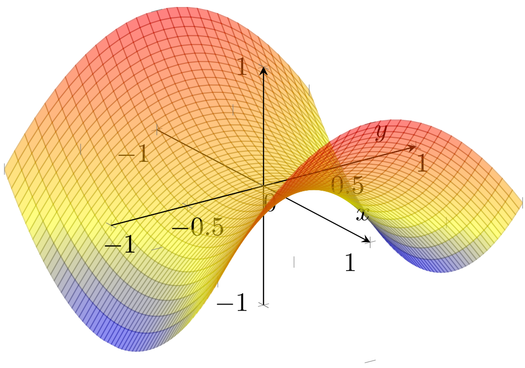


FIGURE 3.4: If $f(x,y) = x^2 - y^2$ then $\nabla f(x,y) = \begin{pmatrix} 2x \\ -2y \end{pmatrix}$ and $\nabla f(0,0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. The point $(0,0)$ is a saddle point for f.

3.3 Hessian matrix

To proceed it is useful to develop the idea of a second order Taylor expansion in this higher dimensional setting. In particular this will allow us to identify the local behaviour close to stationary points. The main object for doing this is the *Hessian matrix*.

Definition 3.8 (Hessian matrix)**.** Let $f : \mathbb{R}^2 \to \mathbb{R}$ be twice differentiable and use the notation $f(x,y)$. The *Hessian matrix* at $\mathbf{a} \in \mathbb{R}^2$ is defined as

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

Observe that the Hessian matrix $\mathbf{H}f(\mathbf{a})$ is a symmetric matrix since we know that $\frac{\partial^2 f}{\partial x\,\partial y}(\mathbf{a}) = \frac{\partial^2 f}{\partial y\,\partial x}(\mathbf{a})$ for twice differentiable functions (Theorem 2.25). The Hessian matrix is defined analogously in any dimensions as follows. Let $f : \mathbb{R}^n \to \mathbb{R}$ be twice differentiable. The *Hessian matrix* at $\mathbf{a} \in \mathbb{R}^n$ is defined as

$$\mathbf{H}f(\mathbf{a}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2}(\mathbf{a}) & \frac{\partial^2 f}{\partial x_1\,\partial x_2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n}(\mathbf{a}) \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1}(\mathbf{a}) & \frac{\partial^2 f}{\partial x_2^2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n}(\mathbf{a}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1}(\mathbf{a}) & \frac{\partial^2 f}{\partial x_n\,\partial x_2}(\mathbf{a}) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(\mathbf{a}) \end{pmatrix}.$$

Observe that the Hessian matrix is a real symmetric matrix in any dimension. If $f : \mathbb{R} \to \mathbb{R}$ then $\mathbf{H}f(a)$ is a 1×1 matrix and coincides with the second derivative of f. In this sense what we know about extrema in $\mathbb{R}$ is just a special case of everything we do here.

Lemma. *If* $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$ *then*[1] $\mathbf{v^t}\,\mathbf{H}f(\mathbf{a})\,\mathbf{v} = \sum_{j,k=0}^{n} \partial_j\partial_k f(\mathbf{a}) v_j v_k \in \mathbb{R}$.

Proof. Multiplying the matrices we calculate that[2]

$$\begin{aligned} \mathbf{v^t}\,\mathbf{H}f(\mathbf{a})\,\mathbf{v} &= \begin{pmatrix} v_1 & \cdots & v_n \end{pmatrix} \begin{pmatrix} \partial_1\partial_1 f(\mathbf{a}) & \cdots & \partial_1\partial_n f(\mathbf{a}) \\ \vdots & \ddots & \vdots \\ \partial_n\partial_1 f(\mathbf{a}) & \cdots & \partial_n\partial_n f(\mathbf{a}) \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \\ &= \sum_{j,k=0}^{n} \partial_j\partial_k f(\mathbf{a}) v_j v_k \end{aligned}$$

as required. □

Example. Let $f(x, y) = x^2 - y^2$ (Figure 3.4). The gradient and the Hessian are respectively

$$\begin{aligned} \nabla f(x,y) &= \begin{pmatrix} \frac{\partial f}{\partial x}(x,y) \\ \frac{\partial f}{\partial y}(x,y) \end{pmatrix} = \begin{pmatrix} 2x \\ -2y \end{pmatrix}, \\ \mathbf{H}f(x,y) &= \begin{pmatrix} \frac{\partial^2 f}{\partial x^2}(x,y) & \frac{\partial^2 f}{\partial x\,\partial y}(x,y) \\ \frac{\partial^2 f}{\partial y\,\partial x}(x,y) & \frac{\partial^2 f}{\partial y^2}(x,y) \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}. \end{aligned}$$

[1] The notation $\mathbf{v^t}$ denotes the transpose of the vector $\mathbf{v}$.

[2] For convenience, here and in many other places of this text, we use the notation $\partial_j\partial_k f(\mathbf{a}) = \frac{\partial^2 f}{\partial x_j\,\partial x_k}(\mathbf{a})$.

The point $(0,0)$ is a stationary point since $\nabla f(0,0) = \left(\begin{smallmatrix}0\\0\end{smallmatrix}\right)$. In this example $\mathbf{H}f$ does not depend on (x,y) but in general we can expect dependence and so it gives a different matrix at different points (x,y).

Second order Taylor formula for scalar fields

First let's recall the first order Taylor approximation from Theorem 2.18. If f is differentiable at $\mathbf{a}$ then $f(\mathbf{x}) \approx f(\mathbf{a}) + \nabla f(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a})$. If $\mathbf{a}$ is a stationary point then this only tells us that $f(\mathbf{x}) \approx f(\mathbf{a})$ so a natural next question is to search for slightly more detailed information.

Theorem 3.9 (second order Taylor)**.** *Let f be a scalar field twice differentiable on $B(\mathbf{a}, r)$. Then,*[a] *for $\mathbf{x}$ close to $\mathbf{a}$,*

$$f(\mathbf{x}) \approx f(\mathbf{a}) + \nabla f(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) + \frac{1}{2}(\mathbf{x} - \mathbf{a})^{\mathbf{t}}\, \mathbf{H}f(\mathbf{a})\, (\mathbf{x} - \mathbf{a})$$

in the sense that the error is $o(\|(\mathbf{x} - \mathbf{a})\|^2)$.

[a] We use the convention that $(\mathbf{x} - \mathbf{a})$ is a vertical vector, equivalently, a $n \times 1$ matrix.

Proof. Let $\mathbf{v} = \mathbf{x} - \mathbf{a}$ and let $g(u) = f(\mathbf{a} + u\mathbf{v})$. The Taylor expansion of g tells us that $g(1) = g(0) + g'(0) + \frac{1}{2}g''(c)$ for some $c \in (0,1)$. Since $g(u) = f(a_1 + uv_1, \ldots, a_n + uv_n)$, by the chain rule,

$$\begin{aligned} g'(u) &= \sum_{j=1}^{n} \partial_j f(a_1 + uv_1, \ldots, a_n + uv_n) v_j = \nabla f(\mathbf{a} + u\mathbf{v}) \cdot \mathbf{v}, \\ g''(u) &= \sum_{j,k=1}^{n} \partial_j \partial_k f(a_1 + uv_1, \ldots, a_n + uv_n) v_j v_k \\ &= \mathbf{v}^{\mathbf{t}}\, \mathbf{H}f(\mathbf{a} + u\mathbf{v})\, \mathbf{v}. \end{aligned}$$

Consequently $f(\mathbf{a} + \mathbf{v}) = f(\mathbf{a}) + \nabla f(\mathbf{a}) \cdot \mathbf{v} + \frac{1}{2}\mathbf{v}^{\mathbf{t}}\, \mathbf{H}f(\mathbf{a} + c\mathbf{v})\, \mathbf{v}$. We define the "error" in the approximation as $\epsilon(\mathbf{v}) = \frac{1}{2}\mathbf{v}^{\mathbf{t}}(\mathbf{H}f(\mathbf{a} + c\mathbf{v}) - \mathbf{H}f(\mathbf{a}))\mathbf{v}$ and estimate that

$$|\epsilon(\mathbf{v})| \leq \sum_{j,k=0}^{n} v_j v_k \left(\partial_j \partial_k f(\mathbf{a} + c\mathbf{v}) - \partial_j \partial_k f(\mathbf{a})\right).$$

Since $|v_j v_k| \leq \|\mathbf{v}\|^2$ we observe that $\frac{|\epsilon(\mathbf{v})|}{\|\mathbf{v}\|^2} \to 0$ as $\|\mathbf{v}\| \to 0$ as required. □

3.4 Classifying stationary points

In order to classify the stationary points we will take advantage of the Hessian matrix and therefore we need to first understand the follow fact about real symmetric matrices.

Theorem 3.10. *Let A be a real symmetric matrix and let $Q(\mathbf{v}) = \mathbf{v}^{\mathbf{t}} A\mathbf{v}$. Then*

$$\begin{aligned} Q(\mathbf{v}) > 0 \text{ for all } \mathbf{v} \neq \mathbf{0} \quad &\iff \quad \text{all eigenvalues of } A \text{ are positive,} \\ Q(\mathbf{v}) < 0 \text{ for all } \mathbf{v} \neq \mathbf{0} \quad &\iff \quad \text{all eigenvalues of } A \text{ are negative.} \end{aligned}$$

Proof. Since A is symmetric it can be diagonalised by matrix B which is orthogonal ($B^{\mathbf{t}} = B^{-1}$) and the diagonal matrix $D = B^{\mathbf{t}}AB$ has the eigenvalues of A as the diagonal. This means that $Q(\mathbf{v}) = \mathbf{v}^{\mathbf{t}}B^{\mathbf{t}}BAB^{\mathbf{t}}B\mathbf{v} = \mathbf{w}^{\mathbf{t}}D\mathbf{w}$ where $\mathbf{w} = B\mathbf{v}$. Consequently $Q(\mathbf{v}) = \sum_j \lambda_j w_j^2$. Observe that, if all $\lambda_j > 0$ then $\sum_j \lambda_j w_j^2 > 0$.

In order to prove the other direction in the "if and only if" statement, observe that $Q(B\mathbf{u}_k) = \lambda_k$. This means that, if $Q(\mathbf{v}) > 0$ for all $\mathbf{v} \neq \mathbf{0}$ then $\lambda_k > 0$ for all k. □

Theorem 3.11 (classification of stationary points)**.** *Let f be a scalar field twice differentiable on $B(\mathbf{a}, r)$. Suppose $\nabla f(\mathbf{a}) = \mathbf{0}$ and consider the eigenvalues of $\mathbf{H}f(\mathbf{a})$. Then*

$$\begin{aligned} \text{All eigenvalues are positive} \quad &\implies \quad \text{relative minimum at } \mathbf{a}, \\ \text{All eigenvalues are negative} \quad &\implies \quad \text{relative maximum at } \mathbf{a}, \\ \text{Some positive, some negative} \quad &\implies \quad \mathbf{a} \text{ is a saddle point.} \end{aligned}$$

Proof. Let $Q(\mathbf{v}) = \mathbf{v}^{\mathbf{t}}\mathbf{H}f(\mathbf{a})\mathbf{v}$, $\mathbf{w} = B\mathbf{v}$ and let $\Lambda := \min_j \lambda_j$. Observe that $\|\mathbf{w}\| = \|\mathbf{v}\|$ and that $Q(\mathbf{v}) = \sum_j \lambda_j w_j^2 \geq \Lambda \sum_j w_j^2 = \Lambda \|\mathbf{v}\|^2$. We have them 2nd-order Taylor

$$\begin{aligned} f(\mathbf{a} + \mathbf{v}) - f(\mathbf{a}) &= \frac{1}{2}\mathbf{v}^{\mathbf{t}}\, \mathbf{H}f(\mathbf{a})\, \mathbf{v} + \epsilon(\mathbf{v}) \\ &\geq \left(\tfrac{\Lambda}{2} - \tfrac{\epsilon(\mathbf{v})}{\|\mathbf{v}\|^2}\right) \|\mathbf{v}\|^2 . \end{aligned}$$

Since $\frac{|\epsilon(\mathbf{v})|}{\|\mathbf{v}\|^2} \to 0$ as $\|\mathbf{v}\| \to 0$, $\frac{|\epsilon(\mathbf{v})|}{\|\mathbf{v}\|^2} < \frac{\Lambda}{2}$ when $\|\mathbf{v}\|$ is small. The argument is analogous for the second part. For final part consider $\mathbf{v}_j$ which is the eigenvector for λ_j and apply the argument of the first or second part. □

3.5 Attaining extreme values

Here we explore the extreme value theorem for continuous scalar fields. The argument will be in two parts: Firstly we show that continuity implies boundedness; Secondly we show that boundedness implies that the maximum and minimum are attained. We use the following notation for *intervals* / *rectangles* / *cuboids* / *tesseracts*, etc. If $\mathbf{a} = (a_1, \dots, a_n)$ and $\mathbf{b} = (b_1, \dots, b_n)$ then we consider the n-dimensional closed Cartesian product

$$[\mathbf{a}, \mathbf{b}] = [a_1, b_1] \times \cdots \times [a_n, b_n].$$

We call this set a *rectangle* (independent of the dimension). As a first step it is convenient to know that all sequences in our setting have convergent subsequences.

Theorem 3.12 (Bolzano–Weierstrass)**.** *If* $\{\mathbf{x}_n\}_n$ *is a sequence in* $[\mathbf{a}, \mathbf{b}]$ *there exists a convergent subsequence* $\{\mathbf{x}_{n_j}\}_j$.

Proof. In order to prove the theorem we construct the subsequence. Firstly we divide $[\mathbf{a}, \mathbf{b}]$ into sub-rectangles of size half the original. We then choose a sub-rectangle which contains infinite elements of the sequence and choose the first of these elements to be part of the sub-sequence. We repeat this process by again dividing the sub-rectangle we chose by half and choosing the next element of the subsequence. We repeat to give the full subsequence. □

Theorem 3.13 (boundedness of continuous scalar fields)**.** *Suppose that* f *is a scalar field continuous at every point in the closed rectangle* $[\mathbf{a}, \mathbf{b}]$. *Then* f *is bounded on* $[\mathbf{a}, \mathbf{b}]$ *in the sense that there exists* $C > 0$ *such that* $|f(\mathbf{x})| \leq C$ *for all* $\mathbf{x} \in [\mathbf{a}, \mathbf{b}]$.

Proof. Suppose the contrary: for all $n \in \mathbb{N}$ there exists $\mathbf{x}_n \in [\mathbf{a}, \mathbf{b}]$ such that $|f(\mathbf{x}_n)| > n$. Bolzano–Weierstrass theorem means that there exists a subsequence $\{\mathbf{x}_{n_j}\}_j$ converges to $\mathbf{x} \in [\mathbf{a}, \mathbf{b}]$. Continuity of f means that $f(\mathbf{x}_{n_j})$ converges to $f(\mathbf{x})$. This is a contradiction and hence the theorem is proved. □

We can now use the above result on the boundedness in order to show that the extreme values are actually obtained.

Theorem 3.14 (extreme value theorem). *Suppose that f is a scalar field continuous at every point in the closed rectangle $[\mathbf{a}, \mathbf{b}]$. There there exist points $\mathbf{x}, \mathbf{y} \in [\mathbf{a}, \mathbf{b}]$ such that*

$$f(\mathbf{x}) = \inf f \quad \textit{and} \quad f(\mathbf{y}) = \sup f.$$

Proof. By the boundedness theorem $\sup f$ is finite and so there exists a sequence $\{\mathbf{x}_n\}_n$ such that $f(\mathbf{x}_n)$ converges to $\sup f$. Bolzano–Weierstrass theorem implies that there exists a subsequence $\{\mathbf{x}_{n_j}\}_j$ which converges to $\mathbf{x} \in [\mathbf{a}, \mathbf{b}]$. By continuity $f(\mathbf{x}_n) \to f(\mathbf{x}) = \sup f$. □

3.6 Extrema with constraints (Lagrange multipliers)

We now consider a slightly different problem to the one earlier in this chapter. There we wished to find the extrema of a given scalar field. Here the general problem is to minimise or maximise a given scalar field $f(x, y)$ under the constraint $g(x, y) = 0$. Subsequently we will also consider the same problem but in higher dimensions. We can visualize this problem as shown in Figure 3.5. For this graphic representation we draw the constraint and also various level sets of the function that we want to find the extrema of. The graphical representation suggests to us that at the "touching point" the gradient vectors are parallel. In other words, $\nabla f = \lambda \nabla g$ for some $\lambda \in \mathbb{R}$. The implementation of this idea is the method of Lagrange multipliers.

Theorem 3.15 (Lagrange multipliers in 2D). *Suppose that a differentiable scalar field $f(x, y)$ has a relative minimum or maximum when it is subject to the constraint*

$$g(x, y) = 0.$$

Then there exists a scalar λ such that, at the extremum point,

$$\nabla f = \lambda \nabla g.$$

In three dimensions a similar result holds.

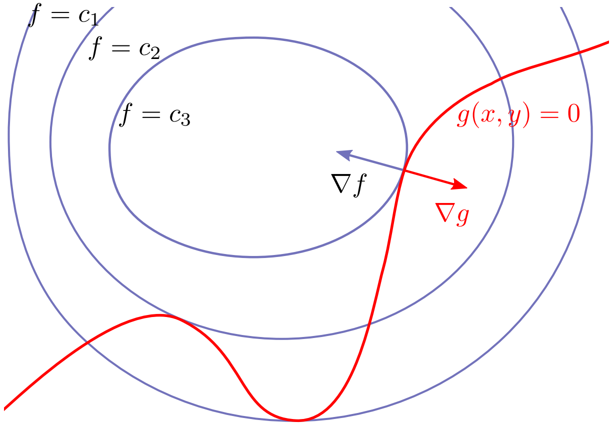


FIGURE 3.5: Searching extrema of f under constraint $g = 0$

Theorem 3.16 (Lagrange multipliers in 3D). *Suppose that a differentiable scalar field $f(x, y, z)$ has a relative minimum or maximum when it is subject to the constraints*

$$g_1(x, y, z) = 0, \quad g_2(x, y, z) = 0$$

and the ∇g_k are linearly independent. Then there exist scalars λ_1, λ_2 such that, at the extremum point,

$$\nabla f = \lambda_1 \nabla g_1 + \lambda_2 \nabla g_2.$$

In higher dimensions and possibly with additional constraints we have the following general theorem.

Theorem (Lagrange multipliers). *Suppose that a differentiable scalar field $f(x_1, \ldots, x_n)$ has an relative extrema when it is subject to m constraints*

$$g_1(x_1, \ldots, x_n) = 0, \ldots, g_m(x_1, \ldots, x_n) = 0,$$

where $m < n$, and the ∇g_k are all linearly independent. Then there exist m scalars $\lambda_1, \ldots, \lambda_m$ such that, at each extremum point,

$$\nabla f = \lambda_1 \nabla g_1 + \cdots + \lambda_m \nabla g_m.$$

The Lagrange multiplier method is often stated and far less often proved. Since the proof is rather involved we will follow this tradition here. See, for example, Chapter 14 of "A First Course in Real Analysis" (2012) by Protter & Morrey for a complete proof and further discussion.

Let us consider a particular case of the method when $n = 3$ and $m = 2$. More precisely we consider the following problem: Find the maxima and minima of $f(x, y, z)$ along the curve C defined as

$$g_1(x, y, z) = 0, \quad g_2(x, y, z) = 0$$

where g_1, g_2 are differentiable functions. In this particular case we will prove the Lagrange multiplier method. Suppose that $\mathbf{a}$ is some point in the curve. Let $\boldsymbol{\alpha}(t)$ denote a path which lies in the curve C in the sense that $\boldsymbol{\alpha}(t) \in C$ for all $t \in (-1, 1)$, $\boldsymbol{\alpha}'(t) \neq \mathbf{0}$ and $\boldsymbol{\alpha}(0) = \mathbf{a}$. If $\mathbf{a}$ is a local minimum for f restricted to C it means that $f(\boldsymbol{\alpha}(t)) \geq f(\boldsymbol{\alpha}(0))$ for all $t \in (-\delta, \delta)$ for some $\delta > 0$. In words, moving away from $\mathbf{a}$ along the curve C doesn't cause $f(\mathbf{x})$ to decrease. Let $h(t) = f(\boldsymbol{\alpha}(t))$ and observe that $h : \mathbb{R} \to \mathbb{R}$ so we know how to find the extrema. In particular we know that $h'(0) = 0$. By the chain rule $h'(t) = \nabla f(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)$ and so

$$\nabla f(\mathbf{a}) \cdot \boldsymbol{\alpha}'(0) = 0.$$

Since we know that $g_1(\boldsymbol{\alpha}(t)) = 0$ and $g_2(\boldsymbol{\alpha}(t)) = 0$, again by the chain rule,

$$\nabla g_1(\mathbf{a}) \cdot \boldsymbol{\alpha}'(0) = 0, \quad \nabla g_2(\mathbf{a}) \cdot \boldsymbol{\alpha}'(0) = 0.$$

To proceed it is convenient to isolate the following result of linear algebra.

Lemma. *Consider* $w, u_1, u_2 \in \mathbb{R}^3$ *and let* $V = \{v : u_k \cdot v = 0, k = 1, 2\}$. *If* $w \cdot v = 0$ *for all* $v \in V$ *then* $w = \lambda_1 u_1 + \lambda_2 u_2$ *for some* $\lambda_1, \lambda_2 \in \mathbb{R}$.

Proof. We can write $w = \lambda_1 u_1 + \lambda_2 u_2 + v_0$ where $v_0 \in V$ because u_1, u_2 together with V must span $\mathbb{R}^3$. Since $v_0 \in V$ and, by assumption, $w \cdot v_0 = 0$,

$$0 = w \cdot v_0 = (\lambda_1 u_1 + \lambda_2 u_2 + v_0) \cdot v_0 = v_0 \cdot v_0 = \|v_0\|^2.$$

This means that $v_0 = 0$ and so $w = \lambda_1 u_1 + \lambda_2 u_2$. □

The above lemma also holds in any dimension with any number of vectors with the analogous proof. Applying this lemma to the vectors $\nabla f(\mathbf{a})$, $\nabla g_1(\mathbf{a})$ and $\nabla g_2(\mathbf{a})$ recovers exactly the Lagrange multiplier method in this setting.

Chapter 4

Curves & line integrals

Curves have played a part in earlier parts of the course and now we turn our attention to precisely what we mean by this notion. Up until now we relied more on an intuition, an idea of some type of 1D subset of higher dimensional space. We will also define how we can integrate scalar and vector fields along these curves. These types of integrals have a natural and important physical relevance. We will then study some of the properties of these integrals. To start let's recall a random selection of curves we have already seen:

Circle	$x^2 + y^2 = 4$
Semi-circle	$x^2 + y^2 = 4, \ x \geq 0$
Ellipse	$\frac{1}{4}x^2 + \frac{1}{9}y^2 = 4$
Line	$y = 5x + 2$
Line (in 3D)	$x + 2y + 3z = 0, \ x = 4y$
Parabola (in 3D)	$y = x^2, \ z = x$

In the above list the curves are written in a way where we are describing a set of points using certain constraint or constraints. In some cases in *implicit* form, in some cases in *explicit* form. For example, for the circle we formally mean the set $\{(x, y) : x^2 + y^2 = 4\}$. We have the idea that the curves should be sets which are single connected pieces and we vaguely have an idea that we need curves that are sufficiently smooth. To proceed we need a precise definition of the 1D objects we can work with. As part of the definition we force a structure which really allows us to work with these objects in a useful way.

4.1 Curves, paths & line integrals

Let $\boldsymbol{\alpha} : [a, b] \to \mathbb{R}^n$ be continuous. For convenience, in components we write $\boldsymbol{\alpha}(t) = (\alpha_1(t), \ldots, \alpha_n(t))$. We say that $\boldsymbol{\alpha}(t)$ is *differentiable* if each component $\alpha_k(t)$ is differentiable on $[a, b]$ and $\alpha_k'(t)$ is continuous (Definition 2.16). We say that $\boldsymbol{\alpha}(t)$ is *piecewise differentiable* if $[a, b] = [a, c_1] \cup [c_1, c_2] \cup \cdots \cup [c_l, b]$ and $\boldsymbol{\alpha}(t)$ is *differentiable* on each of these intervals.

Definition 4.1. If $\boldsymbol{\alpha} : [a, b] \to \mathbb{R}^n$ is piecewise differentiable then we call it a *path*.

Note that different functions can trace out the *same* curve in different ways. Also note that a path has an inherent direction. We say that this is a *parametric representation* of a given curve. We already saw examples of paths in Figure 2.4 and Figure 2.5. A few examples of paths are as follows.

$$\begin{aligned}
\boldsymbol{\alpha}(t) &= (t, t), & t &\in [0, 1] \\
\boldsymbol{\alpha}(t) &= (\cos t, \sin t), & t &\in [0, 2\pi] \\
\boldsymbol{\alpha}(t) &= (\cos t, \sin t), & t &\in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}] \\
\boldsymbol{\alpha}(t) &= (\cos t, -\sin t), & t &\in [0, 2\pi] \\
\boldsymbol{\alpha}(t) &= (t, t, t), & t &\in [0, 1] \\
\boldsymbol{\alpha}(t) &= (\cos t, \sin t, t), & t &\in [-10, 10]
\end{aligned}$$

Observe how some of these paths represent the same curve, perhaps traversed in a different direction.

Let $\boldsymbol{\alpha}(t)$ be a (piecewise differentiable) path on $[a, b]$ and let $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ be a continuous vector field. Recall that we consider $\boldsymbol{\alpha}'(t)$ and $\mathbf{f}(\mathbf{x})$ as n-vectors. I.e., in the case $n = 2$, then $\boldsymbol{\alpha}'(t) = \begin{pmatrix} \alpha_1'(t) \\ \alpha_2'(t) \end{pmatrix}$ and $\mathbf{f}(\mathbf{x}) = \begin{pmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{pmatrix}$.

Definition 4.2 (line integral of a vector field)**.** The *line integral* of the vector field $\mathbf{f}$ along the path $\boldsymbol{\alpha}$ is defined as

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_a^b \mathbf{f}(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)\, dt.$$

Sometimes the same integral is written as $\int_C \mathbf{f} \cdot d\boldsymbol{\alpha}$ to emphasize that the integral is along the curve C. Alternatively the integral is sometimes written as $\int f_1 \, d\alpha_1 + \cdots + f_n \, d\alpha_n$ or $\int f_1 \, dx_1 + \cdots + f_n \, dx_n$. Each of these different notations are in common usage in different contexts but the underlying quantity is always the same.

Example. Consider the vector field $\mathbf{f}(x, y) = \begin{pmatrix} \sqrt{y} \\ x^3+y \end{pmatrix}$ and the path $\boldsymbol{\alpha}(t) = (t^2, t^3)$ for $t \in (0, 1)$. Evaluate $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$.

Solution. We start by calculating

$$\boldsymbol{\alpha}'(t) = \begin{pmatrix} 2t \\ 3t^2 \end{pmatrix}, \quad \mathbf{f}(\boldsymbol{\alpha}(t)) = \begin{pmatrix} t^{\frac{3}{2}} \\ t^6 + t^3 \end{pmatrix}.$$

This means that $\mathbf{f}(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t) = 2t^{\frac{5}{2}} + 3t^8 + 3t^5$ and so

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_0^1 (2t^{\frac{5}{2}} + 3t^8 + 3t^5) \, dt = \frac{59}{42}. \qquad \square$$

4.2 Basic properties of the line integral

Having defined the line integral, the next step is to clarify its behaviour, in particular the following key properties.

Linearity: Suppose $\mathbf{f}, \mathbf{g}$ are vector fields and $\boldsymbol{\alpha}(t)$ is a path. For any $c, d \in \mathbb{R}$, then

$$\int (c\mathbf{f} + d\mathbf{g}) \cdot d\boldsymbol{\alpha} = c \int \mathbf{f} \cdot d\boldsymbol{\alpha} + d \int \mathbf{g} \cdot d\boldsymbol{\alpha}.$$

Joining / splitting paths: Suppose $\mathbf{f}$ is a vector field and that

$$\boldsymbol{\alpha}(t) = \begin{cases} \boldsymbol{\alpha}_1(t) & t \in [a, c] \\ \boldsymbol{\alpha}_2(t) & t \in [c, b] \end{cases}$$

is a path. Then

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int \mathbf{f} \cdot d\boldsymbol{\alpha}_1 + \int \mathbf{f} \cdot d\boldsymbol{\alpha}_2.$$

Alternatively, if we write C, C_1, C_2 for the corresponding curves, then

$$\int_C \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_{C_1} \mathbf{f} \cdot d\boldsymbol{\alpha} + \int_{C_2} \mathbf{f} \cdot d\boldsymbol{\alpha}.$$

As already mentioned, for a given curve there are many different choices of parametrization. For example, consider the curve $C = \{(x,y) : x^2 + y^2 = 1, y \geq 0\}$. This is a semi-circle and two possible parametrizations are $\boldsymbol{\alpha}(t) = (-t, \sqrt{1-t^2})$, $t \in [-1,1]$ and $\boldsymbol{\beta}(t) = (\cos t, \sin t)$, $t \in [0,\pi]$. These are just two possibilities among many possible choices. For a given curve, to what extent does the line integral depend on the choice of parametrization?

Definition 4.3 (equivalent paths)**.** We say that two paths $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ are *equivalent* if there exists a differentiable function $u : [c,d] \to [a,b]$ such that $\boldsymbol{\alpha}(u(t)) = \boldsymbol{\beta}(t)$. Furthermore, we say that $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ are

- ▷ *in the same direction* if $u(c) = a$ and $u(d) = b$,
- ▷ *in the opposite direction* if $u(c) = b$ and $u(d) = a$.

With this terminology we can precisely describe the dependence of the integral on the choice of parametrization.

Theorem 4.4 (change of parametrization)**.** *Let* $\mathbf{f}$ *be a continuous vector field and let* $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ *be equivalent paths. Then*

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \begin{cases} \int \mathbf{f} \cdot d\boldsymbol{\beta} & \textit{if the paths are in the same direction}, \\ -\int \mathbf{f} \cdot d\boldsymbol{\beta} & \textit{if the paths are in the opposite direction}. \end{cases}$$

Proof. Suppose that the paths are continuously differentiable path, decomposing if required. Since $\boldsymbol{\alpha}(u(t)) = \boldsymbol{\beta}(t)$ the chain rule implies that $\boldsymbol{\beta}'(t) = \boldsymbol{\alpha}'(u(t))\, u'(t)$. In particular

$$\int \mathbf{f} \cdot d\boldsymbol{\beta} = \int_c^d \mathbf{f}(\boldsymbol{\beta}(t)) \cdot \boldsymbol{\beta}'(t)\, dt = \int_c^d \mathbf{f}(\boldsymbol{\alpha}(u(t))) \cdot \boldsymbol{\alpha}'(u(t))\, u'(t)\, dt.$$

Changing variables, adding a minus sign if path is opposite direction because we need to swap the limits of integration, completes the proof. □

Gradients & work

Let $h(x,y)$ be a scalar field in $\mathbb{R}^2$ and recall that the gradient $\nabla h(x,y)$ is a vector field. Let $\boldsymbol{\alpha}(t)$, $t \in [0,1]$ be a path. Now let $g(t) = h(\boldsymbol{\alpha}(t))$, consider the derivative

$g'(t) = \nabla h(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)$ and evaluate the line integral

$$\int \nabla h \cdot d\boldsymbol{\alpha} = \int_0^1 \nabla h(\boldsymbol{\alpha}(t)) \cdot \alpha'(t)\, dt$$
$$= \int_0^1 g(t)\, dt = g(1) - g(0) = h(\boldsymbol{\alpha}(1)) - h(\boldsymbol{\alpha}(0)).$$

This equality has the following intuitive interpretation if we suppose for a moment that h denotes altitude. In this case the line integral is the sum of all the infinitesimal altitude changes and equals the total change in altitude.

As a first example of work in physics let's consider gravity. The gravitational field on earth is $\mathbf{f}(x, y, z) = \begin{pmatrix} 0 \\ 0 \\ mg \end{pmatrix}$. If we move a particle from $\mathbf{a} = (a_1, a_2, a_3)$ to $\mathbf{b} = (b_1, b_2, b_3)$ along the path $\boldsymbol{\alpha}(t)$, $t \in [0, 1]$ then the work done is defined as $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$. We calculate that

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_0^1 \mathbf{f}(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)\, dt = \int_0^1 mg\, \alpha_3'(t)\, dt$$
$$= mg\, [\alpha_3(t)]_0^1 = mg(b_3 - a_3).$$

This coincides we what we know, work done depends only on the change in height.

As a second example of work in physics let's consider a particle moving in a force field. Let $\mathbf{f}$ be the force field and let $\mathbf{x}(t)$ be the position at time t of a particle moving in the field. Let $\mathbf{v}(t) = \mathbf{x}'(t)$ be the velocity at time t of the particle and define kinetic energy as $\frac{m}{2} \|\mathbf{v}(t)\|^2$. According to Newton's law $\mathbf{f}(\mathbf{x}(t)) = m\mathbf{x}''(t) = m\mathbf{v}'(t)$ and so the work done is

$$\int \mathbf{f} \cdot d\mathbf{x} = \int_0^1 \mathbf{f}(\mathbf{x}(t)) \cdot \mathbf{v}(t)\, dt = \int_0^1 m\mathbf{v}'(t) \cdot \mathbf{v}(t)\, dt$$
$$= \int_0^1 \tfrac{d}{dt} \left(\tfrac{m}{2} \|\mathbf{v}(t)\|^2 \right) = \left(\tfrac{m}{2} \|\mathbf{v}(1)\|^2 - \tfrac{m}{2} \|\mathbf{v}(0)\|^2 \right)$$

In this case we see, as expected, the work done on the particle moving in the force field is equal to the change in kinetic energy.

4.3 The second fundamental theorem

Recall that, if $\varphi : \mathbb{R} \to \mathbb{R}$ is differentiable then $\int_a^b \varphi'(t)\, dt = \varphi(b) - \varphi(a)$. This is called the second fundamental theorem of calculus and is one of the ways in which we see that differentiation and integration are opposites. The analog for line integrals is the following.

Theorem 4.5 (2nd fundamental theorem in $\mathbb{R}^n$). *Suppose that φ is a continuously differentiable scalar field on $S \subset \mathbb{R}^n$ and suppose that $\boldsymbol{\alpha}(t)$, $t \in [a, b]$ is a path in S. Let $\mathbf{a} = \boldsymbol{\alpha}(a)$, $\mathbf{b} = \boldsymbol{\alpha}(b)$. Then*

$$\int \nabla\varphi \cdot d\boldsymbol{\alpha} = \varphi(\mathbf{b}) - \varphi(\mathbf{a}).$$

Proof. Suppose that $\boldsymbol{\alpha}(t)$ is differentiable. By the chain rule $\frac{d}{dt}\varphi(\boldsymbol{\alpha}(t)) = \nabla\varphi(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)$. Consequently

$$\int \nabla\varphi \cdot d\boldsymbol{\alpha} = \int_0^1 \nabla\varphi(\boldsymbol{\alpha}(t)) \cdot \boldsymbol{\alpha}'(t)\, dt = \int_0^1 \tfrac{d}{dt}\varphi(\boldsymbol{\alpha}(t))\, dt.$$

By the 2nd fundamental theorem in $\mathbb{R}$ we know that $\int_0^1 \frac{d}{dt}\varphi(\boldsymbol{\alpha}(t))\, dt = \varphi(\boldsymbol{\alpha}(b)) - \varphi(\boldsymbol{\alpha}(a))$. □

Example (potential energy). Our earth has mass M with centre at $(0, 0, 0)$. Suppose that there is a small particle close to earth which has mass m. The force field of gravitation and potential energy are, respectively,

$$\mathbf{f}(\mathbf{x}) = \frac{-GmM}{\|\mathbf{x}\|^3}\mathbf{x}, \quad \varphi(\mathbf{x}) = \frac{GmM}{\|\mathbf{x}\|}.$$

We can calculate $\nabla\varphi(\mathbf{x})$ and see that it is equal to $\mathbf{f}(\mathbf{x})$.

4.4 The first fundamental theorem

First we need to consider a basic topological property of sets. In particular we want to avoid the possibility of the set being several disconnected pieces, in other words we want to guarantee that we can get from one point to another in the set in a way without every leaving the set (see Figure 4.1).

Definition 4.6 (connected). The set $S \subset \mathbb{R}^n$ is said to be *connected* if, for every pair of points $\mathbf{a}, \mathbf{b} \in S$, there exists a path $\boldsymbol{\alpha}(t), t \in [a, b]$ such that

- ▷ $\boldsymbol{\alpha}(t) \in S$ for every $t \in [a, b]$,
- ▷ $\boldsymbol{\alpha}(a) = \mathbf{a}$ and $\boldsymbol{\alpha}(b) = \mathbf{b}$.

Sometimes this property is called "path connected" to distinguish between different notions.

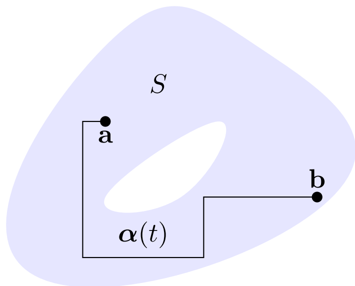


FIGURE 4.1: A connected set.

Recall that, if $f : \mathbb{R} \to \mathbb{R}$ is continuous and we let $\varphi(x) = \int_a^x f(t)\, dt$ then $\varphi'(x) = f(x)$. This is called the first fundamental theorem of calculus and is the other way in which we see that differentiation and integration are opposites. Again we have an analog for the line integral but here it becomes a little more subtle since there are many different paths along which we can integrate between any two points.

Theorem (1st fundamental theorem in $\mathbb{R}^n$). *Let* $\mathbf{f}$ *be a continuous vector field on a connected set* $S \subset \mathbb{R}^n$*. Suppose that, for* $\mathbf{x}, \mathbf{a} \in S$*, the line integral* $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$ *is equal for every path* $\boldsymbol{\alpha}$ *such that* $\boldsymbol{\alpha}(a) = \mathbf{a}$, $\boldsymbol{\alpha}(b) = \mathbf{x}$*. Fix* $\mathbf{a} \in S$ *and define* $\varphi(\mathbf{x}) = \int \mathbf{f} \cdot d\alpha$*. Then* φ *is continuously differentiable and* $\nabla\varphi = \mathbf{f}$.

Sketch of proof. As before let $\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $\mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, $\mathbf{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$. Observe that, if we define the paths $\boldsymbol{\beta}_k(t) = \mathbf{x} + t\mathbf{e}_k, t \in [0, h]$, then

$$\varphi(\mathbf{x} + h\mathbf{e}_k) - \varphi(\mathbf{x}) = \int \mathbf{f} \cdot d\boldsymbol{\beta}_k.$$

Moreover $\boldsymbol{\beta}_k'(t) = \mathbf{e}_k$. Consequently

$$\frac{\partial \varphi}{\partial x_k}(\mathbf{x}) = \lim_{h \to 0} \frac{1}{h}(\varphi(\mathbf{x} + h\mathbf{e}_k) - \varphi(\mathbf{x}))$$

$$= \lim_{h \to 0} \frac{1}{h} \int_0^h \mathbf{f}(\boldsymbol{\beta}_k(t)) \cdot \mathbf{e}_k \, dt = f_k(\mathbf{x}).$$

In other words, we have shown that $\nabla\varphi(\mathbf{x}) = \mathbf{f}(\mathbf{x})$. □

Definition 4.7 (closed path)**.** We say a path $\boldsymbol{\alpha}(t)$, $t \in [a, b]$ is *closed* if $\boldsymbol{\alpha}(a) = \boldsymbol{\alpha}(b)$.

Observe that, if $\boldsymbol{\alpha}(t)$, $t \in [a, b]$ is a closed path then we can divided it into two paths: Let $c \in [a, b]$ and consider the two paths $\boldsymbol{\alpha}(t)$, $t \in [a, c]$ and $\boldsymbol{\alpha}(t)$, $t \in [c, b]$. On the other hand, suppose $\boldsymbol{\alpha}(t)$, $t \in [a, b]$ and $\boldsymbol{\beta}(t)$, $t \in [c, d]$ are two path starting at $\mathbf{a}$ and finishing at $\mathbf{b}$. The these can be combined to define a closed path (by following one backward).

Definition 4.8 (conservative vector field)**.** A vector field $\mathbf{f}$, continuous on $S \subset \mathbb{R}^n$ is *conservative* if there exists a scalar field φ such that, on S,

$$\mathbf{f} = \nabla\varphi.$$

Note that some authors call such a vector field a *gradient* (i.e., the vector field is the gradient of some scalar). If $\mathbf{f} = \nabla\varphi$ then the scalar field φ is called the *potential* (associated to $\mathbf{f}$). Observe that that the potential is not unique, $\nabla\varphi = \nabla(\varphi + C)$ for any constant $C \in \mathbb{R}$.

Theorem 4.9 (conservative vector fields)**.** *Let $S \subset \mathbb{R}^n$ and and consider the vector field $\mathbf{f} : S \to \mathbb{R}^n$. The following are equivalent:*

(i) $\mathbf{f}$ *is conservative, i.e.,* $\mathbf{f} = \nabla\varphi$ *on S for some φ,*
(ii) $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$ *does not depend on $\boldsymbol{\alpha}$, as long as* $\boldsymbol{\alpha}(a) = \mathbf{a}$, $\boldsymbol{\alpha}(b) = \mathbf{b}$,
(iii) $\int \mathbf{f} \cdot d\boldsymbol{\alpha} = 0$ *for any closed path $\boldsymbol{\alpha}$ contained in S.*

Proof. In the previous theorems (the two fundamental theorems) we proved that (i) is equivalent to (ii).

Now we prove that (ii) implies (iii): Let $\boldsymbol{\alpha}(t)$ be a closed path and let $\boldsymbol{\beta}(t)$ be the same path in the opposite direction. Observe that $\int \mathbf{f} \cdot d\boldsymbol{\alpha} = -\int \mathbf{f} \cdot d\boldsymbol{\beta}$ but that $\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int \mathbf{f} \cdot d\boldsymbol{\beta}$ and so $\int \mathbf{f} \cdot d\boldsymbol{\alpha} = 0$.

It remains to prove that (iii) implies (ii): The two paths between $\mathbf{a}$ and $\mathbf{b}$ can be combined (with a minus sign) to give a closed path. □

Theorem 4.10 (mixed derivatives in 2D). *Suppose that $S \subset \mathbb{R}^2$ and that $\mathbf{f} : S \to \mathbb{R}^2$ is a differentiable vector field and write $\mathbf{f} = \left(\begin{smallmatrix} f_1 \\ f_2 \end{smallmatrix}\right)$.*
If $\mathbf{f}$ is conservative then, on S,

$$\frac{\partial f_1}{\partial y} = \frac{\partial f_2}{\partial x}.$$

The above result is a special case of the following general statement which holds in any dimension.

Theorem 4.11 (mixed derivatives). *Suppose that $\mathbf{f}$ is a differentiable vector field[a] on $S \subset \mathbb{R}^n$. If $\mathbf{f}$ is conservative then, for each l, k,*

$$\frac{\partial f_l}{\partial x_k} = \frac{\partial f_k}{\partial x_l}.$$

[a] As before $f_k(x_1, \ldots, x_n)$ denotes the k^{th} component of the vector field $\mathbf{f}$.

Proof. By assumption the second order partial derivatives exist and so

$$\frac{\partial f_l}{\partial x_k} = \frac{\partial^2 \varphi}{\partial x_k \partial x_l} = \frac{\partial^2 \varphi}{\partial x_l \partial x_k} = \frac{\partial f_k}{\partial x_l}.$$ □

Example. Consider the vector field

$$\mathbf{f}(x, y) = \begin{pmatrix} -y(x^2+y^2)^{-1} \\ x(x^2+y^2)^{-1} \end{pmatrix}$$

on $S = \mathbb{R}^2 \setminus (0, 0)$. Calculating we verify that $\frac{\partial f_1}{\partial y} = \frac{\partial f_2}{\partial x}$ on S. We now evaluate the line integral $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$ where $\boldsymbol{\alpha}(t) = (a \cos t, a \sin t)$, $t \in [0, 2\pi]$. We calculate that $\boldsymbol{\alpha}'(t) = \left(\begin{smallmatrix} -a \sin t \\ a \cos t \end{smallmatrix}\right)$ and $\mathbf{f}(\boldsymbol{\alpha}(t)) = \frac{1}{a^2}\left(\begin{smallmatrix} -a \sin t \\ a \cos t \end{smallmatrix}\right)$. This means that

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_0^{2\pi} (\sin^2 t + \cos^2 t)\, dt = 2\pi.$$

Observe that in the above example S is somehow not a "nice" set because of the "hole" in the middle. Moreover, observe that the line integral is the same for any circle, independent of the radius.

Theorem 4.11 isn't really useful in showing that a vector field is conservative because it is possible for the mixed partial derivatives to all be equal but still the field fail to be conservative. On the other hand, if a pair of mixed derivatives is not equal then $\mathbf{f}$ is *not* conservative and so it is useful for proving the negative. Later in this chapter we will return to this topic.

4.5 Potentials & conservative vector fields

We now turn our attention to the following question: Suppose we are given a vector field $\mathbf{f}$ and we know that $\mathbf{f} = \nabla\varphi$ for some φ. How can we find φ? For this we consider two methods in the following paragraphs. First we describe the method which we call

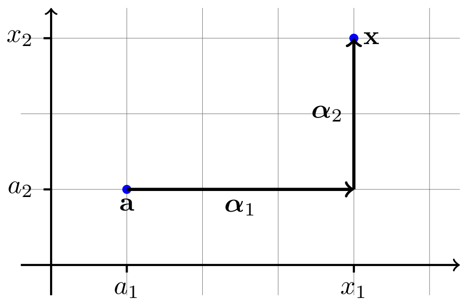


Figure 4.2: The paths $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$.

constructing a potential by line integral. Suppose that $\mathbf{f}$ is a conservative vector field on the rectangle $[a_1, b_1] \times [a_2, b_2]$. We define $\varphi(\mathbf{x})$ as the line integral $\int \mathbf{f} \cdot d\boldsymbol{\alpha}$ where $\boldsymbol{\alpha}$ is a path between $\mathbf{a} = (a_1, a_2)$ and $\mathbf{x}$. For any $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$ consider the two paths:

$$\boldsymbol{\alpha}_1(t) = (t, a_2), t \in [a_1, x_1],$$
$$\boldsymbol{\alpha}_2(t) = (x_1, t), t \in [a_2, x_2].$$

Let $\boldsymbol{\alpha}(t)$ denote the concatenation of the two paths. We calculate that

$$\int \mathbf{f} \cdot d\boldsymbol{\alpha} = \int_{a_1}^{x_1} \mathbf{f}(\boldsymbol{\alpha}_1(t)) \cdot \boldsymbol{\alpha}_1'(t)\, dt + \int_{a_2}^{x_2} \mathbf{f}(\boldsymbol{\alpha}_2(t)) \cdot \boldsymbol{\alpha}_2'(t)\, dt.$$

This means that $\varphi(\mathbf{x}) = \int_{a_1}^{x_1} f_1(t, a_2)\, dt + \int_{a_2}^{x_2} f_2(x_1, t)\, dt$.

Now we describe a different method which we describe as *constructing a potential by indefinite integrals*. Again suppose that $\mathbf{f} = \nabla\varphi$ for some scalar field $\varphi(x, y)$ which we wish to find. Observe that $\frac{\partial\varphi}{\partial x} = f_1$ and $\frac{\partial\varphi}{\partial y} = f_2$. This means that

$$\int_a^x f_1(t, y)\, dt + A(y) = \varphi(x, y) = \int_b^y f_2(x, t)\, dt + B(x)$$

where $A(y)$, $B(x)$ are constants of integration. Calculating and comparing we can then obtain a formula for $\varphi(x, y)$.

Example. Find a potential for $\mathbf{f}(x, y) = \begin{pmatrix} e^x y^2 + 1 \\ 2e^x y \end{pmatrix}$ on $\mathbb{R}^2$.

Solution. We calculate that

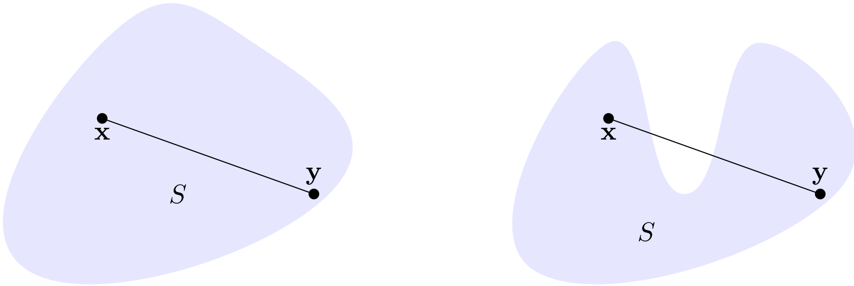
$$\int_a^x f_1(t, y)\, dt + A(y) = e^x y^2 + x + A(y) = \varphi(x, y),$$

$$\int_b^y f_2(x, t)\, dt + B(x) = e^x y^2 + B(x) = \varphi(x, y).$$

From this we see that we can choose $A(y) = 0$ and $B(x) = x$ to obtain equality of the above quantities. Consequently we obtain the potential $\varphi(x, y) = e^x y^2 + x$. □

Theorem 4.11 concerning conservative fields and the mixed partial derivatives was somewhat less than satisfactory since the converse wasn't possible. In order to get a more satisfactory result we need to look at another topological details of the domain of the vector field. This concept is somewhat suggested by the methods of constructing potentials which were described above.

Definition 4.12 (convex set)**.** A set $S \subset \mathbb{R}^n$ is said to be *convex* if for any $\mathbf{x}, \mathbf{y} \in S$ the segment $\{t\mathbf{x} + (1 - t)\mathbf{y}, t \in [0, 1]\}$ is contained in S.



(A) A convex set. (B) A set which is not convex.

FIGURE 4.3: Convex and non-convex sets.

This extra property permits the following sufficient condition for a vector field to be conservative.

Theorem 4.13 (conservative fields on convex sets)**.** *Let*[a] $\mathbf{f}$ *be a differentiable vector field on a convex region* $S \subset \mathbb{R}^n$*. Then* $\mathbf{f}$ *is conservative if and only if*

$$\frac{\partial f_l}{\partial x_k} = \frac{\partial f_k}{\partial x_l}, \quad \textit{for each } l, k.$$

[a] As usual $f_k(x_1, \ldots, x_n)$ denotes the k^{th} component of the vector field $\mathbf{f}$.

Sketch of proof. We have already proved that $\mathbf{f}$ being conservative implies the equality of partial derivatives (Theorem 4.11) and therefore we need only assume that $\partial_g f_l = \partial_l f_k$ and construct a potential. Let $\varphi(\mathbf{x}) = \int \mathbf{f} \cdot d\boldsymbol{\alpha}$ where $\boldsymbol{\alpha}(t) = t\mathbf{x}$, $t \in [0, 1]$. Since $\boldsymbol{\alpha}'(t) = \mathbf{x}$, $\varphi(\mathbf{x}) = \int_0^1 \mathbf{f}(t\mathbf{x}) \cdot \mathbf{x}\, dt$. Also (needs proving)

$$\frac{\partial \varphi}{\partial x_k}(t\mathbf{x}) = \int_0^1 (t\partial_k \mathbf{f}(t\mathbf{x}) \cdot \mathbf{x} + f_k(t\mathbf{x}))\ dt.$$

This is equal to $\int_0^1 (t\nabla f_k(t\mathbf{x}) \cdot \mathbf{x} + f_k(t\mathbf{x}))\ dt$ because $\partial_g f_l = \partial_l f_k$; By the chain rule applied to $g(t) = t\nabla f_k(t\mathbf{x})$ this is equal to $f_k(\mathbf{x})$ as required. $\square$

The above gives us a useful tool to check if a given vector field is conservative. Using the idea of "gluing together" several convex regions this result can be manually extended to some more general settings. Later, in Theorem 5.7, we will take advantage of some further ideas in order to significantly extend this result.

Application to exact differential equations

Let $S \subset \mathbb{R}^2$ be simply-connected and open. The differential equation, considered on S,

$$p(x, y) + q(x, y)y'(x) = 0$$

is called *exact* if there exists $\varphi : S \to \mathbb{R}$ such that $p = \frac{\partial \varphi}{\partial x}$ and $q = \frac{\partial \varphi}{\partial y}$. Exact differential equations are closely related to conservative vector fields.

Theorem 4.14. *Let $S \subset \mathbb{R}^2$ be connected and open.*

- ▷ *Suppose that $\varphi : S \to \mathbb{R}$ satisfies $\nabla\varphi = \left(\begin{smallmatrix} p \\ q \end{smallmatrix}\right)$. Then the solution $y(x)$ of the equation $p(x, y) + q(x, y)y'(x) = 0$ satisfies $\varphi(x, y(x)) = C$ for some $C \in \mathbb{R}$.*
- ▷ *Conversely, if $\varphi : S \to \mathbb{R}$ is such that $\varphi(x, y(x)) = C$ defines implicitly a function $y(x)$, then $y(x)$ is a solution to the equation $p(x, y) + q(x, y)y'(x) = 0$.*

Proof. If $y(x)$ satisfies $\varphi(x, y(x)) = C$, then by the chain rule and the fact that $\nabla\varphi = \left(\begin{smallmatrix} p \\ q \end{smallmatrix}\right)$, we see that $p(x, y(x)) + y'(x)q(x, y(x)) = 0$. Conversely, if $y(x)$ is a solution, $\varphi(x, y(x))$ must be constant in x. □

Example. Solve $y^2 + 2xyy' = 0$. Let $p(x, y) = y^2$, $q(x, y) = 2xy$ and find $\varphi(x, y) = xy^2$ so $\nabla\varphi = \left(\begin{smallmatrix} p \\ q \end{smallmatrix}\right)$. Solutions satisfy $\varphi(x, y(x)) = xy(x)^2 = C$, i.e., $y(x) = \sqrt{\frac{C}{x}}$.

4.6 Line integrals of scalar fields

Up until now this chapter has been devoted to line integrals of vector fields but there is also the obvious question of defining the line integral for scalar fields. This we do now. Such a line integral allows us also to define the *length of a curve* in a meaningful way. Let $\boldsymbol{\alpha}(t)$, $t \in [a, b]$ be a path in $\mathbb{R}^n$ and let $f : \mathbb{R}^n \to \mathbb{R}$.

Definition 4.15 (line integral of a scalar field)**.** The *line integral* of the scalar field f along the path $\boldsymbol{\alpha}$ is defined as

$$\int f \, d\alpha = \int_a^b f(\alpha(t)) \, \|\boldsymbol{\alpha}'(t)\| \, dt.$$

This integral shares the same basic properties of the line integral of a vector field and the proofs are essentially the same. Namely it is linear and also respects how a path can be decomposed or joined with other paths which changing the value of the integral. Moreover, the value of the integral along a given path is independent of the choice of parametrization of the curve. In this case, even if the curve is parametrized in the opposite direction then the integral takes the same value. Consequently it makes sense to define the length of the curve as the line integral of the unit scalar field, i.e., the length of a curve parametrized by the path $\boldsymbol{\alpha}$ is $\int_a^b \|\boldsymbol{\alpha}'(t)\| \, dt$.

As a simple application, consider that the path represents a wire and the wire has density $f(\boldsymbol{\alpha}(t))$ at the point $\boldsymbol{\alpha}(t)$. Then the mass of the wire is equal to $\int f \, d\alpha$.

Chapter 5

Multiple integrals

The extension to higher dimension of differentiation was established in the previous chapters. We then defined line integrals which are, in a sense, one dimensional integrals which exist in a high dimensional setting. We now take the next step and define higher dimensional integrals in the sense of how to integrate a scalar field defined on a subset of $\mathbb{R}^n$. The first step will be to rigorously define which scalar fields are integrable and to define the integral. Then we need to fine reasonable ways to evaluate such integrals. Among other applications we will use this multiple integrals to calculate volumes and moment of inertia. In Green's Theorem we find a connection between multiple integrals and line integrals. We also develop the important topic of change of variables which takes advantate of the Jacobian determinant and is often invaluable for actually working with a given problem.

5.1 Definition of the integral

First we need to find a definition of integrability and the integral. Then we will proceed to study the properties of this higher dimensional integral. Recall that, in the one-dimensional case integration was defined using the following steps:

1. Define the integral for step functions,
2. Define integral for "integrable functions",
3. Show that continuous functions are integrable.

For higher dimensions we follow the same logic. We will then show that we can evaluate higher dimensional integrals by repeated one-dimensional integration.

Definition (partition)**.** Let $R = [a_1, b_1] \times [a_2, b_2]$ be a rectangle. Suppose that $P_1 = \{x_0, \ldots, x_m\}$ and $P_2 = \{y_0, \ldots, y_n\}$ such that $a_1 = x_0 < x_2 < \cdots < x_m = b_1$

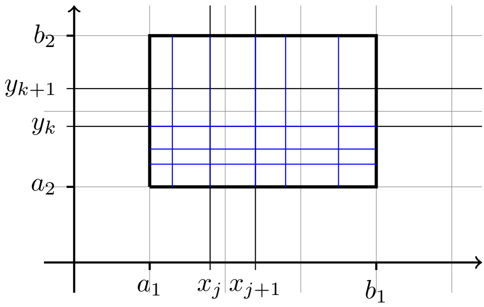


FIGURE 5.1: A partition of a rectangle R.

and $a_2 = y_0 < y_2 < \cdots < y_n = b_2$. $P = P_1 \times P_2$ is said to be a partition of R.

Observe that a partition divides R into nm sub-rectangles. If $P \subseteq Q$ then we say that Q is a finer partition than P. Partitions are constructed in higher dimension, for $\mathbb{R}^n$, in an analogous way. Before defining integration for general functions it is convenient to make the definition for a special class of functions called step functions.

Definition (step function)**.** A function $f : R \to \mathbb{R}$ is said to be a *step function* if there is a partition P of R such that f is constant on each sub-rectangle of the partition.

If f and q are step functions and $c, d \in \mathbb{R}$, then $cf + dg$ is also a step function. Also note that the area of the sub-rectangle $Q_{jk} := [x_j, x_{j+1}] \times [y_k, y_{k+1}]$ is equal to $(x_{j+1} - x_j)(y_{k+1} - y_k)$.

We can now define the integral of a step function in a reasonable way. The definition here is for 2D but the analogous definition holds for any dimension.

Definition (integral of a step function)**.** Suppose that f is a step function with value c_{jk} on the sub-rectangle $(x_j, x_{j+1}) \times (y_k, y_{k+1})$. Then we define the integral as

$$\iint\limits_R f\, dxdy = \sum_{j=0}^{m-1} \sum_{k=0}^{n-1} c_{jk}(x_{j+1} - x_j)(y_{k+1} - y_k).$$

Observe that the value of the integral is independent of the partition, as long as the function is constant on each sub-rectangle. In this sense the integral is well-defined (not dependent on the choice of partition used to calculate it).

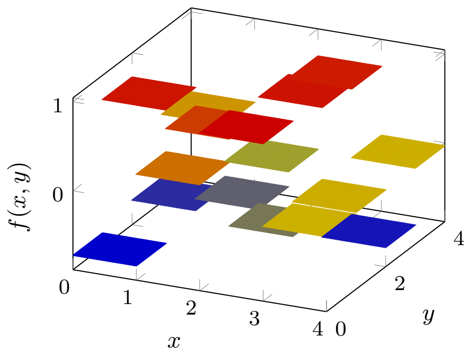


FIGURE 5.2: Graph of a step function.

Theorem 5.1 (basic properties of the integral). *Let f, g be step functions. Then*

$$\iint\limits_R (af + bg)\, dxdy = a \iint\limits_R f\, dxdy + b \iint\limits_R g\, dxdy \quad \text{for all } a, b \in \mathbb{R},$$

$$\iint\limits_R f\, dxdy = \iint\limits_{R_1} f\, dxdy + \iint\limits_{R_2} f\, dxdy \quad \text{if } R \text{ is divided into } R_1 \text{ and } R_2,$$

$$\iint\limits_R f\, dxdy \leq \iint\limits_R g\, dxdy \quad \text{if } f(x, y) \leq g(x, y).$$

Proof. All properties follow from the definition by basic calculations. □

We are now in the position to define the set of integrable functions. In order to define integrability we take advantage of "upper" and "lower" integrals which "sandwich" the function we really want to integrate.

Definition 5.2 (integrability). Let R be a rectangle and let $f : R \to \mathbb{R}$ be a bounded function. If there is one and only one number $I \in \mathbb{R}$ such that

$$\iint\limits_R g(x, y)\, dxdy \leq I \leq \iint\limits_R h(x, y)\, dxdy$$

for every pair of step functions g, h such that, for all $(x, y) \in R$,

$$g(x, y) \leq f(x, y) \leq h(x, y).$$

This number I is called the integral of f on R and is denoted $\iint_R f(x, y)\, dxdy$.

All the basic properties of the integral of step functions, as stated in Theorem 5.1, as holds for the integral of any integrable functions. This can be shown by considering the limiting procedure of the upper and lower integral of step functions which are part of the definition of integrability.

5.2 Evaluation of multiple integrals

Now we have a definition we can rigorously work with integrals but it is essential to also have a way to practically evaluate any given integral.

Theorem (evaluating by repeated integration)**.** *Let f be a bounded integrable function on $R = [a_1, b_1] \times [a_2, b_2]$. Suppose that, for every $y \in [a_2, b_2]$, the integral $A(y) = \int_{a_1}^{b_1} f(x, y)\, dx$ exists. Then $\int_{a_2}^{b_2} A(y)\, dy$ exists and,*

$$\iint_R f\, dxdy = \int_{a_2}^{b_2} \left[\int_{a_1}^{b_1} f(x, y)\, dx \right] dy.$$

Proof. We start by choosing step functions g, h such that $g \leq f \leq h$. By assumption $\int_{a_1}^{b_1} g(x, y)\, dx \leq A(y) \leq \int_{a_1}^{b_1} h(x, y)\, dx$. We then observe that $\int_{a_1}^{b_1} g(x, y)\, dx$ and $\int_{a_1}^{b_1} h(x, y)\, dx$ are step functions (in y) and so $A(y)$ is integrable. Moreover,

$$\int_{a_2}^{b_2} \left[\int_{a_1}^{b_1} g(x, y)\, dx \right] dy \leq \int_{a_2}^{b_2} A(y)\, dy \leq \int_{a_2}^{b_2} \left[\int_{a_1}^{b_1} h(x, y)\, dx \right] dy.$$

This both proves the existence of $\int_{a_2}^{b_2} A(y)\, dy$ and the value of the integral. □

The conditions of the above theorem aren't immediately easy to check and so it is convenient to now investigate the integrability of continuous functions.

Theorem 5.3 (integral of continuous functions)**.** *Suppose that f is a continuous function defined on the rectangle R. Then f is integrable and*

$$\iint_R f(x, y)\, dxdy = \int_{a_2}^{b_2} \left[\int_{a_1}^{b_1} f(x, y)\, dx \right] dy = \int_{a_1}^{b_1} \left[\int_{a_2}^{b_2} f(x, y)\, dy \right] dx.$$

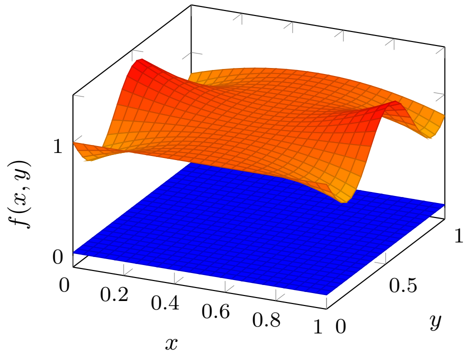


FIGURE 5.3: Set enclosed by xy-plane and $f(x, y)$.

Proof. Continuity implies boundedness and so upper and lower integrals exist. Let $\epsilon > 0$. Exists $\delta > 0$ such that $|f(\mathbf{x}) - f(\mathbf{y})| \leq \epsilon$ whenever $\|\mathbf{x} - \mathbf{y}\| \leq \delta$. We can choose a partition such $\|\mathbf{x} - \mathbf{y}\| \leq \delta$ whenever $\mathbf{x}, \mathbf{y}$ are in the same sub-rectangle Q_{jk}. We then define the step functions g, h s.t. $g(\mathbf{x}) = \inf_{Q_{jk}} f$, $h(\mathbf{x}) = \sup_{Q_{jk}} f$ when $\mathbf{x} \in Q_{jk}$. To finish the proof we observe that $\left|\inf_{Q_{jk}} f - \sup_{Q_{jk}} f\right| \leq \epsilon$ and $\epsilon > 0$ can be made arbitrarily small. □

This integral naturally allows us to calculate the volume of a solid. Let $f(x, y) \leq z \leq g(x, y)$ be defined on the rectangle $R \subset \mathbb{R}^2$ and consider the 3D set defined as

$$V = \{(x, y, z) : (x, y) \in R, f(x, y) \leq z \leq g(x, y)\}.$$

The volume of the set V is equal to $\mathrm{Vol}(V) = \iint_R [g(x, y) - f(x, y)]\ dxdy$.

Up until now we have considered step function and continuous functions. Clearly we can permit some discontinuities and we introduce the following concept to be able to control the functions with discontinuities sufficiently to guarantee that the integrals are well-defined.

Definition (content zero set)**.** A bounded subset $A \subset \mathbb{R}^2$ is said to have content zero if, for every $\epsilon > 0$, there exists a finite set of rectangles whose union includes A and the sum of the areas of the rectangles is not greater than ϵ.

Examples of content zero sets include: finite sets of points; bounded line segments; continuous paths.

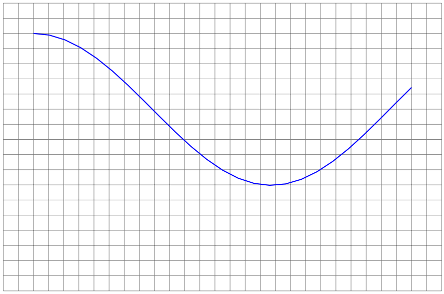


FIGURE 5.4: The graph of a continuous function has content zero.

Theorem. *Let f be a bounded function on R and suppose that the set of discontinuities $A \subset R$ has content zero. Then the double integral $\iint_R f(x,y)\,dxdy$ exists.*

Proof. Take a cover of A by rectangles with total area not greater than $\delta > 0$. Let P be a partition of R which is finer than the cover of A. We may assume that $\left|\inf_{Qjk} f - \sup_{Qjk} f\right| \leq \epsilon$ on each sub-rectangle of the partition which doesn't contain a discontinuity of f. The contribution to the integral of bounding step functions from the cover of A is bounded by $\delta \sup |f|$. □

5.3 Regions bounded by functions

A major limitation is that we have only integrated over rectangles whereas we would like to integrate over much more general different shaped regions. This we develop now.

Suppose $S \subset R$ and f is a bounded function on S. We extend f to R by defining

$$f_R(x,y) = \begin{cases} f(x,y) & \text{if } (x,y) \in S \\ 0 & \text{otherwise.} \end{cases}$$

We use this notation in the following definition.

Definition (integral on general regions)**.** We say that f is integrable if f_R is integrable and define

$$\iint_S f(x,y)\,dxdy = \iint_R f_R(x,y)\,dxdy.$$

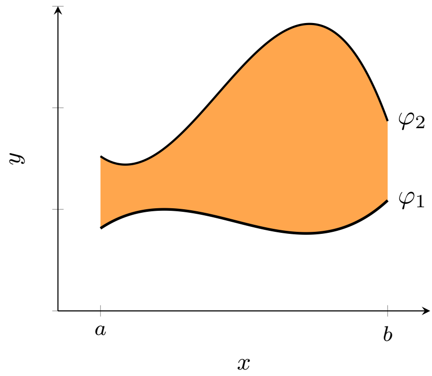


FIGURE 5.5: A region defined by two continuous functions. The "projection" of the region onto the x-axis is the interval $[a, b]$

Suppose that there are continuous functions φ_1, φ_2 on $\mathbb{R}$ and consider the set (see Figure 5.5)

$$S = \{(x, y) : a \leq x \leq b, \varphi_1(x) \leq y \leq \varphi_2(x)\} \subset \mathbb{R}^2.$$

Not all sets can be written in this way but many can and such a way of describing a subset of $\mathbb{R}^2$ is convenient for evaluating integrals. Observe that we could also consider the following set

$$S = \{(x, y) : a \leq y \leq b, \varphi_1(y) \leq x \leq \varphi_2(y)\}.$$

In the first case we could describe the representation as projecting along the y-coordinate whereas in the second case we are projecting along the x-coordinate. Observe that it doesn't make a different to the integral if we use $<$ or $\leq$ in the definition of S since the difference would be a content zero set.

Theorem. *Suppose that φ is a continuous function on $[a, b]$. Then the graph $\{(x, y) : x \in [a, b], y = \varphi(x)\}$ has zero content.*

Proof. By continuity, for every $\epsilon > 0$, there exists $\delta > 0$ such that $|\varphi(x) - \varphi(y)| \leq \epsilon$ whenever $|x - y| \leq \delta$. We then take partition of $[a, b]$ into subintervals of length less than δ. Using this partition we generate a cover of the graph which has area not greater than $2\epsilon |b - a|$. □

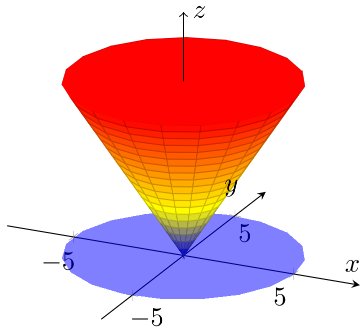


FIGURE 5.6: Upside-down cone of height 5 with tip at the origin. The solid is bounded by the surfaces $z = \sqrt{x^2 + y^2}$ and $z = 5$. This solid can be “projected” onto the xy-plane.

Theorem 5.4. *Let $S = \{(x, y) : x \in [a, b], \varphi_1(x) \le y \le \varphi_2(x)\}$ where φ_1, φ_2 are continuous and let f be a bounded continuous function of S. Then f is integrable on S and*

$$\iint_S f(x, y)\, dxdy = \int_a^b \left[\int_{\varphi_1(x)}^{\varphi_2(x)} f(x, y)\, dy \right] dx.$$

Proof. The set of discontinuity of f_R is the boundary of S in $R = [a, b] \times [\tilde{a}, \tilde{b}]$ which consists of the graphs of φ_1, φ_2. These graphs have zero content as we proved before. For each x, $f(x, y)$ is integrable since it has only two discontinuity points. Additionally $\int_{\tilde{a}}^{\tilde{b}} f_R(x, y)\, dy = \int_{\varphi_1(x)}^{\varphi_2(x)} f(x, y)\, dy$. □

A similar result holds for type 2 regions but with x and y swapped. For higher dimensions we need to also have an understanding of how to represent subsets of $\mathbb{R}^n$. Take for example a 3D solid then we would hope to be able to “project” along one of the coordinate axis and so describe it using the 2D “shadow” and a pair of continuous functions. For example, consider the upside-down cone of Figure 5.6 which has base of radius 5 lying in the plane $\{z = 5\}$ and has tip at the origin. In order to describe this set it is convenient to imagine how it projects down onto the xy-axis. We then describe it as

$$V = \{(x, y, z) : (x, y) \in S, \gamma_1(x, y) \le z \le \gamma_2(x, y)\}$$

where $S \subset \mathbb{R}^2$ is the "shadow" and the functions represent the control we need in the vertical direction. In this case we must choose $S = \{(x, y) : x^2 + y^2 \le 5^2\}$since the base of the cone, at the top of the picture, it the largest part in terms of the shadow. We also must choose $\gamma_1(x, y) = \sqrt{x^2 + y^2}$ and $\gamma_2(x, y) = 5$ to correspond to the sloped lower surface and the horizontal upper surface.

5.4 Applications of multiple integrals

Multiple integrals can be used to calculate the area or volume of a given set. Suppose that

$$S = \{(x, y) : x \in [a, b], \varphi_1(x) \le y \le \varphi_2(x)\} \subset \mathbb{R}^2$$

where φ_1, φ_2 are continuous functions. The the area of S is

$$\iint_S \, dxdy = \int_a^b \left[\int_{\varphi_1(x)}^{\varphi_2(x)} dy \right] dx = \int_a^b [\varphi_2(x) - \varphi_1(x)] \, dx.$$

This corresponds to the usual notion of the integral of a function on $\mathbb{R}$ determining the area under the curve. The same idea extends to arbitrary dimension. Suppose that $\gamma_1(x, y) \le \gamma_2(x, y)$ are continuous functions on S and let
$V = \{(x, y, z) : x \in [a, b], \varphi_1(x) \le y \le \varphi_2(x), \gamma_1(x, y) \le z \le \gamma_2(x, y)\} \subset \mathbb{R}^3$.
The volume of V is

$$\begin{aligned} \iiint_V \, dxdydz &= \int_a^b \left[\int_{\varphi_1(x)}^{\varphi_2(x)} \left[\int_{\gamma_1(x,y)}^{\gamma_2(x,y)} dz \right] dy \right] dx \\ &= \int_a^b \left[\int_{\varphi_1(x)}^{\varphi_2(x)} [\gamma_2(x, y) - \gamma_1(x, y)] dy \right] dx. \end{aligned}$$

Multiple integrals also allow us to calculate the mass and centre of mass of solids. Suppose we have several particles[1] each with mass m_k and located at point (x_k, y_k).

[1]In general, mass m_k at point $\mathbf{x}_k$, the centre of mass is point $\mathbf{X}$ such that $M\mathbf{X} = \sum_k m_k \mathbf{x}_k$.

The total mass would then be $M = \sum_k m_k$ and the centre of mass is the point (p, q) such that

$$pM = \sum_k m_k x_k \quad \text{and} \quad qM = \sum_k m_k y_k.$$

Suppose an object has the shape of a region S and the density of the material is $f(x, y)$ at point (x, y). Then, similar to the discrete case above, the total mass is $M = \iint_S f(x, y)\, dxdy$ and the centre of mass is the point (p, q) such that

$$pM = \iint_S x\, f(x, y)\, dxdy \quad \text{and} \quad qM = \iint_S y\, f(x, y)\, dxdy.$$

By tradition, if the density is constant, then the centre of mass is called the *centroid*.

5.5 Green's theorem

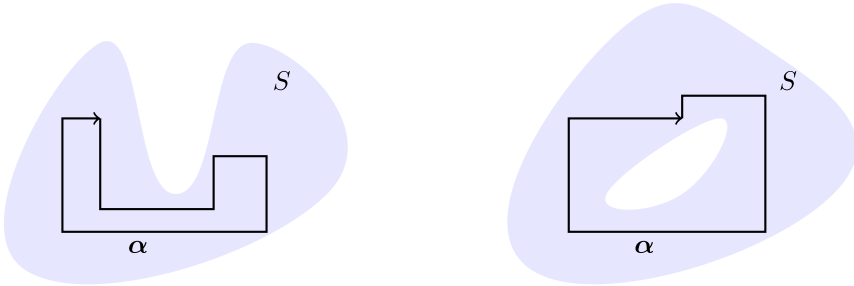
We can now establish a connection between multiple integrals and the line integrals of the previous chapter.

Theorem 5.5 (Green's theorem). *Let $C \subset \mathbb{R}^2$ be a piecewise-smooth simple (no intersections) curve and $\boldsymbol{\alpha}$ a path that parametrizes C in the counter-clockwise direction. Let S be the region enclosed by C. Suppose that $\mathbf{f}(x, y) = \begin{pmatrix} P(x,y) \\ Q(x,y) \end{pmatrix}$ is a vector field continuously differentiable on an open set containing S. Then*

$$\iint_S \left(\tfrac{\partial Q}{\partial x} - \tfrac{\partial P}{\partial y} \right)\, dxdy = \int_C \mathbf{f} \cdot d\boldsymbol{\alpha}.$$

Proof of Green's theorem. To start we assume that S is a type 1 region and that $Q = 0$, Since $S = \{(x, y) : x \in [a, b], \varphi_1(x) \le y \le \varphi_2(x)\}$,

$$\begin{aligned} \iint_S \left(\tfrac{\partial Q}{\partial x} - \tfrac{\partial P}{\partial y} \right)\, dxdy &= \int_a^b \left[\int_{\varphi_1(x)}^{\varphi_2(x)} \left(-\tfrac{\partial P}{\partial y}\right) dy \right] dx \\ &= \int_a^b (P(x, \varphi_1(x)) - P(x, \varphi_2(x)))dx, \end{aligned}$$



(A) Simply connected.

(B) Not simply connected.

FIGURE 5.7: A set is simply-connected if every closed path can be contracted to a point.

It is then natural to choose four paths $\boldsymbol{\alpha}_1(t) = (t, \varphi_1(t))$, $\boldsymbol{\alpha}_2(t) = (a, t)$, $\boldsymbol{\alpha}_3(t) = (t, \varphi_2(t))$, $\boldsymbol{\alpha}_4(t) = (b, t)$. We can calculate that $\int_C \mathbf{f} \cdot d\boldsymbol{\alpha} = \int \mathbf{f} \cdot d\boldsymbol{\alpha}_1 - \int \mathbf{f} \cdot d\boldsymbol{\alpha}_3 = \int_a^b P(t, \varphi_1(t))\, dt - \int_a^b P(t, \varphi_2(t))\, dt$. If S is also type 2 then this works for $P = 0$ and linearity means it works for $\mathbf{f} = \left(\begin{smallmatrix} P \\ 0 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ Q \end{smallmatrix}\right)$, More general regions can be formed by "glueing" together simpler regions of the above type to complete the argument. $\square$

The quantity $\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}$ is reminiscent of something we saw with conservative vector fields and we take advantage of this with the following application. We previously introduced the concept of *connected sets* but now we need a slight refinement of the idea.

Definition 5.6 (simply-connected set)**.** A connected set $S \subset \mathbb{R}^n$ is said to be *simply-connected* if any closed path $\boldsymbol{\alpha}$, contained within S, can be contracted to a point. (This is in the sense that there exists a continuous map $F : D^2 \to S$, where $D^2 \subset \mathbb{R}^2$ denotes the unit disk, such that F restricted to the unit circle is $\boldsymbol{\alpha}$.)

The following result extends Theorem 4.13 which was limited to convex sets.

Theorem 5.7 (conservative vector fields on simply connected regions)**.** *Let S be a simply connected region and suppose that $\mathbf{f} = \left(\begin{smallmatrix} P \\ Q \end{smallmatrix}\right)$ is a vector field, continuously differentiable on S. Then $\mathbf{f}$ is conservative if and only if $\frac{\partial Q}{\partial x} = \frac{\partial P}{\partial y}$.*

Proof. In Theorem 4.11 we already proved that $\frac{\partial Q}{\partial x} = \frac{\partial P}{\partial y}$ whenever $\mathbf{f}$ is conservative so we need only prove the other direction of the statement. Suppose that $\frac{\partial Q}{\partial x} = \frac{\partial P}{\partial y}$ and consider any closed path $\boldsymbol{\alpha}$ in S. By Green's (Theorem 5.5),

$$\int_C \mathbf{f} \cdot d\boldsymbol{\alpha} = \iint_S \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) \, dxdy = 0.$$

This implies that $\mathbf{f}$ is conservative because the fact that the line integral around every closed curve is zero (Theorem 4.9). □

A crucially important consequence of the above result is that it implies the invariance of a line integral under deformation of a path when the vector field is conservative. Observe that the result can be extended to multiply connected regions by adding additional "cuts" and keeping track of the additional line integrals.

5.6 Change of variables

When we want to identify a point in space it is common, particularly if we are pirates recording the position of tresure, that there are many alternative ways we can describe this point. For example we could write the number of steps north and the number of steps east from the central palm tree. Alternatively we can specify that we stand at the palm tree looking in a specific direction and then walk a particular number of steps. Often is is really convenient to swap from one coordinate to another and in this section we show how multiple integrals behave under change of coordinates.

To start, we recall the 1D case. If $g : [a, b] \to [g(a), g(b)]$ is onto with continuous derivative and f is continuous then

$$\int_{g(a)}^{g(b)} f(x) \, dx = \int_a^b f(g(u)) \, g'(u) \, du.$$

In higher dimension we obtain a similar result but g' must be replaced by a type of derivative which works in higher dimension.

For the 2D case we have the following result.

Theorem 5.8 (change of variable in 2D). *Suppose that* $(u,v) \mapsto (X(u,v), Y(u,v))$ *maps* T *to* S *one-to-one and* X, Y *are continuously differentiable. Then*

$$\iint\limits_S f(x,y)\, dxdy = \iint\limits_T f(X(u,v), Y(u,v))\ |J(u,v)|\ dudv.$$

Here $J(u,v) = \left(\begin{smallmatrix} \partial_u X & \partial_u Y \\ \partial_v X & \partial_v Y \end{smallmatrix}\right)$ is the Jacobian matrix as used previously. Note that the Jacobian represents the scaling of volume in the sense that $\iint_S\, dxdy = \iint_T |J(u,v)|\ dudv$.

Polar coordinates

Polar coordinates correspond to the coordinate mapping

$$\begin{cases} x = r\cos\theta \\ y = r\sin\theta. \end{cases}$$

In this case the Jacobian determinant is

$$|J(r,\theta)| = \left|\left(\begin{smallmatrix} \partial_u X & \partial_u Y \\ \partial_v X & \partial_v Y \end{smallmatrix}\right)\right| = \left|\left(\begin{smallmatrix} \cos\theta & \sin\theta \\ -r\sin\theta & r\cos\theta \end{smallmatrix}\right)\right| = r(\cos^2\theta + \sin^2\theta) = r.$$

Consequently, the change of variable in the integral gives that

$$\iint\limits_S f(x,y)\, dxdy = \iint\limits_T r\, f(r\cos\theta, r\sin\theta)\, drd\theta.$$

Linear transformations

In this case the coordinate mapping is

$$\begin{cases} x = Au + Bv \\ y = Cu + Dv \end{cases}$$

where $A, B, C, D \in \mathbb{R}$ are chosen fixed. The Jacobian determinant is equal to

$$|J(u,v)| = \left|\left(\begin{smallmatrix} \partial_u X & \partial_u Y \\ \partial_v X & \partial_v Y \end{smallmatrix}\right)\right| = \left|\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)\right| = |AD - BC|.$$

Consequently the change of coordinates for the integral is

$$\iint\limits_S f(x,y)\, dxdy = |AD - BC| \iint\limits_T f(Au + Bv, Cu + Dv)\, dudv.$$

Extension to higher dimensions

The exact analog of Theorem 5.8 holds in any dimension. In particular, in 3D, if we consider the change of variables $(u, v, w) \mapsto (X(u, v, w), Y(u, v, w), Z(u, v, w))$, then $\iiint_S f(x, y, z)\, dxdydz$ is equal to

$$\iiint_T f(X(u, v, w), Y(u, v, w), Z(u, v, w))\ |J(u, v, w)|\ dudvdw$$

where $J(u, v)$ is now the Jacobian matrix of dimension (3×3).

Cylindrical coordinates

Cylindrical coordinates corresponds to the mapping (require $r > 0, 0 \leq \theta \leq 2\pi$)

$$\begin{cases} x = r\cos\theta \\ y = r\sin\theta \\ z = z \end{cases}$$

and, in this case, the Jacobian determinant is

$$|J(r, \theta, z)| = \left| \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -r\sin\theta & r\cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \right| = \left| r(\cos^2\theta + \sin^2\theta) \right| = r$$

and so the change of variables in the integral gives

$$\iiint_S f(x, y, z)\, dxdydz = \iiint_T r\, F(r, \theta, z)\, drd\theta dz.$$

where $F(r, \theta, z) = f(r\cos\theta, r\sin\theta, z)$. Note that cylindrical coordinates are closely related to polar coordinates in the sense that we don't touch the z coordinate and use polar coordinates for x and y.

Spherical coordinates

Spherical coordinates correspond to how we use lattitude, longitude and altitude to specify a position on earth. It is the coordinate mapping (require $\rho > 0, 0 \leq \theta \leq 2\pi$, $0 \leq \varphi < \pi$)

$$\begin{cases} x = \rho\cos\theta\sin\varphi \\ y = \rho\sin\theta\sin\varphi \\ z = \rho\cos\varphi. \end{cases}$$

In this case the Jacobian determinant is

$$|J(\rho,\theta,\varphi)| = \left| \begin{pmatrix} \cos\theta\sin\varphi & \sin\theta\sin\varphi & \cos\varphi \\ -\rho\sin\theta\sin\varphi & \rho\cos\theta\sin\varphi & 0 \\ \rho\cos\theta\cos\varphi & \rho\sin\theta\cos\varphi & -\rho\sin\varphi \end{pmatrix} \right| = \left|-\rho^2\sin\varphi\right| = \rho^2\sin\varphi.$$

Consequently the change of variables in the integral gives that

$$\iiint\limits_S f(x,y,z)\,dxdydz = \iiint\limits_T F(\rho,\theta,\varphi)\rho^2\sin\varphi\,d\rho d\theta d\varphi.$$

where $F(\rho,\theta,\varphi) = f(\rho\cos\theta\sin\varphi, \rho\sin\theta\sin\varphi, \rho\cos\varphi)$.

Chapter 6

Surface integrals

In this section we consider surfaces and how to define integral of vector fields over these surfaces. This is similar in many ways to line integrals but a higher dimensional version. Curves (for line integrals) are 1D subsets of higher dimensional space whereas surfaces are 2D subsets of higher dimensional space. Identically to line integrals, the first step is to understand a practical way to represent the surfaces, just like with curves we used paths as the parametric representation of the curve. Once we have clarified the parametric representation of surface we can define the surface integral (of a vector field) and show that it satisfies various properties which we would expect, including that the integral is independent of the choice of parametrization. Similar to how we were able to use a line integral (of a scalar) to calculate the length of a curve we can use a surface integral (of a scalar) to calculate the area of a surface.

We then introduce two important operators that act on vector fields, namely *curl* and *divergence*. Using these operators and the surface integral we introduce two theorems, Gauss' Theorem and Stokes' Theorem. These theorems connect line integrals with surface integrals and with volume integrals.

6.1 Representation of a surface

Before developing parametric representations of surfaces let's recall an example of parametric representation of a curve (path). For example, the half circle $C = \{(x, y) : x^2 + y^2 = 1, y \geq 1\}$ can be parametrized in many ways, including the following two paths.

$$\boldsymbol{\alpha}(x) = (x, \sqrt{1 - x^2}), \quad x \in [-1, 1],$$
$$\boldsymbol{\alpha}(t) = (\cos t, \sin t), \quad t \in [0, \pi].$$

In a similar way, now in 2D we can have a parametric representation of a hemisphere.

Example (hemisphere)**.** The hemisphere $S = \{(x, y, z) : x^2+y^2+z^2 = 1, z \geq 0\}$ can be represented parametrically in many ways, including

$$\begin{aligned} \mathbf{r}(x, y) &= (x, y, \sqrt{1 - x^2 - y^2}), \quad (x, y) \in \{x^2 + y^2 \leq 1\}, \\ \mathbf{r}(u, v) &= (\cos u \cos v, \sin u \cos v, \sin v), \quad (u, v) \in [0, 2\pi] \times [0, \pi/2]. \end{aligned}$$

Observe that the second form above can be deduced from spherical coordinates (fixed distance from the origin).

Example (cone)**.** The cone $S = \{(x, y, z) : z^2 = x^2 + y^2, z \in [0, 1]\}$ can be represented parametrically in many ways, including

$$\begin{aligned} \mathbf{r}(x, y) &= (x, y, \sqrt{x^2 + y^2}), \quad (x, y) \in \{x^2 + y^2 \leq 1\}, \\ \mathbf{r}(u, v) &= (v \cos u, v \sin u, v), \quad (u, v) \in [0, 2\pi] \times [0, 1]. \end{aligned}$$

Observe that the second form can be deduced from spherical coordinates (fixed angle from z-axis).

Fundamental vector product

A key notion for parametric surfaces and natural geometric object is the *fundamental vector product*. Consider the parametric surface, denoted $\mathbf{r}(T)$, and suppose it has the form

$$\mathbf{r}(u, v) = (X(u, v), Y(u, v), Z(u, v)), \quad (u, v) \in T.$$

Definition 6.1 (fundamental vector product)**.** The vector-valued function defined as

$$\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} = \begin{pmatrix} \partial_u X \\ \partial_u Y \\ \partial_u Z \end{pmatrix} \times \begin{pmatrix} \partial_v X \\ \partial_v Y \\ \partial_v Z \end{pmatrix}$$

is called the *fundamental vector product* of the representation $\mathbf{r}$.

By definition, the vector-valued functions $\frac{\partial \mathbf{r}}{\partial u}$ and $\frac{\partial \mathbf{r}}{\partial v}$ are tangent to the surface. As such, assuming that they are linearly independent, the fundamental vector product $\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v}$ is normal to the surface (orthogonal to every curve which passes through the surface). Moreover the norm of the vector represents the local scaling of area (small parallelograms).

As always we need to take some care about smoothness of the objects we work with.

Definition (regular point). If (u, v) is a point in T at which $\frac{\partial \mathbf{r}}{\partial u}$ and $\frac{\partial \mathbf{r}}{\partial v}$ are continuous and the fundamental vector product is non-zero then $\mathbf{r}(u, v)$ is said to be a *regular point* for that representation.

Definition (smooth surface representation). A surface $\mathbf{r}(T)$ is said to be smooth if all its points are regular points.

Just like we saw with paths to represent curves, there are many different ways we can find the parametric representation of a given surface. If the surface S has the form $z = f(x, y)$ (the surface in written in explicit form) then we can use x, y as the parameters and have the representation

$$\mathbf{r}(x, y) = (x, y, f(x, y)), \quad (x, y) \in T.$$

The region T is the projection of S onto the xy-plane. For such a surface we compute

$$\frac{\partial \mathbf{r}}{\partial x} = \begin{pmatrix} 1 \\ 0 \\ \partial_x f \end{pmatrix}, \quad \frac{\partial \mathbf{r}}{\partial y} = \begin{pmatrix} 0 \\ 1 \\ \partial_y f \end{pmatrix},$$

and consequently

$$\frac{\partial \mathbf{r}}{\partial x} \times \frac{\partial \mathbf{r}}{\partial y} = \begin{pmatrix} 1 \\ 0 \\ \partial_x f \end{pmatrix} \times \begin{pmatrix} 0 \\ 1 \\ \partial_y f \end{pmatrix} = \begin{pmatrix} -\partial_x f \\ -\partial_y f \\ 1 \end{pmatrix}.$$

An example of such a representation is as follows for the hemisphere.

Example (hemisphere representation 1). Let $T = \{x^2 + y^2 \le 1\}$, and let

$$\mathbf{r}(x, y) = (x, y, \sqrt{1 - x^2 - y^2}).$$

The surface $\mathbf{r}(T)$ is the unit hemisphere $\{(x, y, z) : x^2 + y^2 + z^2 = 1\}$. The fundamental vector product of this representation is

$$\frac{\partial \mathbf{r}}{\partial x} \times \frac{\partial \mathbf{r}}{\partial y}(x, y) = \begin{pmatrix} x(1-x^2-y^2)^{-1/2} \\ y(1-x^2-y^2)^{-1/2} \\ 1 \end{pmatrix} = z^{-1}\, \mathbf{r}(x, y).$$

In this case, all points are regular except the equator.

Example (hemisphere representation 2). Let $T = [0, 2\pi] \times [0, \pi/2]$ and let

$$\mathbf{r}(u, v) = (\cos u \cos v, \sin u \cos v, \sin v).$$

The surface $\mathbf{r}(T)$ is the unit hemisphere $\{(x, y, z) : x^2 + y^2 + z^2 = 1\}$. This is the representation which is connected to spherical coordinates. We calculate that

$$\frac{\partial \mathbf{r}}{\partial u}(u, v) = \begin{pmatrix} -\sin u \cos v \\ \cos u \cos v \\ 0 \end{pmatrix}, \quad \frac{\partial \mathbf{r}}{\partial v}(u, v) = \begin{pmatrix} -\cos u \sin v \\ -\sin u \sin v \\ \cos v \end{pmatrix},$$

and so the fundamental vector product of this representation is

$$\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v}(u, v) = \cos v \, \mathbf{r}(u, v).$$

In this case many points map to the north pole $(0, 0, 1)$ and the north pole is not a regular point. Additionally there are two points which map to each point on the line between equator and north pole $\{(x, y, z) \in \mathbf{r}(T) : y = 0\}$.

6.2 Surface integral of scalar field

Mirroring the process for line integrals we will define surface integrals both for scalar fields and for vector fields. The surface integral of a scalar field is closely related to the area of a parametric surface, just like the length of a curve is closely related to the line integral of a scalar field.

Definition 6.2 (area of a parametric surface)**.** The area of the parametric surface $S = \mathbf{r}(T)$ is defined as the double integral

$$\text{Area}(S) = \iint_T \left\| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right\| \, du dv.$$

Observe that the definition is in terms of a multiple integral over the region T, and the quantity being integrated is the norm of the fundamental vector product.

Later we will show that $\text{Area}(S)$ is *independent* of the choice of representation as we require for such a definition, it would be unreasonable if the area of a surface depended on the choice of representation.

We will check that this definition corresponds to a fact that we already know by computing the surface area of a hemisphere. Let, as before, $T = [0, 2\pi] \times [0, \pi/2]$ and let $\mathbf{r}(u, v) = (\cos u \cos v, \sin u \cos v, \sin v)$. The norm of the fundamental vector product (which we computed earlier) is

$$\left\| \frac{\partial \mathbf{r}}{\partial x} \times \frac{\partial \mathbf{r}}{\partial y}(u, v) \right\| = \cos v \ \|\mathbf{r}(u, v)\| = \cos v.$$

This means, by Definition 6.2 and evaluating the multiple integral, that

$$\text{Area}(S) = \iint_T \cos v \, du dv = \int_0^{2\pi} \left[\int_0^{\pi/2} \cos v \, dv \right] du = 2\pi.$$

The surface integral of a scalar field is defined in a way similar to the area of a surface.

Definition 6.3 (surface integral)**.** Let $S = \mathbf{r}(T)$ be a parametric surface and let f be a scalar field defined on S. The surface integral of f over S is defined as

$$\iint\limits_{\mathbf{r}(T)} f \, dS = \iint\limits_{T} f(\mathbf{r}(u,v)) \left\| \tfrac{\partial \mathbf{r}}{\partial u} \times \tfrac{\partial \mathbf{r}}{\partial v}(u,v) \right\| \, dudv$$

whenever the double integral on the right exists.

Observe that, if we choose $f \equiv 1$, that is we choose the scalar field identically equal to 1, then we obtain the formula for the area of the surface (Definition 6.2). This is just the same as the line integral of a scalar and the length of the corresponding curve.

From the point of view of applications, we could take f as the density of thin material which has the shape of the surface S and then $\iint_S f \, dS$ is the total mass of this piece of material. Extending this idea we could also calculate the centre of mass of this piece of material.

6.3 Change of surface parametrization

In order to validate the definition of a surface integral and consequently that of the area of a surface, we will now show that the the value of the evaluated integral doesn't depend on the choice of representation for any given surface.

Theorem 6.4 (change of surface parametrization)**.** *Suppose that $\mathbf{q}(A)$ and $\mathbf{r}(B)$ are both representations of the same surface, and that $\mathbf{r} = \mathbf{q} \circ G$ for some differentiable $G : B \to A$. Then*

$$\iint\limits_{A} f \circ \mathbf{q} \left\| \tfrac{\partial \mathbf{q}}{\partial s} \times \tfrac{\partial \mathbf{q}}{\partial t} \right\| \, dsdt = \iint\limits_{B} f \circ \mathbf{r} \left\| \tfrac{\partial \mathbf{r}}{\partial u} \times \tfrac{\partial \mathbf{r}}{\partial v} \right\| \, dudv.$$

Proof. Since $\mathbf{r}(u,v) = \mathbf{q}(S(u,v), T(u,v))$ we calculate (chain rule and vector product) that

$$\left[\tfrac{\partial \mathbf{r}}{\partial u} \times \tfrac{\partial \mathbf{r}}{\partial v} \right](u,v) = \left[\left(\tfrac{\partial \mathbf{q}}{\partial s} \times \tfrac{\partial \mathbf{q}}{\partial t} \right) \left(\tfrac{\partial S}{\partial u} \tfrac{\partial T}{\partial v} - \tfrac{\partial S}{\partial v} \tfrac{\partial T}{\partial u} \right) \right] (S(u,v), T(u,v)).$$

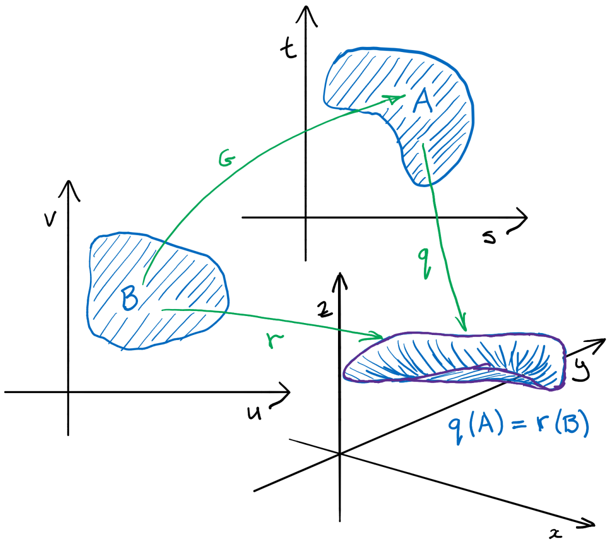


FIGURE 6.1: Two different representations for a given surface.

Observe that $\frac{\partial S}{\partial u}\frac{\partial T}{\partial v} - \frac{\partial S}{\partial v}\frac{\partial T}{\partial u}$ is the Jacobian determinant associated to change of variables $(u, v) \mapsto (S(u, v), T(u, v))$. Consequently, by the change of variables theorem,

$$\iint_A f \circ \mathbf{q} \left\| \frac{\partial \mathbf{q}}{\partial s} \times \frac{\partial \mathbf{q}}{\partial t} \right\| dsdt = \iint_B f \circ \mathbf{r} \left\| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right\| dudv$$

as announced in the theorem. □

6.4 Surface integral of a vector field

In preparation for defining the surface integral of a vector field we need the notion of the *normal* vector of a surface. This is a natural geometric notion, for each point in the surface it is the unit vector field which is orthogonal to the surface.

Definition 6.5 (normal vector)**.** Let $S = \mathbf{r}(T)$ be a parametric surface. At each regular point the two unit normals are

$$\mathbf{n}_1 = \frac{\frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v}}{\left\| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right\|} \quad \text{and} \quad \mathbf{n}_2 = -\mathbf{n}_1.$$

By definition $\|\mathbf{n}_1\| = \|\mathbf{n}_2\| = 1$. That there are two normal vectors is expected because there are two sides to the surface at each point, one is just the opposite direction to the other. If $\mathbf{f}$ is a vector field then $\mathbf{f} \cdot \mathbf{n}$ is the component of the flow in direction of $\mathbf{n}$.

Definition 6.6 (surface integral of a vector field)**.** Let $S = \mathbf{r}(T)$ be a parametric surface and $\mathbf{f}$ a vector field. The integral

$$\iint_S \mathbf{f} \cdot \mathbf{n} \, dS$$

is said to be the *surface integral of* $\mathbf{f}$ *with respect to the normal* $\mathbf{n}$.

For convenience let $\mathbf{N} = \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v}$ and $\mathbf{n} = \mathbf{N} / \|\mathbf{N}\|$. Observe that

$$\iint_S \mathbf{f} \cdot \mathbf{n} \, dS = \iint_T (\mathbf{f} \circ \mathbf{r}) \cdot \mathbf{n} \left\| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \right\| dudv = \iint_T (\mathbf{f} \circ \mathbf{r}) \cdot \mathbf{N} \, dudv$$

and so for evaluating the surface integral of a vector field there is typically no need to evaluate the norm of the fundamental vector product. Also note that $\iint_S \mathbf{f} \cdot \mathbf{n}_1 \, dS = -\iint_S \mathbf{f} \cdot \mathbf{n}_2 \, dS$ because $\mathbf{n}_1 = -\mathbf{n}_2$. This means that choose one normal or the other simply corresponds to a minus sign in the evaluated integral. This is the notion that there is a choice of orientation inherent with a surface. As a tangible example imagine that the surface has a flow passing it and this flow is determined by a vector field. Then the surface integral would represent the total flow passing the given surface in a given direction.

6.5 Curl and divergence

Suppose that $\mathbf{f} = \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}$ is a differentiable vector field.

Definition 6.7 (curl)**.** The *curl* of $\mathbf{f}$ is defined as

$$\nabla \times \mathbf{f} = \begin{pmatrix} \frac{\partial f_z}{\partial y} - \frac{\partial f_y}{\partial z} \\ \frac{\partial f_x}{\partial z} - \frac{\partial f_z}{\partial x} \\ \frac{\partial f_y}{\partial x} - \frac{\partial f_x}{\partial y} \end{pmatrix}.$$

Definition 6.8 (divergence)**.** The *divergence* of $\mathbf{f}$ is defined as

$$\nabla \cdot \mathbf{f} = \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z}.$$

Often the notation $\operatorname{curl} \mathbf{f} = \nabla \times \mathbf{f}$ and $\operatorname{div} \mathbf{f} = \nabla \cdot \mathbf{f}$ is used instead. Note that the symbols"$\times$" and "$\cdot$" used in the notation for curl and divergence are not truly representing the vector and scalar product but are more a convenient way to remember the definitions. These quantities satisfy the following basic properties which can all be proved by the basic calculation.

- ▷ If $\mathbf{f} = \nabla\varphi$ then $\nabla \times \mathbf{f} = \mathbf{0}$,
- ▷ $\nabla \cdot (\nabla \times \mathbf{f}) = 0$,
- ▷ $\nabla \times (\nabla \times \mathbf{f}) = \nabla(\nabla \cdot \mathbf{f}) - \nabla^2 \mathbf{f}$.

The quantity defined as $\nabla^2\varphi = \nabla \cdot (\nabla\varphi) = \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2}$ is called the Laplacian and occurs in many applications of physics and mathematics.

Example. If $\mathbf{f}(x, y, z) = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ then $\nabla \times \mathbf{f} = \mathbf{0}$, $\nabla \cdot \mathbf{f} = 3$.

Example. If $\mathbf{f}(x, y, z) = \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}$ then $\nabla \times \mathbf{f} = \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}$, $\nabla \cdot \mathbf{f} = 0$.

Theorem 6.9. *Let $S \subset \mathbb{R}^3$ be convex. Then $\nabla \times \mathbf{f} \equiv \mathbf{0}$ on S if and only if $\mathbf{f}$ is conservative on S.*

The above result implies Theorem 5.7 (the 2D vector fields can be written as 3D vector fields with a zero component).

6.6 Theorems of Stokes and Gauss

Theorem 6.10 (Stokes). *Let $S = \mathbf{r}(T)$ be a parametric surface. Suppose that T is simply connected and that the boundary of T is mapped to C, the boundary of S. Let $\boldsymbol{\beta}$ be a counter clockwise parametrization of the boundary of T and let $\boldsymbol{\alpha}(t) = \mathbf{r}(\boldsymbol{\beta}(t))$. Then*

$$\iint_S (\nabla \times \mathbf{f}) \cdot \mathbf{n} \, dS = \int \mathbf{f} \cdot d\boldsymbol{\alpha}.$$

Sketch of proof. Write $\mathbf{f} = \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}$ and suppose that $f_y = f_z = 0$. This effectively reduces the full problem to the lower dimensional version that we previously consider. As such, we can then apply Green's theorem (Theorem 5.5). Finally we conclude for general $\mathbf{f}$ by linearity of the integral. □

Just as Green's Theorem holds for regions which can contain holes, as long as they are correctly accounted for, we can extend Stokes' theorem to more general surfaces with the idea of "cutting and gluing" the surface. In particular this allows the extension to surfaces with holes, cylinders, spheres, etc. On the other hand the theorem can't be extended to the Möbius band because the topology of this surface prevents a similar process being completed.

Theorem 6.11 (Gauss). *Let $V \subset \mathbb{R}^3$ be a solid with boundary the parametric surface S and let $\mathbf{n}$ be the outward normal unit vector. If $\mathbf{f}$ is a vector field then*

$$\iiint_V \nabla \cdot \mathbf{f} \, dxdydz = \iint_S \mathbf{f} \cdot \mathbf{n} \, dS.$$

Sketch of proof. We start by writing

$$\iiint_V \left(\frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z} \right) dxdydz = \iint_S (f_x n_x + f_y n_y + f_z n_z) \, dS.$$

As such, it suffices to show that $\iiint_V \left(\frac{\partial f_x}{\partial x} \right) dxdydz = \iint_S (f_x n_x) \, dS$. If we suppose the solid V is xy-projectable then we can explicitly write the integral (later to be extended to general solids). We then use basic calculus to express f_x as the integral of the derivative. □

Stokes' Theorem allows us to connect surface integrals (2D) to line integrals (1D). On the other hand Gauss' Theorem allows us to connect volume integrals (3D) to surface integrals (2D). In this way they are similar to each other, the integral goes decreases dimension and also there is the loss of a derivative. Indeed the fundamental theorem of calculus for line integral also fits into this same pattern. The branch of mathematics called "differential geometry" provides a framework in which all these results can be described in a unified way by the statement

$$\int_{\partial\Omega} \omega = \int_{\Omega} d\omega.$$

This result is called the "generalized Stokes theorem".

Note that Gauss' Theorem is often called the "divergence theorem". We can use this theorem for the following interpretation of divergence as a limit, similar to the way other versions of derivatives are defined.

Theorem. *Let V_t be the ball of radius $t > 0$ centred at $\mathbf{a} \in \mathbb{R}^3$ and let S_t be its boundary with outgoing unit normal vector $\mathbf{n}$. Then*

$$\nabla \cdot \mathbf{f} = \lim_{t \to 0} \frac{1}{\operatorname{Vol}(V_t)} \iint_{S_t} \mathbf{f} \cdot \mathbf{n} \, dS.$$

Proof. Using Gauss' theorem. □

Curl can also be written as a similar limit. Given the similarity of all the terms, it is not unexpected that there is a relation between curl and divergence with the Jacobian matrix. Recall that

$$\operatorname{Jac}(\mathbf{f}) = \begin{pmatrix} \frac{\partial f_x}{\partial x} & \frac{\partial f_x}{\partial y} & \frac{\partial f_x}{\partial z} \\ \frac{\partial f_y}{\partial x} & \frac{\partial f_y}{\partial y} & \frac{\partial f_y}{\partial z} \\ \frac{\partial f_z}{\partial x} & \frac{\partial f_z}{\partial y} & \frac{\partial f_z}{\partial z} \end{pmatrix}$$

We can immediately see that divergence is the trace of the Jacobian matrix. In order to see the connection with curl, recall that every real matrix A can be written as the sum of a symmetric matrix $\frac{1}{2}(A + A^T)$ and a skew-symmetric matrix $\frac{1}{2}(A - A^T)$. In this case we have that

$$\frac{1}{2}(\mathrm{Jac}(\mathbf{f}) - \mathrm{Jac}(\mathbf{f})^T) = \begin{pmatrix} 0 & \frac{\partial f_x}{\partial y} - \frac{\partial f_y}{\partial x} & \frac{\partial f_x}{\partial z} - \frac{\partial f_z}{\partial x} \\ \frac{\partial f_y}{\partial x} - \frac{\partial f_x}{\partial y} & 0 & \frac{\partial f_y}{\partial z} - \frac{\partial f_z}{\partial y} \\ \frac{\partial f_z}{\partial x} - \frac{\partial f_x}{\partial z} & \frac{\partial f_z}{\partial y} - \frac{\partial f_y}{\partial z} & 0 \end{pmatrix}$$

and can see that the terms of the skew-symmetric part of the matrix are exactly the terms of curl.