MATHEMATICS FOR QUANTUM CHEMISTRY

LECTURE NOTES

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About these lectures and lecture notes

These lecture notes were prepared as part of the European Summerschool in Quantum Chemistry (ESQC) 2022. This is my first round of lecturing at ESQC, with all that implies. The lectures themselves necessarily covers much less than the lecture notes, due to the time constraints.

Given that ESQC is an intense summer school for quantum chemistry students, and only 5 lectures are devoted to the broad theme "mathematics", the content must be chosen carefully. The balance is difficult: some students may not know much at all, having maybe only one or two undergraduate courses of uncertain freshness, while others may be quite proficient in a wide range of mathematical topics. I therefore do not assume too much mathematical background, and I certainly won't present theorems with full statements or proofs, but instead give a very broad overview. I think that most students will find something they can understand and like.

Successful research in quantum chemistry invariably requires delving into mathematics: from the theory of complex functions, integration, linear algebra, Fourier analysis, through topics like calculus of variations, functional analysis, optimization theory, and numerical analysis. The goal of the lectures is *not* to teach mathematics, but to give the students some tools for where to look for information on relevant topics, in addition to a rough idea about what different concepts are about, and how they are interconnected. The exercises that accompany the lectures are varied, from basic exercises training the fingers to do matrix-vector multiplication, so small projects, also with some programming. There should be something for everyone.

Unfortunately, it is not possible to *learn* mathematics by watching a lecturer state definitions and some facts. Understanding comes with extensive experience, careful reading and understanding of proofs, doing exercises, and practice. One should therefore consider these lectures as a *starting point*. One should not worry if the material seems difficult, or if what being said is hard to understand. Instead, one should do the exercises oney can, collaborate with co-students, and take note of topics that seem interesting. When the school is over, at least one should have some overview of how topics are connected and used in quantum chemistry research.

Contents

The fundamentals: Sets and numbers

1.1 Introduction

1.1.1 Why learn mathematics?

Doing successful research in quantum chemistry invariably requires the researcher to use mathematical tools. These range from elementary topics like real and complex analysis, and linear algebra, but, especially in method development of manybody theory, topics like functional analysis, convex analysis, nonlinear partial differential equations, and so on, pop up. Moreover, computer implementation of quantum chemistry methods require a good command of numerical analysis and optimization theory. Furthermore, even if the researchers ambition is *not* to do advanced research in quantum chemistry method development, application of the methods also require an understanding of where they come from and how they work.

1.1.2 What is mathematics?

In science, we build models to describe observations made by experiments. The language of models is mathematics. Mathematics itself can be said to model nature: The integers model counting of discrete objects, the real numbers model lengths and time intervals, and euclidean geometry models (non-relativistic) space-time. Functions of real variables model observable quantities. Hilbert spaces model the states of matter in the quantum mechanical regime. Partial differential equations model natural laws. Mathematics is also used to interpret the outcome of experiments via statistics, i.e., the dichotomy between theory and experiment is not so clear.

Isn't it strange, and wonderful, that mathematics is able to accurately describe reality? Isn't it fascinating, that humans have made *mental models* built on logic, that is able to model reality? Isn't it strange, that whenever we need to refine our scientific models, then mathematics is malleable enough to provide the correct ones, and even make predictions of what new experiments may observe?

But what *is* mathematics? Here is a quote from the Wikipedia article on Mathematics:[1]

> Mathematics (from Ancient Greek μαθημα; máthēma: 'knowledge, study, learning') is an area of knowledge that includes such topics as numbers (arithmetic and number theory), formulas and related structures (algebra), shapes and the spaces in which they are contained (geometry), and quantities and their changes (calculus and analysis). Most mathematical activity involves the use of pure reason to discover or prove the properties of abstract objects, which consist of either abstractions from nature or—in modern mathematics—entities that are stipulated with certain properties, called axioms. A mathematical proof consists of a succession of applications of some deductive rules to already known results, including previously proved theorems, axioms and (in case of abstraction from nature) some basic properties that are considered as true starting points of the theory under consideration.

[1] Wikipedia. http://en.wikipedia.org/w/index.php?title=Mathematics&oldid=1103972043. [Online; accessed 17-August-2022]. 2022.

Thus, mathematics is a kind of tower built with the human capacity for abstract thought alone. Theories are built on more fundamental theories, branching out like a tree. But is there something at *the root*? Can we know *for sure* that no mistake has been made, destroing swathes of centuries-old work in a moment, once the mistake is discovered?

In the late 19th and early 20th century, the quest for a common foundation of mathematics, based on mathematics alone, led to a crisis: the foundational crisis of mathematics.[2] Paradoxes like the famous Russell's paradox questioned whether mathematics could be formulated consistently with mathematics alone. Most of us are used to mathematical sets being rather informally defined, e.g., via a list,

$$\mathbb{N} = \{0, 1, 2, 3, \ldots\}, \tag{1.1}$$

or via some condition,

$$C = \{x \mid x \text{ is a cat}\} \tag{1.2}$$

While this informal point of view ("naive" set theory) is often fine (mathematicians use it all the time), Russell's paradox shows what can go wrong. A certainly intuitive "fact" about sets is the *axiom schema of comprehension* due to Frege (1893):[3]

> If φ is a property, then there exists a set $Y = \{X \mid \varphi(X)\}$ of all elements having property φ.

However, this principle is false:

> *Russell's paradox* (1902): By a set, we mean any collection of objects — for example the set of all even integers or the set of all saxophone players in Brooklyn. The objects that make up a set are called its members or elements. Sets may themselves be members of sets; for example the set of all sets of integers has sets as its members. Most sets are not members of themselves; the set of cats, for example, is not a member of itself because the set of cats is not a cat. However, there may be sets that do not belong to themselves—perhaps, for example, a set containing all sets. Now, consider the set A of all those sets X such that X is not a member of X. Clearly, by definition, A is a member of A if and only if A is not a member of A. So, if A is a member of A, then A is also not a member of A; and if A is not a member of A, then A is a member of A. In any case, A is a member of A and A is not a member of A.

Thus, mathematicians found that they cannot always rely on their intuition.

Today, the foundational crisis of mathematics is mostly settled. Virtually all of mathematics can be formulated in terms of Zermelo–Fraenkel (ZF) set theory with the axiom of choice added (ZFC).

Example: In ZF theory, the natural numbers is defined recursively in terms of the empty set $\emptyset = \{\}$ (due to von Neumann):

$$0 := \emptyset, \quad 1 := \{\emptyset\}, \quad 2 := \{\emptyset, \{\emptyset\}\} \tag{1.3}$$

$$3 := \{\emptyset, \{\emptyset\}, \{\emptyset, \{\emptyset\}\}\} \tag{1.4}$$

$$\vdots \tag{1.5}$$

$$n + 1 = S(n) = n \cup \{n\} \tag{1.6}$$

The set $\mathbb{N}$ is now defined as the smallest set that contains all n while being closed under the successor function S. The *system* $\langle \mathbb{N}, 0, S \rangle$ is now a *model* of the Peano axioms for natural numbers and their

[2] Wikipedia. http://en.wikipedia.org/w/index.php?title=Foundations%20of%20mathematics&oldid=1097188669. [Online; accessed 17-August-2022]. 2022; J. Ferreiros. In: *The Princeton Companion to Mathematics*, p. 142. ISBN: 978-0-691-11880-2.

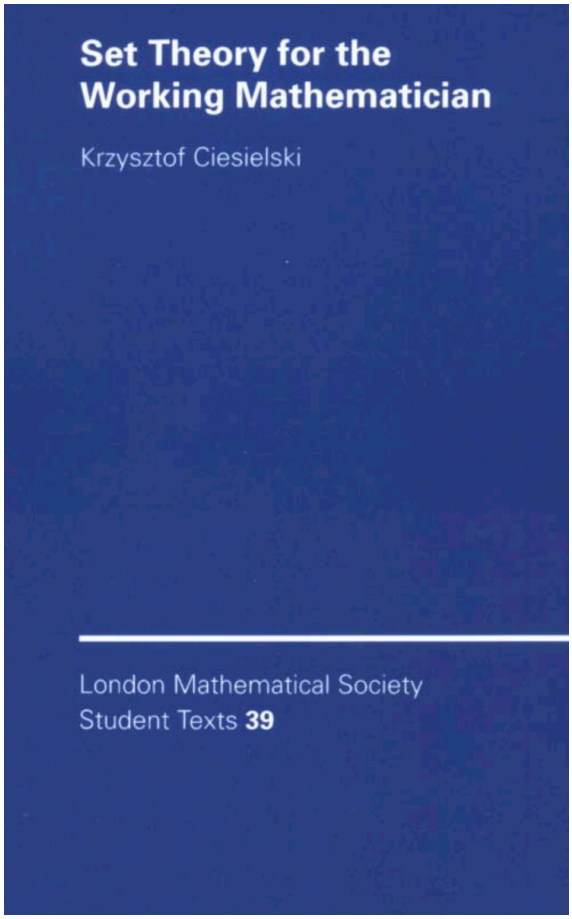
[3] K. Ciesielski. *Set Theory for the Working Mathematician*. London Mathematical Society Student Texts. Cambridge University Press, 1997. ISBN: 978-0-521-59441-7 978-0-521-59465-3.

arithmetic. The Peano axioms define natural numbers and their arithmetic operations *recursively* in terms of a successor function S acting on natural numbers to produce the next natural numbers. Thus, the natural numbers and their axioms can be exhibited in terms of sets and their axioms.

In a similar manner, axioms for the *rational numbers* $\mathbb{Q}$ can be built on the Peano axioms. And so on.

Recommended reading

This book is a widely recommended text on Zermelo–Fraenkel set theory with the axiom of choice (ZFC). It describes, in particular, encodings of "all" classical mathematical structures in terms of ZFC set theory.



1.2 Preliminary notes

1.2.1 Basic set notation

A set S is an unordered collection of its elements, e.g.,

$$S = \{1, 2, 3\}. \tag{1.7}$$

When x is an element, we write $x \in S$. Here, $1 \in S$ but $0 \notin S$. There is no limit to the number of elements a set can have. In particular $\emptyset = \{\}$ denotes the empty set. An infinite set is the set of natural numbers.

When all elements of one set S are also elements of another set T, we write $S \subset T$.

From two sets S and T we can construct new sets: The union $S \cup T$ consists of all elements of either set. The intersection $S \cap T$ consists of the elements common to both sets. The set difference $S \setminus T$ consists of S with the elements of T taken away.

We can also specify sets using a *condition* on a set S, i.e., a rule $P(x)$ for every $x \in S$ that evaluates to true or false. We then define

$$T = \{x \in S \mid P(x)\} \tag{1.8}$$

to denote the set of those $x \in S$ such that $P(x)$ is true. We can also use more complicated conditions, by either using English language, or mathematical symbols. For example,

$$P = \{\frac{1}{p} \mid p \text{ is prime}\}, \tag{1.9}$$

$$C^0[0,1] = \{f : [0,1] \to \mathbb{R} \mid f \text{ is continuous}\} \tag{1.10}$$

The *cardinality* of a set, $|S|$, is the number of elements of the set S. The cardinality of the natural numbers is denoted $\aleph_0$ ("aleph naught"). Two sets have the same cardinality if and only if they can be mapped one-to-one onto each other.

It is common to denote a set of sets a *family of sets*. Mathematically, there is (almost) no difference, since all mathematical objects are sets, but in everyday maths usage, we usually do not consider a number as a set, for example.

We can build *cartesian products of sets*. The cartesian product $S \times T$ is the set of ordered pairs (x, y), where $x \in S$ and $y \in T$. Note that an ordered pair is not the same as the set $\{x, y\}$, which is *unordered*. Similarly, cartesian products of n sets is an ordered n-tuple. A useful example is $\mathbb{R}^3 = \mathbb{R} \times \mathbb{R} \times \mathbb{R} = \{(x, y, z) \mid x, y, z \in \mathbb{R}\}$, that is, space.

Basic set operations include:

1. Union: $A \cup B = \{x \mid x \in A \text{ or } x \in B\}$
2. Intersection: $A \cap B = \{x \mid x \in A \text{ and } x \in B\}$
3. $A \setminus B = \{x \in A \mid x \notin B\} = B^{\complement}$

A mnemonic for remembering what is union and what is section, is that in the union, the symbol is a cup, that gathers everything from A and B.

1.2.2 Functions

A *function* or *map* $f : S \to T$ from a set S (the domain) to a set T (codomain) is a rule that assigns to every $x \in S$ precisely one element $f(x) \in T$. The set $\{f(x) \mid x \in S\}$ is a subset of T, and called the *range* of f.

The domain is the set of possible input, the codomain is what can possibly come out, and the range is what actually comes out.

If for every $y \in T$ there is an $x \in S$ such that $f(x) = y$, i.e., all elements of T are reached, we say that f is *surjective*, or *onto*. If $f(x) = f(x')$ implies that $x = x'$, then f is *injective* or *one-to-one*. If f is both surjective and injective, we say that f is *bijective*, or *one-to-one and onto*.

1.3 Numbers

1.3.1 The integers, the rationals, and the reals

The natural numbers are the counting numbers,

$$\mathbb{N} = \{0, 1, 2, \ldots\}. \tag{1.11}$$

It is a set of cardinality $\aleph_0$, the "smallest" infinity. The integers are the numbers ("Zahlen")

$$\mathbb{Z} = \{\ldots, -3, -2, -1, 0, 1, 2, \ldots\}, \tag{1.12}$$

which has the *same* cardinality as $\mathbb{N}$. Next, the rational numbers ("quotients"),

$$\mathbb{Q} = \left\{ \frac{p}{q} \mid p, q \in \mathbb{Z},\ q \neq 0 \right\}. \tag{1.13}$$

The cardinality is again $\aleph_0$.

[Exercise: prove that these sets have the same cardinality, and that the reals have a greater cardinality.]

Next up is the set of real numbers, but the precise definition of these in terms of $\mathbb{Q}$ is subtle. Let us therefore be very imprecise, and denote the reals by the set of all infinite decimal expansions,

$$\mathbb{R} = \{ \text{infinite decimal expansions of numbers} \} \tag{1.14}$$

$$= \mathbb{R} = \left\{ (-1)^s 10^p \times 0.a_1 a_2 a_3 a_4 \cdots \mid s \in \{0,1\},\ p \in \mathbb{Z},\ \forall j \in \mathbb{N},\ a_j \in \mathbb{Z}_{10} \right\}, \tag{1.15}$$

where $\mathbb{Z}_{10} = \{0,1,2,3,4,5,6,7,8,9\}$. The symbol "$\forall$" means "for all". Strictly speaking, this definition of $\mathbb{R}$ does not make sense, since we have to define what an infinite decimal expansion means. The correct answer is that it is a *limit* of rational number approximations, or rather an *equivalence class* of such.

We will not dig deeper into the real numbers. It is common to simply view the reals in an informal manner as a continuous infinite line, with the integers and rationals marked off, and the "gaps" denoting *irrational numbers* being those numbers that need infinitely many decimal places in any base, i.e., those reals which are not in $\mathbb{Q}$.

The real numbers have a special property: They are *complete* in the Cauchy sense. Informally, all sequences that "ought to converge" actually converges. We will talk more about this later.

The basic properties of the real numbers are usually formalized as a theorem:

Theorem 1

There is a unique number system called the real number system which is a complete ordered field.

By "ordered" we mean that it is always true that $a \leq b$ or $b \leq a$ for any $a, b \in \mathbb{R}$. By "unique" we mean that all other constructions that satisfy the axioms of fields, and is ordered, can be put into a one-to-one correspondence, this correspondence being compatible with the rules of multiplication, addition, and the ordering. In fact, this theorem justifies the mental picture of the reals as, indeed, the "real line".

These number sets are fairly easy to get a grasp on, and we note that they are included in one another, written

$$\mathbb{N} \subset \mathbb{Z} \subset \mathbb{Q} \subset \mathbb{R}. \tag{1.16}$$

The sets $\mathbb{Q}$ and $\mathbb{R}$ are also *fields*. Fields are abstractions of, well, numbers, with the following axioms:

Definition 1: Field

Let $\mathbb{F}$ be a set, together with binary operations + (addition) and · (multiplication) such that the following holds:

1. Commutativity of addition: $x + y = y + x$
2. Associativity of addition: $x + (y + z) = (z + y) + z$
3. Identity element for addition: There is a zero element $0 \in \mathbb{F}$ such that $0 + x = x$ for all $x \in \mathbb{F}$
4. Inverses for addition: For every $x \in \mathbb{F}$ there is a $y \in \mathbb{F}$ such that $x + y = 0$.
5. Commutativity of multiplication: $x \cdot y = y \cdot x$
6. Associativity of multiplication: $x \cdot (y \cdot z) = (z \cdot y) \cdot z$
7. Identity element for multiplication: There is a unit element 1 such that $1 \cdot x = x$
8. Inverse for multiplication: For every $x \neq 0$ there is a y such that $x \cdot y = 1$.
9. Distributive law: $x \cdot (y + z) = x \cdot y + x \cdot z$.

In short, numbers in a field can be manipulated using *all* the usual operations of real numbers. What distinguishes the rationals from the reals, is that the reals are complete.

1.3.2 Complex numbers

Besides $\mathbb{R}$, the complex numbers $\mathbb{C}$ are extremely important for us. The complex numbers are defined in terms of the real numbers by adjoining to $\mathbb{R}$ a special element i that satisfies

$$\mathrm{i}^2 = -1. \tag{1.17}$$

Adding this element alone does not generate a field, because a field must be closed under addition and multiplication. The smallest field that contains $\mathbb{R}$ and i is the set

$$\mathbb{C} = \{a + \mathrm{i}b \mid a, b \in \mathbb{R}\}, \tag{1.18}$$

which is also a field, but no longer an ordered field!

Important unary operations: Let $z = a + \mathrm{i}b \in \mathbb{C}$. Real part, $\mathrm{Re}\, z = a$. Imaginary part, $\mathrm{Im}\, z = b$. Complex conjugate, $\bar{z} = z^* = a - \mathrm{i}b$. Modulus, $|z| = \sqrt{a^2 + b^2}$.

Example 1: Multiplication and addition of complex numbers

Given two complex numbers $z_1 = x_1 + \mathrm{i}y_1$ and $z_2 = x_2 + \mathrm{i}y_2$. We compute the sum of the complex numbers:

$$z_1 + z_2 = (x_1 + \mathrm{i}y_1) + (x_2 + \mathrm{i}y_2) = (x_1 + x_2) + \mathrm{i}(y_1 + y_2). \tag{1.19}$$

We compute the product:

$$z_1 z_2 = (x_1 + \mathrm{i}y_1)(x_2 + \mathrm{i}y_2) = x_1 x_2 - y_1 y_2 + \mathrm{i}(y_1 x_2 + x_1 y_2), \tag{1.20}$$

where we used $\mathrm{i}^2 = -1$.

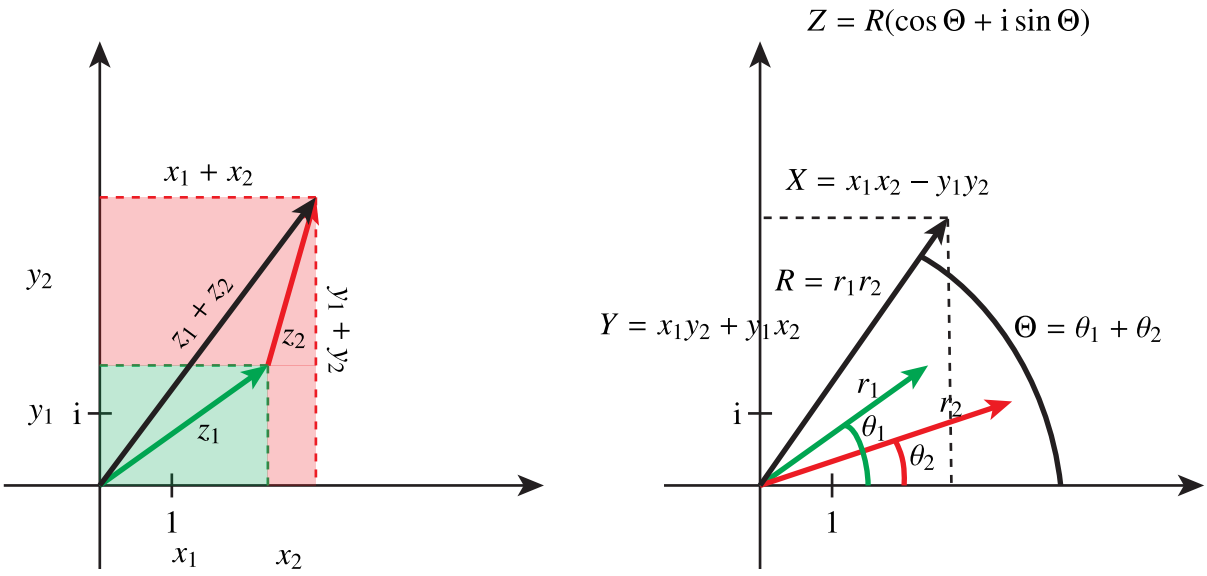


Figure 1.1: Geometric interpretation of addition and multiplication of complex numbers. Left: Addition $Z = z_1 + z_2$ of $z_1 = x_1 + \mathrm{i}y_1$ and $z_2 = x_2 + \mathrm{i}y_2$. Right: multiplication $Z = z_1 + z_2$.

1.3.3 Geometric interpretation

A geometric interpretation of the complex numbers was first given by the Norwegian cartographer and mathematician Caspar Wessel, who used complex numbers in his cartography work. The interpretation is as follows: Draw a two-dimensional coordinate system. The horizontal axis is the real line, while the vertical axis is the purely imaginary numbers $\mathrm{i}\mathbb{R}$. A point in the plane with coordinates (x, y) now corresponds to the complex number $z = x + \mathrm{i}y$. The rules of addition become the usual plane vector addition rules (componentwise addition/putting the tip of one arrow at the end of another arrow), while the rules of multiplication becomes multiplication of the moduli (lengths). and addition of the angles, between the points and the positive real line. See Figure 1.1.

1.3.4 Fundamental theorem of algebra

The complex numbers set $\mathbb{C}$ a kind of Columbi egg to solve the problem that a polynomial of degree n over the real numbers may not have a full set of n roots.

Theorem 2: Fundamental theorem of algebra

Every polynomial p of degree n over $\mathbb{C}$ have exactly n roots in $\mathbb{C}$, i.e., there is a nonzero $C \in \mathbb{C}$ and n numbers $r_i \in \mathbb{C}$, such that

$$p(z) = C(z - r_1)(z - r_2)\cdots(z - r_n).$$

Descartes used the term "imaginary" about the complex numbers. It was not because it was imaginative or similar, but rather in a pejorative sense: these numbers provide solutions to the root equations, but the roots are useless, since they don't exist anyway.

Well, do the complex numbers exist or not? Maybe he would have changed his mind if he saw the geometric interpretation – who knows?

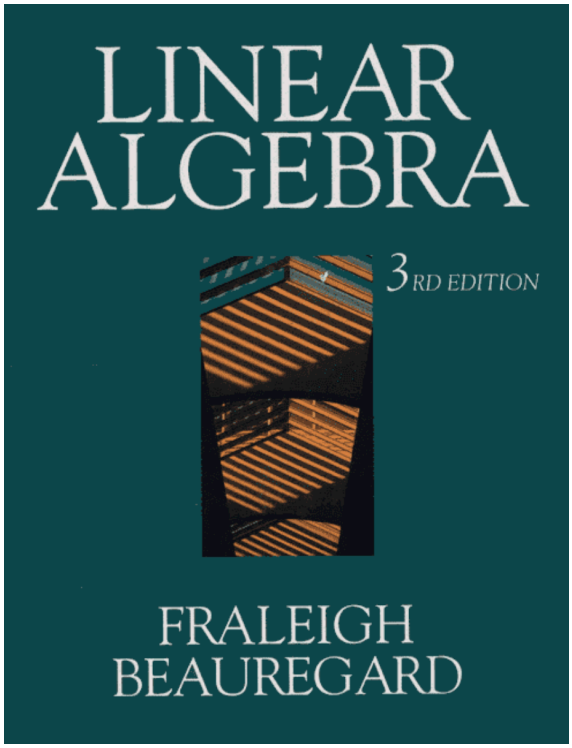
Linear algebra

2.1 Finite dimensional vector spaces

Linear algebra is perhaps the most important tool for modern science: quantum mechanics, data analysis, machine learning, …All use linear algebra in one way or another.

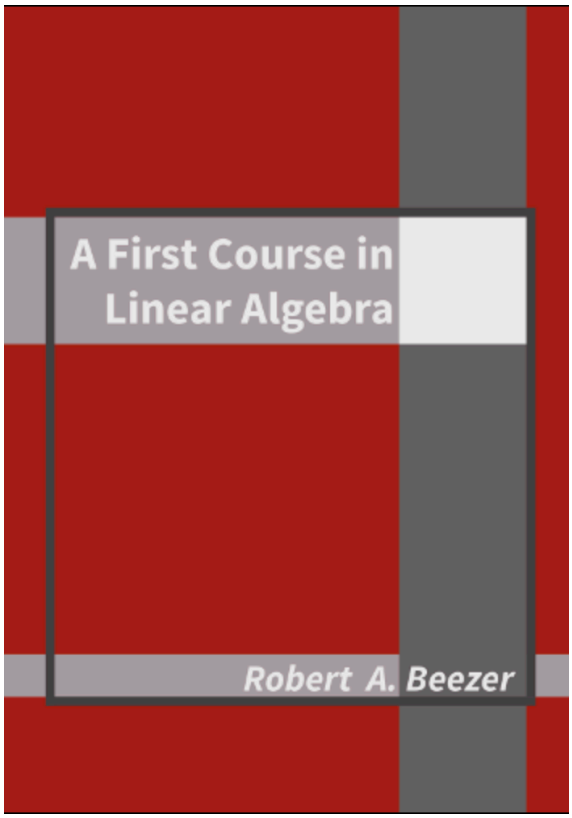
Recommended reading

This was my curriculum in the first linear algebra course I took. I think it is a very good book, and highly readable. What it lacks, is the consideration of general finite dimensional linear vector spaces.



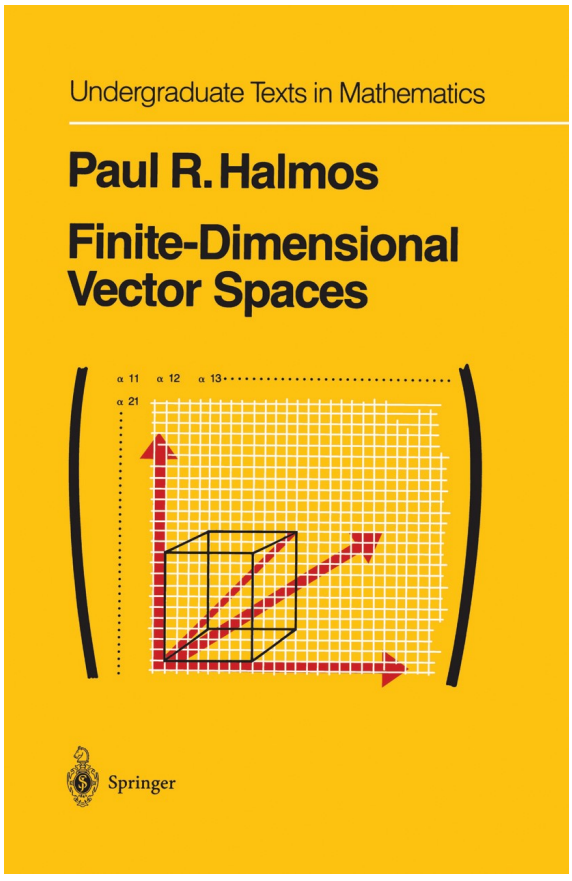
Recommended reading

An online textbook in linear algebra by Robert A. Beezer can be found here: http://linear.ups.edu/. It is free, and also has great sets of exercises. PDF versions here: http://linear.ups.edu/download.html



Recommended reading

This book by the great Paul Halmos is old, by very comprehensive. I find it quite readable, and have used it many times. I would consider the level to be more advanced than Fraleigh and Beauregard.



2.1.1 Euclidean space

Much of what we do in quantum chemistry is in the context of the spaces $\mathbb{R}^n$ or $\mathbb{C}^n$. These are examples of *vector spaces*. We will define general vector spaces later, but for the moment it is easier to concentrate on $\mathbb{F}^n$.

Definition 2: Euclidean space

Let $\mathbb{F}$ be either $\mathbb{R}$ or $\mathbb{C}$. Let $\mathbb{F}^n$ be the set of n-tuples of $\mathbb{F}$-numbers $\mathbf{x} = (x_1, \cdots, x_n)$, on which we define the following operations: For $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$ define

$$\mathbf{x} + \mathbf{y} \in \mathbb{F}^n, \quad (\mathbf{x} + \mathbf{y})_i = x_i + y_i \qquad \textbf{\textit{addition}}, \tag{2.1}$$

for all $1 \leq i \leq n$. and for any $\alpha \in \mathbb{F}$,

$$\alpha\mathbf{x} \in \mathbb{F}^n, \quad (\alpha\mathbf{x})_i = \alpha x_i \qquad \textbf{\textit{scalar multiplication}}. \tag{2.2}$$

We also define the Euclidean *inner prooduct*

$$\langle \mathbf{x}, \mathbf{y} \rangle = \bar{\mathbf{x}} \cdot \mathbf{y} = \sum_i \bar{x}_i y_i \in \mathbb{F} \qquad \textbf{\textit{Euclidean inner product}} \tag{2.3}$$

and the Euclidean norm

$$\|\mathbf{y}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} \in \mathbb{R}. \qquad \textbf{\textit{Euclidean norm}} \tag{2.4}$$

The two first axioms give $\mathbb{F}^n$ the structure of a vector space, while the two next axioms define a *topology*. We will see the formal definition of general vector spaces later. We will say more on topology later.

The boldface symbol for vectors in Euclidean space is very common in linear algebra. Less common, but not unusual, is the notation $\vec{r}$. This notation is more common in $\mathbb{R}^2$ and $\mathbb{R}^3$. It is also common to simply use plain letters u, v, etc., for vectors. Some like to put a tilde under the letters, $\underset{\sim}{u}$.

It is common to write vectors in $\mathbb{F}^n$ as *column vectors*, i.e.,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}. \tag{2.5}$$

It is also common to simply list the elements as a tuple,

$$\mathbf{x} = (x_1, x_2, \cdots, x_n). \tag{2.6}$$

You will see both versions in the literature, and one must get used to the different notations.

A *basis* is a set of vectors in which we may linearly expand every vector. We begin with the *standard basis*:

Definition 3: Standard basis

The *standard basis* for $\mathbb{F}^n$ is the set of vectors $\{\mathbf{e}_i \mid 1 \leq i \leq n\}$ such that

$$(\mathbf{e}_i)_j = \delta_{ij}, \qquad \textit{Kronecker delta symbol} \tag{2.7}$$

i.e.,

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \quad \text{etc.} \tag{2.8}$$

It now follows that for every $\mathbf{x} \in \mathbb{F}^n$,

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i. \tag{2.9}$$

You should convince yourself by doing calculations, that

$$x_i = \langle \mathbf{e}_i, \mathbf{x} \rangle . \tag{2.10}$$

2.1.2 Visualization in the plane

TODO: Illustrate vector addition, scalar multiplication, using arrows in the plane. Compare with componentwise addition and scalar multiplication.

2.1.3 Linear transformations

A very important class of functions on vector spaces are *linear transformations*, also known as *linear maps or functions*.

Definition 4: Linear transformation

Let $A : \mathbb{F}^n \to \mathbb{F}^m$ be a function. We say that A is a *linear transformation* if it conserves the vector addition and scalar multiplication laws, i.e., for all $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$

$$A(\mathbf{x} + \mathbf{y}) = A(\mathbf{x}) + A(\mathbf{y}), \tag{2.11}$$

and for all $\alpha \in \mathbb{F}$,

$$A(\alpha \mathbf{x}) = \alpha A(\mathbf{x}). \tag{2.12}$$

If a $n = m$, i.e., the special case when domain and codomain both are the same space, we often say that A is a *linear operator*

Any linear transformation $A : \mathbb{F}^n \to \mathbb{F}^m$ is determined uniquely by a *matrix*, i.e., there are unique coefficients $A_{ij} \in \mathbb{F}$, $1 \leq i \leq m$, $1 \leq j \leq n$, such that

$$A(\mathbf{x})_i = \sum_{j=1}^{n} A_{ij} x_j. \tag{2.13}$$

The first index i on A_{ij} is called the *row index*, and the second index j the *column index*. Thus, we think of A as a table:

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,m} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n,1} & A_{n,2} & \cdots & A_{n,m} \end{bmatrix} \tag{2.14}$$

Linear transformations form a vector space in a natural way (see later for definition):

$$(A + B)(\mathbf{x}) := A(\mathbf{x}) + B(\mathbf{x}), \quad (\alpha A)(\mathbf{x}) := \alpha A(\mathbf{x}). \tag{2.15}$$

In fact this vector space can be thought of as $\mathbb{F}^{nm}$, since the matrix elements behave just like nm vector components under addition and scalar multiplication. On the other hand, a matrix has a *shape*, so merely saying "$A \in \mathbb{F}^{nm}$" is ambigous.

Example 2

$$\begin{bmatrix} 1 & 4 & 6 \end{bmatrix} \in \mathbb{R}^{1\times 3} \quad \begin{bmatrix} 1 & 4 \\ -3 & \sqrt{3} \\ 8 & 0 \end{bmatrix} \in \mathbb{R}^{3\times 2} \quad \begin{bmatrix} 0 \\ \pi \end{bmatrix} \in \mathbb{R}^{2\times 1} \tag{2.16}$$

Definition 5: Matrix

Formally, a matrix $A \in M(n, m, \mathbb{F}) = \mathbb{F}^{n\times m}$ is a function $A : \{1, 2, \cdots, n\} \times \{1, 2, \cdots, m\} \to \mathbb{F}$. Informally, A is a table with n rows and m columns with entries in $\mathbb{F}$.

The space $\mathbb{F}^n$ is identified with $M(n, 1, \mathbb{F}) = \mathbb{F}^{n\times 1}$, the set of *column vectors*.

If we have two linear maps $A \in M(n, m; \mathbb{F})$ and $B \in M(m, o, \mathbb{F})$, the *composition* of the maps is again a linear map, and must have a matrix! That is, there must be some $C \in M(n, o, \mathbb{F})$ such that for all $\mathbf{x} \in \mathbb{F}^o$,

$$A(B(\mathbf{x})) = C(\mathbf{x}). \tag{2.17}$$

The solution is the matrix product:

Definition 6: Matrix product

Let $A \in M(n, m, \mathbb{F})$ and $B \in M(m, o, \mathbb{F})$. Then the *matrix product* $C = AB \in M(n, o; \mathbb{F})$ is defined by the formula

$$C_{ik} = \sum_{j=1}^{n} A_{ij} B_{jk}. \tag{2.18}$$

The matrix product satisfies:

1. $A(BC) = (AB)C$ ***associativity***
2. $(A + B)C = AC + BC$ and $A(B + C) = AB + AC$ ***distributivity***

However, the matrix product is *not commutative*, i.e., $AB \neq BA$ in general!

Note that the only instances where the matrix product $C = AB$ is defined is when the column dimension of A and row dimension of B match.

We observe that $\mathbb{F}^n = \mathbb{F}^{n\times 1}$ can be thought of as matrices, i.e., linear maps $\mathbf{x} : \mathbb{F} \to \mathbb{F}^n$. Therefore, $A(\mathbf{x})$ is a matrix product, and it is customary to drop the parenthesis, and just write $A(\mathbf{x}) = A\mathbf{x}$. *From now on we will do this*.

Definition 7: Dual space

The *dual space* of $\mathbb{F}^n = M(n, 1, \mathbb{F})$ is the set of linear functions $\omega : \mathbb{F}^n \to \mathbb{F}$, i.e., the set $M(1, n, \mathbb{F})$ of *row vectors*. The dual space is often written $(\mathbb{F}^n)'$.

The distinction between a vector space and its dual is subtle, but in finite dimensional Euclidean space things become very simple: Dual space is the space of row vectors.

Definition 8: Matrix transpose

For $A \in M(n, m, \mathbb{F})$ with matrix elements A_{ij}, the matrix transpose $A^T \in M(m, n, \mathbb{F})$ is defined by the matrix elements $(A^T)_{ij} = A_{ji}$, i.e., the table is reflected along the diagonal.

Example 3

$$\begin{bmatrix} 0 & 1 \\ -1 & \mathrm{i} \\ -2 & \pi \end{bmatrix}^T = \begin{bmatrix} 0 & -1 & -2 \\ 1 & \mathrm{i} & \pi \end{bmatrix} \tag{2.19}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}^T = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \tag{2.20}$$

For all matrices A, $(A^T)^T = A$.

Since a matrix $A \in M(n, m, \mathbb{F})$ is a linear map from $\mathbb{F}^n$ to $\mathbb{F}^m$, the matrix transpose is a unique linear transformation from $\mathbb{F}^m$ to $\mathbb{F}^n$. This transformation satisfies,

$$\forall \omega \in (\mathbb{F}^n)', \mathbf{x} \in \mathbb{F}^m, \quad \omega A\mathbf{x} = (A^T\omega)\mathbf{x}. \tag{2.21}$$

In this sense, the transpose of a matrix is an associated linear map on the dual space.

We do not need the notion of inner product to have the notion of dual. They are independent. However, since the inner product associates a number with two vectors, they are related. We note that

$$\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\mathbf{x}^T}\mathbf{y}.$$

and moreover that

$$\forall \mathbf{y} \in \mathbb{F}^n, \mathbf{x} \in \mathbb{F}^m, \quad \langle \mathbf{y}, A\mathbf{x} \rangle = \langle \overline{A}^T\mathbf{y}, \mathbf{x} \rangle \tag{2.22}$$

This leads to the definition

Definition 9: Hermitian adjoint

For $A \in M(n, m, \mathbb{F})$ with matrix elements A_{ij}, the Hermitian adjoint $A^H \in M(m, n, \mathbb{F})$ is defined by $A^H = \overline{A^T}$, i.e., the table is reflected along the diagonal and complex conjugated. In the case $\mathbb{F} = \mathbb{R}$ transpose and Hermitian conjugation are the same.

Example 4

$$A = \begin{bmatrix} 1+\mathrm{i} & 2-2\mathrm{i} \\ 1 & 0 \\ 0 & 0 \end{bmatrix} \quad A^H = \begin{bmatrix} 1-\mathrm{i} & 1 & 0 \\ 2+2\mathrm{i} & 0 & 0 \end{bmatrix} \tag{2.23}$$

For all matrices compatible with mutiplication,

$$(AB)^H = B^H A^H \tag{2.24}$$

A result which is non-trivial in the infinite dimensional case, is Riesz' representation theorem, that relates a Hilbert space and its dual. We mention it here, since it is easy to visualize in the finite dimensional case, and since you may come across this theorem in the more abstract infinite dimensional setting:

Theorem 3: Riesz' representation theorem

To every $\mathbf{x} \in \mathbb{F}^n$ there is an associated unique $\omega_{\mathbf{x}} \in (\mathbb{F}^n)'$ given by

$$\omega_{\mathbf{x}} = \langle \mathbf{x}, \cdot \rangle = \mathbf{x}^H. \tag{2.25}$$

Conversely, to every $\omega \in (\mathbb{F}^n)'$ there is a unique vector $\mathbf{x}_\omega = \omega^H$. In other words, the Hermitian conjugate is a one-to-one mapping between $\mathbb{F}^n$ and $(\mathbb{F}^n)'$.

The one-to-one mapping between $\mathbb{F}^n$ and its dual $(\mathbb{F}^n)'$ is *antilinear* in the case when $\mathbb{F} = \mathbb{C}$. A transformation $B : \mathbb{F}^n \to \mathbb{F}^m$ is antilinear if $B(\mathbf{x} + \mathbf{y}) = B(\mathbf{x}) + B(\mathbf{y})$ but $B(\alpha\mathbf{x}) = \bar{\alpha} B(\mathbf{x})$.

2.1.4 General vector spaces

The spaces $\mathbb{F}^n$ are archetypal finite-dimensional vector spaces. However, it is very useful to consider abstract vector spaces that are not manifestly the same as $\mathbb{F}^n$.

Here is the definition of a *general* vector space. Such spaces may have any dimension, even infinite:

Definition 10: Vector space

A *vector space over the field* $\mathbb{F}$ is a set V together with a binary *vector addition* $+ : V \times V \to V$ and *scalar multiplication* $\cdot : \mathbb{F} \times V \to V$ such that, for all $x, y, z \in V$ and all $\alpha, \beta \in \mathbb{F}$, the following axioms are true:

1. There exists a $0 \in V$ such that $0 + x = x$ for all $x \in V$ — ***identity element for addition***
2. $x + (y + z) = (x + y) + z$ — ***associativity for addition***
3. $x + y = y + x$ — ***commutativity for addition***
4. There exists x' such that $x + x' = 0$ — ***inverse element for addition***
5. $(\alpha\beta) \cdot x = \alpha \cdot (\beta \cdot x)$ — ***compatibility of scalar and field multiplications***
6. $1 \cdot x = x$ — ***identity for scalar multiplication***
7. $(\alpha + \beta) \cdot x = \alpha \cdot x + \beta \cdot x$ — ***distributivity of scalar multiplication***
8. $\alpha \cdot (x + y) = \alpha \cdot x + \alpha \cdot y$ — ***distributivity of scalar multiplication***

These are quite a few axioms, but this stems from the fact that a vector space structure is the combination of *two* general algebraic structures: an abelian group (addition), amd a ring homomorphism from $\mathbb{F}$ to the ring of endomorphisms of the given abelian group. For the example $V = \mathbb{F}^n$, some of the axioms are not necessary to state, since they follow from the definition of elementwise operations. Can you identify these extra axioms?

Vector spaces are very general, but we will be interested in *finite dimensional spaces* for the moment. In $\mathbb{F}^n$, the dimension was defined by n. But we need to characterize it abstractly, without reference to $\mathbb{F}^n$ as example.

We introduce the notion of *linear independence* and *dimension*.

Definition 11: Linear independence

Let V be a vector space, and $L \subset V$ a subset. The set L is *linearly indepdenent* if for any finite subset $\{v_i \mid 1 \leq i \leq k\} \subset L$, we have

$$\sum_{i=1}^{k} a_i v_i = 0 \implies a_i = 0 \text{ for all } i$$

The *dimension* of V is the cardinality of the largest linearly independent subset of V.

From this, we read that V has finite dimension n if and only if one can find at most n linearly dependent elements.

Note that linear independence in particular means that one of the v_i cannot be decomposed in terms of the other v_j.

Not all vector spaces are finite dimensional! Consider for example the space of all functions $f : S \to \mathbb{R}$, where S is an infinite set. The dimension of this space is the cardinality of S, which can be pretty big!

Consider now the space $\mathbb{F}^n$, with the standard basis. The standard basis vectors are all linearly independent in the sense of the definition above (see the Exercises). Any vector $\mathbf{x} \in \mathbb{F}^n$ can be *uniquely*

written

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i. \tag{2.26}$$

Thus, there cannot be subsets of $\mathbb{F}^n$ that are both linearly independent *and* have more elements than the standard basis! Thus, the dimension of $\mathbb{F}^n$ is n.

We apply these notions to general finite-dimensional spaces. Note that there is no notion of a "standard basis" in general.

Definition 12: Basis

Let V be a vector space of finite dimension n. A basis is a linearly independent set of vectors $\{b_1, \cdots, b_n\}$, with exactly n elements.

Theorem 4

If $B = \{b_1, \cdots, b_n\}$ is a basis for a the vector space V, $\dim(V) < +\infty$, then any $v \in V$ can be uniquely decomposed as

$$v = \sum_{i=1}^{n} v_i b_i. \tag{2.27}$$

The proof is not difficult: If there was some vector $v \in V$ that could *not* be decomposed like this, then $B \cup \{v\}$ is linearly independent with $n + 1$ elements, but this is not possible.

Definition 13: Dual basis

Let V be a vector space of finite dimension n, and let V' be its dual space. Let $B = \{b_1, \cdots, b_n\}$ be a basis, and let $\tilde{b}_i \in V'$ be defined by

$$\tilde{b}_i(b_j) = \delta_{ij}.$$

This basis $\tilde{B} = \{\tilde{b}_1, \cdots, \tilde{b}_n\}$ for V' is uniquely given by the basis B for V, and is called the dual basis to V (of V').

We now make the connection between finite dimensional vector spaces and $\mathbb{F}^n$.

Theorem 5: Isomorphism between finite dimensional spaces

Let V be a vector space over $\mathbb{F}$ of finite dimesion n, and let $B = \{b_i\}$ be a basis for V. Then, to every $v \in V$ there is a unique $\mathbf{x} \in \mathbb{F}^n$ such that

$$v = \sum_{i=1}^{n} x_i b_i. \tag{2.28}$$

Conversely, any $\mathbf{x} \in \mathbb{F}^n$ describes a unique $v \in V$ by the same formula. Thus, V and $\mathbb{F}^n$ are in one-to-one correspondence,

Moreover, let v and w have expansion coefficients $\mathbf{x}$ and $\mathbf{y}$, respectively. Then, $v + w$ has coefficients $\mathbf{x} + \mathbf{y}$, and αv has coefficients $\alpha\mathbf{x}$, for any $\alpha \in \mathbb{F}$.

In other words, V and $\mathbb{F}^n$ are *isomorphic* as vector spaces: There is a (basis-dependent) linear function $U : \mathbb{F}^n \to V$ such that

$$v = U\mathbf{x},$$

and such that U has an inverse as a function, *which is also linear*.

This may seem trivial. However finite-dimensional vector spaces are not always easily seen as identical to $\mathbb{F}^n$.

Example 5: Space of polynomials of bounded degree

Let V be the space of polynomials of degree less than or equal to n, $p \in V$ if and only if $p : \mathbb{F} \to \mathbb{F}$ has the form

$$p(x) = a_0 + a_1 x^1 + \cdots a_n x^n. \tag{2.29}$$

A basis, which may be considered "standard", is the basis of monomials x^k, for $0 \le k \le n$. The dimension of V is $n + 1$.

But we have not defined an inner product on the space of polynomials! Thus, it does not make sense to simply say that V' is identified with V. On the other hand, pick $n + 1$ distinct points $x_j \in \mathbb{F}$, and consider the operation of evaluation at x_j,

$$\omega_j(p) := p(x_j). \tag{2.30}$$

Then $\omega_j \in V'$ is a linear function on p in a natural way. One can show that all the ω_j are linearly independent, and thus form a basis for V'! But this basis does not satisfy $\omega_j(x^k) = \delta_{jk}$, so it is not dual to the monomial basis. But we can transform them by taking linear combinations to a dual basis.

TODO: Write exercise on the polynomials and the dual basis
TODO: Write up example of C*-algebra

Theorem 6: Linear transformations between finite dimensional spaces

Let V and W be vector spaces over $\mathbb{F}$ of finite dimensions n and m, respectively. Let $\hat{A} : V \to W$ be a linear transformation, i.e., $\hat{A}(v + v') = \hat{A}v + \hat{A}v'$, and $\hat{A}(\alpha v) = \alpha\hat{A}v$. We denote by $L(V, W)$ the set of such linear functions, which is a vector space, cf. (2.15).

The linear vector spaces $L(V, W)$ and $M(m, n, \mathbb{F})$ are isomorphic as vector spaces. That is, given bases for V and W, there is a linear one-to-one correspondence between $L(V, W)$ and $M(m, n, \mathbb{F})$.

We prove this as follows:
Let $B = \{b_i\}$ be a basis for V, and $C = \{c_i\}$ a basis of W, with dual basis $\{\tilde{c}_i\}$.
Let $v \in V$, and $w = \hat{A}v \in W$, with coefficients $\mathbf{v} \in \mathbb{F}^n$ and $\mathbf{w} \in \mathbb{F}^m$, respectively. Then

$$w_i = \sum_{j=1}^{n} A_{ij} v_j, \tag{2.31}$$

with

$$A_{ij} = \tilde{c}_i(\hat{A} b_j). \tag{2.32}$$

Conversely, any matrix $A \in \mathbb{F}^{m \times n}$ defines a unique $\hat{A} \in L(V, W)$.

This simple result is striking, in that for the finite dimensional case, and given that we have chosen a basis, we can think in terms of $\mathbb{F}^n$ and $M(n, m, \mathbb{F})$. All finite dimensional vectors spaces are "the same", and also the linear transformations will be "the same" by way of their matrix representations.

2.2 Inner product spaces

What actually distinguish finite dimensional spaces is their *topology*, i.e., how points are considered to be close to each other. Note that we did *not* use any inner product to make correspondences between a vector space V and $\mathbb{F}^n$. Indeed, there is no inner product on a general finite dimensional vector space V.

Example 6: Space of planets

Suppose we characterize a planet by its mass, diameter, and average distance from the sun, all measured in SI units. These three numbers are gathered in a vector $\mathbf{u} = [u_1, u_2, u_3]$, but the components refer to different units of measurements. Does it make sense to define the inner product between two planets as $\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + u_3 v_3$?

If we supply an inner product on V, we say that V is an inner product space, and since V is finite dimensional, it will also be *complete* and hence a *Hilbert space*. **TODO:** Refer to functional analysis section

Definition 14: Inner product

Let V be a vector space. An *inner product* $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ is a map which satisfies the following axioms:

1. $\langle x, x \rangle \geq 0, \quad \langle x, x \rangle = 0$ if and only if $x = 0$ — ***non-negative***
2. $\langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle$ — ***linearity***
3. $\langle \alpha y + \beta z, x \rangle = \bar{\alpha} \langle y, x \rangle + \bar{\beta} \langle z, x \rangle$ — ***conjugate linearity***
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$ — ***hermiticity***

Let V be a finite-dimensional Hilbert space, and let $B = \{b_i\}$ be a basis for V. Consider arbitrary vectors $v = \sum_{i=1}^{n} b_i v_i$ and $v' = \sum_{i=1}^{n} b_i v'_i$, and compute the inner product:

$$\langle v, v' \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} \bar{x}_i \langle b_i, b_j \rangle x'_j \equiv \sum_{i=1}^{n} \sum_{j=1}^{n} \bar{x}_i S_{ij} x'_j = \mathbf{x}^H S \mathbf{x}'. \tag{2.33}$$

The matrix S is often called the *overlap matrix of the basis* B. We see that that since we start with an inner product on V, the latter equation defines an inner product on $\mathbb{F}^n$ – but it is not the Euclidean inner product!

However, if S has matrix elements δ_{ij}, then we get the Euclidean inner product.

Definition 15: Orthonormal basis

Let V be a finite dimensional Hilbert space, and let $B = \{b_i\}$ be a basis. We say that B is an orthonormal basis if, for all i and j, $\langle b_i, b_j \rangle = \delta_{ij}$.

In finite dimensional Hilbert spaces (and indeed infinite dimensional separable Hilbert spacs), orthonormal bases are not very special: they always exist, and can be constructed using *Gram–Schmidt orthogonalization*.

Theorem 7: Existence of orthonormal basis

Any finite dimensional Hilbert space V has an orthonormal basis.

Theorem 8

Let V be a vector space of finite dimension n, and let $B = \{b_i\}$ be an orthonormal basis.

For any $v \in V$,

$$v = \sum_i v_i b_i, \quad v_i = \langle b_i, v \rangle . \tag{2.34}$$

Let $\hat{A} \in L(V)$ be a linear operator. The matrix of $\hat{A}$ has elements

$$A_{ij} = \langle b_i, \hat{A} b_j \rangle . \tag{2.35}$$

Definition 16: Hermitian adjoint

Let V, W be finite-dimensional Hilbert spaces, and let $\hat{A} \in L(V, W)$. The *Hermitian adjoint* $\hat{A}^\dagger$ is an operator in $L(W, V)$ defined by the criterion that for all $v \in W$ and all $w \in W$,

$$\langle w, \hat{A} v \rangle = \langle \hat{A}^\dagger w, v \rangle . \tag{2.36}$$

For a $v \in V$, we also define $v^\dagger \in V'$ by the criterion that for all $v' \in V$,

$$v^\dagger v' = \langle v, v' \rangle . \tag{2.37}$$

For a $\omega \in V'$ we define $\omega^\dagger \in V$ by the criterion that for all $v \in V$,

$$\omega v = \langle \omega^\dagger, v \rangle \tag{2.38}$$

Remark 1

This definition is compatible with the Hermitian adjoint of matrices. The definition of $v^\dagger$ and $\omega^\dagger$ is a one-to-one mapping between V and V', just like for vectors in $\mathbb{F}^n$. In particular $(v^\dagger)^\dagger = v$, and the inner product can be written

$$\langle v, w\rangle = v^\dagger w. \tag{2.39}$$

The matrix element of an operator $\hat{A} : V \to W$ becomes

$$\langle w, \hat{A}v\rangle = w^\dagger \hat{A} v = (\hat{A}^\dagger w)^\dagger v. \tag{2.40}$$

Thus, *just like for matrices, row vectors and column vectors*, whenever the product XY is defined, then $(XY)^\dagger = Y^\dagger X^\dagger$.

We are now in the situation, that, using an orthonornal basis, inner products are preserved when moving to coefficient space: If $\mathbf{u}, \mathbf{v} \in \mathbb{F}^n$ are the components of $u, v \in V$ in some orthonormal basis, then

$$\langle u, v\rangle = \langle \mathbf{u}, \mathbf{v}\rangle = \mathbf{u}^H \mathbf{v}. \tag{2.41}$$

This means that, as inner product spaces, there is nothing that distinguishes the Hilbert spaces V from $\mathbb{F}^n$.

Theorem 9: Finite dimensional Hilbert spaces are basically all the same

Finite dimensional Hilbert spaces over $\mathbb{F}$ of dimension n are all *isometrically isomorphic* to $\mathbb{F}^n$, and hence to each other. The word "isometricall" means that the inner product can be considered the same for both spaces.

Note that spaces over $\mathbb{R}$ and $\mathbb{C}$ are still different!

Remark 2

In order to study (the vector space structure of) finite dimensional Hilbert spaces, including the linear operators over these spaces, it suffices to $\mathbb{F}^n$ and matrices $M(n, m, \mathbb{F})$.

This is a very important fact!

2.2.1 Linear subspaces

We generalize the notion of a linear subspace to general vector spaces spaces (also infinite dimensional ones):

Definition 17: Linear subspace

Let V be a vector space over $\mathbb{F}$. A subset $W \subset V$ is a *linear subspace* if it is closed under vector addition and scalar multiplication, i.e., if

$$\forall w \in W, \quad \alpha w \in W, \quad w_1 + w_2 \in W, \tag{2.42}$$

and if $0 \in W$.

Linear subspaces are also vector spaces.

In the finite dimensional case V, we must have that $W \subset V$ is finite dimensional, too. In particular W has a basis of vectors $b_i \in V$, $1 \leq m \leq n$, and m is the dimension of W.

Conversely, any linearly independent set $\{b_i\}$ of m vectors of V define a subspace of all possible linear combinations, written:

$$W = \text{span}\{b_1, \ldots, b_m\}. \tag{2.43}$$

2.2.2 Dirac's bra-ket notation

Dirac introduced the bra-ket notation in his celebrated book on quantum mechanics. The notation, which is very useful, has some problems when one works in infinite dimensions. The interested student can have a look at the paper by Gieres **TODO:** add citation.

In the present case, we will use the bra-ket notation, since we work in finite dimensions, and since it is very intuitive and transparent.

Bras and kets The basic premise is that we write the inner product with a bar instead of a comma:

$$\langle u|v\rangle := \langle u, v\rangle \tag{2.44}$$

The idea is now that this is a scalar product between a vector $v \in V$ and a *dual element* $u^\dagger \in V'$, denoted

$$\langle u|v\rangle := \langle u, v\rangle = u^\dagger v. \tag{2.45}$$

We now define

$$|v\rangle := u \in V \quad (\text{“ket”}) \qquad \langle u| := |u\rangle^\dagger \in V' \quad (\text{“bra”}). \tag{2.46}$$

Thus, we interpret the bra-ket as a product between a bra and a ket,

$$\langle u|v\rangle = \langle u| \cdot |v\rangle\,. \tag{2.47}$$

Remark 3

The abstract juggling we did earlier with the daggers can be summarized as follows: We may think of kets as column vectors, and bras as row vectors. The dagger and the Hermitian adjoint are essentially the same operations:

$$|u\rangle \quad \longleftrightarrow \quad \mathbf{u} \in \mathbb{F}^{n\times 1} \tag{2.48}$$

$$\langle u| \quad \longleftrightarrow \quad \mathbf{u}^H \in \mathbb{F}^{1\times n} \tag{2.49}$$

Orthonormal basis Let $B = \{b_i\}$ denote an orthonormal basis for V. We denote the corresponding kets simply by $|i\rangle$. We may use any name we like, and simply using the index reduces clutter. Recall the expansion

$$|u\rangle = \sum_i^n u_i\,|i\rangle\,, \tag{2.50}$$

and that the coefficients were

$$u_i = \langle b_i, u\rangle = \langle i|u\rangle\,. \tag{2.51}$$

Inserting this expression gives

$$|u\rangle = \sum_i^n \langle i|u\rangle\,|i\rangle = \sum_i^n |i\rangle\,\langle i| \cdot |u\rangle\,. \tag{2.52}$$

We can pull $|u\rangle$ outside the sum, to get

$$|u\rangle = \left(\sum_i^n |i\rangle\langle i|\right)|u\rangle = |u\rangle\,. \tag{2.53}$$

Thus, the *identity operator* can be written using an orthonormal basis as

$$\mathbb{1} = \sum_i^n |i\rangle\langle i|\,. \tag{2.54}$$

More generally, consider the expression

$$|i\rangle\langle j|\,. \tag{2.55}$$

When acting on a basis vector, we see that it takes $|j\rangle$ and transforms it to $|i\rangle$. Watch this, where we use the $\mathbb{1}$ trick:

$$\hat{A} = \mathbb{1}\hat{A}\mathbb{1} = \sum_i^n\sum_j^n |i\rangle\langle i|\hat{A}|j\rangle\langle j| = \sum_{i,j}^n |i\rangle A_{ij}\langle j|\,. \tag{2.56}$$

We have derived the fact that the set $\{|i\rangle\langle j| \;:\; 1 \le i, j \le n\}$ is a basis for the linear space of operators over V!

This statement can of course be generalized to operators between different spaces V and W with their own orthonormal basis.

Another important operator tool is the following construction: Let $B = \{b_1, \cdots, b_m\} \subset V$, with $\dim(V) = n$, be a set of vectors. They may or may not be linearly independent. Let $|i\rangle$ be a standard basis vector for $\mathbb{F}^m$. Consider the operator $\hat{B} : \mathbb{F}^m \to V$ given by

$$\hat{B} = \sum_{i=1}^m |b_i\rangle\langle i|\,. \tag{2.57}$$

Let now $\mathbf{x} \in \mathbb{F}^m$, and compute

$$\hat{B}|\mathbf{x}\rangle = \sum_{i=1}^m |b_i\rangle x_i, \tag{2.58}$$

that is $\hat{B}$ *generates linear combinations*. One can think of $\hat{B}$ as a generalized matrix, where each "column" is a ket,

$$\hat{B} = [|b_1\rangle\ |b_2\rangle\ \cdots\ |b_m\rangle]. \tag{2.59}$$

Since V is n-dimensional, we can think of each ket as an n-dimensional vector in $\mathbb{F}^n$, i.e., $\hat{B}$ is like a matrix in $\mathbb{F}^{n\times m}$.

2.3 Matrices

We know that all linear transformations between finite dimensional spaces are naturally expressed with matrices. Therefore, the manipulation of matrices and understanding their behavior is essential for any quantum chemist.

2.3.1 Column space, row space, rank

A matrix $A \in \mathbb{F}^{n\times m}$ has a set of *columns*, the jth column is denoted $A_{:,j}$ and a set of *rows*, the ith row denoted $A_{i,:}$. This notation can remind us about the Python or Matlab notations for taking slices.

Example:

$$A = \begin{bmatrix} 1+\mathrm{i} & 2-2\mathrm{i} \\ 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad A_{:,1} = \begin{bmatrix} 1+\mathrm{i} \\ 1 \\ 0 \end{bmatrix}, \quad A_{:,2} = \begin{bmatrix} 2-2\mathrm{i} \\ 0 \\ 0 \end{bmatrix}, \quad A_{1,:} = [1+\mathrm{i},\ 2-2\mathrm{i}], \quad A_{2,:} = [1,\ 0], \quad A_{3,:} = [0,\ 0]. \tag{2.60}$$

Note the comma notation on the rows. This is for clarity.

The significance of the columns is the following: Let $\mathbf{a}_i = A_{i,:}$ be the ith column. We write

$$A = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n].$$

We now act with A on some $\mathbf{x} \in \mathbb{F}^n$, and it is straightforward to see, that the answer is:

$$A\mathbf{x} = \mathbf{a}_1 x_1 + \mathbf{a}_2 x_2 + \cdots + \mathbf{a}_n x_n. \tag{2.61}$$

Thus: The result is a linear combination of the columns, the coefficient being given by $\mathbf{x}$.

Similarly, the rows are significant when acting *to the left* on some row vector.

Definition 18: Column space

For a matrix $A = [\mathbf{a}_1, \cdots, \mathbf{a}_n] \in \mathbb{F}^{n\times m}$, the *column space* is the set of all linear combinations of the columns $\mathbf{a}_i$. This is also denoted *the range* or *image* of A, since it is the set of all vectors $A\mathbf{x}$.

The column space is a linear vector space, written

$$\mathrm{span}\{\mathbf{a}_1,\ \mathbf{a}_2,\ \cdots, \mathbf{a}_n\}. \tag{2.62}$$

The *rank* of the matrix is the dimension of the column space.

The row space is defined similarly.

(It is a fact that the dimension of the row space is the same as the dimension of the column space.)

Facts: Any linear subspace of $\mathbb{F}^n$ is the column space of some matrix (not unique). The columns form a basis for the subspace.

2.3.2 Systems of linear equations

Consider a matrix $A \in M(n, m, \mathbb{F})$. Consider the *linear equation*: Find $\mathbf{x} \in \mathbb{F}^n$ such that, for a given $\mathbf{y} \in \mathbb{F}^m$,

$$A\mathbf{x} = \mathbf{y}. \tag{2.63}$$

This is one of the basis uses of matrices: to solve linear systems of equations.

Written out in terms of matrix elements and vector components,

$$A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n = y_1 \tag{2.64}$$
$$A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n = y_2 \tag{2.65}$$
$$\vdots \tag{2.66}$$
$$A_{m1}x_1 + A_{m2}x_2 + \cdots + A_{mn}x_n = y_m \tag{2.67}$$

Given this setup, several things can happen:

1. No solutions exist. This may only happen if $m \geq n$, and we say that the equations are *inconsistent* or *overdetermined*.

2. Exactly one solution exists for every $\mathbf{y}$. If $m > n$, some equations can be eliminated and can be reduced to a square system with $n = m$.

3. An infinite number of solutions exist, and we say that the system is *underdetermined*. This may happen both for $n \neq m$ and $n = m$.

Suppse A is square, and that $\mathbf{x}$ can be found for *any* $\mathbf{y} \in \mathbb{F}^n$, then this solution defines a linear map $\tilde{A} : \mathbb{F}^n \to \mathbb{F}^n$ such that

$$\tilde{A}A\mathbf{x} = \tilde{A}\mathbf{y} = \mathbf{x}.$$

This map is the *inverse function* of A. Thus, it is natural to write $\tilde{A} = A^{-1}$ for the solution operator.

In some cases, there is no unique solution. This happens precisely when the rank of A is smaller than n. The set of $\mathbf{x}$ such that $A\mathbf{x} = 0$ is the *null space* of A. This is a linear subspace. Its dimension is the *nullity*.

Theorem 10: Rank/nullity theorem

Let $A \in \mathbb{F}^{m \times n}$. Rank of A + nullity of A equals n.

2.3.3 Gaussian elimination

A classic way to solve a linear system of equations is by *gaussian elimination*. Given a linear equation $A\mathbf{x} = \mathbf{y}$, we expand it in order to see better:

$$A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n} = y_1 \tag{2.68}$$
$$A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n} = y_2 \tag{2.69}$$
$$\vdots \tag{2.70}$$
$$A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nn} = y_n \tag{2.71}$$
$$\tag{2.72}$$

Thus, A_{ij} is the coefficient of x_j in the ith equation, the right-hand side of which is y_i. Now, we can produce an equivalent linear system by *multiplying equations by (nonzero) numbers* or *adding pairs of equations*. That is *taking linear combinations of equations*.

In gaussian elimination, one proceeds systematically. First, we write down the *augented matrix*

$$B = [A|\mathbf{y}] \in \mathbb{F}^{n \times (n+1)}. \tag{2.73}$$

We then use using *elementary row operations* to bring the system to *row echelon form*.

Definition 19: Row echelon form

A matrix $T \in \mathbb{F}^{n \times m}$ is on row echelon form if $T_{ij} = 0$ whenever $i > j$, and if the *leading coefficient* (first nonzero) of row number i is always to the left of the leading coefficient of row number $i + 1$. The leading coefficient is also called a *pivot*

The elementary matrix operations are:

- Multiply a row by a nonzero number
- Swap two rows
- Add one row to another (includes subtraction by first multiplying by nonzero scalar)

Example 7

This matrix is in row echelon form. The pivots are in squares.

$$\begin{bmatrix} \boxed{1} & 2 & 0 & 0 \\ 0 & \boxed{2} & -4 & -1 \\ 0 & 0 & 0 & \boxed{1} \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.74}$$

We say that two matrices are *equivalent* if they are related by one or more elementary operations, written $A \sim A'$.

The leading coefficients can all be taken to be 1, by a final scaling operation if necessary.

When the row echelon form has been obtained, we will be able to find a unique solution to the linear system *if and only if the diagonal of the row echelon form is nonzero*. Assuming the diagonal elements to be 1, solving the system is trivial *by backsubstitution*: the last equation says y_n =something, and by substituting into the $n-1$th equation, we get y_{n-1}, etc.

Alternatively, we may bring the matrix to the form $B = [I|\mathbf{x}]$ by further elementary operations.

To compute the matrix inverse, we start with the augmented matrix $B = [A|I]$ and use elementary operations to bring it to the form $\tilde{B} = [I|A^{-1}]$.

Example 8

Solve the linear system

$$x_1 + x_2 + x_3 = 0, \quad x_1 - 2x_2 + 3x_3 = 1, \quad 4x_1 - x_3 = 2. \tag{2.75}$$

Augmented matrix:

$$B = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & -2 & 3 & 1 \\ 4 & 0 & -1 & 2 \end{bmatrix} \tag{2.76}$$

We begin by subtracting the first row from the second, and 4 times the first row from the third:

$$B \sim \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & -3 & 2 & 1 \\ 4 & 0 & -1 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & -3 & 2 & 1 \\ 0 & -4 & -5 & 2 \end{bmatrix} \tag{2.77}$$

We now multiply the second row by $-1/3$ and the third by $-1/4$:

$$B \sim \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & -2/3 & -1/3 \\ 0 & 1 & 5/4 & -1/2 \end{bmatrix} \tag{2.78}$$

Finally, we subtract row 2 from row 3 to get the row echelon form

$$B \sim \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & -2/3 & -1/3 \\ 0 & 0 & 23/12 & -1/6 \end{bmatrix} \tag{2.79}$$

We simplify a bit and multiply the last row by $12/23$

$$B \sim \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & -2/3 & -1/3 \\ 0 & 0 & 1 & -12/138 \end{bmatrix} \tag{2.80}$$

Solving the linear system is now easy: $x_3 = -12/138$ from the last equation. We insert back into the second equation:

$$x_2 = (2/3)x_3 - 1/3, \tag{2.81}$$

and finally

$$x_1 = -x_2 - x_3. \tag{2.82}$$

2.3.4 Matrix powers

We may compose A with itself, which gives a matrix power,

$$AA\mathbf{x} = A^2\mathbf{x}.$$

Higher powers are defined similarly.

How about negative powers?

The *matrix inverse* defined above satisfies

$$AA^{-1} = A^{-1}A = I,$$

where I is the common notation for the *identity matrix*, with elements $I_{ij} = \delta_{ij}$. The identity matrix is such that $I\mathbf{x} = \mathbf{x}$ for all $\mathbf{x} \in \mathbb{F}^n$.

We define $A^{-k} = (A^{-1})^k$, and we now have, with the definition $A^0 = I$,

$$A^{k+l} = A^k A^l = A^l A^k, \quad \forall k, l \in \mathbf{Z}.$$

2.3.5 Classes of operators

We now consider some important classes of operators.

Definition 20

Let V be a Hilbert space over $\mathbb{F}$ of finite dimension n, and let $\hat{A} \in L(V)$ be a linear operator. We say that A is …

1. Hermitian if $\langle u, \hat{A}v\rangle_V = \langle \hat{A}u, v\rangle_V$ for all $u, v \in V$. Equivalently, the matrix of $\hat{A}$ in any orthonormal basis satisfies $A^H = A$.
2. Unitary if it preserves inner products, i.e., $\langle u, v\rangle_V = \langle \hat{A}u, \hat{A}v\rangle_V$. Equivalently, the matrix satisfies $A^H = A^{-1}$.
3. Normal if it *commutes* with its adjoint, $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}$
4. Invertible if $\hat{A}^{-1}$ exists

2.3.6 The eigenvalue decomposition

Given a linear operator $\hat{A} \in L(V)$, consider the *eigenvalue equation*: Find $\lambda \in \mathbb{F}$ and a nonzero $v \in V$ such that

$$\hat{A}v = \lambda v. \tag{2.83}$$

We call λ an *eigenvalue*, v an *eigenvector*, and (λ, v) an *eigenpair*. Clearly, if v is an eigenvector, then αv is an eigenvector for any $\alpha \neq 0$. So an eigenvector is defined only up to a multiplicative constant.

Suppose (λ', v') is another eigenpair. Then,

$$\langle u|\hat{A}|v\rangle = \lambda \langle u|v\rangle = \lambda' \langle u|v\rangle . \tag{2.84}$$

If $\lambda' \neq \lambda$, then we must have $\langle u|v\rangle = 0$. So if we have a set of n different eigenvalues, then we can build an orthonormal basis of eigenvectors! This is significant, because it tells us that there exists a basis for V in which $\hat{A}$ is very easy to describe!

All normal operators have such orthonormal bases:

Theorem 11: Spectral theorem for normal operators

Suppose $\hat{A} \in L(V)$ is a normal operator. Then, there exists an orthonormal basis $\{v_1, \cdots, v_n\}$ such that

$$\hat{A} = \sum_{i=1}^{n} |v_i\rangle \lambda_i \langle v_i| . \tag{2.85}$$

In terms of the matrices relative to some orthonormal basis, there exists a unitary matrix U such that

$$A = \sum_{i=1}^{n} \mathbf{u}_i \lambda_i \mathbf{u}_i^H = U \Lambda U^H \tag{2.86}$$

where $\mathbf{u}_i$ is the ith column of U, and where Λ is a diagonal matrix with elements $\Lambda_{ij} = \lambda_i \delta_{ij}$

2.3.7 Singular value decomposition

One of the most striking matrix factorizations is *the singular-value decomposition* (SVD). It decomposes a matri A as follows:

Theorem 12: Singular value decomposition

Let $A \in M(n, m, \mathbb{F})$ be a matrix, and let $k = \min(n, m)$. There exists k *singular values* $\sigma_i \geq 0$ and k *left singular vectors* $\mathbf{u}_i$, and k *right singular vectors* $\mathbf{v}_i$, such that

$$A = \sum_{i=1}^{k} \mathbf{u}_i \sigma_i \mathbf{v}_i^H = U \Sigma V^H,$$

where $U = [\mathbf{u}_1, \cdots, \mathbf{u}_k]$, $V = [\mathbf{v}_1, \cdots, \mathbf{v}_k]$, $\Sigma = \mathrm{diag}(\sigma_1, \cdots, \sigma_k)$. Equivalently,

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i.$$

The rank of A is the number of nonzero singular values. The decomposition is unique if all the singular values are distinct.

Interpreting the SVD: $V^\dagger \mathbf{x}$ decomposes $\mathbf{x}$ along k orthonormal vectors. The matrix Σ scales the vectors by a constant amount, and finally U maps rotates the scaled vectors to a new orthonormal set of k vectors.

Since the decomposition always exists, the SVD is a universal geometric interpretation of *any* matrix!

It is customary to arrange the singular values in descending order. If we *truncate* the expansion after $\ell < k$ terms,

$$A_\ell = \sum_{i=1}^{\ell} \mathbf{u}_i \sigma_i \mathbf{v}_i^\dagger, \tag{2.87}$$

we obtain an approximation to A which is *optimal* in the so-called Frobenius, or Hilbert–Schmidt norm on matrices,

$$\|A\|_{\mathrm{F}} = \left(\sum_{ij} |A_{ij}|^2 \right)^{1/2}, \tag{2.88}$$

i.e., the space of matrices $M(n, m, \mathbb{F})$ is viewed as Euclidean nm-dimensional space, a Hilbert space.

The SVD is a powerful tool in data analysis, since it identifies the most important components of a matrix.

Topologies on vector spaces

3.1 The notion of a topology

In our discussion of Euclidean space and finite-dimensional Hilbert spaces in Sec. 2.1.4, we had an *inner product* at our disposal. The inner product could be used to define a *norm*, that measured length. Appealing to the linear structure of the space, we could measure distances, $d(x, y) = \|x - y\|$.

A distance measure gives us the ability to talk about *closeness* between points, i.e., a *topology*. In the field of topology, one makes these concepts abstract. In particular, we get axioms for *open and closed subsets*. These sets are used, for example, to define various concepts of functions $f : U \to V$ being *continuous*.

Not all topologies are equal. By carefully choosing the topology when describing a problem, one can obtain results on convergence of, say, a quantum chemical calculation as the number of basis functions increase.

3.2 Metric space hierarchy

We are now motivated to look closer at metric spaces, and open and closed sets in metric spaces. In this section, we look at metric spaces, and these will be the most general topological spaces we discuss.

A vector space with a topology is called a *topological vector space* (TVS).

3.2.1 Inner product spaces

Definition 21: Inner product

Let V be a vector space. An *inner product* $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ is a map which satisfies the following axioms:

1. $\langle x, x \rangle \geq 0, \quad \langle x, x \rangle = 0$ if and only if $x = 0$ — ***non-negative***
2. $\langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle$ — ***linearity***
3. $\langle \alpha y + \beta z, x \rangle = \bar{\alpha} \langle y, x \rangle + \bar{\beta} \langle z, x \rangle$ — ***conjugate linearity***
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$ — ***hermiticity***

We say that the pair $(V, \langle \cdot, \cdot \rangle)$ is an *inner-product space*.

3.2.2 Normed spaces

In Euclidean space, the length of a vector $\mathbf{v} \in \mathbb{F}^n$ is $\|\mathbf{v}\| = \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}$. This is but one out of many possible *norms* on Euclidean space. Norms are abstractions of the notions of *length* of elements of

vector spaces:

Definition 22: Norm

Let V be a vector space. A *norm* $\|\cdot\| : V \to \mathbb{R}_+ = [0, +\infty[$ is a function that satisfies the following axioms:

1. $\|x\| \geq 0$, and $\|x\| = 0$ if and only if $x = 0$. ***positivity***
2. $\|\alpha x\| = |\alpha| \|x\|$ ***absolute homogeneity***
3. $\|x + y\| \leq \|x\| + \|y\|$ ***triangle inequality***

The pair $(V, \|\cdot\|)$ is called a *normed vector space*.

You should convince yourself that the axioms indeed correspond to what we expect from a useful concept of length.

3.2.3 Angles between vectors

Returning to the inner product, we can now obtain some intuition using the associated norm. The inner product measures *angles between vectors*. Indeed, any inner product satisfies the Cauchy–Schwarz inequality:

Lemma 1: Cauchy--Schwarz inequality

Let $(V, \langle \cdot, \cdot \rangle)$ be an inner product space, and let $\|\cdot\|$ be the induced norm. Then, for any $x, y \in V$, it holds that

$$\langle x, y \rangle \leq \langle x, x \rangle^{1/2} \langle y, y \rangle^{1/2} = \|x\| \, \|y\|. \tag{3.1}$$

The Cauchy–Schwarz inequality implies that

$$0 \leq \frac{|\langle x, y \rangle|}{\|x\| \|y\|} \leq 1 \tag{3.2}$$

so that we may define the *angle* between the vectors as the unique $\theta \in [0, \pi/2]$ such that

$$\cos \theta = \frac{|\langle x, y \rangle|}{\|x\| \|y\|}. \tag{3.3}$$

Note in particular that if $\langle x, y \rangle = 0$, then $\theta = \pi/2$, coinciding with the notion of x and y being orthogonal to each other.

3.2.4 Metric spaces

Norms can be used to measure *distance* in Euclidean space and in inner product spaces in general. Given two elements $\mathbf{u}, \mathbf{v} \in \mathbb{F}^n$, the distance is given by $\|u - v\|$. This is a special case of a *metric*, whose definition gives axioms that encapsulate the notion of distance:

Definition 23: Metric

Let M be a set. A function $f : S \times S \to \mathbb{R}$ is a *metric* if it satisfies the following axioms:

1. $d(x, y) = d(y, x)$ ***symmetry***
2. $d(x, y) \geq 0$, and $d(x, y) = 0$ if and only if $x = y$ ***positivity and nondegeneracy***
3. $d(x, y) \leq d(x, z) + d(z, y)$ ***triangle inequality***

The pair (M, d) is a *metric space*. If M is a vector space, we say that (M, d) is a *metric vector space*.

In this definition, note that we are not starting with a vector space, since none of the axioms actually *use* vector space properties of the set!

Again, make sure that you understand how the axioms embody essential properties expected from a distance measure.

3.2.5 Metric spaces include normed spaces and inner product spaces

When a vector space V has an inner product, a norm, or a metric, we say that V is a *topological vector space*. The concept of a *topological space* is more general than a metric space (which is the most general space we are going to define in these notes). A topological space axiomates the concept of open sets, while for metric spaces, the open sets are defined in terms of the metric. (The open sets defined using the metric satisfies the axioms of general topology.)

Before we move on to the topology of metric spaces, we merely observe that everything we say is also valid in normed vector spaces and inner product spaces due to the hierarchical manner in which these are defined:

An inner product space is a normed space, and a normed space is a metric space.

3.3 Some topological concepts

A topology gives structure to a point set, e.g., which points are nearby other points. This allows the notion of *convergence of sequences* and *continuous functions*. With the vector space structure, we can also study *differentiation* from a very general point of view.

3.3.1 Sequences and limits

Definition 24: Sequence

Let S be a set. A *sequence* is a function $a : \mathbb{N} \to S$, i.e., an infinite "vector" $(x_1, x_2, x_3, \cdots)$, with $x_j = a(j) \in S$. It is common to suppress the actual function a and simply write "(x_j) is a sequence in S," or "let $(x_j) \subset S$ be a sequence," or other similar variants.

Warning: Do not confuse the notation x_j here with the jth component of a vector in $\mathbb{F}^n$! If we have a sequence in $\mathbb{F}^n$, we will have n sequences of $\mathbb{F}$-numbers, $(\mathbf{x}_j)_i \in \mathbb{F}$.

Sometimes, the index is not a natural number, but some other countable set. This still defines a sequence, since countable sets can be be brought into 1-to-1 correspondence with the natural numbers. Somtimes the index is even more general, such as a real mumber ε that goes to zero from above. In topology this is called a *net*. We will not discuss nets here.

If (M, d) is a metric space, we can study the convergence of the sequence.

Definition 25: Convergent sequence

Let (M, d) be a metric space, and let $(x_i) \subset M$ be a sequence. If there is some $x \in M$ such that for all $\varepsilon > 0$, there is an N_ε such that $i > N_\varepsilon$ implies $d(x_i, x) < \varepsilon$, we say that (x_i) is convergent, and that it converges to x, written $x_i \to x \in M$, or $\lim_{i \to +\infty} x_i = x$.

TODO: Elaborate with pictorial examples
Which sequences converge?

Definition 26: Cauchy sequence

We say that (x_i) is *Cauchy convergent* if for every $\varepsilon > 0$ there is an $N_\varepsilon \in \mathbb{N}$ such that $i, j > N_\varepsilon$ implies

$$d(x_i, x_j) < \varepsilon. \tag{3.4}$$

Thus, the elements of the sequence get closer and closer in a uniform manner. After the index N_ε, no two elements *ever* get further apart than a distance ε.

Such sequences *should* converge: It is inescapable that the distance between successive elements approach zero the further into the sequence one gets. In fact, the opposite assertion is true:

Theorem 13

If a sequence converges, it is Cauchy convergent.

Note that Cauchy convergence does not refer to the potential limit. Only elements at various positions in the sequence are referred to in the definition.

Example 9: Non-convergent Cauchy sequence

Consider a sequence $(x_i) \in \mathbb{Q}$ of *rational numbers*. Let $x = \sqrt{2} \in \mathbb{R} \setminus \mathbb{Q}$ (an irrational number), and let x_i be the decimal expansion of x to i significant digits after the decimal points. Thus, $x_1 = 1.4$, $x_2 = 1.41$, etc. If this sequence converges, it should be to x. It is straightforward to see that for $i > j$, $|x_i - x_j| = |(x - x_j) - (x - i_j)| \leq |x - x_j| + |x - x_i| \leq 10^{-i} + 10^{-j} \leq 2 \cdot 10^{-j}$. So if we choose $\varepsilon > 0$, find j such that $2 \cdot 10^{-j} < \varepsilon$. We then see that (x_i) is a Cauchy sequence. But the sequence does not converge to a rational number, beacuse we know the limit to be irrational.

The example demonstrates that a space can be incomplete, in that it lacks certain limits.

Definition 27: Complete metric space

We say that (M, d) is *(Cauchy) complete* if every Cauchy sequence is convergent.

From the construction of the real numbers $\mathbb{R}$, Cauchy completeness is built in as a fundamental property. Using the Euclidean metric in $\mathbb{R}^n$, one can then show the very important fact that:

Theorem 14

Euclidean space $\mathbb{F}^n$ is complete.

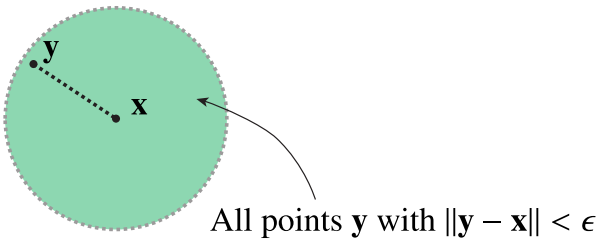


Figure 3.1: The open ball $B_\varepsilon(\mathbf{x})$ of radius ε around $\mathbf{x}$.

Why is completeness important? The completeness of a metric space ensures that limits of Cauchy sequences exist within the space, providing a solid foundation for many important theorems and applications in analysis, physics, and applied mathematics, including quantum chemistry. Without completeness, the analysis would be prone to gaps and inconsistencies.

3.3.2 Topologically important sets

The metric defines ε-*balls*:

Definition 28: ε-ball

Let (M, d) be a metric space. Let $x \in M$. The ε-ball around x is the set

$$B_\varepsilon(x) = \{y \in M \mid d(x, y) < \varepsilon\}. \tag{3.5}$$

The ε-ball is the archetypal *open set*, and illustrated in Fig. 3.1. In Fig. 3.2 subsets that are open, closed, and neither open nor closed are illustrated. Open sets are needed to understand the concepts of limits, continuity, and differentiation of functions.

Example 10: Two metrics on $\mathbb{R}^2$

Let us consider $\mathbb{R}^2$ with the usual Euclidean metric. Denote by $\mathbf{x} = (x_1, x_2)$ and $\mathbf{y} = (y_1, y_2)$ two points in $\mathbb{R}^2$. Then the Euclidean distance between these points is

$$d_{\text{Euclidean}}(\mathbf{x}, \mathbf{y}) = [(x_1 - y_1)^2 + (x_2 - y_2)^2]^{1/2}.$$

Furthermore, the open ball of radius r around the origin is the set

$$B_\varepsilon(0, \text{Euclidean}) = \left\{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 < \varepsilon^2\right\}.$$

This is the geometric description of the interior of a circle with radius ε centered at the origin.

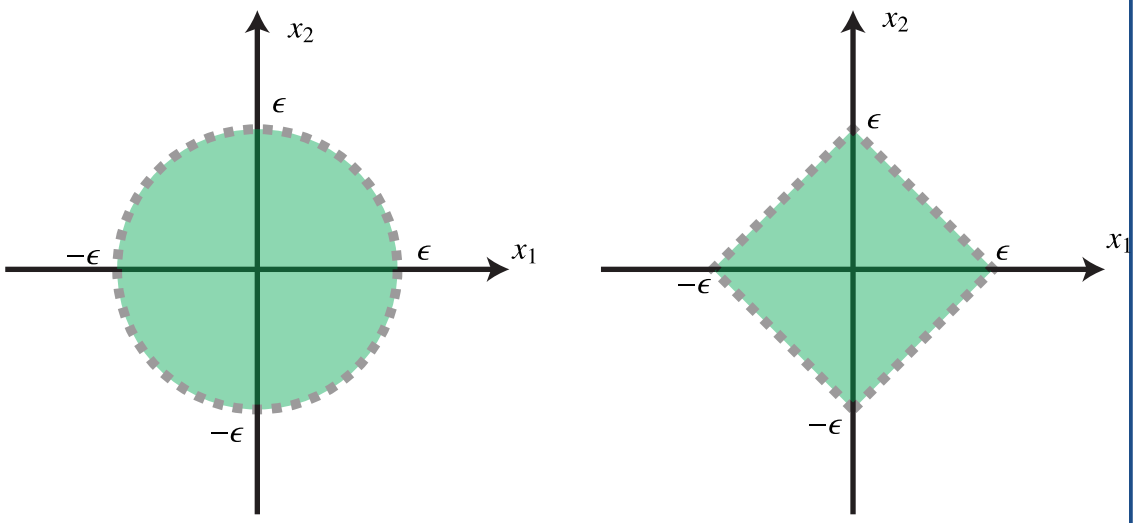
Let us consider an alternative metric, the *Manhattan metric*, named so because it is the relevant metric from the point of view of a taxicab driving along perfectly straight streets that cross each other at right angles:

$$d_{\text{Manhattan}}(\mathbf{x}, \mathbf{y}) = |x_1 - y_1| + |x_2 - y_2|.$$

The open ball of raius ε around the origin is now:

$$B_\varepsilon(0, \text{Manhattan}) = \left\{(x, y) \in \mathbb{R}^2 \mid |x| + |y| < \varepsilon\right\}.$$

The Euclidean ε-ball is illustrated below to the left, while the Manhattan unit ball is illustrated to the right:



Open sets can be used to redefine convergence of sequences.

Theorem 15: Convergence in terms of open sets

Let $(x_i) \subset M$ be a sequence in a metric space (M, d). Then x_i converges to $x \in M$, if and only if for every ε-ball $B_\varepsilon(x)$, (x_i) is *eventually in that ball*, i.e., there is an $N_U \in \mathbb{N}$, such that $x_i \in B_\varepsilon(x)$ whenever $i > N_U$.

The phrase "for all ε-balls" can be replaced with "for all neighborhoods of x".

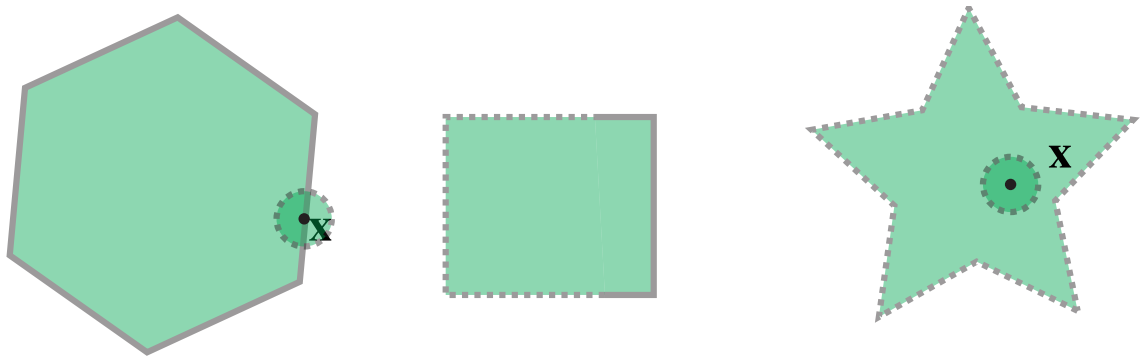


Figure 3.2: Illustration of open set (right), closed set (left), and neither open nor closed (middle) in the plane $\mathbb{R}^2$. The dashed lines indicate boundaries that are *not* included in the set, while the full lines indicate boundaries that *are* in the set. The rightmost set is open, since for every point in the set there is a finite distance to the edge. The leftmost set includes the boundary. If we select a point on the boundary, any ε-ball will be partially outside the set. On the other hand, the complement of the set is open, since it has no boundary! The middle set contains parts of its boundary, but not all, so it cannot be closed.

Definition 29: Neighborhood

Let (M, d) be a metric space, and let $x \in M$. A *neighborhood* N of x is any $N \subset M$ that contains x.

Definition 30: Open and closed sets, complements

Let (M, d) be a metric space. A subset $S \subset M$ is *open* if, for every $x \in S$, there exists an ε-ball completely contained in S.

The *complement* of S is defined as

$$S^{\complement} = \{x \in M \mid x \notin A\} = M \setminus S. \tag{3.6}$$

We say that S is *closed* if $S^{\complement}$ is open. (There are sets that are both open and closed, and neither open nor closed.)

Definition 31: Boundary and interior

A point $\mathbf{x} \in A$ is called *a boundary point* if every neighborhood of $\mathbf{x}$ both contains a point in A and a point in $A^{\complement}$.

The *boundary* ∂A is the set of boundary points of A.

The *interior* of A is the set of all points $\mathbf{x} \in A$ such that for some $\varepsilon > 0$, $B_\varepsilon(\mathbf{x}) \subset A$.

The *closure* of A is the smallest closed set containing A, and is equal to $A \cup \partial A$.

The concept of Cauchy completeness can be reformulated using open and closed sets:

Definition 32: Complete metric space

A metric space (M, d) is *complete* if for any open set $U \subset M$ (such as an ε-ball $B_\varepsilon(x) \subset M$), then $\mathrm{cl}(U) \subset M$.

Intuitively, the boundary of every open ball should be contained in the set.
The following definition/theorem stresses the link between completeness and closed sets:

Definition 33: Limit points

Let (M, d) be a metric space, and let $S \subset M$ be a subset. The closure $\mathrm{cl}(S)$ is the set of limit points of S: If $(x_i) \subset S$ is a sequence, and if $\lim x_i = x \in M$, then in actually $x \in \mathrm{cl}(S)$. Conversely, if $x \in \mathrm{cl}(S)$, there exists a sequence in S that converges to x. The closure $\mathrm{cl}(S)$ is the *smallest* set that contains all the limit points of S.

3.3.3 Continuity

Take a function $f : [0, 1] \to \mathbb{R}$, where $[0, 1] = \{x \in \mathbb{R} \mid 0 \leq x \leq 1\}$. You should be familiar, at least intuitively, with the notion of f being continuous, perhaps differentiable (at a point or everywhere), or even smooth. These notions are defined using topology, since we somehow need to study the behavior of f in the vicinity of some $x \in [0, 1]$.

Definition 34: Continuity

Let (M_1, d_1) and (M_2, d_2) be complete metric spaces. Let a function $f : M_1 \to M_2$ be given, and let $x \in M_1$, $y = f(x) \in M_2$. We say that f is *continuous* at x if for every $\varepsilon > 0$, there is a $\delta > 0$, such that $f[B_\delta(x)] \subset B_\varepsilon(y)$. Equivalently, for every neighborhood V_2 of y, there is a neighborhood V_1 of x such that $f[V_1] \subset V_2$.

This may seem complicated, but using words, the definition simply says: f is continuous at x if points that are nearby $f(y)$ in the image come from points nearby x. For our function $f : [0, 1] \to \mathbb{R}$, this states that you should be able to draw the graph without removing the pen from the paper.

That picture is useful, but not entirely accurate – when you move the pen, this must be in a smooth manner! But there are continuous functions that would require, say, infinite acceleration or an "infinite amount of ink."

TODO: Make illustration of Weierstrass function

3.3.4 Compactness

An important notion in metric spaces is that of *compactness*.

Definition 35: Compact sets

Let (M, d) be a metric space, and let $S \subset M$. We say that S is *compact* if every sequence $(x_i) \subset S$ has a convergent subsequence. That is, there is an increasing function $f : \mathbb{N} \to \mathbb{N}$ of indices such that $y_j := x_{f(i)}$ is a convergent sequence, $y_j \to y \in S$. Usually, subsequences are written informally as $y_j = x_{i_j}$.

Compactness may be hard to get a grasp on from the get go, but the intuition is that S behaves a little like a finite set. There is not too much "room" for the sequence x_i to wander around. Eventually, it must revisit the same neighborhood (of y) infinitely many times, getting infinitely closer.

An important consequence of compactness is the following:

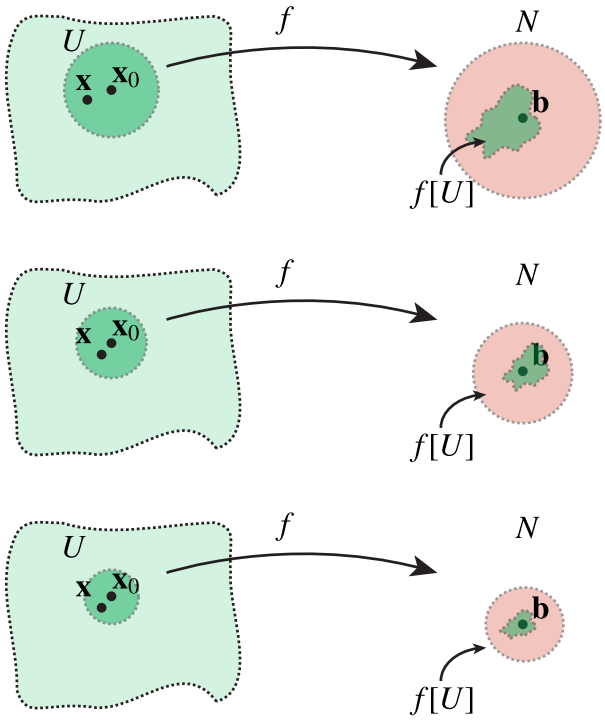


Figure 3.3: Illustration of the concept of continuity, using a function $f : \mathbb{R}^2 \to \mathbb{R}^2$ as an example. For every neighborhood N, taken to be an ε-ball, there shoud be an open set U such that $f[U] \subset N$. The ball N becomes smaller and smaller, but we can always find a corresponding U. Then, f is continuous.

Theorem 16: Images of compact sets

If $f : M \to N$ is a function between metric spaces, and if $S \in M$ is a compact set, then $f[S] \subset N$ is compact.

In finite dimensional vector spaces with a metric, compactness becomes easy to characterize:

Theorem 17: Compact sets in finite dimensions

If (M, d) is a finite dimensional metric vector space, then every compact subset is closed and bounded. The converse is also true.

3.3.5 Move me

TODO: Move this section!

In Figure 3.3, the concept of a continuous function is illustrated, using a function $f : \mathbb{R}^2 \to \mathbb{R}^2$ as an example.

Theorem 18

Let $f : \mathbb{F}^n \to \mathbb{F}^m$ be a function. Thus, we have m functions $f_i : \mathbb{F}^n \to \mathbb{F}$, $f_i(\mathbf{x}) = f_i(x_1, \cdots, x_n)$. Then f is continuous at $\mathbf{x} \in \mathbb{F}^n$ if and only if all the components f_i are continuous in all the n variable separately.

3.3.6 Limits and continuity

In Euclidean space, we are assigned a *topology* defined by the norm. That is, we can measure distances,

$$d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|. \tag{3.7}$$

The metric (here, our norm) defines ε-*balls*:

Definition 36: ε-ball

Ket $\mathbf{x}_0 \in \mathbb{R}^n$. The ε-ball around $\mathbf{x}_0$ is the set

$$B_\varepsilon(\mathbf{x}_0) = \{\mathbf{x} \in \mathbb{R}^n \mid \|\mathbf{x} - \mathbf{x}_0\| < \varepsilon\}. \tag{3.8}$$

The ε-ball is the archetypal *open set*. Open sets are needed to understand the concepts of limits, continuity, and differentiation of functions.

Definition 37: Open and closed sets

A subset $A \subset \mathbb{R}^n$ is *open* if, for every $\mathbf{x} \in A$, there exists an ε-ball completely contained in A.

The *complement* of A is defined as

$$A^\complement = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \notin A\} = \mathbb{R}^n \setminus A. \tag{3.9}$$

We say that A is *closed* if $A^\complement$ is open.

[Illustration]

Definition 38: Neghborhood

Let $\mathbf{x} \in \mathbb{R}^n$. A *neighborhood* of $\mathbf{x}$ is any open subset that contains $\mathbf{x}$.

Definition 39: Boundary and interior

A point $\mathbf{x} \in A$ is called *a boundary point* if every neighborhood of $\mathbf{x}$ both contains a point in A and a point in $A^\complement$.

The *boundary* ∂A is the set of boundary points of A.

The *interior* of A is the set of all points $\mathbf{x} \in A$ such that for some $\varepsilon > 0$, $B_\varepsilon(\mathbf{x}) \subset A$.

The *closure* of A is the smallest closed set containing A, and is equal to $A \cup \partial A$.

[Illustration]
[Exercises]

Definition 40: Limit

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, where Ω is open. Let $\mathbf{x}_0 \in \Omega \cup \partial\Omega$, and let N be a neighborhood of $\mathbf{b} \in \mathbb{R}^m$.

We say that f is *eventually in N as $\mathbf{x}$ approaches $\mathbf{x}_0$*, if there exists a neighborhood U of $\mathbf{x}_0$, such that $\mathbf{x} \in U$ but $\mathbf{x} \neq \mathbf{x}_0$ and $\mathbf{x} \in \Omega$ imply $f(x) \in N$.

We say that $f(\mathbf{x})$ *approaches* $\mathbf{b}$ *as* $\mathbf{x}$ *approaches* $\mathbf{x}_0$,

$$\lim_{\mathbf{x}\to\mathbf{x}_0} f(\mathbf{x}) = \mathbf{b} \quad \text{or} \quad f(\mathbf{x}) \to \mathbf{b} \text{ as } \mathbf{x} \to \mathbf{x}_0, \tag{3.10}$$

when, given any neighborhood N of $\mathbf{b}$, f is eventually in N as $\mathbf{x}$ approaches $\mathbf{x}_0$.

Interpretation: $f(\mathbf{x})$ is close to $\mathbf{b}$ if $\mathbf{x}$ is close to $\mathbf{x}_0$.
Important to note that *limits are unique*.

Definition 41: Continuity

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$. Let $\mathbf{x}_0 \in \Omega$. We say that f is *continuous at* $\mathbf{x}_0$ if

$$\lim_{\mathbf{x}\to\mathbf{x}_0} f(\mathbf{x}) = f(\mathbf{x}_0). \tag{3.11}$$

This is the multidimensional version of the notion that the graph of a continuous function is unbroken, does not make jumps.

[Examples]
[Exercises]

Theorem 19: Properties of continuous functions

Let $f, g : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be functions with a common domain Ω, continuous at $\mathbf{x}_0$: Then:

1. $f + g$ and αf for any $\alpha \in \mathbb{R}$ are continuous at $\mathbf{x}_0$.
2. In the scalar-valued case $m = 1$, the product fg is continuous at $\mathbf{x}_0$
3. If $f \neq 0$ in all of Ω, then $1/f$ is continuous at $\mathbf{x}_0$
4. The component functions $f_i : \Omega \to \mathbb{R}$ are all continuous at $\mathbf{x}_0$. The converse is also true.

Theorem 20: Compositions of functions

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be continuous at $\mathbf{x}_0 \in \Omega$, and $g : \Omega' \subset \mathbb{R}^m \to \mathbb{R}^o$. Suppose $f[\Omega] \subset \Omega'$, and let g be continuous at $\mathbf{y}_0 = f(\mathbf{x}_0)$. Then $h : \Omega \subset \mathbb{R}^n \to \mathbb{R}^o$,

$$h(\mathbf{x}) = g(f(\mathbf{x}_0)$$

is continuous at $\mathbf{x}_0$.

[Exercises]
We have an equivalent characterization of continuity using an ε-δ argument:

Theorem 21: ε-δ continuity

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$. Then f is continuous at $\mathbf{x}_0 \in \Omega$ if and only if for every $\varepsilon > 0$ there is a $\delta > 0$ such that

$$\mathbf{x} \in \Omega \text{ and } \|\mathbf{x} - \mathbf{x}_0\| < \delta \quad \Longrightarrow \quad \|f(\mathbf{x}) - f(\mathbf{x}_0)\| < \varepsilon. \tag{3.12}$$

The norm and inner product spaces encountered earlier are specializations of the general concept of *topological vector spaces (TVS)*. We have the chain,

$$\text{TVS} > \text{metric vector space} > \text{normed vector space} > \text{inner product space}$$

The spaces to the right are less general than the spaces to the left. The fact that we have a *topology*, means that we can talk about continuous functions between the spaces. (This is very different from saying that the functions in function spaces are continuous!)

Example 11

The Sobolev space $H^2([0,1])$ of twice weakly differentiable functions in $L^2([0,1])$ with derivatives in $L^2([0,1])$. Let $T = -\frac{1}{2}\partial^2/\partial x^2$ be the Laplace operator. This function is a linear continuous function from $H^2([0,1])$ to $L^2([0,1])$.

Topological vector space. A translationally invariant definition of *open sets* is given. In topology, open sets are much more general than those defined by metrics. A *locally convex* TVS, for example, is given by a *family of seminorms*. The perhaps most prominent example of a TVS are the spaces of *test functions* and *distributions*, e.g., objects like the Dirac δ-function.

Metric vector space. The open sets are given by ε-balls defined by a metric. Thus, a metric space is a TVS.

Definition 42: Metric

Let M be a set. A function $f : S \times S \to \mathbb{R}$ is a *metric* if it satisfies the following axioms:

1. $d(x,y) = d(y,x)$ — ***symmetry***
2. $d(x,y) \geq 0$, and $d(x,y) = 0$ if and only if $x = y$ — ***positivity and nondegeneracy***
3. $d(x,y) \leq d(x,z) + d(z,y)$ — ***triangle inequality***

The pair (M,d) is a *metric space*.

The intuition behind the metric is that is an abstraction of computing distances between points. However, there are many different ways of measuring distance than the Euclidean distance. Indeed, many spaces are not Euclidean at all.

Normed vector space. The metric is given by a *norm*,

$$d(x,y) = \|x - y\| \tag{3.13}$$

If a normed vector space is complete, it is called a *Banach space*.

Inner product space. The norm is given by an *inner product*, An inner product induces a norm:

$$\|x\| = \sqrt{\langle x, x \rangle}. \tag{3.14}$$

If the inner product space is complete, it is called a *Hilbert space*.

Definition 43: Inner product

An *inner product* $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ is a map which satisfies the following axioms:

1. $\langle x, x \rangle \geq 0, \quad \langle x, x \rangle = 0$ if and only if $x = 0$ — ***non-negative***
2. $\langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle$ — ***linearity***
3. $\langle \alpha y + \beta z, x \rangle = \bar{\alpha} \langle y, x \rangle + \bar{\beta} \langle z, x \rangle$ — ***conjugate linearity***
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$ — ***hermiticity***

Measure and integration theory

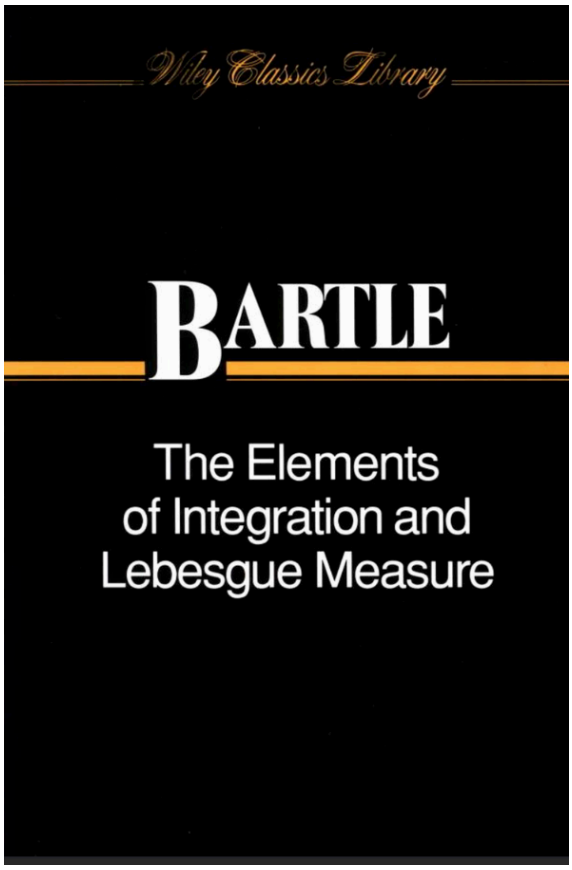
Most (all?) laws of nature are formulated using *differential equations*, and in general, partial differential equations (PDEs) form a class of problems of great value to any scientist.

The Schrödinger equation for a molecule is a PDE. Its mathematically rigorous formulation relies on abstract vector spaces of *Lebesgue integrable functions*. Moreover, computing and manipulating integrals is an important task in theoretical chemistry. Thus, we here give an overview of the field *measure and integration*.

The Lebesgue integral is a generalization of the Riemann integral. Admittedly, it is rather more complicated to define, but the result is powerful results that allow us to define such things as Hilbert spaces of square integrable functions.

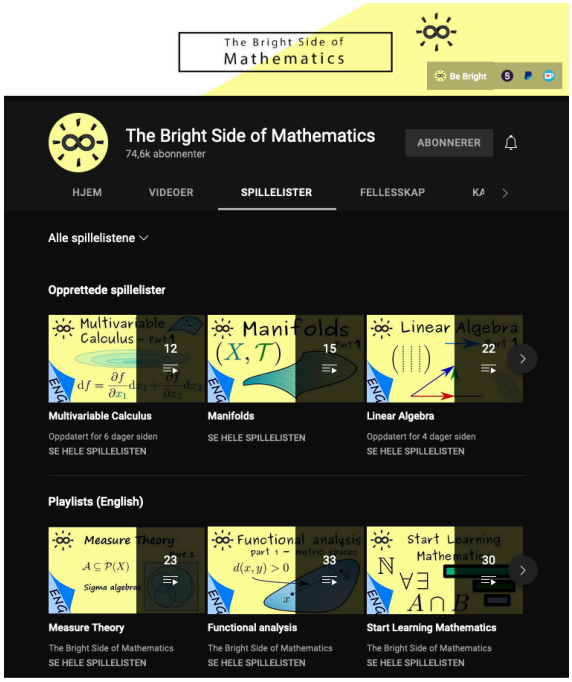
Recommended reading

The slim book by Bartle is a classic in measure and integration theory. It contains all you need.



Recommended reading

An excellent YouTube channel is *The Bright Side of Mathematics*, created by Dr. Julian P. Grossmann. Fantastic pedagogical presentation of many topics, well suited to give an intuitive impression and even more. Check out the videos on measure and integration! In fact, I based parts of my presentation of this topic on the videos.



4.1 Measurable sets

Measure theory tries to assign *measure* to subsets of some set X. This can be lengths of intervals of $\mathbb{R}$, areas in $\mathbb{R}^2$, et.c. A little thought shows that we need to consider quite general subsets. For example, I expect to be able to measure the area of a circle, but also the circle with a single point, or a countable number of points, punched out. Moreover, when integrating functions, we compute areas under a curve. Changing a function at a single point in $\mathbb{R}$, or a whole surface in $\mathbb{R}^3$, does not change the value of the integral of the function. We need to have a more rigorous understanding of measure.

Consider the real line $\mathbb{R}$. Our intuition tells us that an interval $[a,b] \subset \mathbb{R}$ has length $\mu([a,b]) = b-a$. The symbol μ means "measure". Similarly, the length of $\mathbb{R}$ must be infinite, $\mu(\mathbb{R}) = +\infty$. We also want the measure of a union of two disjoint intervals to be the sum of the lengths, $\mu([a,b] \cup [c,d]) = \mu([a,b]) + \mu([c,d])$, with $a < b \leq c < d$. And the measure of a single point should be zero, $\mu(\{x\}) = 0$. The measure of finitely many points should also be zero, but what about infinitely many points? If the set is *contably infinite*, we expect the measure to be zero, but the interval is an *uncountably infinite* set, with positive measure.

This leads to the notion of a σ-algebra; an all-important notion in measure theory:

Definition 44: σ-algebra

et X be a set. A σ-algebra $\boldsymbol{X}$ is a family of subsets of X such that:

1. $\emptyset, X \in \boldsymbol{X}$ — ***empty set and X***
2. $A \in \boldsymbol{X}$ if and only if $A^{\complement} = X \setminus A \in \boldsymbol{X}$ — ***complements***
3. $A_i \in \boldsymbol{X}$ for $i \in I \subset \mathbb{N}$ implies that $\bigcup_{i \in I} A_i \subset \boldsymbol{X}$ — ***countable unions***

The pair $(X, \boldsymbol{X})$ is called a measurable space, and $A \in \mathcal{X}$ is called a measurable (sub)set.

Reading between the lines, so to speak, we dont't expect to be able to measure *all* subsets of X. Indeed, it turns out it is not possible in general to define a measure on all subsets of, say, $\mathbb{R}$. *There will be non-measurable sets, to which we cannot assign a meaningful measure.*

Example 12

The smallest possible σ-algebra:

$$\boldsymbol{X} = \{\emptyset, X\} \tag{4.1}$$

The largestpossible σ-algebra:

$$\boldsymbol{X} = 2^X = \{\text{all subsets of } X\} \tag{4.2}$$

Interesting cases lie between these.

The following lemma is useful, because it shows that one can always find a *smallest* σ-algebra fulfilling some condition:

Lemma 2: Intersections of σ-algebras

Let I be a set, and let $\{\boldsymbol{X}_i \mid i \in I\}$ be a family of σ-algebras. Then the intersection of all the σ-algebras is again a σ-algebra:

$$\boldsymbol{X} = \{A \mid A \in \boldsymbol{X}_i \text{ for all } i \in I\} \tag{4.3}$$

Turning to Euclidean space, or any other metric space, *the open sets* form subsets that we wisth to make measurable.

Definition 45: Borel σ-algebra

Let X be a metric space. The Borel σ-algebra $\boldsymbol{B}(X)$ is the smallest σ-algebra that contain all open subsets of X. (It is enough to require that it contains all ε-balls.)

Such a smallest σ-algebra exists by the above lemma. We say that the Borel σ-algebra is *generated* by the open sets.

Which subsets are included in the Borel σ-algebra?

- All open sets
- All closed sets
- Countable unions of open and closed sets
- Complements of countable unions of open and closed sets
- …

Example 13

Consider $\mathbb{R}$, and its Borel σ-algebra. It contains all subsets consisting of a single point, since $\{x\} = (]-\infty, x[\cup]x, +\infty[)^{\complement}$. But then we can take countable unions of such points, e.g., the rational numbers $\mathbb{Q}$, which is also measurable. But then we can take the complement, to get the irrational numbers $\mathbb{R} \setminus \mathbb{Q}$, also measurable.

We can also consider the Cantor set: Start with an interval, and remove the middle third. Remove the middle third of those two again, and continue. It is not hard to see that this produces a measurable set, and in fact a *fractal*.

So the Borel σ-algebra $\boldsymbol{B}(\mathbb{R})$ contains quite complicated sets.

4.2 Measure

We now add the next ingredient: a measure.

Definition 46: Measure, measure space

Let $(X, \mathcal{X})$ be a mesurable space. A *measure* is a function $\mu : \boldsymbol{X} \to [0, +\infty[\cup \{+\infty\}$ that satisfies

1. $\mu(\emptyset) = 0$
2. For a countable family of disjoint subsets $\{A_i\} \subset \mathcal{X}$, i.e., $A_i \cap A_j = 0$, we have

$$\mu\left(\bigcup_i^{\infty} A_i\right) = \sum_i^{\infty} \mu(A_i) \qquad \textbf{\textit{σ-additive}} \tag{4.4}$$

We then say that $(X, \boldsymbol{X}, \mu)$ is a measure space.

The definition of the measure μ encapsulate some intuitive notions about measuring volumes. Volume of nothing is zero, and volume of unions of sets is the sum of the volume. Finally, the infinite union allows for *approximation* of volumes. Note that a similar idea was present in the definition of the σ-algebra.

An example that shows how measure can be used differently, consider counting measure:

Example 14: Counting measure

Let N be a finite set, and let $\boldsymbol{N} = 2^N$, the set of all subsets of N. This is a σ-algebra, and since N is finite, we can define counting measure:

$$\mu(A) = |A| \quad \text{(number of elements)} \tag{4.5}$$

Having a measure theoretic concept of counting is more useful that one would think! For example, it will allow us to rigorously define square integrable functions over electron configuration space $\mathbb{R}^3 \times \{\uparrow, \downarrow\}$ in a manner which does not artificially distinguish between discrete and continuous degrees of freedom.

We next introduce the notion of a *measurable function*. These are functions that we later can define the integral for.

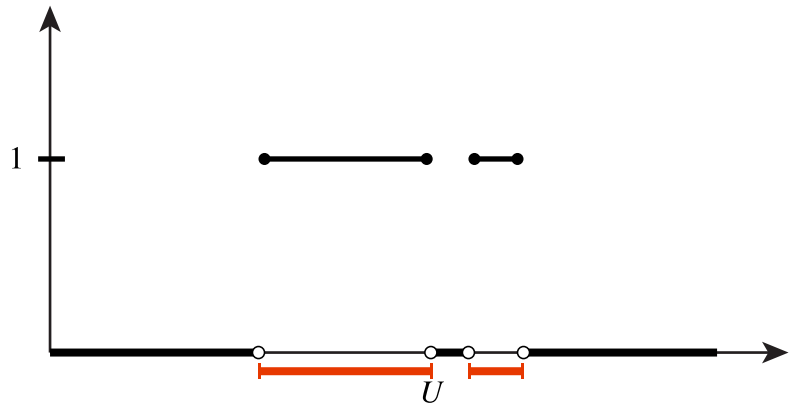


Figure 4.1: Characteristic function of a subset U of $\mathbb{R}$ consisting of two intervals.

Definition 47: Measurable function

Let $(X, \boldsymbol{X})$ and $(Y, \boldsymbol{Y})$ be measurable spaces. A function

$$f : X \to Y \tag{4.6}$$

is called *measurable* if, for all $U \in \boldsymbol{Y}$,

$$f^{-1}[U]\,\{x \in X \mid f(x) \in U\} \in \boldsymbol{X} \tag{4.7}$$

Note the close analogy with the definition of continuous functions between metric (or more generally topological) spaces: The inverse image of an open set must be open. Measurability of a function is certainly less restrictive: The inverse image of an open set need only be measurable – and we saw that there are "complicated" measurable sets.

Just like for continuous functions, when $f : X \to Y$ with $Y = \mathbb{F}^n$, we get that linear combinations of measurable functions are again measurable. We can also multiply or take absolute values of masurable functions, and still get measurable functions. [Perhaps formulate as theorem]

Example 15

Why is this a definition that can be useful? Consider the *characteristic function* χ_U of some subset $U \subset Y$, defined by

$$\chi_U(y) = \begin{cases} 1 & y \in U \\ 0 & y \notin U \end{cases} \tag{4.8}$$

See Fig. 4.1. Then the inverse image $\chi_U^{-1}[1]$ is exactly U. If U is actually measurable, this means that we can measure it with a measure $\mu : \boldsymbol{Y} \to [0, +\infty[$.

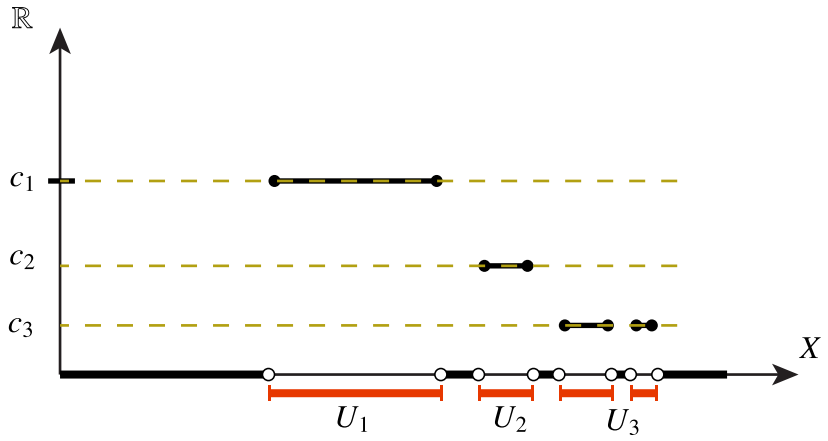


Figure 4.2: A non-negative simple function.

Example 16

Consider the function

$$f(x) = \begin{cases} 1 & x \in \mathbb{Q} \\ 0 & x \in \mathbb{R} \setminus \mathbb{Q} \end{cases} \tag{4.9}$$

This function is not Riemann integrable, since the upper and lower Riemann sums will converge to different numbers. However, since $f = \chi_{\mathbb{Q}}$ we now expect it to be integrable. But what will be the integral? Since $\mu(\mathbb{Q}) = 0$ we expect that $f^{-1}(1) = \mathbb{Q}$ will not contribute, i.e., the integral is 0.

4.3 The integral

We now turn to actually defining the integral of a measurable function. One begins by defining the integral of *simple functions*.

Definition 48: Simple functions

Let $(X, \boldsymbol{X})$ be a measurable space. Let $f : X \to \mathbb{R}$ be a measurable function. We say that f is a *simple function* if it takes on only finitely many function values. The set of simple functions is denoted $\mathcal{S}$. The set of non-negative simple functions is denoted $\mathcal{S}^+$.

A simple measurable function has a *unique* decomposition as

$$f = \sum_{i=1}^{n} c_i \chi_{U_i}, \quad U_i \in \boldsymbol{X}, \quad U_i \cap U_j = \emptyset. \tag{4.10}$$

A simple function is illustrated in Fig. 4.2. What should the integral of this simple function be? Clearly, the integral of the characteristic function χ_U of some measurable U should be the volume, or measure, of U! We have to be careful, since the measure of U can be infinite.

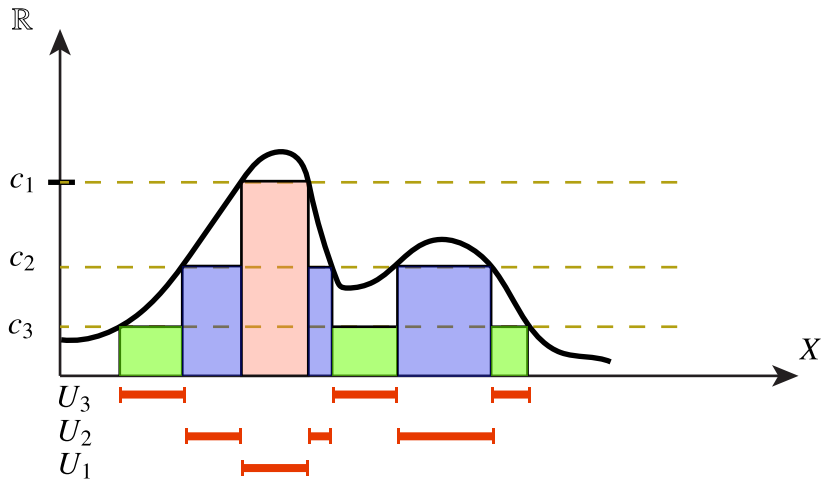


Figure 4.3: Approximation of a function from below by simple functions.

Definition 49: Integral of non-negative simple function

Let $(X, \boldsymbol{X}, \mu)$ be a measure space. Let $f : X \to \mathbb{R}$ be simple and non-negative. We *define* the integral of f to be the *extended valued function* $I : \mathcal{S}^+ \to \mathbb{R} \cup \{+\infty\}$ given by,

$$\int_X f \, \mathrm{d}\mu = I\left(\sum_i c_i \chi_{U_i}\right) = \sum_i c_i \, \mu(U_i). \tag{4.11}$$

The function I is linear and *monotone*,

$$f, g \in \mathcal{S}^+, \quad f \leq g \implies I(f) \leq I(g). \tag{4.12}$$

Let now $f : X \to [0, +\infty[$ be a non-negative measurable function. It is implicit here, that we have the Borel σ-algebra on the real numbers. How do we define the integral? The idea is to *approximate* f by simple functions from below, and indeed this can always be done.

Definition 50: Integral of non-neagative functions

Let $(X, \boldsymbol{X}, \mu)$ be a measure space, and let $f : X \to [0, +\infty[$ be measurable. We define the integral of f to be

$$\int_X f \, \mathrm{d}\mu = \sup\{I(h) \mid h \in \mathcal{S}^+, \, h \leq f\} \in [0, \infty]. \tag{4.13}$$

The function f is *integrable* if $\int_X f \, \mathrm{d}\mu < +\infty$.

Thus, we take every non-negative simple function that lies below f, compute the integral, and maximize over all such simple functions. If f can be approximated by simple functions, which it can, then the integral could and should converge. (The technical result that allows approximation from below in this way is *the monotone convergence theorem*.)

In Fig. 4.3, the approximation of f by simple functions is illustrated. From this illustration we take home perhaps the most important intuition: Whereas the Riemann integral is defined in terms of approximating the are below the graph by vertical strips, the measure-theoretic integral instead consider horizontal strips!

In the next result, the phrase μ-almost everywhere, abbreviated μ-a.e., means that the condtion holds for every $x \in X$ *except possibly* at a set of measure zero.

Theorem 22: Properties of the integral

Let $(X, \boldsymbol{X}, \mu)$ be a measure space, and let $f \geq 0$ be a measurable function $f : X \to \mathbb{R}$. The integral on such functions satisfies: Monotone:

$$f \leq g \quad \text{measurable functions} \implies \int_X f \, \mathrm{d}\mu \leq \int_X f \, \mathrm{d}\mu \tag{4.14}$$

Vanishing on set of measure zero:

$$f = 0 \quad \mu\text{-a.e.} \iff \int_X f \, \mathrm{d}\mu = 0. \tag{4.15}$$

Irrelevant on set of measure zero:

$$f = g \quad \mu\text{-a.e.} \implies \int_X f \, \mathrm{d}\mu = \int_X \mathrm{d}\mu \tag{4.16}$$

The concept of "almost everywhere" is very important when Lebesgue integrals are considered. Whenever a function is only "used" to define integrals, it does not matter what the function values are at a set of measure zero. As we have seen, such sets can be fairly large!

We can now define the integral of arbitrary measurable functions.

Definition 51: Integral

Let $(X, \boldsymbol{X}, \mu)$ be a measure space, and let $f : X \to \mathbb{R}$ be measurable. Let f_+ and f_- be the positive, resp., negative part of f. We define f to be integrable if f_+ and f_- are ingegrable, and we define

$$\int_X f \, \mathrm{d}\mu = \int_X f_+ \, \mathrm{d}\mu - \int_X f_- \, \mathrm{d}\mu. \tag{4.17}$$

s

4.4 Lebesgue measure and the Lebesgue integral

Although we have defined the Borel σ-algebra on $\mathbb{R}^n$, and indicated how we would like the measure to be, we have not yet defined the measure.

The key technical result that allows the existence and uniqueness of a measure on the Borel σ-algebra $\boldsymbol{B}(\mathbb{R}^n)$ is *Carathéodoty's extension theorem*. We will not describe this theorem in any detail, but just note that when we have defined our measure on a sufficiently large subset of $\boldsymbol{B}(\mathbb{R}^n)$, it can be *extended* to the whole algebra in a unique fashion to an actual measure.

The subset of a σ-algebra needed is called a *semiring*: we have the empty set and X, as for the σ-algebra, and we also have intersevtions $A \cap B$ of oairs sets in the semiring. Finally, when we consider $A \setminus B$, this should be decomposable in a finite number of sets from the ring. Nothing more, no complements or unions. The reader can check that these conditions hold for the set of all half-open intervals $[a, b[\subset \mathbb{R}$, which is the most important examle. Now, the half-open intervals generate the Borel algebra of $\mathbb{R}$, and this is key.

For $\mathbb{R}^n$, take the set of Cartesian products of half-open intervals as a semiring. A box is $B = [a_1, b_1[\times \cdots \times [a_n, b_n[$, with measure $\mu(B) = (b_1 - a_1) \cdots (b_n - a_n)$. Now, the boxes generate the Borel algebra. The Carathéodory exension theorem now guarantees the existence of a *unique* measure on $\boldsymbol{B}(\mathbb{R}^n)$ such that it correctly reproduces the measure of all boxes.

This measure is called *the Lebesgue measure* on $\mathbb{R}^n$, and together with the integral defined earlier, it makes for a very powerful integral. This integral generalizes the Riemann integralm in the sense that every Riemann integrable function is also Lebesgue integrable, with the same integral of course. But there are also many functions that "should" have an integral but for which the Riemann integral fails. For example, exhanging limits and integrals is more often valid with the Lebesgue integral. The Lebesgue integral is also needed to produce the Hilbert space of square-integrable wavefunctions in quantum mechanics!

4.5 Lebesgue spaces

As claimed, the theory of PDEs are formulated using function spaces. These function spaces are in general called *Lebesgue spaces*, and are based on the Lebesgue integral.

In this section, let $(X, \boldsymbol{X}, \mu)$ be a fixed measure space, for example a measurable subset $\Omega \subset \mathbb{R}^n$ with Lebesgue measure, and we consider $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ a measure space with the Lebesgue measure. For complex functions, we consider really $\mathbb{C}$ as $\mathbb{R}^2$.

The reader may have encountered square integrable functions before, i.e., functions $f : X \to \mathbb{C}$ that satisfies

$$\int_\Omega |f(x)|^2 \, \mathrm{d}x < +\infty. \tag{4.18}$$

Here, $\mathrm{d}x$ is short for the Lebesgue measure. The reader may also be used to thinking of f as a point in Hilbert space $L^2(\Omega)$. However, it is not hard to see, that we can have $f \neq g$ but

$$\int |f - g|^2 \, \mathrm{d}^n x = 0 \quad ! \tag{4.19}$$

So, are the functions really different?

In quantum mechanics, the wavefunction $\psi(x)$ fo a particle defines a probability density $P(x) = |\psi(x)|^2$. The theory of probability *also* work with measurable spaces, and the probability of locating the particle in a subset $A \subset \Omega$ is given by $\int_A P(x) \, \mathrm{d}x$, where A is measurable. The pointwise definition of a probability density is therefore only meaningful up to a set of measure zero, i.e., "almost everywhere".

Let $f : X \to \mathbb{F}$ be a measurable function. Recall that $\int_X f \, \mathrm{d}\mu = 0$ if and only if $f(x) = 0$ "almost everywhere". An example is the function over $\mathbb{R}^n$ which is zero except for at the points with rational coordinates. As the integral concerned, this function is zero!

To define function spaces with integrals involved in norms and inner products rigorously, we need the following:

Definition 52: Equivalence classes of measurable functions

Let $f, g : X \to \mathbb{F}$ be measurable functions. We say that f and g are equivalent, written $f \sim g$, if $f = g$ almost everywhere. We write

$$[f] = \{g \mid f \sim g\} \tag{4.20}$$

for the *equivalence class* of functions that are almost everywhere the same.

Definition 53: Lebesgue spaces

Let $p \geq 1$, and define the p-norm

$$\|[f]\|_p = \|f\|_p = \left(\int_X |f(x)|^p \, \mathrm{d}^n x \right)^{1/p} \tag{4.21}$$

The space $L^p(X)$ is defined as

$$L^p(X) = \left\{ [f] \mid f : X \to \mathbb{F} \text{ measurable}, \ \|f\|_p < +\infty \right\}. \tag{4.22}$$

Theorem 23

The Lebesgue spaces $L^p(X)$ are *complete* normed spaces, i.e., *Banach spaces*. (See Chapter 5.)

The space $L^2(X)$ is a Hilbert space with inner product

$$\langle f, g \rangle_{L^2(X)} = \int \overline{f(x)} g(x) \, \mathrm{d}^n x. \tag{4.23}$$

The fact that L^p spaces are *complete* is of great importance. It guarantees that if we consider Cauchy sequences in these spaces, they are converge *to something in the space*. This is extremely useful when studying PDEs.

To close this section, we demonstrate just how general the Lebesgue spaces are, and how "wild" integrable functions can be.

Example 17: A wild function

Let $X = \mathbb{R}^3$ with Lebesgue measure. Let $u(\mathbf{x}) = \|\mathbf{x}\|^{-1} e^{-\|\mathbf{x}\|}$. This function is square integrable. (Can you prove it?) The function is also unbounded as $\|\mathbf{x}\| \to 0$.

Now let $\mathbb{Q}^3$ be the set of rational coordinates in $\mathbb{R}^3$. It is a countable set, so we may write it as a sequence $\mathbf{y}_i$, $i \in \mathbb{N}$. Consider the function

$$f(\mathbf{x}) = \sum_{i=1}^{\infty} 2^{-i} u(\mathbf{x} - \mathbf{y}_i), \tag{4.24}$$

i.e., at every rational point, we place a singularity.

It now follows, that for every ε-ball in $\mathbb{R}^3$, no matter how small, the function is unbounded. Yet,

$$\|f\|_{L^2} \leq \sum_{i=1}^{\infty} 2^{-i} \|u\|_{L^2} < +\infty. \tag{4.25}$$

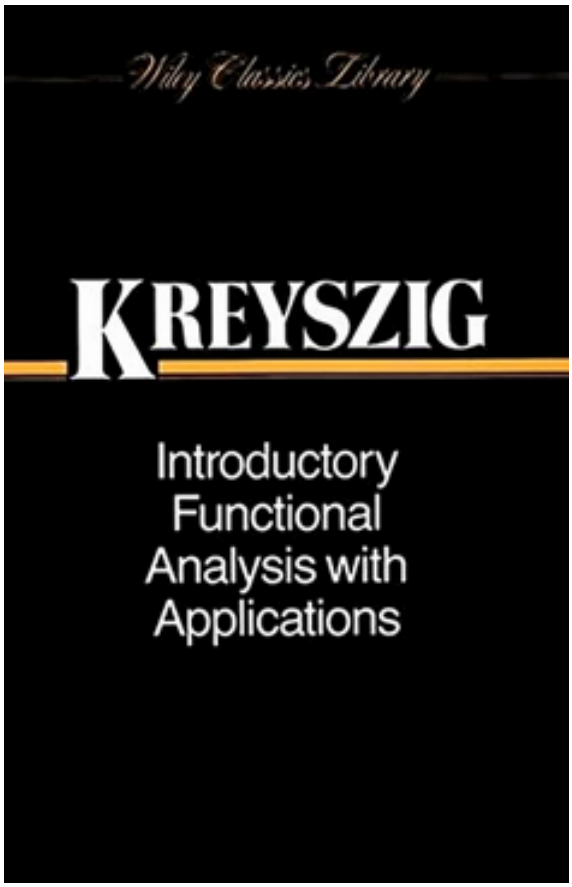
Not only is the norm finite, but since L^2 is complete, the series actually converges to an element in $L^2(X)$. This function is unbounded in every arbitrarily small region.

Functional analysis

5.1 Infinite dimensions

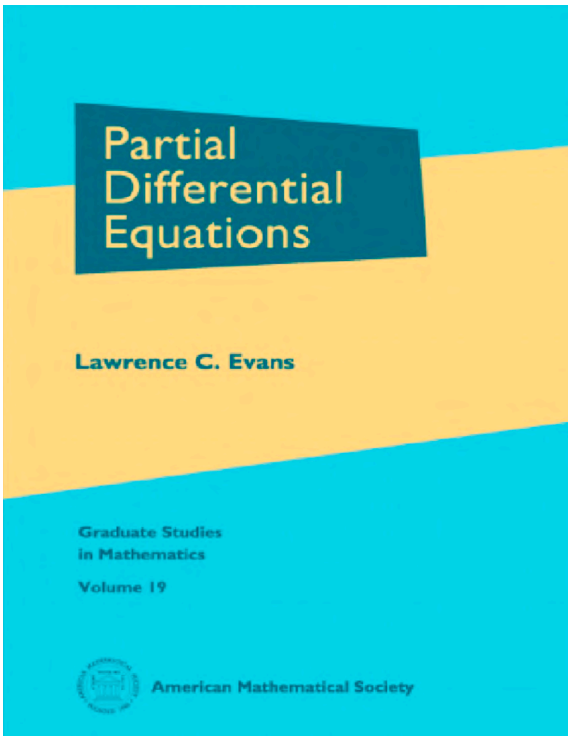
Recommended reading

A very pedagogical text. Covers metric spaces, Banach spaces, Hilbert spaces, the fundamental theorems like the Hahn–Banach theorem, open mapping theorem, closed graph theorem. Spectral theory of self-adjoint operators, applications to quantum mechanics. (This makes the book special, together with its pedagogical level.)



Recommended reading

A classic in PDE theory. Used in many graduate courses all over the world.

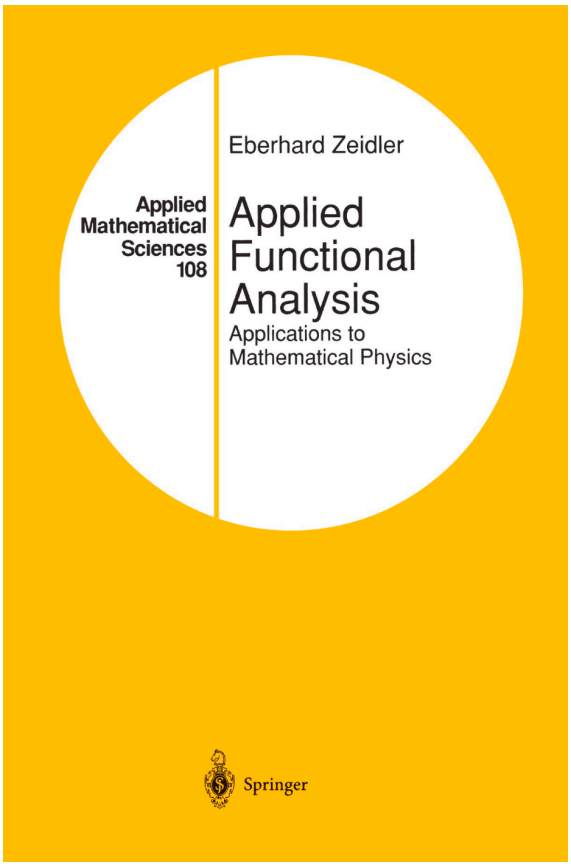


Recommended reading

A classic. Maybe not the most accessible text, but it is very much geared towards mathematical physics.

Recommended reading

Eberhard Zeidler was a giant of nonlinear functional analysis, and enormously productive. Many of his volumes focus greatly on pedagogical exposition and motivation for study. This book is no exception.



We now enter the realm of inifinite dimensional vector spaces. The mathematical field that studies such objects is called *Functional Analysis*. Infinite dimensional vector spaces are often spaces of *functions*. We know that operators like the derivative acts linearly on differentiable functions. Hence, *functional analysis is the mathematical language of analysis of partial differential equations*.

In quantum chemistry, our laws of nature are *linear*, e.g., the time-independent Schrödinger equation is a *linear partial differential equation*. On the other hand, many of our approximation methods are *nonlinear* in nature. Such methods comprise self-consistent field methods like Hartree–Fock and density-functional theory, complete-active space self-consistent field theory, and coupled-cluster theory. Hartrr–Fock, for example, can be viewed as a coupled set of nonlinear integro-partial differential equations. The mathematical analysis of these methods then needs *nonlinear functional analysis*. Since most methods are formulated in terms of optimization of some energy function, we must deal with *nonlinear optimization* in infinite dimensions. There are also methods, like many-body perturbation theory, that are not variational, but instead needs the abstract theory of *perturbation theory* in order to be studied.

All these topics are fairly advanced, and usually encountered only after a few semesters' mathematics studies. The published mathematics papers that study quantum chemical methods mathematically are brilliant and truly inspiring works of famous mathematicians such as P.-L. Lions, E.H. Lieb, B. Simon, and T. Kato, to name a few. Hence, this section will only mention some concepts and try to draw some lines, to get a feel for the concepts that the mathematician works with. Maybe it can be a help to read and understand mathematics papers on quantum chemistry methods, and to bridge a language barrier that certainly is present.

5.1.1 Introducing infinite dimensions

We have previously studied finite-dimensional vector spaces. However, quantum mechanics is formulated with an infinite dimensional vector space – a separable Hilbert space. The quantum chemist may say, "but we always introduce a basis set, and then we are in finite dimensions!" True, but the underlying physical model can *not* be formulated in finite dimensions. For example, if we consider quantum mechanics in one spatial dimension, the canonical commutator relation

$$[\hat{x}, \hat{p}_x] = \mathrm{i}\hbar\mathbb{1} \tag{5.1}$$

requires infinite dimensions. Furthermore, in order to prove error estimates of some quantum chemical model, one needs to in some way compare the finite dimensional model with the infinite dimensional "exact" model. This is best done by basically working in the infinite dimensional setting all the time, considering instead finite dimensional subspaces of the function spaces involved. [Quantum chemists are used to talking about the full-configuration interaction limit as "exact". It is not! One still has the basis set error. This can not be eliminated in finite dimensions.]

In Definition 10, Section 2.1.4, we introduced a general vector space. There is no reason why a general vector space should have a finite dimension. Here are some examples of vector spaces that have infinite dimension:

Example 18: Space of all functions over a set

Let S be a set. The space of all functions $f : S \to \mathbb{F}$ is a vector space, with addition and scalar multiplication defined pointwise,

$$[f + g](x) = f(x) + g(x), \quad [\alpha f](x) = \alpha f(x). \tag{5.2}$$

The dimension of this space is at least as large as the cardinality of S. To see this, let $y \in S$ be arbitrary, and let $f_y : S \to \mathbb{F}$ be the function defined by $f_y(x) = 0$ if $x \neq y$ and $f_y(y) = 1$. These functions are linearly independent. Thus every point in S gives a linearly independent vector.

Special cases: $S = \mathbb{N}$ gives the set of all sequences. $S = \{1, 2, \cdots, N\}$ gives $\mathbb{F}^n$ (without the inner product, which is extra information).

Example 19: Space of all polynomials

The space of all polynomials $p : \mathbb{F} \to \mathbb{F}$ with coefficients in $\mathbb{F}$ is a vector space. If we set $S = \mathbb{F}$ in the previous example, the space of all polynomials is a subspace of the space of all functions from $\mathbb{F}$ to $\mathbb{F}$. An arbitrary element of our vector space can be written as

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots a_n x^n$$

for a vector $\mathbf{a} = [a_0, \cdots, a_n] \in \mathbb{F}^{n+1}$. Note that n depends on p, and is not bounded, so the dimension is infinite. In particular the monomials x^n are linearly independent, and there are infinitely many of these.

Example 20: Space of continuous functions

Let $\Omega \subset \mathbb{R}^n$ be a bounded, closed domain, such as a box $[0,1]^n$ which includes its boundary. Consider the set $C^k(\Omega)$ of functions that are continuous at all points in Ω, with continuous partial derivatives of order $\leq k$. (See Chapter 6.3.2.) Consider in particular the special case $k = 0$. We can supply a norm on this space,

$$\|f\|_\infty = \max\{|f(x)| \mid x \in \Omega\}. \tag{5.3}$$

The maximum can be shown to be attained, since Ω is bounded and closed, and hence compact. (We have not covered compactness so far in the lecture notes.) It is a fact that C^0 is complete with this norm. This means. that if $f_k \in C^0(\Omega)$ is a sequence of continuous functions, and if

$$\|f_j - f_k\|_\infty = \max\{|f_j(x) - f_k(x)| \mid x \in \Omega\} \tag{5.4}$$

is a Cauchy sequence, then it converges to some $f \in C^0(\Omega)$, a continuous function. The completeness can be generalized to C^k, but we have to modify the norm accordingly.

TODO: Add plots illustrating the norm and convergence.

Example 21: N-electron Hilbert space

This is the main vector space of quantum chemistry, and a central ingredient in the mathematical formulation of molecular problems in the Born–Oppenheimer approximation. This space is constructed as follows: Let $X = \mathbb{R}^3 \times \{\uparrow, \downarrow\}$ be two copies of Euclidean space. Here, $\uparrow$ and $\downarrow$ are simply symbols that we associate with spin up and down ("α" and "β" spin). The set X is made into a measure space by assigning the product of Lebesgue measure and counting measure (see Chapter 4). We now can define *single-electron space* $\mathcal{H}_1 = L^2(X;\mathbb{C})$. For multiple electrons, we take *the antisymmetric tensor product N times*,

$$\mathcal{H}_N = \mathcal{H}_1 \wedge \mathcal{H}_1 \cdots \wedge \mathcal{H}_1 \quad (N \text{ times}). \tag{5.5}$$

The elements of $\mathcal{H}_N$ now become antisymmetric upon permutation of the particle indices, i.e., for all pairs (i, j),

$$\psi(x_1, \cdots, x_j, \cdots, x_i, \cdot, x_N) = -\psi(x_1, \cdots, x_i, \cdots, x_j, \cdots, x_N).$$

By theorems on spaces of square integrable functions, we have the alternative characterization: $\psi \in \mathcal{H}_N$ if and only of $\psi \in L^2(X^N)$ and is antisymmetric. Since X^N can be viewed as 2^N copies of $\mathbb{R}^{3N}$ associated with the 2^N unique arrangements of N spins, we also have $\psi \in L^2(\mathbb{R}^{3N})^N$, i.e., ψ is a *vector of functions*. These functions are *not necessarily* antisymmetric, since they isolate the spatial coordinate.

The infinite dimensional spaces we meet in functional analysis are often *spaces of functions*. These spaces, when supplied with a suitable topological structure, are designed to deal with partial differential equations. Here is an example that shows how this is done for a simple PDE:

Example 22: Poisson equation

(For this example, we use nomenclature from Chapter 6.) Let $\Omega =]0,1[^3 \subset \mathbb{R}^3$ be an open box, a typical domain with a well-behaved boundary $\partial\Omega$. Consider the Poissin equation, a PDE, formulated "classically": Find $u : \Omega \to \mathbb{R}$ such that

$$\nabla^2 u(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega \tag{5.6}$$
$$u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial\Omega \tag{5.7}$$

where $f : \mathbb{R}^3 \to \mathbb{R}$ is some function, and such that $u(\mathbf{x}) = 0$ on $\partial\Omega$. What is meant by a solution to this equation? Should we require u to have continuous derivatives up to and including second order? Is it enough that the second order derivatives exist? What are the properties of the "data" f? These questions must be answered, such that one can provide a sound theory for existence and uniqueness of solutions.

If we introduce the Sobolev space $H_0^1(\Omega)$ of twice weakly differentiable functions over Ω that vanishes on the boundary, this is a Hilbert space. In fact the Laplace operator ∇^2 is a continuous operator from $H_0^1(\Omega)$ into the space $H_0^{-1}(\Omega)$, which is a set that also contains some generalized functions, i.e., functions that are not really functions, but make sense when we integrate them. It is big! Then, the PDE can be formulated as: Given $f \in H_0^{-1}(\Omega)$, find $u \in H_0^1(\Omega)$ such that

$$\hat{A}u = f. \tag{5.8}$$

Now, one can show that $\nabla^2 = \hat{A} : H_0^1 \to H_0^{-1}$ is in fact not only continuous, but also invertible, with a continuous inverse. Then, there exists a unique solution $u = \hat{A}^{-1} f$ that depends *continuously* on f.

Now, one can introduce the *Galerkin method*: Choose a finite dimensional subspace $V \subset H_0^1(\Omega)$ with basis $\{b_i\}$. For example, a finite element space. This space is suitable for approximation, in the sense that we can refine the finite element mesh and obtain approximations of any accuracy of elements in H_0^1. The PDE becomes a linear algebra problem,

$$A\mathbf{u} = \mathbf{f}, \tag{5.9}$$

with $A_{ij} = \langle b_i, \hat{A} b_j \rangle = \langle \nabla b_i, \nabla b_j \rangle_{L^2}$ and $f_j = \langle b_k, f \rangle_{L^2}$.

From the structure of the function spaces and the Galerkin space, we know that this approximation is convergent as the mesh becomes finer. We even have error estimates.

This methodology is quite powerful, and amply motivates the study of functional analysis for studying PDEs.

TODO: Elevate this example to a section.

5.1.2 Banach spaces and Hilbert spaces

In Section 3.1, we introduced the inner product spaces and normed spaces. However, the spaces that are most useful in analysis are *complete spaces*: Accroding to Definition 27 a space is complete if all sequences that "ought to converge" actually converges. All possible limits of sequences are present, and there are no holes, so to speak, in the space.

Definition 54: Banach and Hilbert space

A *Banach space* is a complete normed vector space. A *Hilbert space* is a complete inner product space.

All Hilbert spaces are Banach spaces, but not vice versa.
Infinite dimensional spaces can be *huge*. Usually, we will be mostly interested in separable spaces:

Definition 55: Separable space

A Banach space X is called *separable* if it contains a dense countable subset, i.e., a countable $A \subset X$ such that the closure of A is X.

Recall that a subset $A \subset V$ is dense if its closure is V. For example, the rationals $\mathbb{Q}$ are dense in $\mathbb{R}$. A space is separable if there exists some *list of elements* that form a dense subset: all elements of the space can be written as limits of sequences of elements taken from this list. This seems rather drastic, but thankfully, most spaces of interest to us are separable.

5.2 L^p spaces (Lebesgue spaces)

Consider some open subset $\Omega \subset \mathbb{R}^n$, with a "nice" boundary (e.g., piecewise smooth) and consider the set of measurable functions $f : \Omega \to \mathbb{F}$. (See Section 4 on measure and integration theory. Measurable functions are roughly those that have an integral, even if it may be infinite.) We have previously encountered the L^p-spaces.

Recall the fact that $[f] \in L^p(\Omega)$ is an equivalence class of almost-everywhere equal functions. We now have the strange situation that *this is almost universally ignored*; one writes things like "Let f be defined as [some definition] be a function, and we now show that $f \in L^p$". Only when there is doubt about some property, e.g., a singularity, one suddenly reintroduce the notion of equivalence class. Talk about abuse of notation! So this is something to be aware of.

We also have the case $p = +\infty$, but then the norm is not defined as an integral, but rather the *essential supremum*:

$$\|f\|_\infty := \operatorname*{esssup}_{x\in\Omega} |f(x)|, \tag{5.10}$$

where the *essential supremum* means

$$\operatorname*{esssup}_{x\in\Omega} |f(x)| := \inf\{ \sup_{x\in\Omega\setminus Z} |f(x)| \mid Z \text{ has zero measure}\}. \tag{5.11}$$

This is a bit of a mouthful, but it essentially means "maximum, but try to take away point sets of zero measure to lower the value". The space L^∞ is not separable.

Definition 56: Almost everywhere

Let f be a measurable function over a measure space. Let $P(f(x))$ be a statement, such as "$|f(x)| < 1$. We say that $P(f(x))$ holds *almost everywhere* if it holds everywhere except for a set of measure zero.

Example 23: Coulomb potential

In the analysis of the molecular Schrödinger equation, we must deal with the singular Coulomb potential between charged particles. For the hydrogen atom in the Born–Oppenheimer approximation,

$$V(\mathbf{r}) = \frac{1}{r} = \frac{1}{\|\mathbf{r}\|} = \frac{1}{\sqrt{x^2 + y^2 + z^2}}. \tag{5.12}$$

As a function $1/r$ does not live in any of the L^p spaces due to the singularity at the origin. On the other hand, the physics of the Coulomb potential has a short-range and a long-range part. The short-range part is responsible for the *nuclear cusp* in the wavefunction, while the long-range part is responsible for the infinite scattering cross section. Thus, we split V into a long-range and a short-range part, by introducing some ball $\Omega = B_R(\mathbb{R}^3)$ and setting

$$V = V_{\text{sr}} + V_{\text{lr}} = \frac{1}{r}\chi_\Omega + \frac{1}{r}\chi_{\Omega^\complement}. \tag{5.13}$$

Now the long range part is clearly bounded by $1/R$,

$$V_{\text{lr}} \in L^\infty(\mathbb{R}^3), \tag{5.14}$$

while the short-range part can be shown to be

$$V_{\text{sr}} \in L^p(\mathbb{R}^3), \quad p \in [1, 2]. \tag{5.15}$$

For analysis, the value $p = 3/2$ is often taken, giving

$$V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3), \tag{5.16}$$

where the right-hand side is defined as the space of functions splittable as a sum with terms from each space. (This is in fact a Banach space when the proper norm is supplied.)

Thus, we see how Banach spaces can be used to handle some singular potentials. This can in turn help with formulating the Schrödinger equation in a rigorous manner.

5.2.1 The weak derivative

Studying PDE, one needs partial derivatives of functions in L^p-spaces. However, we have seen that such functions are only defined up to a set of measure zero. In order to define partial derivatives of L^p functions, we need a strategy that deals with this. The solution is the *weak derivative*.

We first need the notion of a test function.

Definition 57: Test functions

Let $\Omega \subset \mathbb{R}^n$ be open. A *test function* is an infinitely differentiable function $f : \Omega \to \mathbb{F}$ with compact support, i.e., there is some closed and bounded set $K \subset \Omega$ such that f is identically zero on $K^\complement$.

The set of test functions is denoted $C_0^\infty(\Omega)$.

Test functions exist. The classic example is the following:

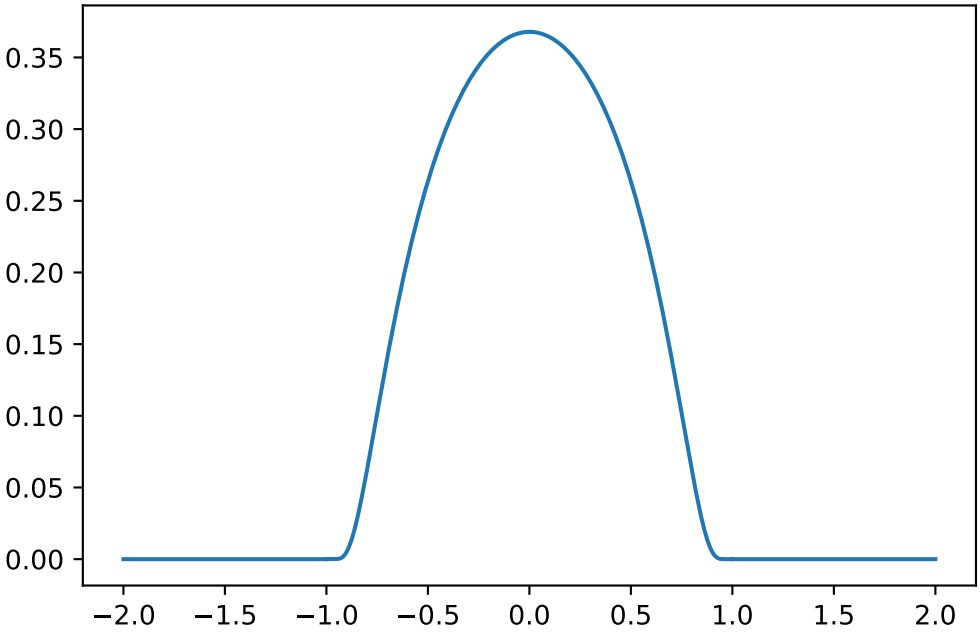


Figure 5.1: The bump function from Example 24 in one dimension.

Example 24: The bump function

Let $u : \mathbb{R}^n \to \mathbb{R}$ be given by

$$u(\mathbf{x}) = \begin{cases} 0 & \|\mathbf{x}\| \geq 1 \\ \exp(-1/(1 - \|\mathbf{x}\|^2)) & \|\mathbf{x}\| < 1 \end{cases} \tag{5.17}$$

Then u is infinitely many times differentiable, in particular across the boundary of the unit sphere, too. See Fig. 5.1.

From the above example, a huge number of test functions can be generated by *convolution*: Let $\eta = u/\int u$, normalizing the bump. Take any integrable function $f : \mathbb{R}^n \to \mathbb{C}$, and take the convolution with η,

$$f_\varepsilon(\mathbf{x}) = \int_{B_1(0)} \varepsilon^{-n} \eta(\mathbf{y}/\varepsilon) f(\mathbf{x} - \mathbf{y}) \, \mathrm{d}\mathbf{y}. \tag{5.18}$$

This process smooths f, and is called *mollification of* f. For small ε, the function is only "slightly" modified, since the bump becomes very concentrated. In particular, if f is supported in K, then f_ε is supported in only a slightly larger K_ε.

In fact the set of test functions is *dense* in all the L^p spaces except L^∞. [Check precise wording of this.] All L^p functions can be arbitrarily well approximated by such functions. Can you guess a construction of the approximate sequence for a given $f \in L^p(\Omega)$?

TODO: Produce a visualization.

Having established the set of test functions, we can now define the weak derivative:

Definition 58: Weak derivative/distributional derivative

Let $f \in L^1_{\text{loc}}(\Omega)$ be a *locally integrable function*. This means that $f \in L^1_{\text{loc}}(K)$ for all bounded subsets $K \subset \Omega$. (This function set is very general, and contains all the L^p spaces!)

A measurable function g_k is called *a weak derivative* of f if, for all test functions $\varphi \in C_0^\infty(\Omega)$,

$$\int \varphi(\mathbf{x}) g_k(\mathbf{x}) \, \mathrm{d}\mathbf{c} = -\int \frac{\partial \varphi(\mathbf{x})}{\partial x_k} f(\mathbf{x}) \, \mathrm{d}\mathbf{x}. \tag{5.19}$$

We see that the weak derivative behaves just like the derivative of f when being under the integral sign and "tested against" a test function.

Weak derivatives of higher order are defined completely analogously. Let $\alpha = (\alpha_1, \cdots, \alpha_k)$ denote a multi-index of nonnegative integers, and define

$$\partial^\alpha = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}} \cdots \frac{\partial^{\alpha_n}}{\partial \alpha_n^{\alpha_n}}, \quad |\alpha| = \sum_{i=1}^n \alpha_i \tag{5.20}$$

$g_\alpha \in L^1_{\text{loc}}$ is a weak partial derivative of mixed order α if

$$\int \varphi(\mathbf{x}) g_\alpha(\mathbf{x}) \, \mathrm{d}\mathbf{x} = (-1)^{|\alpha|} \int \partial^\alpha \varphi(\mathbf{x}) f(\mathbf{x}) \, \mathrm{d}\mathbf{x}. \tag{5.21}$$

Mixed weak derivatives are symmetric. The weak derivative is unique up to a set of measure zero.

5.2.2 Sobolev spaces

A very important class of function spaces are Sobolev spaces.

Definition 59: Sobolev space

Let $\Omega \subset \mathbb{R}^n$ be open. Let $p \in [1, +\infty]$ (incliuding infinite). Let $u \in L^p(\Omega)$, and suppose u has weak derivatives up to order $k \geq 1$ that are *also* in $L^p(\Omega)$. Then we say that $u \in W^{k,p}(\Omega)$, a Sobolev space. The Sobolev space $W^{k,p}(\Omega)$ is a Banach space with norm

$$\|u\|_{W^{k,p}} = \|u\|_p + \sum_{\alpha, |\alpha| \leq k} \|\partial_\alpha u\|_p, \tag{5.22}$$

where α denotes a partial derivative of order $\leq k$. [For example, order 1 means $\alpha \in \{1, \cdots, n\}$, order 2 means $\alpha = (\alpha_1, \alpha_2)$ with $\alpha_i \in \{1, \cdots, n\}$, and so on.]

For encoding *boundary conditions*, it is useful to consider Sobolev spaces of functions that in some "integrable sense" vanish on $\partial\Omega$.

Definition 60: Sobolev space, homogenous boundary conditions

Let $\Omega \subset \mathbb{R}^n$ with piecewise smooth boundary. The space $W_0^{k,p}(\Omega)$ is defined as the clousure in the $W^{k,p}(\Omega)$ norm of the set of test functions $C_0^\infty(\Omega)$.

The definition may seem arbitrary, but the denseness of the test functions in $W^{k,p}(\mathbb{R}^n)$ implies that this makes sense, and indeed corresponds to functions that vanish near the boundary, when $k > 0$.

When $k = 0$ we just get $L^p(\Omega)$.

5.3 Hilbert spaces

5.3.1 L^2 -- the square integrable functions

For a quantum chemist, the most important L^p space is $L^2(\Omega)$, where Ω is a measure space, such as $\mathbb{R}^3$, or $X = \mathbb{R}^3 \times \{\uparrow, \downarrow\}$. Previously, we saw that this was a Banach space with the L^2 norm, but this norm comes from an inner product:

$$\langle f, g \rangle_{L^2} := \int_\Omega \overline{f(x)} g(x) \, \mathrm{d}x, \tag{5.23}$$

where the complex conjugate is relevant only if $\mathbb{F} = \mathbb{C}$. Again, functions that agree on sets of measure zero are identified.

5.3.2 ℓ_2 -- the archetypal separable Hilbert space

Consider the following situation: Let $u = (u_i) \subset \mathbb{F}$ be a real or complex-valued sequence. Let $p \in [1, +\infty)$. We can define a norm given by

$$\|u\|_p := \left(\sum_{i \in \mathbb{N}} |u_i|^p \right)^{1/p}. \tag{5.24}$$

The set of sequences such that $\|u_p\|$ is a convergent sum is called ℓ_p. For $p = +\infty$, we set $\|u\|_{+\infty} = \max_i |u_i|$. The spaces ℓ_p are all Banach spaces.

In particular, the space ℓ_2 is a Hilbert space when we use the inner product

$$\langle u, v \rangle = \sum_{i \in \mathbb{N}} \overline{u_i} v_i. \tag{5.25}$$

This Hilbert space is an archetypal Hilbert space, as we will next see.

5.3.3 Existence of orthonormal bases

TODO: This section needs more work.

The following fact is significant, because it tells us that $\ell_2(\mathbb{N}; \mathbb{F})$ is an archetypal separable Hilbert space, much in the same manner as $\mathbb{F}^n$ is the archetypal finite-dimensional Hilbert space.

Definition 61: Orthnormal basis for separable Hilbert space

An orthonormal basis for an infinite dimensional separable Hilbert space V is a linearly independent orthonormal set $\{b_i\} \subset V$ (i.e., $\langle b_i, b_j \rangle = 0$ whenever $i \neq j$, and $\langle b_i, b_i \rangle = 1$), such that for every $u \in V$, there exist numbers $c_i \in \mathbb{F}$ such that

$$u = \sum_{i=1}^{\infty} c_i b_i. \tag{5.26}$$

The infinite sum is to be interpreted as a *series*, i.e., $u \in V$ means

$$\|u - \sum_{i=1}^{N} c_i b_i\| \to 0 \quad \text{as} \quad N \to +\infty. \tag{5.27}$$

The space of sequences equipped with the Euclidean inner product is denoted $\ell_2(\mathbb{N})$,

$$\langle c, d \rangle_{\ell_2} = \sum_{i=1}^{\infty} \overline{c_i} d_i. \tag{5.28}$$

We see that V and ℓ_2 are *isometrically isomorphic* when a basis is given, since if $v = \sum_i d_i b_i$ then $\langle u, v \rangle = \langle c, d \rangle_{\ell_2}$.

An fundamental result is the following:

Theorem 24

Any separable Hilbert space has an orthonormal basis.

Thus any separable Hilbert space is essentially $\ell_2(\mathbb{N})$ after a basis has been chosen.

5.4 Linear transformations

We now scratch the surface on linear transformations on infinite dimensional Banach and Hilbert spaces.

Let V be a separable Hilbert space. We now know that we may think of this space as the coneptually simpler space $\ell_2 = \ell_2(\mathbb{N})$, the space of square summable sequences. In particular, there is no notion of having to consider equivalence classes of functions defined almost everywhere.

In the finite dimensional case, linear transformations between vector spaces became matrices. How about in the separable Hilbert space case? Do linear transformations and operators become infinite matrices?

Yes and no. One can certainly define a class of linear transformations using infinite matrices, if one is careful. However, the set of linear transformations on a Hilbert space is much richer than the corresponding finite dimensional linear transformations. For a given basis choice a linear transformation may or may not have a well-defined matrix representation.

Perhaps the most important fact is that *transformations need not be continuous*. In the finite-dimensional case, all linear transformations were continuous, even though we did not discuss this fact: In finite dimensions, there is no way for a linear transformation to produce rips or tears or jumps. Moreover, even if linear transformations is continuous, there are some that are "more continuous" than others, such as compact operators, Hilbert–Schmidt operators, trace-class operators, and merely

continuous operators.

Since the topology on a Banach or Hilbert space is translationally invariant, a linear transformation $T : V \to W$ between two Banach spaces is continuous at $x \in V$ if and only if it is continuous at 0, and then continuity is equivalent to *boundedness*, i.e., a finite operator norm:

Definition 62: Bounded linear transformations

Let V and W be Banach spaces over $\mathbb{F}$, and let $D(T) \subset V$ be a linear subspace.Let $T : V \to W$ be a linear transformation, i.e., for all $u, v \in D(T)$ and all $\alpha \in \mathbb{F}$,

$$T(\alpha u) = \alpha T u,$$

and

$$T(u + v) = Tu + Tv.$$

The linear space $D(T)$ is called the *domain of* T, and it may or may not be all of T. Let $\|T\|_{L(V,W)}$ be the norm ("operator norm") defined by

$$\|T\|_{L(V,W)} = \sup \left\{ \frac{\|Tu\|_W}{\|u\|_V} \mid 0 \neq u \in D(T) \right\}. \tag{5.29}$$

If $\|T\|_{L(V,W)} < +\infty$ and $D(T) = V$, then T is a *bounded, or countinuous, linear transformation from* V *to* W.

In the definition, note that we introduce the domain $D(T)$ of $T : V \to W$. The reason is that operators that are not bounded usually cannot be defined on all of V. On the other hand, if T is bounded on $D(T)$ the *bounded linear transformation theorem* states that T can be unuqiely *extended* to all of V. This is why we eliminate the domain in the definition of the space $L(V, W)$ of bounded linear transformations.

Theorem 25: Bounded linear transformations are continuous

Any $T \in L(V, W)$ is a continuous function.

We now give an examples of linear transformations that are *unbounded*, i.e., not bounded.

Example 25: Example of unbounded linear transformation

Let $\ell_2(\mathbb{N}, \mathbb{R})$ be the space of square summable sequences of real numbers, i.e., $u = (u_n) \subset \mathbb{R}$ with

$$\sum_{n=1}^{\infty} u_n^2 < +\infty.$$

Let A be the operator that is defined by

$$(Au)_n = nu_n,$$

i.e., each element in the sequence is multiplied by n. Let $(e_m)_n = \delta_{m,n}$ be the sequence which is zero everywhere except for the m'th position, where we have a 1. Then $Ae_m = (0, 0, 0, \cdots, m, \cdots)$ where the m is in the m'th position. We have $\|Ae_m\| = m$, which grows to infinity as $m \to +\infty$. Therefore A is not bounded.

Furthermore, the sequence given by $u_n = n^{-1}$ is square summable, that is,

$$\|u\|^2 = \sum_n n^{-2} < +\infty.$$

However, $Au = (1, 1, 1, 1, \dots)$ which is clearly not square summable. So A cannot be defined on all of $\ell_2(\mathbb{N}, \mathbb{R})$.

This example illustrates an important fact for unbounded operators: They are typically *not* everywhere defined.

Here is another example relevant for quantum chemistry:

Example 26: Unbounded operator

Let $u_\alpha \in L^2(\mathbb{R})$ be given by

$$u_\alpha(x) = N(\alpha) \exp(-\alpha x^2/2). \tag{5.30}$$

Here, $N(\alpha) = (\alpha/\pi)^{1/4}$ is such that $\|u_\alpha\| = 1$. Let $\hat{D} = \partial_x$, and compute

$$\partial_x u_\alpha(x) = -\alpha x u_\alpha(x). \tag{5.31}$$

We obtain

$$\frac{\|\partial_x u_\alpha\|}{\|u_\alpha\|} = \sqrt{\frac{\alpha}{\pi}} \alpha^2 \int x^2 \exp(-\alpha x^2)\, \mathrm{d}x. \tag{5.32}$$

It is an easy exercise to compute that this goes to infinity as $\alpha \to 0$. Thus, ∂_x is unbounded. Similarly, it is easy to show that the kinetic energy operator $-\nabla^2/2$ for a single particle is unbounded.

5.4.1 Compact operators

In finite dimensions, all linear transformations are bounded, and hence continuous. Furthermore, in finite dimensions, all bounded and closed sets are *compact*, see Chapter 3.

Compact linear transformations are "more than continuous". They are such that closed and bounded subsets are mapped to compact sets.

Definition 63: Compact linear transformation

Let V and W be Banach spaces over $\mathbb{F}$, and let $T \in B(V, W)$. The linear transformation T is called *compact* if the closed unit ball $U = \{x \in V \mid \|x\|_V \leq 1\}$ is mapped to a compact subset $T[U] \subset W$.

5.4.2 Eigenvalues and the spectrum

For finite dimensional Banach spaces, the concept of an *eigenvalue* of a linear operator is well-known. If V is a finite-dimensional Banach space over $\mathbb{F}$, and $T \in L(V)$ is a bounded linear operator, then the eigenvalue problem reads:

$$\text{Find nonzero } u \in V \text{ and } \lambda \in V, \text{ such that } Tu = \lambda u. \tag{5.33}$$

In finite dimensions, the eigenvalue problem *always* has a solution if $\mathbb{F} = \mathbb{C}$, since it can be reduced to finding a root of a finite-degree polynomial, and we can appeal to the Funamental Theorem of Algebra to find our eigenvalue.

In *infinite dimensions*, however, this is no longer true. Why? The concept of determinant is not valid for these operators, and one must use more abstract means to show existence of an eigenvalue problem. The followine example is illustrative:

Example 27: Shift operator

Let $V = \ell_2(\mathbb{N}; \mathbb{C})$, the space of square summable sequencess $u = (u_i) \subset \mathbb{C}$ with complex coefficients. Let T be the *shift operator*:

$$T(u_0, u_1, \cdots) = (0, u_0, u_1, \cdots).$$

This operator has no eigenvalues, and it is an instructive exercise to show this. (See the exercises.)

For infinite dimensional Banach spaces, the *spectrum* of an operator is a generalization of the set of eigenvalues that we have in the finite dimensional case.

Definition 64: Spectrum and resolvent of bounded operators

Let V be a Banach space over $\mathbb{C}$, and let $T \in L(V)$ be a bounded operator. The *resolvent* of T is the set

$$\rho(T) = \{\lambda \in \mathbb{C} \mid T - \lambda I \text{ has a bounded inverse}\}. \tag{5.34}$$

Here, I is the identity operator, $Iu = u$. That X has a bounded inverse means that there is an operator $\tilde{X} \in L(V)$ such that $\tilde{X}X = X\tilde{X} = I$ on V. We then write $\tilde{X} = X^{-1}$.

The *spectrum* of T is defined as:

$$\sigma(T) = \{\lambda \in \mathbb{C} \mid T - \lambda I \text{ does not have a bounded inverse}\}. \tag{5.35}$$

The set $\rho(T) \subset \mathbb{C}$ is a closed (in fact compact) set, and $\sigma(T) \subset \mathbb{C}$ is an open set.

The spectrum can be quite general, but at least it is compact, i.e., closed *and* bounded. For unbounded operators the situation is more complicated.

5.5 Operators over separable Hilbert spaces

Separable Hilbert spaces are central to quantum chemistry: The space of N-electron wavefunctions, and the subspace of those wavefunctions that have finite kinetic energy are examples. Let us therefore briefly mention some types of operators that can be encountered.

5.5.1 Bounded operators

Definition 65: Adjoint operator

Let $(V, \langle\cdot,\cdot\rangle_V)$, $(W, \langle\cdot,\cdot\rangle_W)$ be separable Hilbert spaces over $\mathbb{F}$, and let $T \in L(V, W)$.

The *Hermitian adjoint* $T^\dagger \in V(W, V)$ is the unique operator that satisfies

$$\langle w, Tv\rangle_W = \langle T^\dagger w, v\rangle_V$$

for all $v \in V$, $w \in W$.

If $H \in L(V, V)$, then $H^\dagger \in L(V, V)$ is an operator over V. We say that H is *Hermitian, or self-adjoint* if $H^\dagger = H$.

The Hermitian adjoint generalizes the corresponding concept for finite dimensional Hilbert spaces. The Hermitian adjoint may also be defined for unbounded operators, but self-adjointness becomes a more strict concept.

5.5.2 Projectors

Definition 66: Orthogonal projector

Let V be a separable Hilbert space over $\mathbb{F}$. A *orthogonal projector* is a Hermitian (self-adjoint) $P \in B(V)$ that satisfies $P^2 = P$.

The set $U = P[V]$ is a closed subspace of V, and any $v \in V$ can be uniquely decomposed as

$$v = v_\parallel + v_\perp,$$

where $v_\parallel = Pv \in U$ and $\langle v_\parallel, v_\perp\rangle = 0$. We have $v_\perp = v - v_\parallel$, and Pythagoras' Theorem

$$\|v\|^2 = \|v_\parallel\|^2 + \|v_\perp\|^2.$$

A projection onto the x_1x_2-plane in $\mathbb{R}^3$ is illustrated in Fig. 5.2.

5.5.3 Spectral theorem

Self-adjointness (equal to Hermiticity for bounded operators) allow the important Spectral Theorem, which for *bounded* operators goes as follows:

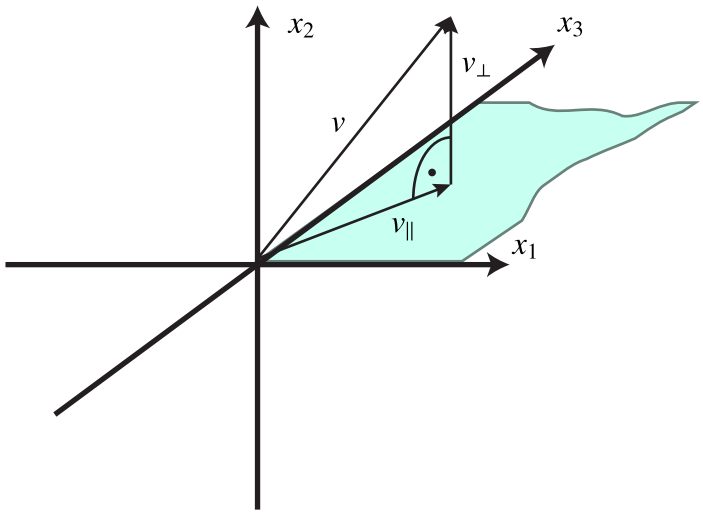


Figure 5.2: Illustration of projection in $\mathbb{R}^3$

Theorem 26: Spectral theorem for bounded self-adjoint operators

Let V be a complex separable Hilbert space, and let $T \in L(V)$ be self-adjoint. The spectrum is real, $\sigma(T) \subset \mathbb{R}$, and compact. We have

$$\|T\|_{L(V)} = \sup\{|\lambda| \mid \lambda \in \sigma(T)|\}.$$

Moreover, T can be decomposed using what is called a *spectral measure* E on the real line $\mathbb{R}$, defined on the Borel subsets of $\mathbb{R}$, such that

$$T = \int_{\mathbb{R}} \lambda dE(\lambda). \tag{5.36}$$

This integral represents T in terms of a integral over the spectrum of T, where λ represents the possible spectral values (e.g., eigenvalues), and $E(\lambda)$ acts as a projection operator that captures how much of Hilbert space corresponds to each value λ. (For each Borel subset of $\mathbb{R}$, such as an interval I, the integral $\int_I dE(\lambda)$ is a projection operator that projects onto the eigenspaces, ina generalized sense.)

The spectral decomposition 5.36 is immensely useful. It can be used to apply functions to the operator to build new operators with well-defined properties, similarly to what one can do in finite dimensions:

Theorem 27: Spectral calculus

Let V be a complex separable Hilbert spae, and let $T \in L(V)$ be self-adjoint with spectral decomposition given by Eq. (5.36). Let $f : \mathbb{R} \to \mathbb{C}$ be any Borel measurable function. We can define a new operator $f(T)$ by the formula

$$f(T) = \int_{\mathbb{R}} f(\lambda) dE(\lambda). \tag{5.37}$$

Example 28: Solving the time-dependent Schrödinger equation

Suppose V is the complex separable Hilbert space of quantum states of a nonrelativistic quantum system, and suppose $H \in L(V)$ is the governing Hamiltonian operator, i.e., the time-dependent Schrödinger equation reads

$$i\hbar \frac{d}{dt}\psi(t) = H\psi(t), \quad \psi(0) = \psi_0.$$

This is an initial value problem and an ordinary differential equation in Hilbert space. (When H is written out it often becomes a partial differential equation formulated in Sobolev spaces.) We have not really defined what we mean by this equation in the infinite dimensional case. However, the spectral theorem allows us to write

$$H = \int_{\mathbb{R}} \lambda dE(\lambda),$$

and we can define a unitary operator by the formula

$$U(t) = \exp(-iHt/\hbar).$$

This operator is well-defined. Assuming that formal differentiation with respect to time works out as in finite dimensional spaces, we see that

$$\psi(t) = U(t)\psi_0$$

solves the time-dependent Schrödinger equation.

For unbounded operators over a separable Hilbert space, self-adjointness is *not the same* as Hermiticity. The spectral theorem and spectral calculus can be extended to unbounded operators, but is more technical.

5.5.4 Unitary operators

Definition 67: Unitary operator

Let V be a separable Hilbert space over $\mathbb{F}$, and let $U \in L(V)$. We say that U is *unitary* if, for every $u, v \in V$,

$$\langle Tu, Tv\rangle = \langle u, v\rangle .$$

An example of a unitary operator is given in Example **??**.

5.5.5 Hilbert Sobolev spaces

The Sobolev spaces $W^{k,2}(\Omega)$:

Definition 68: The spaces $H^k(\Omega)$ and $H_0^k(\Omega)$

The Sobolev spaces $W^{k,2}(\Omega)$ are denoted $H^k(\Omega)$. Similarly, $W_0^{k,2}(\Omega) = H_0^k(\Omega)$. They are Hilbert spaces with inner product:

$$\langle u, v\rangle_{H^k} = \langle u, v\rangle_{L^2} + \sum_{\alpha,|\alpha|\leq k} \langle \partial_\alpha u, \partial_\alpha v\rangle\,, \tag{5.38}$$

where the sum over α again is a sum over partial derivatives of order $\leq k$.

The special case $k = 1$,

$$\langle u, v\rangle_{H^1} = \langle u, v\rangle_{L^2} + \langle \nabla u, \nabla v\rangle_{L^2}\,. \tag{5.39}$$

Remark 4: Kinetic energy and Sobolev spaces

In quantum mechanics, the kinetic energy operator is $\hat{T} = -\frac{1}{2}\nabla^2$, an unbounded but Hermitian operator. When supplied with the domain $D(\hat{T}) = H_0^2$, then it is in fact self-adjoint.

Suppose $u \in H_0^1(\Omega)$. Then we see that

$$\langle u, \hat{T}u\rangle = \frac{1}{2}\langle \nabla u, \nabla u\rangle < +\infty. \tag{5.40}$$

Here, we assumed that integration by parts is allowed with the weak derivative. Indeed it is in $H_0^1(\Omega)$! Thus, $H_0^1(\Omega)$ is precisely the set of normalizable wavefuctions that has finite kinetic energy and vanish at $\partial\Omega$. This is one of the main steps of the "weak formulation" of the Schrödinger equation.

5.6 Weak formulation of the Schrodinger equation

We have now amassed a set of tools that allow us to formulate the Schrödinger equation using Sobolev spaces. This formulation is often called *the weak formulation*, since we do not require solutions to be *classical* in the sense that any derivative that occurs is of the weak type.

For simplicity, we consider a single spinless particle in $\mathbb{R}^3$, with Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\nabla^2 + V(\vec{r}), \tag{5.41}$$

where $V(\vec{r})$ is a multiplicative potential operator, assumed for the moment to be measurable and in $L^1_{\text{loc}}(\mathbb{R}^3)$. For the moment we let the potential be otherwise unknown. The calligraphic $\mathcal{H}$ is to distinguish it from an actual Hilbert-space operator. It is *formal*, a term mathematicians use about physics formulas that are not rigorous mathematics. Sometimes, but not always, it's just because they don't understand it. (It is also a term that physicists use about mathematics they don't understand, so mathematicians and physicists are really not that different.)

Physicists now want to solve the eigenvalue problem of $\mathcal{H}$, i.e., find nonzero $\psi : \mathbb{R}^3 \to \mathbb{C}$ and $E \in \mathbb{R}$ such that

$$\mathcal{H}\psi = E\psi. \tag{5.42}$$

This equation is also *formal*, because we don't know what kinds of functions $\mathcal{H}$ can operate on.

In order to connect with spectral theory of self-adjoint operators on Hilbert space, we must find a self-adjoint $\hat{H} : D(\hat{H}) \to L^2$ with domain $D(\hat{H})$ that somehow represents $\mathcal{H}$. If we don't do this properly, we may end up "missing" eigenfunctions, or even create complex eigenvalues, which is nonsense.

So let $\phi : \mathbb{R}^3 \to \mathbb{C}$ be a $C_0^\infty(\mathbb{R}^3)$ function. This is a dense set of L^2, and it is typical in functional analysis to study such well-behaved sets first, then take limits or closures afterwards. With such a ϕ, $\mathcal{H}\phi$ is a measurable function; $\nabla^2\phi \in C_0^\infty(\mathbb{R}^3)$, and $V\phi$ is a measurable function (since products of measurable functions are measurable). Requiring $\mathcal{H}\phi$ to be actually in L^2 might be too strong, so let us consider the energy expectation value,

$$\mathcal{E}(\phi) = \frac{\langle \phi, \mathcal{H}\phi \rangle}{\langle \phi, \phi \rangle}. \tag{5.43}$$

This is now a well-defined function on all nonzero elements of $C_0^\infty(\mathbb{R}^3)$. To see this, note that the denominator is certainly well-defined. The numerator is

$$\langle \phi, \mathcal{H}\phi \rangle = \int \frac{-1}{2}\bar{\phi}\nabla^2\phi + \bar{\phi}V\phi. \tag{5.44}$$

Since $V\phi$ is measurable,

$$\left| \int |\phi|^2 V \right| \leq \|\phi\|_\infty^2 \int_K |V| < +\infty, \tag{5.45}$$

where $K \subset \mathbb{R}^3$ is the support of ϕ. Thus, the numerator is well-defined as well.

We now *define* the ground-state energy of $\mathcal{H}$ to be

$$E_0 = \inf\{\mathcal{E}(\phi) \mid \phi \in C_0^\infty(\mathbb{R}^3), \phi \neq 0\} \tag{5.46}$$

where the infimum is the *greatest lower bound* of the function, i.e., E_0 is the largest number such that there is no ϕ that gives $\mathcal{E}(\phi) < E_0$.

As chemists, we know that the elctronic wavefunction has *cusps*. Thus, the space C_0^∞ cannot be large enough to capture our eigenfunctions. We need to *extend* the energy function to a properly large space.

Using integration by parts, we write the kinetic energy as

$$-\frac{1}{2}\langle \phi, \nabla^2\phi \rangle = \frac{1}{2}\langle \nabla\phi, \nabla\phi \rangle . \tag{5.47}$$

This is one out of two locations where the term *weak formulation* is relevant, because we no longer differentiate *twice*, but only once. The second location is the following: We would like to define $\mathcal{E}$ on a *complete* vector space, because we would like to say something about existence of a minimizer, i.e., existence of the eigenfunction of the energy, e.g., since we know about cusps, and also that the exact eigenfunction does not suddenly come zero, such as is the case with C_0^∞. Our enlarged space should be a subspace of L^2 due to the fact that we want a probability interpretation. (See also de denominator.) The *largest* subspace of L^2 where the kinetic energy is finite is the Sobolev space H^1. This space is a space of *weak derivatives*.

So our candidate space is H^1. What assumptions do we need on V in order to make the potential energy well-defined? We also need to make sure that if we find a minimizer of $\mathcal{H}$, this will be an eigenfunction of a self-adjoint operator $\hat{H} : D(\hat{H}) \to L^2$, because this is needed to define quantum mechanics.

Suppose V is such that it is *relatively form-bounded from below by kinetic energy*, in the following manner: Suppose that there exists $\varepsilon \in [0, 1[$ and a $C_\varepsilon \geq 0$, such that for all $\phi \in H^1$,

$$|\langle \phi, V\phi \rangle| \leq \varepsilon\frac{1}{2}\langle \nabla\phi, \nabla\phi \rangle + C_\varepsilon\|\phi\|^2. \tag{5.48}$$

Then we see that

$$\langle \phi, \mathcal{H}\phi \rangle \geq \frac{1}{2}(1-\varepsilon)\langle \nabla\phi, \nabla\phi \rangle - C_\varepsilon\|\phi\|^2. \tag{5.49}$$

Thus,

$$\mathcal{E}(\phi) \geq \frac{1}{2}(1-\varepsilon)\frac{\langle \nabla\phi, \nabla\phi\rangle}{\langle \phi, \phi\rangle} - C_\varepsilon \geq -C_\varepsilon, \tag{5.50}$$

and therefore *the function $\mathcal{E}$ is defined on H^1 and bounded from below*.

Not only that, but we also get

$$\langle \phi, \mathcal{H}\phi\rangle \leq \frac{1}{2}(1+\varepsilon)\|\nabla\phi\|^2 + C_\varepsilon\|\phi\|^2 \leq C'_\varepsilon\|\phi\|^2_{H^1}, \tag{5.51}$$

i.e., that $\mathcal{E}$ is also *bounded above*.

It turns out that the following is true:

Lemma 3: Form boundedness of a class of potentials

Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then V is relatively form bounded in the sense of Eq. (5.48).

There is a powerful representation theorem for quadratic forms such as $h(\phi) = \langle \phi, \mathcal{H}\phi\rangle$. Note that we have proven (or at least outlined the proof) that $|h(\phi)| \leq C\|\phi\|_{H^1}$ for some constant C. Them, the representation theorem says that there is a unique self-adjoint operator $\hat{H} : D(\hat{H}) \to L^2$ such that $D(\hat{H}) \subset H^1$ (a dense subset), and such that for all $\phi \in D(\hat{H})$,

$$h(\phi) = \langle \phi, \hat{H}\phi\rangle\,. \tag{5.52}$$

We are almost done, because now we *can* differentiate the function $\mathcal{E} : H^1 \to \mathbb{R}$ to form the eigenvalue equation

$$\hat{H}\psi = E\psi, \quad E = \mathcal{E}(\psi). \tag{5.53}$$

The question is: what is $D(\hat{H})$? A remarkable fact is that for $V \in L^2 + L^\infty$, then $D(\hat{H}) = H^2(\mathbb{R}^3)$.

Note that even if we have a *weak formulation* of the Schrödinger equation, that only assumes one weak derivative in the variational principle, we actually get eigenfunctions that are twice weakly differentiable!

We summarize as a theorem:

Theorem 28: Weak formulation of the Schrödinger equation

Let $V \in L^2 + L^\infty$ (which includes the Coulomb potential of the hydroge atom). Then the operator $\hat{H} : H^2 \to L^2$ given by

$$\hat{H} = -\frac{1}{2}\nabla^2 + V \tag{5.54}$$

is self-adjoint. Its eigenfunctions are critical points of the energy function $\mathcal{E} : H^1 \to \mathbb{R}$ given by

$$\mathcal{E}(\phi) = \frac{\frac{1}{2}\langle \nabla\phi, \nabla\phi\rangle + \langle \phi, V\phi\rangle}{\langle \phi, \phi\rangle}. \tag{5.55}$$

We note in passing, that even for functions $\phi \in H^1$ we *can* defined $\nabla^2\phi$ as a *distribution*, i.e., a generalized function. This distribution is such that $\langle \phi, -\nabla^2\phi\rangle = \langle \nabla\phi, \nabla\phi\rangle$.

We also note that the construction can be generalized to N-electron Hamiltonians with Coulomb interactions between pairs of electrons and between electrons and nuclei.

5.7 The Fourier transform

The Fourier transform of a square-integrable function is a very useful tool for the study of quantum chemistry. It phrases in mathematical terms the idea that a function can be decomposed into plane wave components with varying weights and frequencies.

5.7.1 Fourier transform for functions over $\mathbb{R}^n$

The Fourier transform is an integral transformation, taking a function into a new function. It is therefore an operator between function spaces.

The transform is most easily defined for L^1 functions, but can be extended to a much larger class of functions, e.g., L^2 functions.

Definition 69: Fourier transform on L^1

We define the *Fourier transform* of $u \in L^1(\mathbb{R}^n)$ as the linear operator $\mathcal{F} \in L(L^1(\mathbb{R}^n), L^\infty(\mathbb{R}^n))$, with an auxiliary notation $\mathcal{F}u = \hat{u} \in L^\infty(\mathbb{R}^n)$, and given by the formula

$$\hat{u}(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\mathbf{k}\cdot\mathbf{x}} u(\mathbf{x})\, d\mathbf{x}. \tag{5.56}$$

We define the *inverse Fourier transform* of $u \in L^1(\mathbb{R}^n)$ as the function $\mathcal{F}^{-1}u = \check{u} \in L^\infty(\mathbb{R}^n)$ given by the formula

$$\check{u}(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i\mathbf{k}\cdot\mathbf{x}} u(\mathbf{x})\, d\mathbf{x}. \tag{5.57}$$

As defined, the inverse transform is actually only defined as a transform on $L^1(\mathbb{R}^n)$, not $L^\infty(\mathbb{R}^n)$. Therefore it is not actually the inverse. However, it can be extended to the actual inverse on $L^\infty(\mathbb{R}^n)$.

To see that the definitions of $\hat{u}$ and $\check{u}$ as integrals make sense, consider a function $u \in L^1(\mathbb{R}^n)$, and the integral in Eq. (5.56). This integral exists for all $\mathbf{k}$, since

$$|\hat{u}(\mathbf{k})| \leq \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} |u(\mathbf{x})|\, d\mathbf{x} = \frac{1}{(2\pi)^{n/2}} \|u\|_1. \tag{5.58}$$

Hence, $\hat{u} \in L^\infty(\mathbb{R}^3)$. The same argument applies to Eq. (5.57).

Can we define the Fourier integral for any $u \in L^\infty(\mathbb{R}^n)$? No, just pick the constant function $u(\mathbf{x}) = 1$. The function $\exp(-i\mathbf{k} \cdot \mathbf{x})$ is measurable but not integrable.

We can, however, extend the definition of the Fourier integral to $L^2(\mathbb{R}^n)$. The classical way to do this, is via *Plancherel's Theorem*. The result is a *unitary operator* $\mathcal{F}$ on $L^2(\mathbb{R}^n)$, and in that case $\mathcal{F}^{-1}$ is actually given by Eq. (5.57):

Theorem 29: Fourier Transform on L^2

For $u \in L^2(\mathbb{R}^n)$, the Fourier integral Eq. (5.56) is almost-everywhere defined, and $\hat{u} \in L^2(\mathbb{R}^n)$. The Fourier transform is *unitary*, i.e., $\|u\|_2 = \|\hat{u}\|_2$. Moreover, we have the following properties: Let $u, v \in L^2(\mathbb{R}^n)$. Then,

1. $\langle u, v\rangle_2 = \langle \hat{u}, \hat{v}\rangle_2 = \langle \check{u}, \check{v}\rangle$ ***unitarity***
2. $\widehat{\partial^\alpha u} = (\mathrm{i}\mathbf{k})^\alpha \hat{u}$ ***partial derivatives***
3. $\widehat{u * v} = (2\pi)^{n/2}\hat{u}\hat{v}$ ***convolutions***
4. $u = (\hat{u})^\vee = (\check{u})^\wedge$ (almost everywhere) ***inverses***

Here, α is a multindex $\alpha = (\alpha_1, \cdots, \alpha_k)$, and

$$\partial^\alpha = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}} \cdots \frac{\partial^{\alpha_n}}{\partial \alpha_n^{\alpha_n}}, \quad \mathbf{k}^\alpha = k_1^{\alpha_1} \cdots k_n^{\alpha_n} \tag{5.59}$$

Example 29: Gaussian

Let $A = A^T$ be an $n \times n$ real invertible matrix, and consider the funtion $u \in L^2(\mathbb{R}^n)$ given by

$$u(\mathbf{x}) = \exp(-\mathbf{x}^T A\mathbf{x}/2) \tag{5.60}$$

Then

$$\hat{u}(\mathbf{k}) = \exp(-\mathbf{k}^T A^{-1}\mathbf{k}/2) \tag{5.61}$$

TODO: Write up some intuition: Smoothness is "dual" to rapid decay. Translation is "dual" to multiplication by phase factor/plane wave. Scaling by λ is dual to scaling by λ^{-1}.

5.7.2 Fourier series and periodic Fourier transform

Another version of the Fourier transform is for square-integrable functions defined on the "unit torus" $\mathbb{T}^n$. The 1D unit torus $\mathbb{T}$ is the interval $[0, 1[$ with periodic boundary conditions, i.e., the points 0 and 1 are identified. (This identification means a certain modification of open sets in $[0, 1[$. Can you describe it?)

Thus we consider functions in $L^2(\mathbb{T}^n)$.

We begin with the case $n = 1$. The Fourier transform of $u \in L^2(\mathbb{T})$ is defined by

$$\hat{u}_k = \int_{\mathbb{T}} e^{-2\pi \mathrm{i} k x} u(x)\, \mathrm{d}x. \tag{5.62}$$

It is readily verifiable that this is equivalent to computing the basis expansion coefficients of the orthonormal set of vectors

$$\phi_k(x) = e^{2\pi \mathrm{i} k x}, \quad k \in \mathbb{Z}. \tag{5.63}$$

(That this is indeed a basis must be shown.) The map $u \mapsto \hat{u}$ is an isometric isomorphism of $L^2(\mathbb{T})$ and $\ell_2(\mathbb{Z})$. The inverse Fourier transform is the *Fourier series*

$$\check{c}(x) = \sum_{k \in \mathbb{Z}} e^{2\pi \mathrm{i} k x} c_k. \tag{5.64}$$

It is a fact that $(\hat{u})^\vee = u$ almost everywhere, and that $\check{c}^\wedge = c$.

The n-dimensional generalization of the Fourier transform is

$$\hat{u}_{\mathbf{k}} = \int_{\mathbb{T}^n} e^{-2\pi i \mathbf{k}\cdot\mathbf{x}} u(\mathbf{x})\, d\mathbf{x}, \tag{5.65}$$

and the Fourier series is

$$\check{c}(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^n} e^{2\pi i \mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k}}\, d\mathbf{x}. \tag{5.66}$$

The transform $u \mapsto c = \hat{u}$ is an isometric isomorphism between $L^2(\mathbb{T}^n)$ and $\ell_2(\mathbb{Z}^n)$.

Theorem 30: Fourier series

1. $\langle u, v\rangle = \langle \hat{u}, \hat{v}\rangle = \sum_{\mathbf{k}\in\mathbb{Z}^n} \hat{u}_{\mathbf{k}}\hat{v}_{\mathbf{k}}$ ***unitarity***
2. $\widehat{\partial^\alpha u} = (2\pi i)^{|\alpha|}\mathbf{k}^\alpha \hat{u}_{\mathbf{k}}$ ***partial derivatives*** **TODO:**
3. a convolution identity, work it out
4. $u = (\hat{u})^\vee$ (almost everyhwere), and $c = (\check{c})^\wedge$ ***inverses***

TODO: Express Fourier series on arbitrary interval/torus, introducing normalization constants.

5.8 Distributions

TODO: Writeup

Functions of several variables and complex variables

6.1 Introductory remarks

We now consider functions over Euclidean space, and more generally Banach and Hilbert spaces. We discuss continuity, differentiability, and integration.

Traditionally, the study of real-valued functions from $\mathbb{R}$ to $\mathbb{R}$ is called calculus, including the study of sequences, series, differentiability, maxima, minima, and integration. It is no understatement to say that calculus is very important to any scientist that deals with calculations of any kind, such as quantum chemists.

The study of functions $f : \mathbb{C} \to \mathbb{C}$ is traditionally called *complex analysis*. The algebraic properties of the complex plane introduce strong and surprising results that it is easy to fall in love with.

It is conventional to call the study of functions $f : \mathbb{R}^n \to \mathbb{R}^m$ *vector calculus*. Moreover, the geometry of $\mathbb{R}^2$ and $\mathbb{R}^3$ is quite important in science, and this special topic is therefore often singled out.

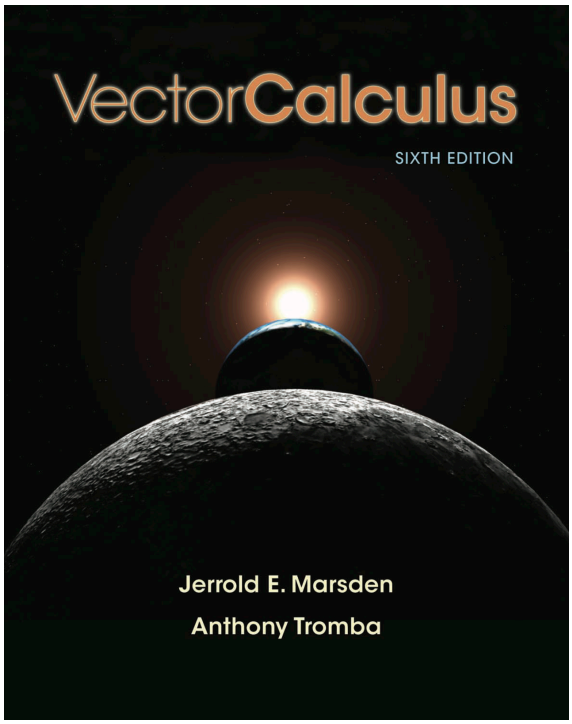
Moving beyond vector calculus, we have the study of functions $f : V \to W$, where V and W are complete normed spaces (Banach spaces). Since quantum mechanics if formulated in Hilbert space, and since many of the quantum chemistry methods are defined in terms of linear or nonlinear partial differential equations, the study of calculus in infinite dimensional spaces hold a certain importance. This topic is often called *non-linear functional analysis*.

6.2 Single-variable functions

6.3 Functions of several variables

Recommended reading

Marsden was a giant in textbok authorship at any level of study. Marsden and Tromba's book is an excellent textbook at the undergraduate level. I find the writing clear and concise, yet engaging. There are many good examples and exercises.



6.3.1 Geometry of real-valued functions

Definition 70: Functions of several variables

Let $\Omega \subset \mathbb{R}^n$, and let $f : \Omega \to \mathbb{R}^m$. The set Ω is the *domain* of f. If $n > 1$, then f is a *function of several (real) variables*. If $m = 1$, then f is *scalar valued*, and if $m > 1$, then f is *vector valued*. A function $f : \Omega \subset \mathbb{R} \to \mathbb{R}^n$ is called a *path* in $\mathbb{R}^n$.

The domains Ω that one is usually interested, are sets that have a nonzero interior, i.e., it contains an open ball of some size, and with a *boundary* $\partial\Omega$ which is sufficiently nice, e.g., piecewise smooth. (We have not defined this notion.)

A notation which is common in order to specify a function "quickly is", e.g.,

$$f : \mathbb{R}^2 \to \mathbb{R}^3, \quad [x, y] \mapsto [\sin(x) + \cos(y), \exp(x + y), -y]. \tag{6.1}$$

Sometimes the domain and codomain are omitted for brevity.

Example 30

A path in $\mathbb{R}^2$:

$$f : [0, 1] \to \mathbb{R}^2, \quad t \mapsto [t^2, \exp(-t)] \tag{6.2}$$

A scalar-valued function:

$$f : \mathbb{R}^2 \to \mathbb{R}, \quad [x, y] \mapsto (x^2 - y^2) \exp(-(x^2 + y^2)) \tag{6.3}$$

Tools for visualizing functions: Graphs, level sets (curves, surfaces …), sections.

The *graph* of $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ is the subset

$$\text{graph}(f) = \{(\mathbf{x}, f(\mathbf{x})) \mid \mathbf{x} \in \Omega\} \subset \mathbb{R}^{n+m}. \tag{6.4}$$

The *level set* of f with value c is

$$\{\mathbf{x} \in \Omega \mid f(\mathbf{c}) = c\}. \tag{6.5}$$

In $\mathbb{R}^2$, this is typically a (union) of curves, and in in $\mathbb{R}^3$, a (union) of surfaces, et.c.

A *section* is obtained by fixing a hyperplane of $\mathbb{R}^n$ and considering f a function only on this plane.

Several exercises.

6.3.2 Differentiability

The idea of the derivative of a function has great use. Locating maxima and minima, understanding the function's behavior, and so on.

Many methods of quantum chemistry are defined in terms of critical point conditions, i.e., that some function $f(\mathbf{x})$ has a vanishing derivative at some point.

To begin with, we define the notion of a *partial derivative*:

Definition 71: Partial derivative

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be a scalar-valued function, Ω open. The *partial derivatives* with respect to the variable x_i are defined by

$$\frac{\partial}{\partial x_i} f(\mathbf{x}) = \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\vec{x})}{h} \tag{6.6}$$

if the limit exists.

In the case $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, the the partial derivatives are defined componentwise, i.e.,

$$\frac{\partial}{\partial x_i} f_j(\mathbf{x}). \tag{6.7}$$

Note that

$$\mathbf{x} + h\mathbf{e}_i = [x_1, x_2, \cdots, x_i + h, \cdots, x_n]^T, \tag{6.8}$$

i.e., we compute the *ordinary* derivative of f with respect to x_i, imagining all the other variables to be fixed.

[Examples and exercises]

The existence of partial derivatives initially seems like a good notion of f being differentiable. However, the following example shows that something is off: We expect a "differentiable function" to behave somewhat nicely.

Example 31

let $f : \mathbb{R}^2 \to \mathbb{R}$, $(x, y) \mapsto x^{1/3}y^{1/3}$. Recall, that the cube root of any real number is well defined. Computing the partial derivatives at $(0, 0)$ gives

$$\frac{\partial}{\partial x} f(0,0) = \lim_{h\to 0} \frac{f(h,0) - f(0,0)}{h} = \lim_{h\to 0} \frac{0-0}{h} = 0, \tag{6.9}$$

and similarly

$$\frac{\partial}{\partial y} f(0,0) = 0. \tag{6.10}$$

But f is far from constant near $(0, 0)$. Indeed, consider f along the line $y = x$,

$$g(x) = f(x, x) = x^{2/3}. \tag{6.11}$$

The derivative of $g(x)$ is

$$g'(x) = \frac{2}{3}x^{-1/3} \tag{6.12}$$

which does not even exist at $x = 0$.

The problem seems to be that the partial derivatives only "see" in two more or less arbitrary directions, and not "all directions".

Definition 72: Differentiable

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, with Ω open. We say that f is *differentiable at* $\mathbf{x}_0 \in \Omega$ if the partial derivatives all exist at $\mathbf{x}_0$, and if

$$\lim_{\mathbf{x}\to\mathbf{x}_0} \frac{\|f(\mathbf{x}) - f(\mathbf{x}_0) - M(\mathbf{x} - \mathbf{x}_0)\|}{\|\mathbf{x} - \mathbf{x}_0\|} = 0, \tag{6.13}$$

where $M = Df(\mathbf{x}_0)$, the *derivative*, is the matrix of partial derivatives,

$$M_{ij} = \frac{\partial f_i(\mathbf{x}_0)}{\partial x_j}. \tag{6.14}$$

and where $M(\mathbf{x} - \mathbf{x}_0)$ is the matrix-vector product applied to $\mathbf{x} - \mathbf{x}_0$.

Intuitively, f is differentiable at $\mathbf{x}_0$ if the function

$$f(\mathbf{x}_0) + Df(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0), \tag{6.15}$$

is a good approximation of f near $\mathbf{x}_0$. The graph of this "first order approximation" is a hyperplane that touches the graph of f at $\mathbf{x}_0$.

In our previous example, the first-order function is *not* a good approximation, and the function was hence not differentiable.

Theorem 31

If f is differetiable at $\mathbf{x}_0$, it is continuous at $\mathbf{x}_0$.

It can be difficult to check the definition of differentiability in many cases. We have a helpful *sufficient* condition for differentiability:

Theorem 32: Condition for differentiability

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, with Ω open. Suppose the partial derivatives all exist at $\mathbf{x}_0$, and furthermore that they are all continuous *in a neighborhood* of $\mathbf{x}_0$. Then f is differentiable at $\mathbf{x}_0$.

Note that we need continuity not only at the point in question, but a whole ε-ball around it, too.

Definition 73: C^1 functions

A function whose partial derivatives exist and are continuous throughout the open domain is said to be of class C^1.

The C^1 functions are differentiable, and can be approximated by first-order polynomials.

We list some properties of the derivative, that aids in computing derivatives of complicated functions:

Theorem 33: Properties of the derivative

1. Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be differentiable at $\mathbf{x}_0 \in \Omega$, and let $c \in \mathbb{R}$. Then $h(\mathbf{x}) = cf(\mathbf{x})$ is differentiable at $\mathbf{x}_0$, and
$$Dh(\mathbf{x}_0) = cDf(\mathbf{x}_0). \tag{6.16}$$
2. Let $g : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be another function differentiable at $\mathbf{x}_0$. Then $h(\mathbf{x}) = f(\mathbf{x}) + g(\mathbf{x})$ is differentiable at $\mathbf{x}_0$, and
$$Dh(\mathbf{x}_0) = Df(\mathbf{x}_0) + Dg(\mathbf{x}_0). \tag{6.17}$$
3. Let $f, g : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be *scalar-valued* functions, differentiable at $\mathbf{x}_0 \in \Omega$. Then $h(\mathbf{x}) = f(\mathbf{x})g(\mathbf{x})$ is differentiable at $\mathbf{x})_0$, and
$$Dh(\mathbf{x}_0) = g(\mathbf{x}_0)Df(\mathbf{x}_0) + f(\mathbf{x}_0)Dg(\mathbf{x}_0). \tag{6.18}$$
4. As in 3, and additionally that $g > 0$ thrughout Ω. Then $h(\mathbf{x}_0) = f(\mathbf{x}_0)/g(\mathbf{x}_0)$ is differentiable at $\mathbf{x}_0$, and
$$Dh(\mathbf{x}_0) = \frac{g(\mathbf{x}_0)Df(\mathbf{x}_0) - f(\mathbf{x}_0)}{[g(\mathbf{x}_0)]^2} \tag{6.19}$$

[Exercises]

Theorem 34: Chain rule

Let $\Omega \subset \mathbb{R}^n$ and $\Omega' \subset \mathbb{R}^m$ be open sets, and let $g : \Omega \to \mathbb{R}^m$ with $g[\Omega] \subset \Omega'$. Let $f : \Omega' \to \mathbb{R}^o$. Thus, $h = f \circ g : \Omega \to \mathbb{R}^o$ is defined. Suppose g is differentiable at $\mathbf{x}_0 \in \Omega$, and f is differentiable at $\mathbf{y}_0 = f(\mathbf{x}_0) \in \Omega'$. Then $f \circ h$ is differentiable at $\mathbf{x}_0$ with derivative

$$D(f \circ g)(\mathbf{x}_0) = Df(\mathbf{y}_0)Df(\mathbf{x}_0), \tag{6.20}$$

i.e., the matrix product of the Jacobian matrices.

Example 32: Function along a path

Let $\mathbf{c} : \mathbb{R} \to \mathbb{R}^3$ be a path tracing out a curve in space, say the flight of a drone with a temperature sensor. The position $\mathbf{c}(t) = [x(t), y(t), z(t)]^T$ is the position of the drone at time f. Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a function, say temperature, in space. The temperature registered by the drone as function of time is $h(t) = (g \circ \mathbf{c})(t) = g(\mathbf{c}(t))$. The rate of change of $h(t)$ is

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{\partial h}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial h}{\partial y}\frac{\partial y}{\partial t} + \frac{\partial h}{\partial z}\frac{\partial z}{\partial t}. \tag{6.21}$$

Example 33: Change-of-variables in space

Let $f : \mathbb{R}^3 \to \mathbb{R}$ be some scalar-valued function in space, say temperature. let $g : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^3$ be *a parameterized surface*. $g(u, v) = [x(u, v), y(u, v), z(u, v)]^T$ is traces out a two-dimensional surface patch in $\mathbb{R}^3$. The temperature over the surface is $h(u, v) = f(g(u, v))$. The rate of change of the temperature along the surface coordinates (u, v) is

$$\begin{bmatrix} \frac{\partial h}{\partial u} & \frac{\partial h}{\partial v} \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial y} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \\ \frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} \end{bmatrix}, \tag{6.22}$$

written out, we get

$$\frac{\partial h}{\partial u} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial u} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial u} \tag{6.23}$$

$$\frac{\partial h}{\partial v} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial v} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial v} \tag{6.24}$$

(6.25)

6.3.3 Higher derivatives

Recall the class C^1 of functions $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ having continuous partial derivatives throughout their domains. In particular, the derivative is a *matrix-valued* function,

$$Df : \Omega \subset \mathbb{R}^n \to \mathbb{R}^{m \times n}, \tag{6.26}$$

since we hace n partial derivatives for each of the m component functions $f_i : \Omega \to \mathbb{R}$.

Suppose now $Df \in C^1$, i.e., each of the mn partial derivatives have continuous partial derivatives throughout Ω. We then say that $f \in C^2$, it is *twice continuously differentiable*. We note that $D^2 f = D(Df) : \Omega \to \mathbb{R}^{m \times n \times n}$, by which we indicate a *three-index symbol*, or *tensor*,

$$[D^2 f(\mathbf{x}_0)]_{ijk} = \frac{\partial}{\partial x_j}\frac{\partial}{\partial x_k} f_i(\mathbf{x}_0). \tag{6.27}$$

It is a theorem, that the mixed partial derivatives are symmetric for C^2 functions,

$$\frac{\partial^2 f_i}{\partial x_j x_k} = \frac{\partial^2 f_i}{\partial x_k x_j}. \tag{6.28}$$

Iterating this argument, we now define:

Definition 74: C^k functions

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, with Ω open. We say that f is of class C^k if, for all partial derivatives of order $\leq k$ exist and are continuous throughout Ω. The ℓth order derivative is denoted

$$D^\ell f : \Omega \to \mathbb{R}^{m\times n\times\cdots\times n}, \tag{6.29}$$

with components

$$D^\ell f(\mathbf{x})_{ij_1j_2\cdots j_\ell} = \frac{\partial^\ell}{\partial x_{i_1}\cdots\partial x_{i_\ell}} f_i(\mathbf{x}). \tag{6.30}$$

Accepting that mixed partial derivatives of order 2 are symmetric, it immediately follows that:

Theorem 35

For a function of class C^k, the mixed partial derivatives are all symmetric with respect to exhange of the order of the differentiation.

Example 34

Let $f(x, y) = x^2 - 4xy$. Compute all partial derivatives up to order 2.

The first-order derivatives are

$$\frac{\partial f}{\partial x} = 2x - 4y, \qquad \frac{\partial f}{\partial y} = -4x. \tag{6.31}$$

The partial derivatives are continuous, hence f is of class C^1. We compute the second-order derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial x\partial y} = \frac{\partial^2 f}{\partial y\partial x} = -4, \quad \frac{\partial^2 f}{\partial y^2} = 0. \tag{6.32}$$

These are also continuous. Hence f is of class C^2.

The next derivatives vanish. Hence, f is of class C^k for every k.

We note the symmetry of the partial derivatives in this simple example.

6.3.4 Taylor's Theorem

Polynomials play an important role in analysis, and they are indispensable for any researcher in quantum chemistry. Polynomials help us define gaussian-type orbital basis sets, helps us approximate difficult functions, derive variational equations, and so on.

For functions of class C^1, the derivative gives an approimation to the function "to first order" near a differentiable point $\mathbf{x}_0$. Indeed, for functions of class C^k this can be generalized: The function can be well-approximated by a multivariable polynomial of degree k near $\mathbf{x}_0$.

Theorem 36: Second-order Taylor formula

et $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be of class C^2. Then we may write

$$f(\mathbf{x}_0 + \mathbf{h}) = f(\mathbf{x}_0) + Df(\mathbf{x}_0)\mathbf{h} + \frac{1}{2}\mathbf{h}^T D^2 f(\mathbf{x}_0)\mathbf{h} + R_2(\mathbf{h}, \mathbf{x}_0), \tag{6.33}$$

where the *remainder* satisfies $R_2(\mathbf{h}, \mathbf{x}_0)/\|\mathbf{h}\|^2 \to 0$ as $\mathbf{h} \to 0$, written

$$R_2(\mathbf{h}, \mathbf{x}_0) = o(\|\mathbf{h}\|^2). \tag{6.34}$$

The symbol $D^2 f(\mathbf{x}_0)$ is the *Hessian* of f, the matrix of second-order mixed partial derivatives, a symmetric matrix.

The above formula can be generalized to polynomials of degree k for C^k functions.
The formula can also be generalized to vector-valued functions whose components are all C^k.

Example 35

Compute the second-order Taylor polynomial of $f(x, y) = \exp(-x^2 - y^2)$ at $(0, 0)$.

$$Df(x, y) = [-2xf(x, y), -2yf(x, y)], \quad D^2 f(x, y) = \begin{bmatrix} (4x^2 - 2)f(x, y) & 4xyf(x, y) \\ 4xyf(x, y) & (4y^2 - 2)f(x, y) \end{bmatrix} \tag{6.35}$$

$$f(0, 0) = 1, \quad Df(0, 0) = [0, 0], \quad D^2 f(0, 0) = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix} \tag{6.36}$$

$$f(x, y) = 1 - (x^2 + y^2) + o(x^2 + y^2). \tag{6.37}$$

6.3.5 Maxima and minima

Suppose $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$, with Ω being an open domain. We wish to find *local minima or maxima* of f:

Definition 75: Local maxima and minima

et $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$, with Ω being an open domain.

1. A *local maximum* is a point $\mathbf{x} \in \Omega$ such that there exists an open ε-ball $B_\varepsilon(\mathbf{x})$ with

$$f(\mathbf{x}) \leq f(\mathbf{y}), \quad \text{for all } \mathbf{y} \in B_\varepsilon(\mathbf{x}). \tag{6.38}$$

2. A *local minimum* is a point $\mathbf{x} \in \Omega$ such that there exists an open ε-ball $B_\varepsilon(\mathbf{x})$ with

$$f(\mathbf{x}) \geq f(\mathbf{y}), \quad \text{for all } \mathbf{y} \in B_\varepsilon(\mathbf{x}). \tag{6.39}$$

For local maxima and minima to be defined, f need not even be continuous.

How do we charaterize local maxima and minima? For a general function f, it can be hard to verify that a candidate point $\mathbf{x} \in \Omega$ is indeed a local maximum or minimum. If, on the other hand f is C^1, then a local maximum or minimum always has a vanishing derivative. This can be proven from

the first-order Taylor polynomial approximation. On the other hand, it can happen that the derivative vanishes, even though we do not have a local maximum or minimum at $\mathbf{x}$.

Definition 76: Critical point, saddle point

Ler $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be of class C^1. Any $\mathbf{x} \in \Omega$ such that $Df(\mathbf{x}) = 0$ is called *a critical point of* f. The function value $f(\mathbf{x})$ is called a *critical value*. If $\mathbf{x}$ is not a local maximum or minimum, we say that $\mathbf{x}$ is a *saddle point*.

If a function is of class C^2, the second derivative matrix $H = D^2 f(\mathbf{x})$, often called the Hessian, is a symmetric matrix, since partial derivatives are symmetric. Thus there is a unitary matrix U with columns $\mathbf{u}_i$ such that

$$H = U\Lambda U^T = \sum_{i=1}^{n} \mathbf{u}_i \lambda_i \mathbf{u}_i^T, \tag{6.40}$$

with Λ being a diagonal matrix of eigenvalues. Recall the second-order Taylor approximation

$$f(\mathbf{x} + \mathbf{h}) = f(\mathbf{x}) + \frac{1}{2}\mathbf{h}^T H \mathbf{h} + o(\|\mathbf{h}\|^3). \tag{6.41}$$

Introducing the spectral form of H, the second order term is

$$\frac{1}{2}\mathbf{h}^T H \mathbf{h} = \sum_{i=1}^{n} h_i^2 \lambda_i, \quad h_i = \mathbf{u}_i^T h. \tag{6.42}$$

This term dominates the remainder if and only if all eigenvalues of H are nonzero. (The examples $f(x) = x^3$, $f(x) = -x^4$, and $f(x) = x^4$ how that this matters, since $f'(0)$ and $f''(0)$ in all cases, so that the second derivative does not diagnose the critical point.) In this case, the behavior of f near the critical point is determined by the sign of the eigenvalues. There are precisely three cases: If all eigenvalues are positive, we have a local minimum, and if all eigenvalues are negative, we have a local maximum. If we have eigenvalues of both signs, then we have a saddle point.

Theorem 37: Classification of critical points

et $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$, with Ω being an open domain. Let f be of class C^2. Let $H = D^2 f(\mathbf{x})$ be the second derivative (Hessian) at a critical point. Assume all eigenvalues of H to be nonzaero. Then we have:

1. If all the eigenvalues of H are positive, then $\mathbf{x}$ is a local minimium.
2. If all the eigenvalues of H are negative, then $\mathbf{x}$ is a local maximum.
3. If there are eigenvalues of H with both positive and negative values, then $\mathbf{x}$ is a saddle point.

When there are one or more eigenvalues that are zero, then we need to analyze the problem further in order to conclude the nature of the critical point.

6.3.6 Integration

The first rigorous definition of a definite integral of a function $f : I \to \mathbb{R}$, $I = [a, b] \subset \mathbb{R}$, is that of the *Riemann ingeral*,

$$\int_a^b f(x)\,\mathrm{d}x. \tag{6.43}$$

Roughly speaking, one defines the integral as the (signed) area under the curve, and approximates this by a *Riemann sum* over areas of N narrow boxes of width $\Delta x = (b-a)/N$,

$$\sum_{i=1}^{N} \Delta x f(x_i), \tag{6.44}$$

where x_i is some point in the interval $[a+(i-1)\Delta x, a+i\Delta x]$, say, the midpoint. As the width Δx of the boxes approaches zero (i.e., $N \to +\infty$), the sum will be a Cauchy sequence with respect to N, under some assumptions on f. It then is a convergent sequence, and we define the integral as the limit.

We will not dig deeper into this topic here. I recommend Morgan (elementary), Lindstrom, and Marsden/Freeman for more details.

Theorem 38: Riemann integrable functions

A function $f : [a,b] \to \mathbb{R}$ is Riemann integrable, i.e., the Riemann integral exists and is finite, if and only if f is bounded on $[a,b]$, and the set of points where f is discontinuous is finite. In that case, the integral is given by

$$\int_a^b f(x)\,\mathrm{d}x = \lim_{N\to+\infty} \frac{b-a}{N} \sum_{i=1}^{N} f(x_i), \quad x_i = a + (i-1/2)\frac{b-a}{N}.$$

A more powerful notion of integrability is that of Lebesgue integrability. The main idea here is that the Riemann sums' vertical boxes are replaced with horizontal boxes.

The Lebesgue integral requires an understanding of *measurable sets and functions*. Measure theory is a powerful theory in itself, but for the average quantum chemist, the Riemann integral will do in most cases.

To read more about measure theory at a pedagogical level, see the book by Lindstrom. Bartle is a classic text on measure theory.

6.4 The tools of calculus [move/edit this material]

In this section, we collect some of the basic facts about manipulating functions.

6.4.1 Differentiation

Differentiation is craft. Integration is art.

We will often use the Leibniz' notation for a derivative

$$f'(x) = \frac{\mathrm{d}}{\mathrm{d}x} f(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x} = \frac{\mathrm{d}f}{\mathrm{d}x}. \tag{6.45}$$

This is indicative of a fraction of infinitesimals, and in fact sometimes they do behave like fractions …

Product rule:

$$(fg)' = f'g + fg' \tag{6.46}$$

Chain rule:

$$f(x(y))' = f'(x(y))y'(x) \tag{6.47}$$

Using Leibniz,

$$\frac{\mathrm{d}}{\mathrm{d}x} f(y(x)) = \frac{\mathrm{d}f}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x}. \tag{6.48}$$

Note "cancellation." Helpful mnemonic device.

Logarithmic differentiation: Sometimes the logarithm of a function is easier to differentiate than the original function. We can then use

$$f' = f \cdot (\ln f)'. \tag{6.49}$$

6.4.2 Integration

An *antiderivative* of a function $f : I \to \mathbb{R}$ is a function $F : I \to \mathbb{R}$ such that $F' = f$. Since the derivative of a constant is zero, such can be added freely. Another notation for the antiderivative is the indefinite integral,

$$F(x) = \int f(x)\,\mathrm{d}x + C, \tag{6.50}$$

with C being a constant.

Antiderivatives are tabulated. But there are basic tricks to evaluate your own.

Variable substitution: Write $x = x(y)$, a function of another variable y.

$$\int_{x_0}^{x_1} f(x)\,\mathrm{d}x = \int_{y_0}^{y_1} f(x(y))\,\frac{\mathrm{d}x}{\mathrm{d}y}\,\mathrm{d}y. \tag{6.51}$$

Here, $x_i = x(y_i)$. Thus, one must be able to invert the function $y(x)$ to get $x(y)$.

Note how the denominator is seemingly "canceled." Helpful mnemonic device.

Integration by parts:

$$\int u'(x)v(x)\,\mathrm{d}x = u(x)v(x) - \int u(x)v'(x)\,\mathrm{d}x. \tag{6.52}$$

Again, an arbitrary constant can be added.

Feynman's differentiation under the integral sign: Let $g(x, \alpha)$ be a function that depends on some parameter α in a smooth manner. Suppose that our function to be integrated i

$$f(x) = \frac{\partial}{\partial\alpha} g(x, \alpha), \tag{6.53}$$

for some value α. Under mild conditions on g,

$$\int f(x)\,\mathrm{d}x = \int \frac{\partial}{\partial\alpha} f(x, \alpha)\,\mathrm{d}x = \frac{\partial}{\partial\alpha} \int f(x, \alpha)\,\mathrm{d}x. \tag{6.54}$$

The latter integral may be easier to compute.

Example: Gaussian integral.

6.5 Complex analysis

6.5.1 Complex algebra

Complex numbers go back to the 16th century, when one tried to solve polynomial root equations. Some equations, like $x^2 + 1 = 0$, did not have roots. On the other hand, by pretending that it *does* have roots, let's call them $\sqrt{-1}$, which was absurd at the time, the Italian mathematician R. Bombelli (ca. 1560) showed that if one used such numbers systematically, one could come up with algorithms for finding roots that were actually real! For example, the equation $x^3 = 15x + 4$ has 4 as a root, which Bombelli found as

$$4 = \sqrt[3]{2 + \sqrt{-121}} + \sqrt[3]{2 - \sqrt{-121}}. \tag{6.55}$$

Descartes famously dubbed the square root of negative numbers *imaginary*, as he seemed to think they did not "exist" like the real numbers. The name stuck, and L. Euler himself coined the notation

$$\mathrm{i} = \sqrt{-1}. \tag{6.56}$$

However, the Norwegian mathematician and cartographer C. Wessel was the first to discover the geometric interpretation of complex numbers as vectors in the plane, around 1797.

Today, complex numbers are everywhere. They are useful in real analysis too: The fundamental Theorem of Algebra, convergence theory of Taylor series, et.c.

For the quantum chemist *why* learn complex analysis?

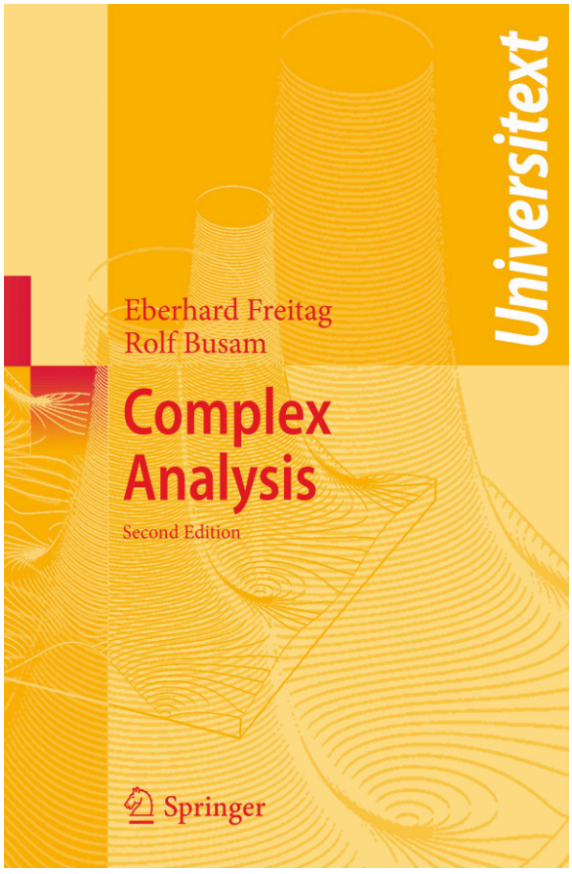
Quantum mechanics is complex-valued, so complex numbers are a natural tool. Analytic functions pop up in many situations. Many of the integrals quantum chemists deal with every day have a natural setting in complex analysis. Complex functions are useful for wave phenomena and oscillations in general, since using complex exponentials, a traveling wave obtains a very transparent form,

$$\cos(kx - \omega t) = \mathrm{Re}\exp(\mathrm{i}(kx - \omega t)). \tag{6.57}$$

In short, complex analysis deals with *differentiable complex functions*. Such functions turn out to be much more than differentiable: they are *infinitely* differentiable, and they can be expanded locally in power series. Hence, "analytic". Moreover, their singularity structire is very rigid, and integration of such functions have many surprising and useful properties. For example, integration of rational functions become straightforward.

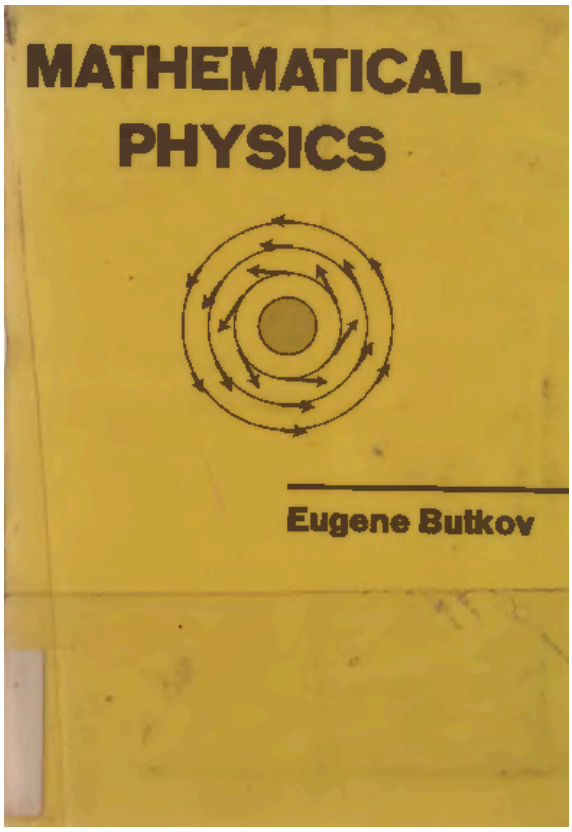
Recommended reading

This is an excellent and modern textbook in complex analysis, and an engaging read.



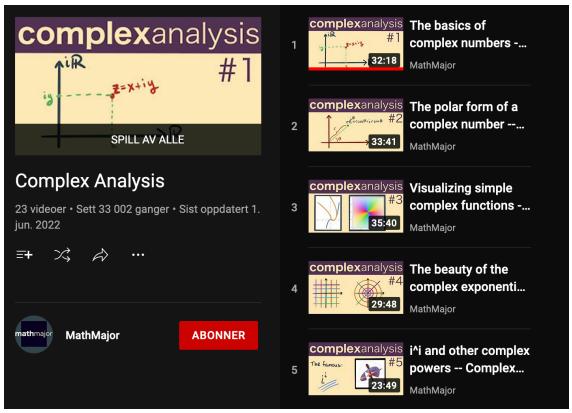
Recommended reading

This book from 1968 is a classic in mathematical physics. It is not a rigorous mathematics book, but gives you many of the tools of the trade. There are also many interesting problems.



Recommended reading

The YouTube channel MathMajor of Michael Penn of Randolph College, Virginia, contains excellent videos on many mathematics topics, and in particular on complex analysis. https://www.youtube.com/playlist?list=PLVMgvCDIRy1wzJcFNGw7t4tehgzhFtBpm



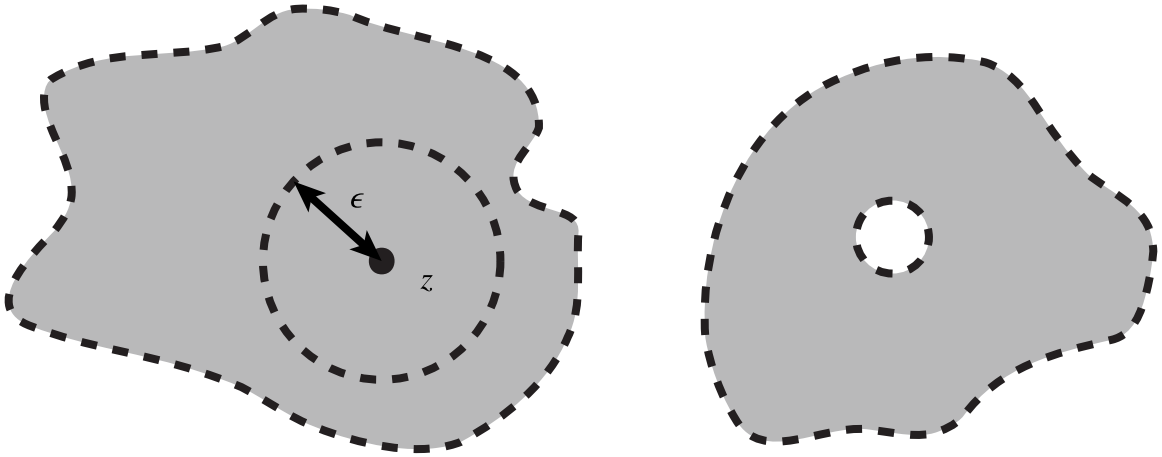


Figure 6.1: Left: Simply connected open domain in the complex plane. An arbitrary point z is surrounded by a small disc of radius ε. Right: Domain with a hole (not simply connected)

Definition 77: Complex number operations

Let $z = x + \mathrm{i}y \in \mathbb{C}$.

- $\operatorname{Re} z = x$, $\operatorname{Im} z = y$ — ***real and imaginary part***
- $\bar{z} = z^* = x - \mathrm{i}y$ — ***complex conjugate***
- $z = re^{i\theta}$, where $e^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$ — ***polar form*** / ***Euler's formula***
- $\operatorname{Arg} z = \theta$ — ***argument/angle/phase***
- $|z|^2 = \bar{z}z = \operatorname{Re} z^2 + \operatorname{Im} z^2 = r^2$ — ***squared modulus/norm***

The complex plane can be regarded as $\mathbb{R}^2$. Indeed, the modulus $|z| = \sqrt{(\operatorname{Re} z)^2 + (\operatorname{Im} z)^2}$ is the Euclidean norm in $\mathbb{R}^2$.

Recall that an ε-ball in $\mathbb{R}^2$ is a small disc centered at some (x, y) with radius ε, excluding its boundary. Thus, convergence of sequences, continuity, the same as in $\mathbb{R}^2$

Throughout, we let $D \subset \mathbb{C}$ be an open domain, i.e., every point $z \in D$ is surrounded by some ε-ball.

A *simply connected* domain is one without any holes. Figure 6.1.

Let $f : \mathbb{C} \to \mathbb{C}$ be a function. By writing $f(z) = u(x, y) + \mathrm{i}v(x, y)$, we can regard f a s a *pair* of real-valued functions defined in the plane region D.

$$f(z) \quad \leftrightarrow \quad u(x, y) + \mathrm{i}v(x, y). \tag{6.58}$$

What are the properties of such functions? What is distinguishes functions like

$$f(z) = z^3 + 1, \quad f(z) = \frac{1}{1 - z},$$

from functions like

$$f(z) = \operatorname{Re} z + \operatorname{Im} z \quad ?$$

The first function is clearly a function of the combination $z = x + \mathrm{i}y$, and not of x and y individually. In an intuitive sense, the first function is "purer" than the second one, it is a "true function of z".

It is useful to note that

$$\operatorname{Re} z = \frac{1}{2}(z + \bar{z}), \quad \operatorname{Im} z = \frac{1}{2\mathrm{i}}(z - \bar{z}). \tag{6.59}$$

Thus, seemingly z and $\bar{z}$ are like independent variables.

Thus, we can rewrite any occurence of $\operatorname{Re} z$ and $\operatorname{Im} z$ in terms of z and $\bar{z}$, i.e., the latter can be used as independent variables (even if they are, strictly speaking, not! When z changes, so do $\bar{z}$!) For example,

$$f(z) = \operatorname{Re} z + \operatorname{Im} z = (\frac{1}{2} + \frac{1}{2\mathrm{i}})z + (\frac{1}{2} - \frac{1}{2\mathrm{i}})\bar{z}. \tag{6.60}$$

It now looks like $f(z)$ is not a "pure" function of z.

Indeed, it turns out that the "pure" functions are the differentiable ones, while the "mixed" functions are never differentiable. And the "pure" functions are always extremely well-behaved!

Example 36

The perhaps simplest complex functions, and among the most important, are *polynomials*

$$p(z) = a_0 + a_1 z + a_2 z^2 + \cdots + a_n z^n. \tag{6.61}$$

The degree of the polynomial is the index of the larges nonzero coefficient $a_n \in \mathbb{C}$. The polynomials are the simplest complex differentiable functions, from which much is derived.

Theorem 39: Fundamental Theorem of Algebra

Any polynomial of degree n can be factorized uniquely (up to reordering of the roots r_i) as

$$p(z) = c(z - r_1)(z - r_2)\cdots(z - r_n). \tag{6.62}$$

6.5.2 Complex differentiability

Complex differentiability is defined in a similar manner as real single-variable differentiability:

Definition 78: Complex differentiability

The function $f : U \to \mathbb{C}$, $U \subset^{\text{open}} \mathbb{C}$, is (complex) differentiable at $z \in U$ if the limit

$$\lim_{h \to 0} \frac{f(z + h) - f(z)}{h} = f'(z) = \frac{\mathrm{d}f}{\mathrm{d}z} \tag{6.63}$$

exists. The expression $h \to 0$ means the same as in the $\mathbb{R}^2$ case.

If D is an open domain in $\mathbb{C}$, and if $f(z)$ is complex differentiable for all $z \in D$, we say that f is *analytic in* D.

The fact that the limit is to exist as $h \to 0$ in the complex sense is *much more restrictive* than the previous limit for real functions from $\mathbb{R}^2 \to \mathbb{R}^2$. Not only can one approach 0 from any direction, but the rules of complex multiplication must also be obeyed.

Example 37: Derivative of monomial

Let us apply the definition of the derivative to $f(z) = z^n$.

$$f(z+h) = (z+h)^n = z^n + hnz^{n-1} + \text{higher order terms.} \tag{6.64}$$

Thus

$$\frac{f(z+h) - f(z)}{h} = \frac{hnz^{n-1} + \text{h.o.t.}}{h} = nz^{n-1} + \text{h.o.t.}, \tag{6.65}$$

so that the limit becomes

$$\frac{\mathrm{d}}{\mathrm{d}z} z^n nz^{n-1}. \tag{6.66}$$

We were able to perform the limit just by doing complex algebra. Notably, $z \in \mathbb{C}$ was completely arbitrary, so the derivative exists everywhere.

Example 38: Derivative of $\bar{z}$ does not exist

Let us try to see if $f(z) = \bar{z}$ is differentiable. Let us consider the limit $h = \delta x \to 0$ in $\mathbb{R}$.

$$\lim_{\delta x \to 0} \frac{f(x + \delta x + \mathrm{i}y) - f(x + \mathrm{i}y)}{\delta x} = \frac{\delta x}{\delta x} = 1. \tag{6.67}$$

However, if we allow $h = \mathrm{i}\delta y \to 0$ instad, with $\delta y \in \mathbb{R}$, then

$$\lim_{\delta y \to 0} \frac{f(x + \mathrm{i}(\delta y + y)) - f(x + \mathrm{i}y)}{\delta y} = \frac{-\mathrm{i}\delta y}{\delta y} = -\mathrm{i}. \tag{6.68}$$

Since the two limits are not the same, the complex limit cannot exist, since limits are unique.

This is in fact a very simple example of a continuous function from $\mathbb{C} \to \mathbb{C}$ which is not differentiable anywhere! Such an exampe is much harder to find for functions $\mathbb{R}^2 \to \mathbb{R}^2$.

Theorem 40: Properties of complex derivative

The complex derivative enjoys the same properties as the usual single-variable derivative: Linearity, product rule, quotient rule, and chain rule.

When viewed as a pair of real functions, we get:

Theorem 41: Cauchy-Riemann equations

Let $f : D \to \mathbb{C}$, D being a simply connected open set. Let $z = z + \mathrm{i}y$, and write $f(z) = u(x,y) + \mathrm{i}v(x,y)$, with $u, v : D \to \mathbb{R}^2$ (where D is viewed as a subset of $\mathbb{R}^2$). If f is complex differentiable at z, then

$$\frac{\partial u(x,y)}{\partial x} = \frac{\partial v(x,y)}{\partial y}, \quad \frac{\partial u(x,y)}{\partial y} = -\frac{\partial v(x,y)}{\partial x} \qquad \textbf{\textit{Cauchy–Riemann equations}} \tag{6.69}$$

Conversely, if the Cauchy–Riemann equations are satisfied in D, then f is complex differentiable in D.

It is important here, that we are not talking about *a single point*, but a whole neighborhood. The

theorem fails if we omit the last fact.

6.5.3 Series of complex numbers

Definition 79: Series

Given a sequence (z_n) of complex numbers, we define the *partial sums*

$$S_N = \sum_{n=0}^{N} z_n. \tag{6.70}$$

If the partual sums converge, $\lim S_N = S \in \mathbb{C}$, then we denote that sum by

$$S = \sum_{n=0}^{\infty} z_n = z_0 + z_1 + z_2 + \cdots \tag{6.71}$$

Example 39: Geometric series

The geometric series,

$$f(z) = \frac{1}{1-z} = 1 + z + z^2 + \cdots \qquad \text{for } |z| < 1. \tag{6.72}$$

The function $f(z)$ is complex differentiable at any $z \neq 1$:

$$f(z+h) = \frac{1}{1-z-h} = \frac{1}{1-z}\frac{1}{1-h/(1-z)} = \frac{1}{1-z}(1 + \frac{h}{1-z} + \text{h.o.t.}), \tag{6.73}$$

so that $f'(z) = \frac{1}{(1-z)^2}$.

We note that f is *divergent* as $z \to 1$, this is an example of a *pole* of f.

Note the slight abuse of notation: The infinite sum is used to denote *both* the limit of the partial sums, if it exists, but also the sequence of partial sums.

Theorem 42: Power series

A *power series* is a series of the type

$$\sum_{n=0}^{\infty} a_n z^n. \tag{6.74}$$

The *radius of convergence* of the power series is given by

$$\frac{1}{R} = \limsup_{n\to\infty} |a_n|^{1/n}. \tag{6.75}$$

In particular, $R > 0$ if $\{|a_n|^{1/n}\}$ stays bounded as n grows.

A power series is complex differentiable inside the radius of convergence, and the derivative is computed term by term,

$$\frac{\mathrm{d}}{\mathrm{d}z}\sum_{n=0}^{\infty} a_n z^n = \sum_{n=1}^{\infty} n a_n z^{n-1}. \tag{6.76}$$

The radius of convergence of the derivative is again R. It follows that a power series is *infinitely differentiable*.

Definition 80: Important functions as power series

We *define*

$$\exp(z) = \sum_{n=0}^{\infty} \frac{1}{n!} z^n \tag{6.77}$$

$$\sin(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n+1} \tag{6.78}$$

$$\cos(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n!)} z^{2n}. \tag{6.79}$$

These series are simply complex generalizations of the corresponding real series. The complex exponential satisfies

$$\exp(x + \mathrm{i}y) = \exp(x)[\cos(y) + \mathrm{i}\sin(y)]. \tag{6.80}$$

See also the exercises, where the complex exponential is derived/defined in a different but equivalent way.

6.5.4 Analyticity

Theorem 43: Infinite differentiability

If f is complex differentiable in an ε-ball U of $z \in \mathbb{C}$, then it is complex differentiable as many times as we like the same ball.

A ruly remarkable result about analytic functions is:

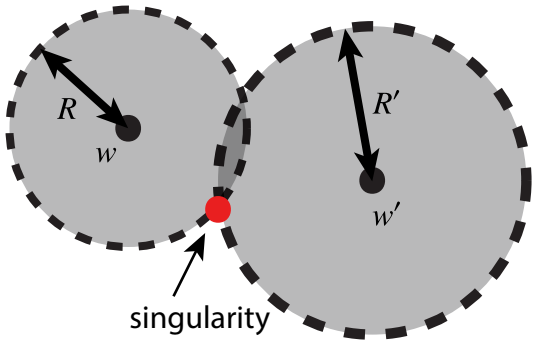


Figure 6.2: Illustration of convergence disk for two different origins w and w' for a Taylor/power series in the presence of a singularity. The series converges inside a disk with radius equal to the distance to the closest singularity of the function.

Theorem 44: Analytic functions are power series

If $f(z)$ is analytic in an open ball around z, then $f(z)$ can be expanded in a power series there.

Example 40: Geometric series

A standard example is the function

$$f(z) = \frac{1}{1-z}, \tag{6.81}$$

with domain $D = \mathbb{C} \setminus \{1\}$. The Taylor expansion/power series of $f(z)$ around $z = 0$ is

$$f(z) = 1 + z + z^2 + \cdots, \tag{6.82}$$

the geometric series. All the $a_n = 1$, so $|a_n|^{1/n} = 1$, and $R = 1$ is the convergence radius. For all $|z| < R$ the series converges. For $|z| = 1$, we don't know, and for $|z| > R$ it always diverges.

The Taylor series around oher points $w \in \mathbb{C}$ can be derived rather easily. The convergence radius will be $R = |w - 1|$. See Fig. 6.2.

6.5.5 Complex line integrals

Consider the problem: Given $f : D \subset^{\text{open}} \mathbb{C} \to \mathbb{C}$. When does f have an antiderivative (aka primitive), a function $F : D \to \mathbb{C}$ such that $F'(z) = f(z)$? In real analysis this question results in the *fundamental theorem of analysis*, which gives the antiderivative of a real function using the definite integral

$$F(x) = \int_{x_0}^{x} f(t)\,\mathrm{d}t.$$

For a complex function, how should one generalize this idea? In the complex plane, there are many ways to go from a point $z_0 \in D$ to a point $z \in D$.

This leads to the idea of a complex *line integral*: the integral of a complex function along a smooth curve in $\mathbb{C}$, see Fig. 6.3. Such a path as previously considered in the section on vector calculus: Let $I = [a, b]$ be a closed interval, and let $\gamma : I \to \mathbb{C}$ be smooth. Smoothness means, that both the real and imaginary parts of γ are differentiable as many times as we like in all of I. The graph of γ is now

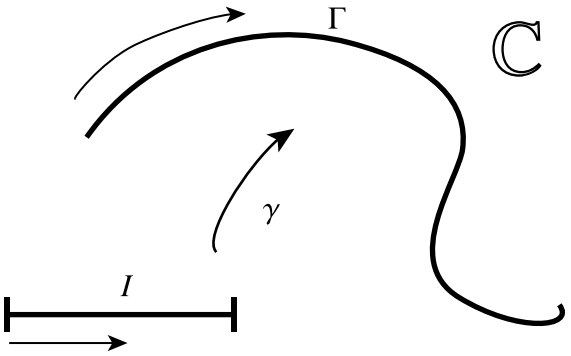


Figure 6.3: A smooth path and curve in $\mathbb{C}$.

a curve Γ in $\mathbb{C}$, and we say that γ is a *smooth parameterization* of Γ. Conversely, we say that a subset $\Gamma \subset \mathbb{C}$ is a smooth curve if there exists a smooth parameterization. There are many parameterizations of a given smooth curve Γ.

We say that Γ is *closed* if the endpoints match, so that we have a *loop*, and Γ is *simple* if the loop does not cross itself.

It is important here, that since our integral is supposed to *start* at one endpoint, and *end at another*, the *direction* of traversal on the curve matters. We say that the curve is *oriented*.

Definition 81: Complex line integral

Let $f : D \to \mathbb{C}$ be continuous, and let Γ be a (piecewise) smooth oriented curve parameterized by $\gamma : I \to \mathbb{C}$. The complex line integral of f along Γ is now defined as

$$\int_\Gamma f(z)\,\mathrm{d}z = \int_I f(\gamma(t))\gamma'(t)\,\mathrm{d}t, \tag{6.83}$$

which is independent of parameterization. Note that $\mathrm{d}z = \gamma'(t)\mathrm{d}t$, an infinitesimally small piece of the curve.

The line integral is a *complex* integral. The real and imaginary parts exist as Riemann integrals. The Cauchy–Riemann equations together with Green's theorem for surface integrals now imply:

Theorem 45: Cauchy theorem

Let $f : D \to \mathbb{C}$, where D is a simply connected open domain. Let Γ be a piecewise smooth simple closed curve in D. Then,

$$\oint_\Gamma f(z)\,\mathrm{d}z = 0. \tag{6.84}$$

Theorem 46: Path independence, antiderivative

Let f and D be as above. In particular, D is simply connected. If two curves Γ and Γ' have the same z_0 and z, then the line integrals have the same value, and hence they depend only on the endpoints. In that case, one may define

$$F(z) = \int z_0^z f(z)\,\mathrm{d}z \tag{6.85}$$

as the common value, which satisfies $F'(z) = f(z)$ for every $z \in D$.

Fix $z_0 \in D$, and choose $\varepsilon > 0$ such that the open disk $B_\varepsilon(z_0) \in D$. Let Γ be the boundary of the disk, traversed counter-clockwise by some parameterization, e.e., $\gamma(t) = z_0 + e^{\mathrm{i}t}\varepsilon$, $0 \le t < 2\pi$.

Theorem 47: Cauchy integral formula

Let the function $f : D \to \mathbb{C}$ be complex differentiable, and $B_\varepsilon(z_0) \subset D$ as above. Then,

$$f(z_0) = \frac{1}{2\pi\mathrm{i}} \oint_\Gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z. \tag{6.86}$$

This result is incredibly powerful and profound. The value *inside* the curve is completely determined by the values *on* the curve. Furthermore, Cauchy integral theorem above, generalize the result to *any* piecewise smooth simple closed loop inside D that contain z in its interior. The Cauchy integral formula is *still valid* for such paths.

The next consequence is the following:

Theorem 48

Let D be simply connected, and let $f : D \to \mathbb{C}$ be complex analytic in D. Then f is *infinitely* many times differentiable, and we have the power series representation

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n, \quad \text{where} \quad a_n = \frac{f^{(n)}(z)}{n!} \tag{6.87}$$

The derivatives are given by the formula

$$f^{(n)}(z) = \frac{1}{2\pi\mathrm{i}} \oint_\Gamma \frac{f(w)}{(w - z)^{n+1}}\,\mathrm{d}w. \tag{6.88}$$

The proof is based on two results; the Weierstrass M-test and Leibniz' rule for differentiation under the integral sign. The latter reads:

Lemma 4: Leibniz' rule

Let C and D be simply connected domains, and let $f : C \times D \to \mathbb{C}$ be complex differentiable in each variable *separately*, i.e.,

$$\frac{\partial f(w,z)}{\partial z} \quad \text{and} \quad \frac{\partial f(w,z)}{\partial w} \quad \text{both exist.} \tag{6.89}$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}z}\oint_{\partial C} f(w,z)\,\mathrm{d}w = \oint_{\partial C}\frac{\partial f(w,z)}{\partial z}\,\mathrm{d}w. \tag{6.90}$$

The fact that a complex differentiable $f : D \to \mathbb{C}$ is infinitely differentiable now follows immediately, when applied to the Cauchy integral formula. To complete the proof, see for example Butkov.

Since power series also are complex differentiable so long as the coefficients do now grow too fast, we have

Theorem 49

Complex differentiablility of $f : D \to \mathbb{C}$ in a simply connected D is equivalent to a convergent power series of f around $z \in D$

This incredibly powerful statement has great consequences for the study of functions of a *real* variable. For example, we know that e^z is complex analytic, so for every $x \in \mathbb{R}$, $e^(x + \Delta x)$ can be developed in a convergent power series for Δx small enough. Conversely, one can show that if we have a convergent power series in a real variable, then this series is *also* convergent for a complex variable. Hence, the real function can be *analytically continued* into the complex plane, and we may use the powerful results of complex analysis. We define the exponential function for complex arguments in this way in the exercies.

6.5.6 Laurent series

Power series in z can be generalized to *negative* powers. This is very useful, as one can show the following:

Theorem 50: Functions from Laurent series

Let a*Laurent series* be given,

$$\sum_{n=-\infty}^{+\infty} c_n(z-w)^n = \sum_{n=1}^{\infty} c_{-n}(z-w)^{-n} + \sum_{n=0}^{\infty} c_n(z-w)^n, \tag{6.91}$$

defined as the sum of two power series, in z^{-1} and z. Then there exists R_1 and R_2 such that the positive power series converges to an analytic function for $|z| < R_1$, and the negative power series converges to an analytic function for $|z| > R_2$. If $R_2 < R_1$, we obtain a unique analytic function in the *annulus*

$$D = \{z \in \mathbb{C} \mid R_2 < |z| < R_1\}, \tag{6.92}$$

with

$$c_n = \frac{1}{2\pi\mathrm{i}}\oint_{\Gamma}\frac{f(w)}{(w-z)^{n+1}}\,\mathrm{d}w. \tag{6.93}$$

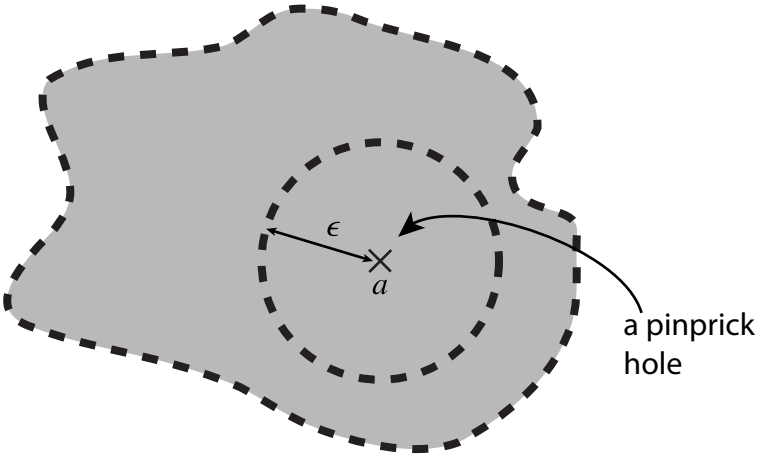


Figure 6.4: A domain with a single point a missing. The domain is still open, but no longer simply connected.

6.5.7 Isolated singularities

Let $f : D \subset^{\text{open}} \mathbb{C} \to \mathbb{C}$ be analytic. Let $a \in D^{\complement}$, and assume that for some $\varepsilon > 0$, the *punctured disc* $\dot{B}_\varepsilon(a) := B_\varepsilon(a) \setminus \{a\}$ is a subset of D. Thus, D has a single-point "hole" at a, it is "punctured", see Fig. 6.4. Since f is not defined at a, this is a *singularity*. It is also *isolated*, since a is surrounded by an open subset in D.

What types of behavior can f have at, or near, a?

Three typical examples are, with $a = 0$:

$$\frac{sinz}{z}, \quad \frac{1}{z}, \quad e^{1/z}. \tag{6.94}$$

The first example has a singularity at $a = 0$ since the denominator vanishes. But one can easily deduce that the limit as $z \to 0$ is 1, and that the function is complex differentiable there. Thus, we can include $z = 0$ in the domain. The singularity is *removable*. It is a fact, that the singularity is removable if $f(z)$ is bounded (absolute value smaller than some constant) inside some punctured disc around a.

The second example is such that it is dominated by a single a negative power of z near $z = 0$. Clearly, the first trick cannot be reused. On the other hand, we obtain an analytic function my multiplying with z^k for some smallest integer $k \geq 1$. Such singularities are called *poles of order k*, and it follows that we have a Laurent series expansion

$$f(z) = \sum_{n=-k}^{\infty} c_n (z-a)^n$$

near a pole of order k, i.e., the negative powers are only finite.

For the third example, this trick does not work. There exist *no power* z^k such that $z^k f(z)$ is analytic. Such singularities are called *essential singularities*.

6.5.8 Algebraic functions

There is a fourth class of singularity: "square-root type" singularities. We have not discussed *algebraic functions*. These are functions defined as roots of polynomials: Let $a_n(w)$ be complex differentiable coefficients, and consider the equation

$$F(w,z) = a_0(w) + a_1(w)z + \cdots + a_n(w)z^n = 0. \tag{6.95}$$

Under mild conditions on the coefficients, we can solve for z using the implicit function theorem and the fundamental theorem of algebra to find n functions $f_i(w)$ such that

$$F(w, f_i(w)) = 0. \tag{6.96}$$

The function f is called *algebraic*, and in general there are n solutions to $F = 0$, so that we have n solution functions! These are called *branches* of the same function.

Example 41: A simple algebraic function

Consider the equation

$$z^2 + w = 0 \tag{6.97}$$

which as the solution

$$z(w) = w^{1/2}. \tag{6.98}$$

We know that there are two distinct complex square roots. Each square root defines a *branch*, and they coincide at $w = 0$, a *branch point*.

Each branch can be made complex analytic in any simply connected region that excludes the origin, i.e., we can draw a (possibly wiggly) line from the origin to infinity. This line is called a *branch cut*.

Algebraic functions are very useful. For example, the eigenvalues of a matrix dependent on a complex parameter,

$$C(z) = A + zB \tag{6.99}$$

are roots of the characteristic polynomial of $C(z)$, and hence algebraic functions! Thus, the study of algebraic functions is relevant for quantum mechanical perturbation theory.

We are of course only scratching the surface here. Butkov is a good place to start for learning more on algebraic functions, branch points etc.