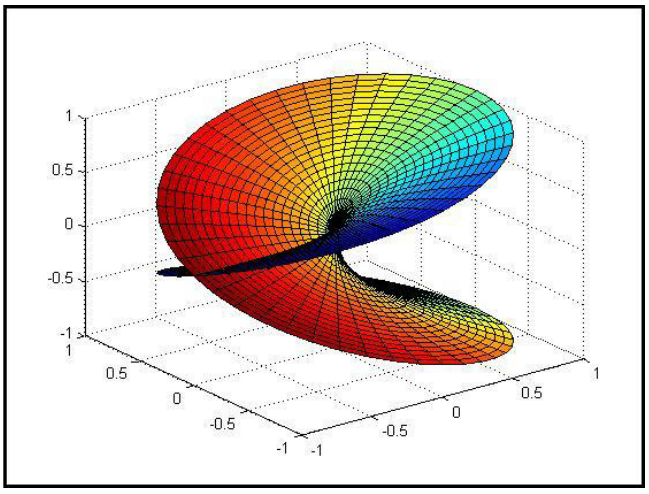
University College Dublin
An Coláiste Ollscoile, Baile Átha Cliath

School of Mathematics and Statistics
Scoil na Matamaitice agus Staitisticí
Survey of Applied and Computational Mathematics
(ACM40690)



Dr Lennon Ó Náraigh

Lecture notes in *Survey of Applied and Computational Mathematics*, January 2017

Survey of Applied and Computational Mathematics (ACM40690)

- Subject: Applied and Computational Mathematics
- School: Mathematical Sciences
- Module coordinator: Dr Lennon Ó Náraigh
- Credits: 5
- Level: 4
- Semester: Second

This module gives a survey of advanced mathematical methods and their application to problems in physics and more generally, in science and engineering. The aim of the module is to equip students to be well-rounded applied mathematicians, capable of tackling problems using closed-form solutions in certain asymptotic limits. Topics will be drawn from the following (non-exhaustive) list: [Review of complex analysis] Cauchy-Riemann conditions, Cauchy's integral theorem, calculus of residues, harmonic functions, Jensen's formula [Laplace transforms] Definition, examples, properties, and inversion via the Bromwich contour [Asymptotic methods for integrals] Laplace's method, Watson's lemma, steepest-descent method, [Writing the solution of an ODE as a contour integral], and the evaluation of the same in asymptotic limits where the steepest-descent method can be used, Airy functions [Singular perturbation theory] The WKB approximation in the far field and near turning points, applications of WKB theory in Quantum Mechanics and Fluid Mechanics

What will I learn?

On completion of this module students should be able to

1. Carry out calculations using Laplace transforms, solve ODEs via Laplace-transform methods
2. Evaluate certain integrals in asymptotic limits using the saddle-point method
3. Formulate the solution of ODEs as contour integrals and evaluate these integrals in certain limits
4. Solve ODEs in limiting cases using WKB theory, including turning points
5. Solve ODEs via power-series solutions, understand the analytical properties of these solutions

Editions

First edition: January 2014
Second edition: January 2015
Third edition: January 2016
This edition: January 2017

Acknowledgements

I have borrowed some theorem and definition statements, as well as some notation, from Dr R. Smith's MATH 30040 notes:

`http://mathsci.ucd.ie/~rsmith/teaching/math30040.shtml`

The chapter on conformal mapping borrows very heavily from the notes of Peter J. Olver:

`http://www.math.umn.edu/~olver/ln_/cml.pdf`

The chapters on ODEs and WKB theory were written by Professor Ottewill. The material in the other chapters came either straight from my head, or from the recommended textbooks.

Contents

Chapter 0

Introduction

0.1 Overview

Here is an executive summary of the module:

> This module involves the study of advanced mathematical techniques in complex analysis, theory of differential equations, asymptotic methods, and computation. The aim of this study is twofold: to learn some interesting and useful mathematics, but also to connect the disparate modules you have hitherto studied so you can obtain a broad *survey of Applied and Computational Mathematics*.

The following is a more detailed list of the topics to be studied in the present semester (January 2016). It differs slightly from the module descriptor.

Part I

1. Review of Complex Analysis (1 weeks).
2. Laplace's equation and the maximum principle (1 weeks).
3. Green's functions for Laplace's equation on finite domains (1 week).
4. Conformal mapping theory (1 week).
5. Laplace transforms (1 week).
6. The steepest-descent method (2 weeks).
7. Writing the solution of an ODE as a contour integral, and the evaluation of the same in asymptotic limits where the steepest-descent method can be used (1 week).

8. The WKB approximation in the far field and near turning points, applications of WKB theory in Quantum Mechanics and Fluid Mechanics (1 week)

Part II

Introduction to Fortran programming and multithreading, with applications in Scientific Computing relating to Part I (3 weeks).

0.2 Learning and Assessment

Learning

- For Part I, teaching will be by way of fairly fast-paced lectures, and there will be only **two** such lectures per week during part I of the module (notice that this is different from previous years).
- Teaching in Part II will be by way of lab sessions, details of which and notes for which will be provided later, after the midterm break.
- As this is an advanced undergraduate module, heavy emphasis is placed on independent study. Only a small amount of the material in the lecture notes will be covered in class. Your independent study will be guided by reading this material, supplementary material from the recommended textbooks, and by a weekly problem sheet.

Assessment

- One final exam, counting for 60%.
- Weekly homework assignments in Part I, counting for 20%, the details of which are given below.
- Computational assignments in Part II, counting for 20%.

Concerning the homework assignments in Part I, there will be nine such assignments, given out weekly during Part I of the module. Complete each problem sheet and submit your answers in the following week. The corrected homeworks will be returned to you promptly. Model answers for the assignments will also be provided promptly. You will be able to reflect on your performance as the module progresses by comparing your work with model answers to be provided on a weekly basis.

Lecturers

I will teach both parts of the module.

Textbooks

For Part I of this module, lecture notes that are more-or-less self-contained will be put on the web. The lecture notes will be based in part on the following books:

- Mathematical Methods for Physicists, G. B. Arfken, H. J. Weber, and F. Harris (Wiley, Fifth Edition).
- Advanced Mathematical Methods for Scientists and Engineers – Asymptotic Methods and Perturbation Theory, Carl M. Bender and S. A. Orzag (Springer edition, 1999).
- Partial Differential Equations of Mathematical Physics and Integral Equations, R. B. Guenther and J. W. Lee (Dover edition, 1996).

Chapter 1

Review of Complex Analysis

"It is too soon to say."

Quote by Zhou Enlai, first Premier of the People's Republic of China. The quote is often, though disputedly, thought to refer to the significance of the French Revolution of 1789, although it has been argued that he was actually referring to the French protests of 1968. In any case, what are the consequences of Cauchy's theorems of complex analysis? Again, it is too soon to say.

Overview

We review the basic concepts and results in the theory functions of a single complex variable. The chapter starts with basic definitions and takes the reader up to the Residue Theorem. Homework examples will involve evaluation of seemingly difficult integrals via the Calculus of Residues. This is an important aspect of Complex Analysis in Applied Mathematics and Mathematical Physics, and it is given its proper place in this module. However, a principal aim of this module is to show the reader that the usefulness of complex-variable theory extends to an unimaginably broad vista beyond this single application. You will begin to comprehend this fact in later chapters. Finally, there will be a brief discussion about non-isolated singularities, leading to branch cuts and the beautiful Riemann surfaces.

1.1 Basic notions – Review

Our review of complex analysis starts with our recalling some familiar definitions. We let D be an open subset of $\mathbb{C}$, and we study complex-valued functions of the single complex variable $z = x + \mathrm{i}y$:

$$\begin{aligned} f : D &\to \mathbb{C}, \\ z &\mapsto f(z). \end{aligned} \tag{1.1}$$

The complex-valued function $f(z)$ can itself be split into its real and imaginary parts:

$$f(z) = u(x, y) + \mathrm{i}v(x, y).$$

Examples of such functions, with $D = \mathbb{C}$ include the polynomials, the complex exponential e^z, and the usual trigonometric functions derived from the complex exponential. The function $f(z)$ in Equation (1.1) is said to be **differentiable** at the point z_0 if the limit

$$\lim_{\delta z \to 0} \frac{f(z_0 + \delta z) - f(z_0)}{\delta z} \tag{1.2}$$

exists and is **independent of the particular approach** to the point z_0. The limit in Equation (1.2) – if it exists – is denoted by $f'(z_0)$, and is called the derivative of the function $f(z)$ at the point z_0. The function $f(z)$ in Equation (1.1) is called **analytic** in the domain D if the derivative $f'(z)$ exists for all points $z \in D$.

If the function $f(z)$ is analytic in D, then the independence-of-approach in the definition (1.2) implies that $f(z)$ should satisfy the famous **Cauchy–Riemann** conditions:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}. \tag{1.3}$$

A partial converse exists: if $u(x, y)$ and $v(x, y)$ are C^1 functions of $(x, y) \in D$, such that u and v satisfy the Cauchy–Riemann functions, then the complex-valued function $f(z) = u(x, y) + \mathrm{i}v(x, y)$ is analytic in D.

The Cauchy–Riemann conditions will prove to be incomparably useful in this module and in the wider mathematical world. For now, by way of example, consider the complex-valued function $f(z) = \overline{z}$. Applying the Cauchy–Riemann conditions, one obtains

$$\frac{\partial u}{\partial x} = 1 \neq \frac{\partial v}{\partial y} = -1.$$

Thus, $f(z) = \overline{z}$ is an example of a function that is everywhere continuous but nowhere (complex) differentiable. Indeed, any complex-valued function involving $\overline{z}$ will fail to be analytic.

1.2 Integral theorems

Throughout this section, a closed, non-intersecting piecewise smooth path is called a contour. In the context of closed curves, a brief discussion of the notion of simply-connectedness is warranted. Loosely, a set is simply connected if it 'contains no holes'. More precise is the following: a set D is simply connected if, for any two contours $C_0 : [0,1] \to D$, $C_1 : [0,1] \to D$ based at $\boldsymbol{x}_0 \in D$, i.e.

$$\boldsymbol{x}_{C_0}(0) = \boldsymbol{x}_{C_1}(0) = \boldsymbol{x}_0,$$

there exists a continuous map

$$H : [0,1] \times [0,1] \to D,$$

such that

$$\begin{aligned} H(t,0) &= \boldsymbol{x}_{C_0}(t), \qquad 0 \le t \le 1, \\ H(t,1) &= \boldsymbol{x}_{C_1}(t), \qquad 0 \le t \le 1, \\ H(0,s) &= H(1,s) = \boldsymbol{x}_0, \qquad 0 \le s \le 0. \end{aligned}$$

Such a map is called a **homotopy** and C_0 and C_1 are called homotopy equivalent. One can think of this map as a 'continuous deformation of one loop into another'. Because a point is, trivially, a loop, in a simply-connected set, a loop can be continuously deformed into a point.

In this context, we consider

$$\begin{aligned} f : D &\to \mathbb{C}, \\ z &\mapsto f(z), \end{aligned} \tag{1.4}$$

where D is open and simply-connected. This enables us to formulate the statement of Cauchy's theorem, the cornerstone of complex analysis:

Theorem 1.1 *Let $f(z)$ be analytic on the domain D given in Equation* (1.4)*. Then, for any contour C contained entirely in D,*

$$\oint_C f(z)\mathrm{d}z = 0.$$

Next up is Cauchy's integral formula:

Theorem 1.2 *Let $f(z)$ be analytic on the domain D given in Equation* (1.4)*, and let C be a contour contained entirely in D. Let $I(C)$ denote the open region whose boundary is the contour C. Then, for any $a \in I(c)$,*

$$f(a) = \frac{1}{2\pi \mathrm{i}} \oint_C \frac{f(z)}{z-a}\mathrm{d}z.$$

1.3 Power series

A power series centred at a is a function of the form

$$f(z) = \sum_{n=0}^{\infty} a_n (z-a)^n, \tag{1.5}$$

where the a_n's are complex numbers. A power series of the form (1.5) satisfies precisely one of the following three possibilities:

1. It converges for all $z \in \mathbb{C}$;
2. It converges only for $z = a$ (all power series converge at their centre!);
3. There is $R > 0$ such that the power series converges (absolutely) whenver $|z-a| < R$ and diverges whenever $|z-a| > R$.

If possibility 3 occurs, the power series converges inside the disc $|z-a| < R$, and R is called the **radius of convergence**. The behaviour on the boundary of the disc can be ambiguous, and should be examined on a case-by-case basis. There are several standard ways of computing the radius of convergence, such as the following:

1. If $|a_{n+1}/a_n| \to \ell$ as $n \to \infty$, then $R = 1/\ell$. Note: if $\ell = 0$, then $R = \infty$.
2. If $|a_n|^{1/n} \to \ell$ as $n \to \infty$ then again, $R = 1/\ell$, and if $\ell = 0$, then $R = \infty$.

By the usual criteria for term-by-term differentiation, all complex power series can be differentiated term-by-term inside their radius of convergence. Hence, all complex power series are complex-differentiable (analytic) inside their radius of convergence.

The converse is also true: all analytic functions can be represented by a power series, at least on some open disc. This is the complex version of Taylor's theorem:

Theorem 1.3 *Let $f(z)$ be analytic on the open disc of centre a and radius R, denoted by $D(a,R)$. Then, for all $z \in D(a,R)$,*

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

where

$$a_n = \frac{1}{2\pi \mathrm{i}} \oint_{C(a,r)} \frac{f(z)}{(z-a)^{n+1}} \mathrm{d}z,$$

where $C(a,r)$ is the circle of centre a and radius r, and $0 < r < R$. Recall, the complex version of Taylor's theorem is by no means a trivial extension of its simpler real cousin. Combined with the facts about term-by-term differentiation of complex-valued power series, it provides necessary and sufficient conditions for a power series to converge to its generating function: it is necessary and sufficient for the generating function to be (complex) differentiable. This contrasts greatly to the real case, where convergence of a Taylor series to its generating function is not guaranteed even if the generating function is differentiable. The function $f(x) = \mathrm{e}^{-1/x^2}$ for $x \neq 0$ and $f(0) = 0$ is the celebrated pathological example from real analysis. No such pathology exists in the complex plane: if a function is differentiable, it will have a power series, and conversely.

Indeed, sometimes, the term **holomorphic** is used to describe complex-differentiable functions, while the term **analytic** is used to describe functions that admit a power-series represenation. Taylor's theorem means that these two notions are interchangeable.

1.4 Isolated singularities

Consider the following punctured disc of centre a and radius r, but with the centre removed:

$$D = \{z \in \mathbb{C} | 0 < |z - a| < r\}. \tag{1.6}$$

For definiteness, the following discussion focuses on the case with $a = 0$, but this is without loss of generality. Let $f(z)$ be a complex-valued function defined on the domain D. If $f(z)$ is analytic in D, but not differentiable at $z = 0$, then the point $z = 0$ is called an **isolated singularity** of f. Isolated singularities are classified by their leading-order behaviour as the limit $\lim_{z\to 0} f(z)$ is approached. Specifically, we write

$$f(z) = f_1(z) + f_2(z),$$

where $|f_1(z)| \gg |f_2(z)|$ as $z \to 0$. Now, the singularities are classified as follows:

1. A removable or cosmetic singularity, whereby the Taylor-series representation of $f(z)$ exhibits no singular behaviour, e.g. $f(z) = \sin(z)/z$.

   Equivalently, we have $f(z) = f_1(z) + f_2(z)$, with $|f_1(z)| \gg |f_2(z)|$ as $z \to 0$, and $f_1(z) = cz^n$, where c is a complex constant and $n \geq 0$ is a non-negative integer

2. A pole, whereby

   $$f(z) = f_1(z) + f_2(z),$$

with $|f_1(z)| \gg |f_2(z)|$ as $z \to 0$, and

$$f_1(z) = \frac{c}{z^n},$$

where c is a complex constant and n is a positive integer called the **order** of the pole. A pole of order one is called **simple**.

3. An essential singularity – all other isolated singularities. More precisely, a function $f(z)$ has an essential singularity at $z = a$ if its **Laurent expansion** there is of the form

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z-a)^n,$$

with infinitely many of the coefficients $\{a_{-1}, a_{-2}, \cdots\}$ nonzero.

For the case of simple poles, the function $f(z)$ on the punctured disc D admits a Laurent expansion, in the following sense:

Theorem 1.4 *Let $f(z)$ be analytic on the punctured disc D given by Equation* (1.6)*, with disc centre at zero. Further, let $f(z)$ have a pole at $z = 0$, of order n. Then $f(z)$ admits the following series expansion, valid for all $z \in D$:*

$$f(z) = \sum_{p=-n}^{\infty} a_p z^p,$$

where

$$a_p = \frac{1}{2\pi \mathrm{i}} \oint_{C(0,\rho)} \frac{f(z)}{z^{p+1}} \mathrm{d}z,$$

where $C(0,\rho)$ is a circle of centre zero and radius ρ, with $0 < \rho < r$.

The particular coefficient a_{-1} will be very important in what follows. It is called the **residue**. Denoting the location of the generic pole by $z = a$, we have

$$a_{-1} = \mathrm{Res}(f, a).$$

Consider

$$f(z) = \frac{a_{-n}}{(z-a)^n} + \cdots + \frac{a_{-2}}{(z-a)^2} + \frac{a_{-1}}{z-a} + a_0 + a_1(z-a) + \cdots .$$

The contour integral of $f(z)$ around a contour C enclosing the point a and contained entirely in the domain D is taken (term-by-term integration is legitimate for convergent power series). Additionally,

C is given an anticlockwise sense. For $p \neq -1$, we have

$$\oint_C a_p(z-a)^p \,\mathrm{d}z = \frac{a_p}{p+1}(z-a)^{p+1}\Big|_{z_{\text{start}}}^{z_{\text{end}}},$$

where we have explicitly computed the complex antiderivative and evaluated the result at the start- and endpoints of the path C. But C is closed, so the start- and end-points are the same, and the integral is zero. On the other hand, for $p = -1$, we have

$$\oint_C \frac{a_{-1}\,\mathrm{d}z}{(z-a)}.$$

By Cauchy's integral formula, the result of this integration is the same for any closed curve C encircling the point a, so we switch to a circular contour of radius ρ:

$$\begin{aligned} \oint_C \frac{a_{-1}\,\mathrm{d}z}{(z-a)} &= a_{-1}\oint_{C(a,\rho)} \frac{\mathrm{d}z}{z-a}, \\ &= a_{-1}\int_0^{2\pi} \frac{\mathrm{d}(\rho \mathrm{e}^{\mathrm{i}\theta})}{\rho \mathrm{e}^{\mathrm{i}\theta}}, \qquad z = a + \rho \mathrm{e}^{\mathrm{i}\theta}, \\ &= 2\pi \mathrm{i} a_{-1}. \end{aligned} \tag{1.7}$$

In summary,

$$\begin{aligned} \oint_C f(z)\mathrm{d}z &= \oint_C \left[\frac{a_{-n}}{(z-a)^n} + \cdots + \frac{a_{-2}}{(z-a)^2} + \frac{a_{-1}}{z-a} + a_0 + a_1(z-a) + \cdots\right]\mathrm{d}z, \\ &= 2\pi \mathrm{i} a_{-1}, \end{aligned}$$

hence

$$\frac{1}{2\pi \mathrm{i}}\oint_C f(z)\mathrm{d}z = \mathrm{Res}(f, a). \tag{1.8}$$

Aside: In Equation (1.7) it was possible to switch between an arbitrary closed contour C enclosing the point a and a circular contour centred at a. This is explained in Figure 1.1. Consider in Figure 1.1 the contour consisting of the segments C, L_1, $\widetilde{C}$, and L_2. Call the region bounded by this contour D. Denote the boundary of the region D by ∂D. Hence,

$$\partial D = C \cup L_1 \cup L_2 \cup \widetilde{C}.$$

Thus, by Cauchy's theorem (1.1),

$$\oint_{\partial D} \frac{1}{z-a}\mathrm{d}z = 0,$$

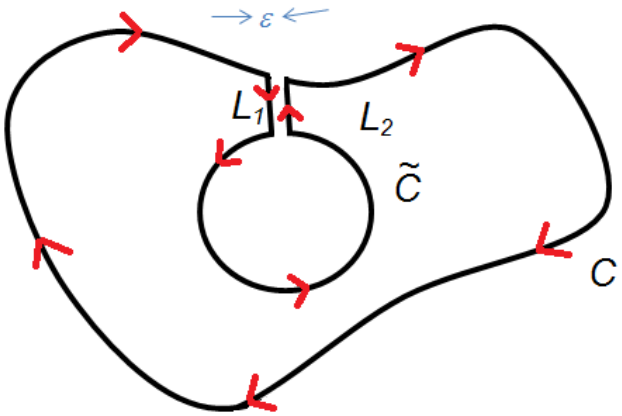


Figure 1.1:

since $(z-a)^{-1}$ has no singularities in the region D. Hence,

$$\int_C \frac{1}{z-a}\mathrm{d}z + \int_{L_1} \frac{1}{z-a}\mathrm{d}z + \int_{L_2} \frac{1}{z-a}\mathrm{d}z + \int_{\widetilde{C}} \frac{1}{z-a}\mathrm{d}z = 0.$$

Let ϵ be the distance separating the two parallel line segments L_1 and L_2, and take $\epsilon \to 0$. Then,

$$\int_{L_1} \frac{1}{z-a}\mathrm{d}z + \int_{L_2} \frac{1}{z-a}\mathrm{d}z = 0,$$

and in the same limit, C is the closed contour of interest and $\widetilde{C}$ is the corresponding circle of interest, hence

$$\int_C \frac{1}{z-a}\mathrm{d}z + \int_{\widetilde{C}} \frac{1}{z-a}\mathrm{d}z = 0.$$

But these contours have opposite senses, hence

$$\int_{C,\ \text{Clockwise}} \frac{1}{z-a}\mathrm{d}z = \int_{\widetilde{C},\ \text{Clockwise}} \frac{1}{z-a}\mathrm{d}z.$$

The result (1.8) extends in a fairly straightforward manner to a function f on domain D such that f has finitely many poles in D. The extension is the celebrated **Cauchy's residue theorem**:

Theorem 1.5 *Let $f(z)$ be analytic in an open set D except at finitely many isolated singularities $z_1, \cdots, z_m$, and let C be an anticlockwise contour contained entirely in D and surrounding the singularities. Then,*

$$\oint_C f(z)\mathrm{d}z = 2\pi\mathrm{i}\sum_{j=1}^{m} \mathrm{Res}(f, z_j).$$

The proof is a fairly straightforward extension of the foregoing discussion.

Finally, the following results are useful as a shortcut for obtaining residues:

Theorem 1.6 *Let $f(z)$ have a simple pole (i.e. order 1) at a. Then,*

$$\mathrm{Res}(f,a) = \lim_{z\to a}\left[(z-a)\,f(z)\right].$$

Be careful! In Dr Smith's words:

> [Theorem 1.6] only works if the pole is simple!! Applying it to a pole of a different order will lead to much upset and embarrassment.

For non-simple poles, we have the following result:

Theorem 1.7 *Let $f(z)$ have a pole of order m at a, and moreover, suppose that $f(z)$ has the following specific form:*

$$f(z) = \frac{g(z)}{(z-a)^m} + h(z)$$

where $g(z), h(z)$ are analytic in some $D(a,r)$, and where $g(a) \neq 0$. Then,

$$\mathrm{Res}(f,a) = \frac{1}{(m-1)!}g^{(m-1)}(a).$$

Example 1: Evaluate the integral

$$I = \int_0^{2\pi} \frac{\mathrm{d}\theta}{1+\epsilon\cos\theta}, \qquad 0<\epsilon<1.$$

Let $z = \rho \mathrm{e}^{\mathrm{i}\theta}$ be a complex number. We are to work on the circle $|z|=1$, hence $\rho = 1$. On this circle

$$\begin{aligned} \mathrm{d}z &= \mathrm{i}\mathrm{e}^{\mathrm{i}\theta}\mathrm{d}\theta, \\ &= \mathrm{i}z\,\mathrm{d}\theta, \end{aligned}$$

hence

$$\mathrm{d}\theta = \frac{\mathrm{d}z}{\mathrm{i}z}.$$

Also, on the circle, $z = \mathrm{e}^{\mathrm{i}\theta}$,

$$\cos\theta = \tfrac{1}{2}\left(\mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta}\right) = \tfrac{1}{2}\left(z + \frac{1}{z}\right).$$

We have

$$\begin{aligned} I &= \frac{1}{\mathrm{i}} \oint_{C(0,1)} \frac{1}{1+\frac{1}{2}\epsilon\left(z+\frac{1}{z}\right)} \frac{\mathrm{d}z}{z}, \\ &= \frac{2}{\mathrm{i}\epsilon} \oint_{C(0,1)} \frac{\mathrm{d}z}{z^2+(2/\epsilon)+1}. \end{aligned}$$

The denominator has roots at

$$z_- = -\frac{1}{\epsilon} - \frac{1}{\epsilon}\sqrt{1-\epsilon^2}, \qquad z_+ = -\frac{1}{\epsilon} + \frac{1}{\epsilon}\sqrt{1-\epsilon^2}.$$

Also,

$$z_+ - z_- = \frac{2}{\epsilon}\sqrt{1-\epsilon^2}$$

The root z_+ is inside the unit circle, while the root z_- is outside. The integrand is now expressed as

$$\begin{aligned} f(z) &:= \frac{1}{z^2+(2/\epsilon)+1}, \\ &= \frac{1}{(z-z_-)(z-z_+)}, \\ &= \frac{1}{z_+-z_-}\left(\frac{1}{z-z_+} - \frac{1}{z-z_-}\right). \end{aligned}$$

It suffices to consider behaviour near the z_+-root. From the partial-fraction decomposition, it follows that $f(z)$ has a simple pole of order 1 at $z = z_+$, and in this instance, the residue can be computed from the formula

$$\begin{aligned} \mathrm{Res}\,(f, z_+) &= \lim_{z\to z_+} \left[(z-z_+)\, f(z)\right], \\ &= \lim_{z\to z_+} \left\{ (z-z_+) \left[\frac{1}{z_+-z_-}\left(\frac{1}{z-z_+} - \frac{1}{z-z_-}\right)\right] \right\}, \\ &= \frac{1}{z_+-z_-}, \\ &= \tfrac{1}{2}\frac{\epsilon}{\sqrt{1-\epsilon^2}}. \end{aligned}$$

Putting it all together,

$$\begin{aligned} I &= \frac{2}{\mathrm{i}\epsilon} \oint_{C(0,1)} \frac{\mathrm{d}z}{z^2+(2/\epsilon)+1}, \\ &= \frac{2}{\mathrm{i}\epsilon} \oint_{C(0,1)} f(z)\mathrm{d}z, \\ &= \frac{2}{\mathrm{i}\epsilon} \left(2\pi\mathrm{i}\mathrm{Res}(f, z_+)\right), \\ &= \frac{2\pi}{\sqrt{1-\epsilon^2}}. \end{aligned}$$

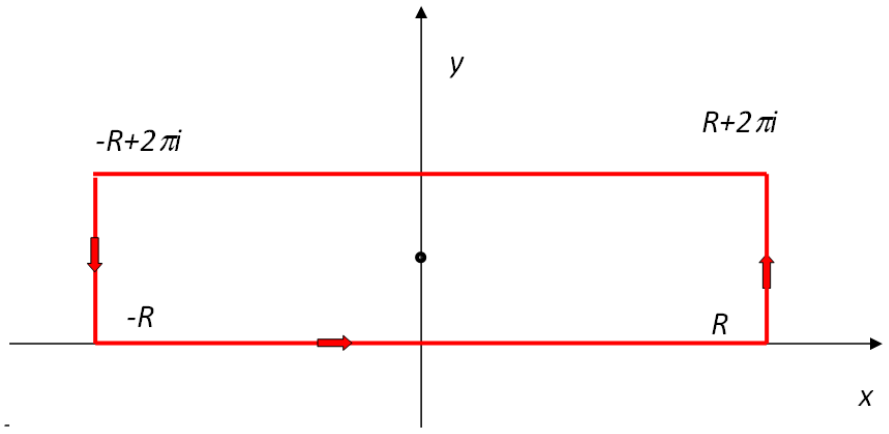


Figure 1.2: Suggested contour for $\int_{-\infty}^{\infty} \mathrm{e}^{ax}(1+\mathrm{e}^{x})^{-1}\mathrm{d}x$, with $0 < a < 1$.

Example 2: Evaluate

$$I = \int_{-\infty}^{\infty} \frac{\mathrm{e}^{ax}}{1+\mathrm{e}^{x}}\mathrm{d}x, \qquad 0 < a < 1.$$

The contour is the one shown in Figure 1.2, with $R \to \infty$ The vertical line-segment contributions vanish as $R \to \infty$. E.g.

$$\begin{aligned}\left[\int \frac{\mathrm{e}^{az}}{1+\mathrm{e}^{z}}\mathrm{d}z\right]_{z=-R+\mathrm{i}t, t\in[0,2\pi]} &= \mathrm{i}\int_0^{2\pi} \frac{\mathrm{e}^{-aR}\mathrm{e}^{\mathrm{i}t}}{1+\mathrm{e}^{-R}\mathrm{e}^{\mathrm{i}t}}\mathrm{d}t, \\ &\to 0, \qquad \text{as } R \to \infty.\end{aligned}$$

Similarly,

$$\begin{aligned}\left[\int \frac{\mathrm{e}^{az}}{1+\mathrm{e}^{z}}\mathrm{d}z\right]_{z=R+\mathrm{i}t, t\in[0,2\pi]} &= \mathrm{i}\int_0^{2\pi} \frac{\mathrm{e}^{aR}\mathrm{e}^{\mathrm{i}t}}{1+\mathrm{e}^{R}\mathrm{e}^{\mathrm{i}t}}\mathrm{d}t, \\ &\sim \mathrm{i}\int_0^{2\pi} \frac{\mathrm{e}^{aR}\mathrm{e}^{\mathrm{i}t}}{\mathrm{e}^{R}\mathrm{e}^{\mathrm{i}t}}\mathrm{d}t, \qquad \text{as } R \to \infty, \\ &= \mathrm{i}\int_0^{2\pi} \mathrm{e}^{\mathrm{i}t}\mathrm{e}^{(a-1)R}\mathrm{d}t, \qquad 0 < a < 1, \\ &\to 0 \ , \qquad \text{as } R \to \infty.\end{aligned}$$

Hence, calling the closed (anticlockwise) contour in Figure 1.2, we have

$$\begin{aligned}\oint_C \frac{\mathrm{e}^{az}}{1+\mathrm{e}^{z}}\mathrm{d}z &= \lim_{R\to\infty}\left[\int_{-R}^{R} \frac{\mathrm{e}^{ax}}{1+\mathrm{e}^{x}}\mathrm{d}x - \mathrm{e}^{2\pi\mathrm{i}a}\int_{-R}^{R} \frac{\mathrm{e}^{ax}}{1+\mathrm{e}^{x}}\right], \\ &= 2\pi\mathrm{i}\sum(\text{enclosed residues}),\end{aligned}$$

where in the second integral here we have used the fact that $\mathrm{e}^{x+2\pi\mathrm{i}} = \mathrm{e}^{x}$.

Consider therefore

$$f(z) = \frac{\mathrm{e}^{az}}{1+\mathrm{e}^{z}}.$$

The singularities are simple poles located at

$$\mathrm{e}^{z} = -1,$$

hence

$$z = \mathrm{i}\pi + 2\pi\mathrm{i}p, \qquad p \in \mathbb{Z}.$$

However, conveniently the contour C encloses only a single simple pole corresponding to $p = 0$ (this is of course more than convenience; the contour has been chosen with perfect hindsight!). But

$$\begin{aligned}
1+\mathrm{e}^{z} &= 1+\mathrm{e}^{z-\mathrm{i}\pi}\mathrm{e}^{\mathrm{i}\pi}, \\
&= 1-\mathrm{e}^{z-\mathrm{i}\pi}, \\
&= -(z-\mathrm{i}\pi)\left[1+\frac{z-\mathrm{i}\pi}{2!}+\frac{(z-\mathrm{i}\pi)^2}{3!}+\cdots\right], \\
\frac{1}{1+\mathrm{e}^{z}} &= -\left(\frac{1}{z-\mathrm{i}\pi}\right)\frac{1}{1+\frac{z-\mathrm{i}\pi}{2!}+\frac{(z-\mathrm{i}\pi)^2}{3!}+\cdots}, \\
\lim_{z\to\mathrm{i}\pi}\left(\frac{1}{1+\mathrm{e}^{z}}\right) &= -\lim_{z\to\mathrm{i}\pi}\left[\frac{1}{1+\frac{z-\mathrm{i}\pi}{2!}+\frac{(z-\mathrm{i}\pi)^2}{3!}+\cdots}\right], \\
&= -1.
\end{aligned}$$

Hence,

$$\mathrm{Res}(f, \mathrm{i}\pi) = -\mathrm{e}^{\mathrm{i}\pi a}.$$

Putting the results together, we have

$$-2\pi\mathrm{i}\mathrm{e}^{\mathrm{i}\pi a} = \underbrace{\left[\int_{-\infty}^{\infty}\frac{\mathrm{e}^{ax}}{1+\mathrm{e}^{x}}\mathrm{d}x\right]}_{=I}\left(1-\mathrm{e}^{2\pi\mathrm{i}a}\right),$$

or

$$-2\pi\mathrm{i} = I\left(1-\mathrm{e}^{2\pi\mathrm{i}a}\right).$$

Algebraic manipulations give the final answer:

$$I = \frac{\pi}{\sin a\pi}.$$

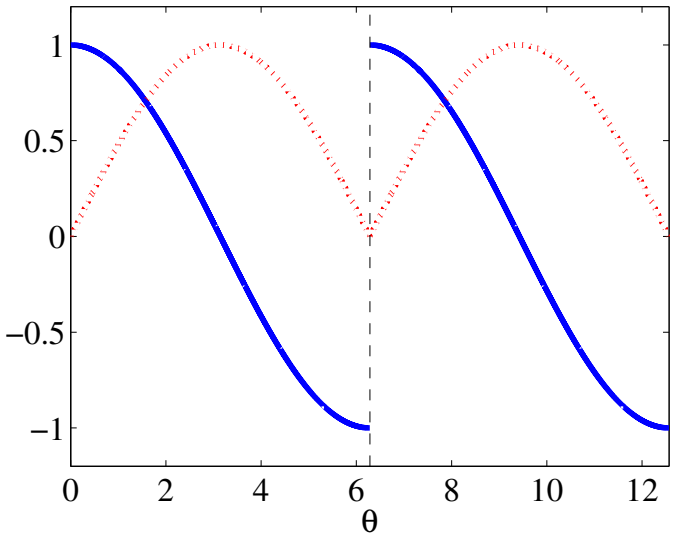


Figure 1.3: Plot of $\cos(\theta/2)$ (continuous blue line) and $\sin(\theta/2)$ (dotted red line) showing the jump discontinuity / cusp at $\theta = 2\pi$.

1.5 Branch cuts – non-isolated singularities

Consider the classic example

$$f(z) = z^{1/2}. \tag{1.9}$$

We restrict first of all to the unit circle $|z| = 1$ and we plot $f(z)$ on this restricted set. Thus, it suffices to plot $\mathrm{e}^{\mathrm{i}\theta/2} = \cos(\theta/2) + \mathrm{i}\sin(\theta/2)$. This is done in Figure 1.3. Consider for example the real part. Starting at $\theta = 0$, we have $\mathrm{Re}(f) = \cos(0/2) = \cos(0) = 1$. Moving around the circle through $\theta = 2\pi$, we have $\mathrm{Re}(f) = \cos(2\pi/2) = \cos(\pi) = -1$. This manifests itself as a jump discontinuity in Figure 1.3, in the interval $[2\pi - \epsilon, 2\pi + \epsilon]$. Because 2π is identified with 0 on the Argand diagram, the real part of function $f(z)$ therefore jumps as the positive real axis is crossed. Consider also the imaginary part. Continuing along the same lines as before, one can see that $\mathrm{Im}(f) = \sin(\theta/2)$ is continuous across the interval $[2\pi - \epsilon, 2\pi + \epsilon]$, but that there is a cusp at $\theta = 2\pi$. Thus, $\mathrm{Im}(f)$ is not differentiable there. Again, because 2π is identified with 0 on the Argand diagram, the function imaginary part of $f(z)$ is not differentiable as the positive real axis is crossed. Thus, the to make $f(z)$ analytic, we must exclude the positive real axis. The point $x = 0, y = 0$ must also be excluded (why?). This line $x \geq 0$ is referred to as a **branch cut**; the square-root function is single-valued and analytic on the open set comprising $\mathbb{C}$, minus the branch cut. Of course, there is something arbitrary about taking $f(z) = |z|^{1/2}\mathrm{e}^{\mathrm{i}\theta/2}$ as we have done. One can equally take $f(z) = |z|^{1/2}\mathrm{e}^{\mathrm{i}\theta/2+\mathrm{i}\pi}$, but this leads again to a branch cut along the positive real axis. Something a bit weirder happens if we do the following. We can 'patch together' a square-root

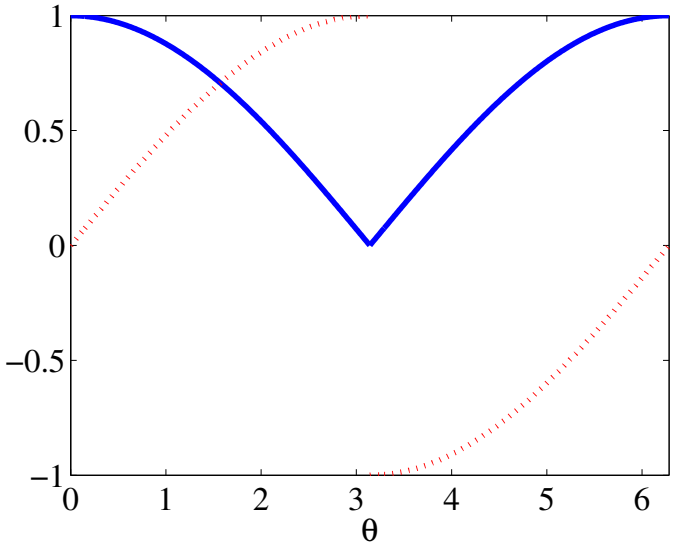


Figure 1.4: Plot of the phases of the square-root function in Equation (1.10). Real part: blue continuous line; Imaginary part: red dotted line. The branch cut is shifted to the negative real line $x \leq 0$, i.e. $\theta = \pi$.

function form the positive- and negative-branch constructions just defined. Thus, let us take[1]

$$\tilde{f}(z) = \begin{cases} |z|^{1/2} \mathrm{e}^{\mathrm{i}\theta/2}, & 0 < \theta < \pi, \\ -|z|^{1/2} \mathrm{e}^{\mathrm{i}\theta/2}, & \pi < \theta \leq 2\pi, \end{cases} \quad , \qquad \theta = \mathrm{Arg}(z). \tag{1.10}$$

This is still a legitimate square-root function, because $[\tilde{f}(z)]^2 = z$. However, by inspecting the phases in Equation (1.10), we see that the jump / cusp has been shifted to $\theta = \pi$. Also, now the real part has the cusp and the imaginary part the jump. Thus, the branch cut for $\tilde{f}(z)$ is located along the half-line $x \leq 0$. The location of the branch cut is therefore rather arbitrary. However, while the location of the branch point is arbitrary, its necessity is ineluctable. The function $\tilde{f}(z)$ is shown plotted in a part of the full complex plane in Figure 1.5 using Matlab. Note that Matlab selects the branch cut to be the negative half-line by default.

Finally, although I said that the presence of the branch cut was unavoidable, this is not quite true. It is unavoidable if one wants to obtain a single-valued square-root function. However, if one is willing to sacrifice single-valuedness, one can glue together the two independent branches of the square-root function into a multi-valued function. A plot of this multi-valued function is then a

[1] In Equation (1.10), I have used $\mathrm{Arg}(z)$ to denote the principal value of the argument of the complex number z, such that $\mathrm{Arg}(z)$ is uniquely determined. I have located the branch cut of $\mathrm{Arg}(z)$ along the positive real axis. I know it is conventional to locate the branch cut along the negative real axis, but the location is somewhat arbitrary and can be shifted as a matter of convenience. There is one convention I do stick with however: I use function names starting with a capital letter to denote principal values, and function names starting with a lower-case letter to denote multivalued functions. E.g. $\mathrm{Arg}(z)$ versus $\arg(z)$, and $\mathrm{Log}(z)$ versus $\log(z)$. This convention is widespread I believe but not universal. Cover your eyes and ears for this final bit: some writers swap around the capital and lowercase letters and adopt the opposite convention for principal values versus multiple values.

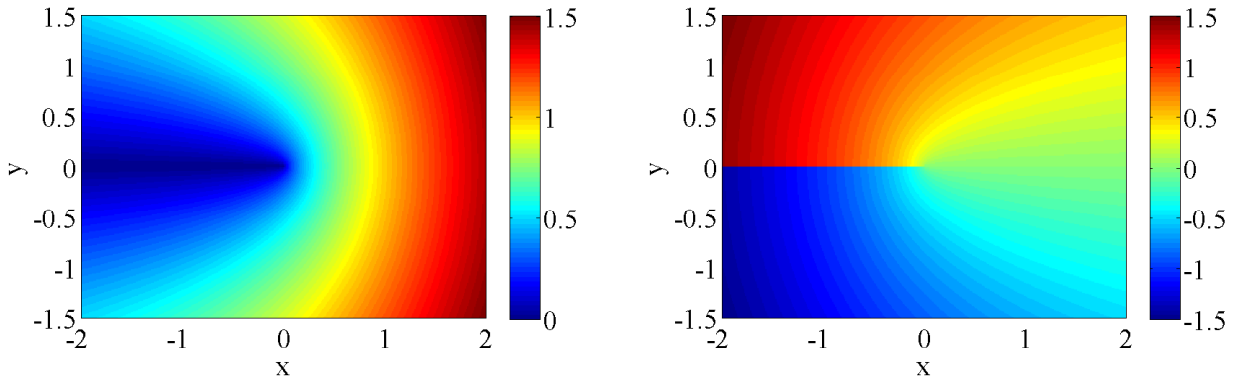


Figure 1.5: Real and imaginary parts of the square-root function $f(z) = (x+\mathrm{i}y)^{1/2}$ with branch cut selected accrding to Matlab's convention.

Riemann surface that intersects itself along an infinitely long line segment. The Riemann surface of the square-root function is shown in Figure 1.6. The line of intersection where the curve crosses itself corresponds precisely to the branch cut. By taking apart the self-intersecting surface, one can reassemble the two branches of the square-root function, which are now single-valued functions, albeit with a branch cut. The taken-apart surfaces are called the **Riemann sheets** of the self-intersecting surface.

Of course, another example of a multivalued function is the inverse of the exponential function e^z. You will have already encountered this in MATH 30040. Recall, one attempts to define the function $f(z) = \log z$ to be the inverse of the exponential function:

$$\begin{aligned} w &= \log z, \\ &= \log(r\mathrm{e}^{\mathrm{i}\theta}), \\ &= \log r + \log \mathrm{e}^{\mathrm{i}\theta}, \\ &= \log r + \mathrm{i}\theta, \\ &= \log|z| + \mathrm{i}\theta. \end{aligned}$$

However, because the complex-valued exponential is not one-to-one, we have $\mathrm{e}^z = \mathrm{e}^{z+2\pi\mathrm{i}p}$, with $p \in \mathbb{Z}$. Thus, we could equally well take

$$\begin{aligned} w &= \log z, \\ &= \log(r\mathrm{e}^{\mathrm{i}\theta+2\pi\mathrm{i}p}), \\ &= \log|z| + \mathrm{i}\theta + 2\pi\mathrm{i}p, \qquad p \in \mathbb{Z}. \end{aligned}$$

Thus, it appears as though the $\log(z)$ is a multi-valued function. One possibility is to define a

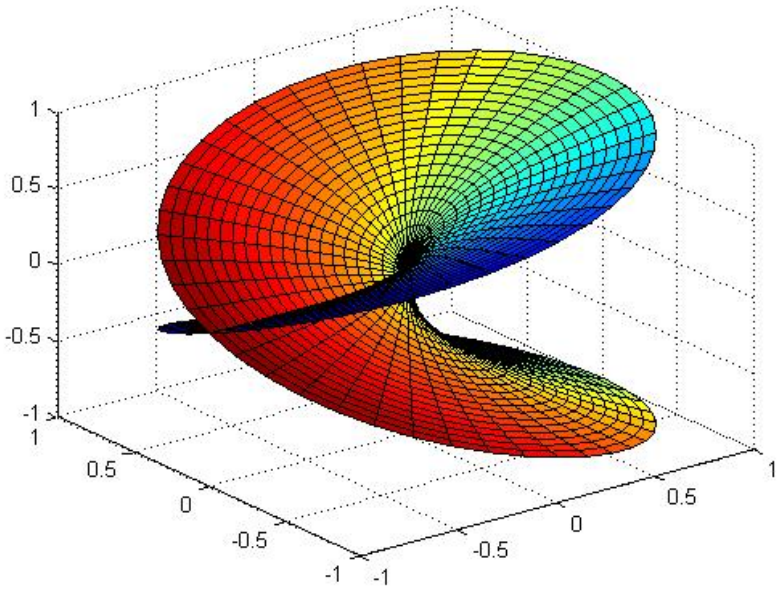


Figure 1.6: (Image courtesy of Wikipedia, page visited 15/01/2014). Riemann surface for the function $f(z) = z^{1/2}$. The two horizontal axes represent the real and imaginary parts of z, while the vertical axis represents the real part of $z^{1/2}$.

logarithm function restricted to $0 \leq \theta < 2\pi$. This is called the **principal value** of the logarithm function, denoted with a capital 'L' as follows:

$$\mathrm{Log}(z) := \log|z| + \mathrm{iArg}(z), \qquad 0 \leq \mathrm{Arg}(z) < 2\pi.$$

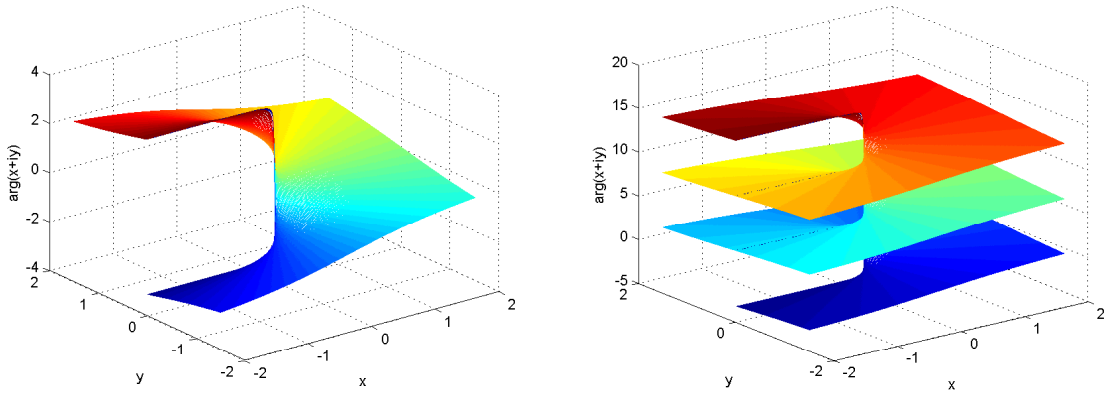
The argument function (and therefore the function $\mathrm{Log}(z)$) therefore has a jump discontuity across the line segment $x > 0$. Also, $\mathrm{Log}(z)$ is not defined for $z = 0$. Thus, on the domain $D = \mathbb{C} - \{x \geq 0\}$, the principal value of the logarithm is an analytic function; one can show easily that

$$\frac{d}{dz}\mathrm{Log}(z) = \frac{1}{z}, \qquad z \in D; \tag{1.11}$$

the segment $\{x \geq 0\}$ is therefore the branch cut chosen to make the inverse-exponential single-valued and analytic.

As in the example of the square-root function, the branch cut can be moved around the complex plane at will. Also, one can get rid of the branch cut altogether, but only by paying the price of making the inverse-exponential multivalued, with countably infinitely many branches. These can be glued together to form the Riemann surface. However, unlike in the square-root case, the different sheets in the surface are non-intersecting. In particular, given $w = u + \mathrm{i}v = \log z$, we have $u + \mathrm{i}v = \log r + \mathrm{i}(\theta + 2p\pi)$, and it is possible to glue together the copies $\theta(x, y) + 2p\pi$ such that each copy connects to its neighbours in a continuous fashion, much as a the ramp in a multistorey

carpark winds its way upwards. I have generated a part of the Riemann surface for $\mathrm{Im}[\log(z)]$ using Matlab. The results are shown in Figure 1.7 and the code is given at the end of this chapter for reference.



(a) (b)

Figure 1.7: (a) Imaginary part of the principal value of the complex logarithm, in other words, $\mathrm{Arg}(z)$, with branch cut along the negative real axis; (b) the same as (a), but superimposed with multiple copies of the argument function, separated by $\pm 2\pi$, in other words, a portion of the Riemann surface of the complex-valued logarithm function (imaginary part).

The theory of Riemann surface has some pretty amazing applications in Applied Mathematics, especially in the theory of complex dispersion relations for problems in linear stability. This is very clearly well beyond the scope of the present module. However, the theory of branch cuts etc. can help us finally to evaluate a further class of tricky definite integrals, an example of which is the following.

Example 3: Show that

$$I = \int_0^\infty \frac{x^a}{x+1}\mathrm{d}x = \frac{\pi}{\sin \pi|a|},$$

with $-1 < a < 0$.

We consider

$$\int_C \frac{z^a}{z+1}\mathrm{d}z,$$

with the contour C to be determined. Plotting the function $g(\theta) = \mathrm{e}^{\mathrm{i}\theta a}$, with $-1 < a < 1$, we see that $g(\theta)$ has a single jump discontinuity between $\theta = 0$ and $\theta = 2\pi$ (Figure 1.8). Thus, the contour C should avoid the segment $x \geq 0$ of the complex plane. This is the branch cut. Additionally, the function $f(z) = z^a/(z+1)$ has a simple pole at $z = -1$. We therefore choose C to be that contour shown in Figure 1.9, such that C encloses no singularities. The result of the integration is not zero, however, because of the phase difference in $f(z)$ across both sides of the branch cut. We obtain several contributions to the integration:

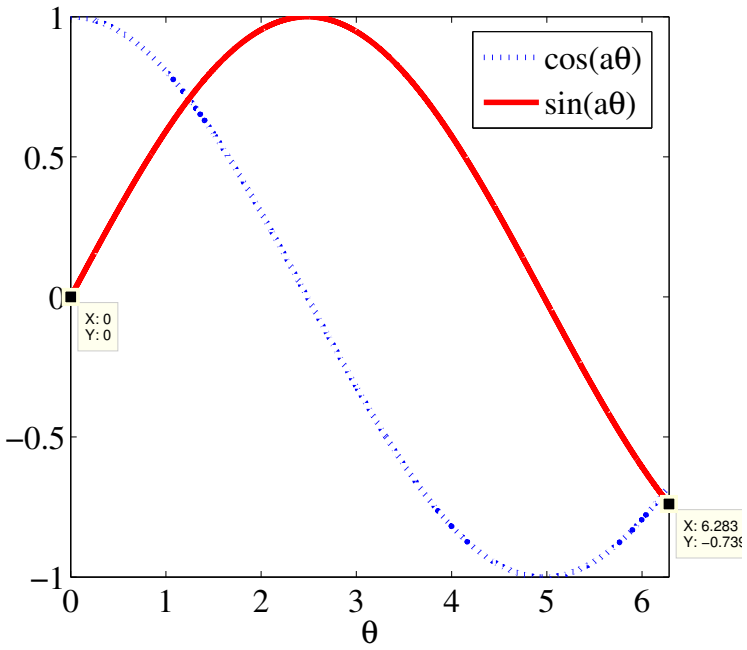


Figure 1.8: Plot of $\cos(\theta)$ and $\sin(a\theta)$, with $a = .6324$.

1. The segment C_1: We have

$$\begin{aligned} I_1 &= \left(\int \frac{z^a}{z+1} \mathrm{d}z \right)_{z=x+\mathrm{i}\epsilon, x\in[\epsilon,\infty)}, \\ &= \int_\epsilon^\infty \frac{(x+\mathrm{i}\epsilon)^a}{x+\mathrm{i}\epsilon+1} \mathrm{d}x, \end{aligned}$$

Consider $z^a = |x+\mathrm{i}\epsilon|^a$ in the integrand. As $\epsilon \to 0$, the argument of the complex $x+\mathrm{i}\epsilon$ tends to zero, hence $z^a \to x^a$ as $\epsilon \to 0$. Thus,

$$I_1 \to \int_0^\infty \frac{x^a}{x+1} \mathrm{d}x, \qquad \epsilon \to 0.$$

2. The segment C_7: Consider next the contribution

$$\begin{aligned} I_7 &= \left(\int \frac{z^a}{z+1} \mathrm{d}z \right)_{z=x-\mathrm{i}\epsilon, x\in[\epsilon,\infty)}, \\ &= \int_\epsilon^\infty \frac{(x-\mathrm{i}\epsilon)^a}{x-\mathrm{i}\epsilon+1} \mathrm{d}x, \end{aligned}$$

As before, we examine $z^a = |x-\mathrm{i}\epsilon|^a$ in the integrand. As $\epsilon \to 0$, the argument of the complex

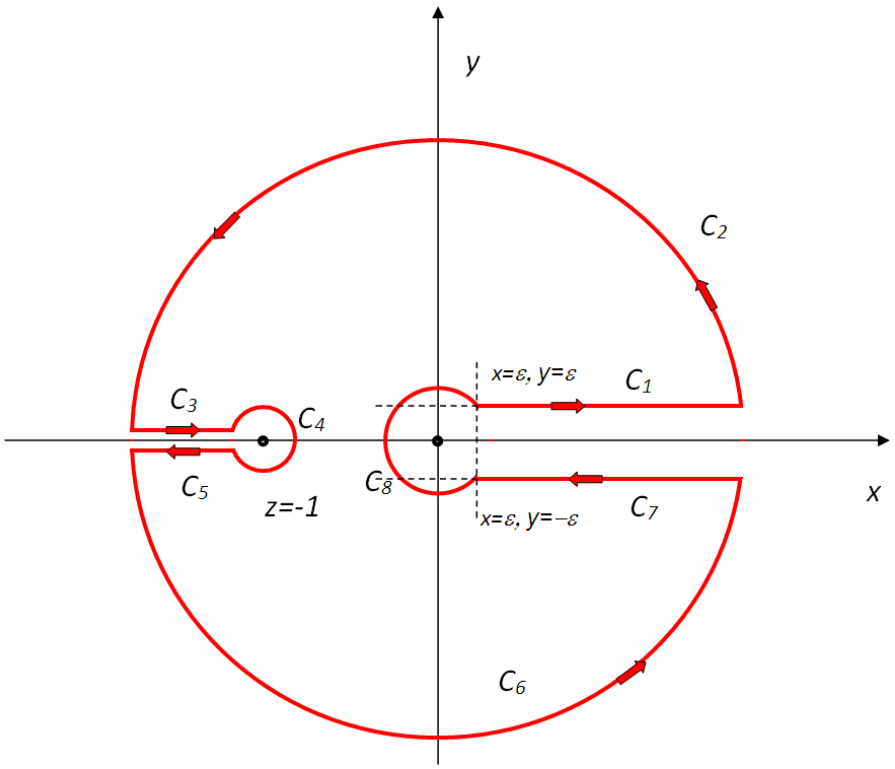


Figure 1.9: Suggested contour for $\int_0^\infty x^a(1+x)^{-1}\mathrm{d}x$, with $-1 < a < 0$.

number $x - \mathrm{i}\epsilon$ tends to 2π, hence $z^a \to x^a \mathrm{e}^{2\pi a}$ as $\epsilon \to 0$. Thus,

$$I_7 \to \mathrm{e}^{2\pi \mathrm{i} a} \int_0^\infty \frac{x^a}{x+1}\mathrm{d}x, \qquad \epsilon \to 0.$$

3. The circlular segment C_8: We have

$$I_8 = \int \frac{\epsilon^a \mathrm{e}^{\mathrm{i}\theta a}}{\epsilon \mathrm{e}^{\mathrm{i}\theta} + 1} \epsilon \mathrm{i} \mathrm{d}\theta,$$

where θ ranges from $\theta = \pi/4$ and proceeds anticlockwise to $\theta = 7\pi/4$. Clearly, $I_8 \to 0$ as $\epsilon \to 0$.

4. The line segments C_3 and C_5: The integrand is continuous across the axis $x \leq 0$. Thus, the contributions from the integrals along the line segments C_3 and C_5 are self-cancelling.

5. The circular segments C_2 and C_6: Consider, for example,

$$I_2 = \int_{\theta=\theta_0}^{\theta=\theta_1} \frac{r^a \mathrm{e}^{\mathrm{i}\theta a}}{r\mathrm{e}^{\mathrm{i}\theta} + 1} \mathrm{i} r \mathrm{e}^{\mathrm{i}\theta}\, \mathrm{d}\theta,$$

where $\theta_0 \to 0$ through positive values, and $\theta_1 \to \pi$ through values strictly less than π. We

have

$$I_2 \to \mathrm{i}r^a \int_0^\pi \mathrm{e}^{\mathrm{i}\theta a}\,\mathrm{d}\theta, \qquad r \to \infty, \qquad \theta_0 \to 0, \qquad \theta_1 \to \pi.$$

Since $a < 0$, we have $I_2 \to 0$ as $r \to \infty$, and similarly for I_6.

6. The circular region C_4:

$$I_4 = \left(\int_{\theta=\theta_0}^{\theta=\theta_2} f(z)\,\mathrm{d}z \right)_{z=-1+r\mathrm{e}^{\mathrm{i}\theta}},$$

where $r > 0$ is a fixed radius $\theta_0 = \pi + \delta$, $\theta_1 = \pi - \delta$, $\delta > 0$, with $\delta \to 0$, and the integral is taken in a clockwise sense. Taking $\delta \to 0$, we obtain

$$I_4 = -\left(\int_0^{2\pi} f(z)\,\mathrm{d}z \right)_{z=-1+r\mathrm{e}^{\mathrm{i}\theta}}$$

Since the integrand has a simple pole at $z = -1$, this becomes

$$\begin{aligned} I_4 &= -\left(\int_0^{2\pi} f(z)\,\mathrm{d}z \right)_{z=-1+r\mathrm{e}^{\mathrm{i}\theta}}, \\ &= = -2\pi\mathrm{i}\left[\mathrm{Res}(f,-1)\right], \\ &= -2\pi\mathrm{i}\mathrm{e}^{\mathrm{i}\pi a}. \end{aligned}$$

Finally now, because the total contour $C = C_1 + \cdots + C_8$ encloses no singularities,

$$0 = \oint_C f(z)\mathrm{d}z = \int_{C_1} f(z)\mathrm{d}z + \cdots + \int_{C_8} f(z)\mathrm{d}z.$$

Putting the results together, we have

$$0 = -2\pi\mathrm{i}\mathrm{e}^{\mathrm{i}\pi a} + I - \mathrm{e}^{2\pi\mathrm{i}a} I.$$

Rearrangement gives

$$\pi = -I\left(\frac{\mathrm{e}^{\mathrm{i}\pi a} - \mathrm{e}^{-\mathrm{i}\pi a}}{2\mathrm{i}} \right),$$

and the result follows.

1.6 Systematic approach to contour integration

Our presentation of contour integration has been a little unfortunate. We have looked at three disparate examples, made an inspired guess for the appropriate contour, and the result followed. This looks a little haphazard. Help is at hand. There is a way to 'classify' definite integrals that can

be evaluated using contour integration. Each class comes with its own techniques. So, to tackle a particular integral, one identifies the class to which the integral belongs, one looks up the tips and tricks for that class in a textbook, and one proceeds from there. For instance, Arfken and Weber classify definite integrals amenable to contour integration into the following categories:

1. Definite integrals of the form
$$\int_0^{2\pi} f(\sin\theta, \cos\theta)\,\mathrm{d}\theta.$$
See [Arfken and Weber], page 451. Also, see example 1 in the present chapter.

2. Definite integrals of the form
$$\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x.$$
See [Arfken and Weber], page 452. Also, see Dr Smith's MATH 30040 notes.

3. Definite integrals of the form
$$\int_{-\infty}^{\infty} f(x)\mathrm{e}^{\mathrm{i}ax}\,\mathrm{d}x, \qquad a \in \mathbb{R}.$$
See [Arfken and Weber], page 453.

4. Singularities on the contour of integration, e.g. $\int_0^{\infty}(\sin x/x)\mathrm{d}x$. See [Arfken and Weber], page 455.

5. Integrands whose complexification involves branch cuts.

   These are the trickiest of them all. Each instance will have its own peculiarities, so that proficiency in this kind of calculation is more of an art than a science. We have already seen an example (example 2 in the present chapter). For more examples, with tips and tricks for the selection of the branch cuts and the contour, see the examples in Section 7.2 of [Arfken and Weber].

1.7 Matlab code to generate Figure 1.7

```
% Create an unambiguous distinction  between x- and y-directions
% by making x- and y-arrays have different sizes.

x=-2:.01:2;
y=-1.5:.01:1.5;
```

```
for i=1:length(x)
  for j=1:length(y)
    u_vec(i,j)=sqrt(x(i)^2+y(j)^2);
    v_vec1(i,j)=angle(x(i)+sqrt(-1)*y(j));
    % don't plot the jump discontinuity!
    if( (y(j)==0)& (x(i)<0))
      v_vec1(i,j)=NaN;
    end
  end
end

mesh(x,y,v_vec1')
xlim('x')
xlabel('x')
ylabel('y')
zlabel('arg(x+iy)')
v_vec2=v_vec1+2*pi;
v_vec3=v_vec1+2*2*pi;
hold on
mesh(x,y,v_vec2')
mesh(x,y,v_vec3')
```

Chapter 2

Maximum Principle for Laplace's Equation

Overview

Throughout this Chapter, we study the following PDE with Dirichlet boundary conditions:

$$\nabla^2 u = 0 \qquad \boldsymbol{x} \in D, \qquad u = f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D, \tag{2.1}$$

where $D \subset \mathbb{R}^n$ is a bounded, simply connected domain with the smooth boundary ∂D, and $f(\boldsymbol{x})$ is a smooth function. The aim of this Chapter is to describe *a priori* the properties of the solutions of Equation (2.1), that is, we **assume** that a smooth solution to Equation (2.1) exists, and deduce the solution propterties in the absence of knowledge of the solution's existence. Throughout this Chapter and elsewhere, functions that satisfy Laplace's equation are called **harmonic**.

Finally, the properties of harmonic functions *a priori* is not so silly, as such *a priori* knowledge can then be turned around to find really existing solutions of the Laplace equation in many situations. We will construct such solutions in the coming chapters.

2.1 The maximum principle

We have the following definitions:

Definition 2.1 *Let D be an open, bounded, and simply connected subset of $\mathbb{R}^n$, and let $U(\boldsymbol{x})$ be harmonic on D. Let $\boldsymbol{x}_0 \in D$. Then, there exists a real number $r > 0$ such that the open ball of radius r and centred at $\boldsymbol{x}_0$ is entirely contained in D. We have some notation:*

- *$B(\boldsymbol{x}_0, r)$ denotes the open ball of radius r and centred at $\boldsymbol{x}_0$ is entirely contained in D. The volume of the ball B is denoted by $|B|$.*

- $S(\boldsymbol{x}_0, r)$ *is the boundary sphere of* $B(\boldsymbol{x}_0, r)$*. The area of the boundary sphere is denoted by* $|S|$*.*

- *The symbol* $\mathrm{d}\Omega_n$ *denotes the differential element of solid angle in* $\mathbb{R}^n$*, and the following identity holds:*

$$\mathrm{d}^n x = r^{n-1}\mathrm{d}r\,\mathrm{d}\Omega_n, \qquad r = |\boldsymbol{x}|, \tag{2.2}$$

- *Integrate both sides of Equation* (2.2) *to obtain* $|B|$*, the volume of the ball in* $\mathbb{R}^n$*, of radius* R*:*

$$|B| = \int_0^R r^{n-1}\mathrm{d}r \int_{\Omega_n} \mathrm{d}\Omega_n,$$

where the subscript in $\int_{\Omega_n}$ *denotes integration over all solid angles. Thus,*

$$|B| = \frac{1}{n}R^n|\Omega_n|,$$

where $|\Omega_n| = \int_{\Omega_n} \mathrm{d}\Omega_n$ *is the area of the unit sphere in* $\mathbb{R}^n$*.*

Example: In $\mathbb{R}^2$, we have $\mathrm{d}\Omega_{n=2} = \mathrm{d}\varphi$, where φ is the polar angle in the usual polar coordinates. Thus, $|\Omega_2| = \int_0^{2\pi} \mathrm{d}\varphi = 2\pi$. Also, $|B_{n=2}| = (1/2)R^2(2\pi) = \pi R^2$.

In $\mathbb{R}^3$, we have $\mathrm{d}\Omega_{n=3} = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$, where again, (θ, φ) denote the usual polar coordinates: θ is the polar angle, and φ is the azimuthal angle. Thus, $|\Omega_3| = \int_0^{\pi} \sin\theta\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi = 4\pi$. Also, $|B_{n=3}| = (1/3)R^3(4\pi) = (4/3)\pi R^3$.

Next, we define boundary-averages and area-averages of $U(\boldsymbol{x})$ as follows:

- Boundary average:

$$\mathrm{av}_{S(\boldsymbol{x}_0,r)}U := \frac{1}{|\Omega_n|}\int_{\Omega_n} U(\boldsymbol{x}_0 + r\hat{\boldsymbol{r}})\,\mathrm{d}\Omega_n$$

  where $\hat{\boldsymbol{r}}$ is the unit radial vector expressed as a function of the pertinent angular variables in $\mathbb{R}^n$.

- Volume average:

$$\mathrm{av}_{B(\boldsymbol{x}_0,r)}U := \frac{1}{|B|}\int_{B(\boldsymbol{x}_0,r)} U(\boldsymbol{x})\mathrm{d}^n x,$$

We have the following theorem:

Theorem 2.1 (Mean-value theorem, harmonic functions) *Let* D *be an open, bounded, and simply-connected subset of* $\mathbb{R}^n$*, and let* $U(\boldsymbol{x})$ *be harmonic on* D*. Specifically, let* $U \in C^2(D) \cap C^0(\overline{D})$*. Let* $\boldsymbol{x}_0 \in D$*. Then, for a ball* $B(\boldsymbol{x}_0, r)$ *contained entirely in* D*,*

$$U(\boldsymbol{x}_0) = \mathrm{av}_{S(\boldsymbol{x}_0,r)}U = \mathrm{av}_{B(\boldsymbol{x}_0,r)}U.$$

Proof: We start with the boundary average. We call

$$\phi(r, \boldsymbol{x}_0) := \mathrm{av}_{S(\boldsymbol{x}_0,r)} U = \frac{1}{|\Omega_n|} \int_{\Omega_n} U(\boldsymbol{x}_0 + r\hat{\boldsymbol{r}})\, \mathrm{d}\Omega_n.$$

We note that $\phi(0, \boldsymbol{x}_0) = U(\boldsymbol{x}_0)$. If we could show that $\partial\phi/\partial r = 0$, then we would be done, since we would then have that

$$\phi(r, \boldsymbol{x}_0) = \phi(0, \boldsymbol{x}_0) = U(\boldsymbol{x}_0).$$

We compute:

$$\begin{aligned}
\frac{\partial \phi}{\partial r} &= \frac{1}{|\Omega_n|} \int_{\Omega_n} \left[\frac{\partial}{\partial r} U(\boldsymbol{x}_0 + r\hat{\boldsymbol{r}}) \right] \mathrm{d}\Omega_n, \\
&= \frac{1}{|\Omega_n|} \int_{\Omega_n} \left[\hat{\boldsymbol{r}} \cdot \nabla U \right]_{\boldsymbol{x}_0 + r\hat{\boldsymbol{r}}} \mathrm{d}\Omega_n, \\
&= \frac{1}{|\Omega_n|} \int_{\Omega_n} \left[(\nabla U)_{\boldsymbol{x}} \right] \cdot \left(\hat{\boldsymbol{r}}\, \mathrm{d}\Omega_n \right), \qquad \boldsymbol{x} = \boldsymbol{x}_0 + r\hat{\boldsymbol{r}}, \\
&= \frac{1}{|\Omega_n| r^{n-1}} \int_{\Omega_n} (\nabla U) \cdot \mathrm{d}\boldsymbol{S}, \qquad \mathrm{d}\boldsymbol{S} = r^{n-1} \mathrm{d}\Omega_n \hat{\boldsymbol{r}}, \\
&= \frac{1}{|\Omega_n| r^{n-1}} \int_B \nabla^2 U\, \mathrm{d}^n x, \qquad \ldots \qquad \text{Gauss's theorem} \\
&= 0.
\end{aligned}$$

Hence, the first part is shown.

For the second part, we also do a direct calculation:

$$\begin{aligned}
\frac{1}{|B|} \int_B U(\boldsymbol{x}) \mathrm{d}^n x &= \frac{1}{|B|} \int_0^r r^{n-1} \mathrm{d}r \int_{\Omega_n} U(\boldsymbol{x}_0 + r\hat{\boldsymbol{r}})\, \mathrm{d}\Omega_n, \\
&= \frac{|\Omega_n|}{|B|} \int_0^r r^{n-1}\, \mathrm{d}r \left[\mathrm{av}_{S(\boldsymbol{x}_0,r)} U \right], \\
&= \frac{n}{r^n} U(\boldsymbol{x}_0) \int_0^r r^{n-1}\, \mathrm{d}r, \\
&= U(\boldsymbol{x}_0).
\end{aligned}$$

Putting it all together, we have the following **mean-value theorem** for harmonic functions:

$$U(\boldsymbol{x}_0) = U(\boldsymbol{x}_0) = \mathrm{av}_{S(\boldsymbol{x}_0,r)} = \mathrm{av}_{B(\boldsymbol{x}_0,r)}.$$

The maximum principle also follows from this result:

Theorem 2.2 (Maximum principle, harmonic functions) *Let D be an open, bounded, and simply-connected subset of $\mathbb{R}^n$ and let $U(\boldsymbol{x})$ be harmonic on D, with $U \in C^2(D) \cap C^0(\overline{D})$. Then*

$$\max_{\overline{D}} U(\boldsymbol{x}) = \max_{\partial D} U(\boldsymbol{x}).$$

Proof: Let $U(\boldsymbol{x})$ attain its maximum over $\overline{D}$ at $\boldsymbol{x}_0$. If $\boldsymbol{x}_0 \in \partial D$, the theorem is proved. Thus, consider the case where $\boldsymbol{x}_0 \in D$, with $M = U(\boldsymbol{x}_0)$. Then, by the topology of the set D, and by the Mean-Value Theorem, we can write

$$U(\boldsymbol{x}_0) = \frac{1}{|B|} \int_{B(\boldsymbol{x}_0, r)} U(\boldsymbol{x}) \mathrm{d}^n x,$$

where $r > 0$ is a positive number. Hence,

$$\max_{B(\boldsymbol{x}_0,r)} U(\boldsymbol{x}) = \mathrm{avg}_{B(\boldsymbol{x}_0,r)} U(\boldsymbol{x}), \tag{2.3}$$

and this result extends to the closed ball $\overline{B(\boldsymbol{x}_0, r)}$ because of the mean value theorem (boundary averages). Thus, the maximum of the function is actually the mean value of the function on $\overline{B(\boldsymbol{x}_0, r)}$, and hence

$$U(\boldsymbol{x}) = M, \qquad \boldsymbol{x} \in \overline{B(\boldsymbol{x}_0, r)}. \tag{2.4}$$

We now extend this result to cover the entire domain D. Thus, choose a point $\boldsymbol{x}_1 \in \partial B(\boldsymbol{x}_0, r)$, with $U(\boldsymbol{x}_1) = M$. Choose a ball $B(\boldsymbol{x}_1, r')$ contained entirely in D and conclude that

$$U(\boldsymbol{x}) = M, \qquad \boldsymbol{x} \in \overline{B(\boldsymbol{x}_1, r')}.$$

By covering the set D with a collection of overlapping balls in this manner, it follows that

$$U(\boldsymbol{x}) = M, \qquad \boldsymbol{x} \in D. \tag{2.5}$$

By continuity (for $U \in C^0(\overline{D})$), we have $U(\boldsymbol{x}) = M$ on $\overline{D}$. Thus, in this second case, the maximum is attained everywhere, in particular, it is attained on the boundary. Therefore, in both cases, we have

$$\boldsymbol{x}_0 \in \partial D,$$

and the result is proved.

Note that this result only holds for D a connected set.

2.2 Maximum principle – heuristics in two dimensions

In the two-dimensional case, there is a heuristic way to understand the maximum principle. We assume that $U(\boldsymbol{x})$ is harmonic on D, an open, bounded, and connected subset of $\mathbb{R}^2$. We consider a stationary point $\boldsymbol{x}_0 \in D$ where

$$U_x(\boldsymbol{x}_0) = U_y(\boldsymbol{x}_0) = 0.$$

We make an expansion of $U(\boldsymbol{x})$ in the neighbourhood of this point

$$\begin{aligned}
\Delta &:= U(\boldsymbol{x}_0 + \boldsymbol{\delta}) - U(\boldsymbol{x}_0), \\
&= \delta_x U_x(\boldsymbol{x}_0) + \delta_y U_y(\boldsymbol{x}_0) + \tfrac{1}{2}\delta_x^2 U_{xx}(\boldsymbol{x}_0) + \tfrac{1}{2}\delta_y^2 U_{yy}(\boldsymbol{x}_0) + \delta_x\delta_y U_{xy}(\boldsymbol{x}_0) + \text{H.O.T.}, \\
&= \tfrac{1}{2}\delta_x^2 U_{xx}(\boldsymbol{x}_0) + \tfrac{1}{2}\delta_y^2 U_{yy}(\boldsymbol{x}_0) + \delta_x\delta_y U_{xy}(\boldsymbol{x}_0) + \text{H.O.T.}, \\
&\approx \tfrac{1}{2}\delta_x^2 U_{xx}(\boldsymbol{x}_0) + \tfrac{1}{2}\delta_y^2 U_{yy}(\boldsymbol{x}_0) + \delta_x\delta_y U_{xy}(\boldsymbol{x}_0).
\end{aligned}$$

Thus, Δ is a quadratic form. We assume that $\boldsymbol{x}_0$ is a **non-degenerate** point:

$$U_{xx}(\boldsymbol{x}_0) \neq 0,$$

and we complete the square as follows:

$$\begin{aligned}
2\Delta &= U_{xx}(\boldsymbol{x}_0)\left[\delta_x^2 + \frac{2U_{xy}(\boldsymbol{x}_0)}{U_{xx}(\boldsymbol{x}_0)}\right] + U_{yy}(\boldsymbol{x}_0)\delta_y^2, \\
&= U_{xx}(\boldsymbol{x}_0)\left(\delta_x + \frac{U_{xy}(\boldsymbol{x}_0)}{U_{xx}(\boldsymbol{x}_0)}\delta_y\right)^2 + \left[U_{yy}(\boldsymbol{x}_0) - \frac{[U_{xy}(\boldsymbol{x}_0)]^2}{U_{xx}(\boldsymbol{x}_0)}\right]\delta_y^2,
\end{aligned}$$

This tidies up as follows:

$$\Delta = \tfrac{1}{2}\text{sign}\left(U_{xx}(\boldsymbol{x}_0)\right)\left[|U_{xx}(\boldsymbol{x}_0)|\left(\delta_x + \frac{U_{xy}(\boldsymbol{x}_0)}{U_{xx}(\boldsymbol{x}_0)}\delta_y\right)^2 + \frac{U_{xx}(\boldsymbol{x}_0)U_{yy}(\boldsymbol{x}_0) - [U_{xy}(\boldsymbol{x}_0)]^2}{|U_{xx}(\boldsymbol{x}_0)|}\delta_y^2\right]$$

We call

$$\mathcal{D}(U(\boldsymbol{x}_0)) := U_{xx}(\boldsymbol{x}_0)U_{yy}(\boldsymbol{x}_0) - [U_{xy}(\boldsymbol{x}_0)]^2$$

the **discriminant**; the quadratic form simplifies to

$$\Delta = \tfrac{1}{2}\text{sign}\left(U_{xx}(\boldsymbol{x}_0)\right)\left[|U_{xx}(\boldsymbol{x}_0)|\left(\delta_x + \frac{U_{xy}(\boldsymbol{x}_0)}{U_{xx}(\boldsymbol{x}_0)}\delta_y\right)^2 + \frac{\mathcal{D}(U)}{|U_{xx}(\boldsymbol{x}_0)|}\delta_y^2\right]$$

The quadratic form Δ is sign-definite if $\mathcal{D} > 0$. Then, the critical point $\boldsymbol{x}_0$ is a definite maximum or minimum. On the other hand, if $\mathcal{D} < 0$, the critical point is a saddle point. The condition for a

non-degenerate critical point to be a saddle is thus

$$U_{xx}(\boldsymbol{x}_0)U_{yy}(\boldsymbol{x}_0) - [U_{xy}(\boldsymbol{x}_0)]^2 < 0.$$

However, for a harmonic function, $U_{xx} = -U_{yy}$, hence, for a non-degenrate critical point of a harmonic function,

$$\mathcal{D}(U) = -[U_{xx}]^2 - [U_{xy}]^2 < 0,$$

(the inequality is strict because $U_{xx}(\boldsymbol{x}_0) \neq 0$). Thus, all non-degenerate critical points are saddle points, hence no maxima or minima exist.

Of course, the very last conclusion here is slightly dodgy, as the critical points could be degenerate; for that reason, such a heuristic argument does not suffice to prove the maximum principle.

2.3 Uniqueness of solutions for Laplace's equation

Theorem 2.3 *Consider Equation* (2.1)*. If this equation has a smooth solution* $u(\boldsymbol{x}) \in C^2(D) \cap C^0(\overline{D})$*, then* $u(\boldsymbol{x})$ *is the unique smooth solution.*

Proof: Suppose that Equation (2.1) has two smooth solutions. Call them u_1 and u_2. Form the difference

$$\delta(\boldsymbol{x}) := u_2 - u_1.$$

By the linearity of Equation (2.1), we have

$$\nabla^2\delta = 0, \qquad \boldsymbol{x} \in D, \qquad \delta = 0, \qquad \boldsymbol{x} \in \partial D.$$

By the maximum principle,

$$\max_{\overline{D}}\delta = \max_{\partial D}\delta = 0.$$

Hence, the maximum value of $\delta(\boldsymbol{x})$ is zero. But the arguments in the maximum principle can also be recycled to show that the minimum of a harmonic function, taken over the closure of the relevant domain, is attained on the boundary, such that

$$\min_{\overline{D}}\delta = \min_{\partial D}\delta = 0.$$

Hence,

$$0 = \min_{\overline{D}}\delta \leq \delta(\boldsymbol{x}) \leq \max_{\overline{D}}\delta = 0,$$

hence $\delta(\boldsymbol{x})$ is zero everywhere in $\overline{D}$, and thus $u_1 = u_2$.

2.4 Laplace's equation in two dimensions – connections to complex analysis

Let $z = x + \mathrm{i}y$ be a complex number, let $D \subset \mathbb{C}$ be an open set, and let

$$\begin{aligned} F : D &\to \mathbb{C} \\ z &\mapsto F(z) = u(x,y) + \mathrm{i}v(x,y) \end{aligned} \tag{2.6}$$

be an analytic function on D (hence $u(x,y)$ and $v(x,y)$ are C^∞ in (x,y)). We have the following remarkable fact:

Theorem 2.4 *Let the function $F(z)$ in Equation (2.6) be analytic. Then the corresponding u and v real-valued functions satisfy Laplace's equation for all points in D:*

$$\nabla^2 u = 0, \qquad \nabla^2 v = 0, \qquad \boldsymbol{x} \equiv (x,y) \in D.$$

where now D is viewed as an open domain in $\mathbb{R}^2$.

The proof of this statement is by direct computation. Because F is analytic, the corresponding u and v real-valued functions are C^∞ in D and satisfy the Cauchy–Riemann conditions:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}.$$

The proof now proceeds by direct computation:

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right), \\ &= \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial y}\left(-\frac{\partial v}{\partial x}\right) \\ &= 0. \end{aligned}$$

The converse is also true, but only for D simply connected:

Theorem 2.5 *Let $u(x,y) : D \to \mathbb{R}$, be harmonic, with and let D be an open, bounded, simply-connected set in $\mathbb{R}^2$, with smooth boundary. Furthermore, let*

$$u \in C^2(D) \cap C^1(\overline{D}).$$

Then there exists a function $v(x,y) : D \to \mathbb{R}$ also harmonic, such that $f(z) = u(x,y) + \mathrm{i}v(x,y)$ is analytic in D; the function v is called the **harmonic conjugate** *to u.*

Note that it is necessary for the function to be in the class $C^1(\overline{D}$ to continue certain integrals up to the boundary of the domain.

Proof: Define a vector field $\boldsymbol{w}(x, y)$ in $\mathbb{R}^2$ as follows:

$$\boldsymbol{w} = \begin{pmatrix} -u_y \\ u_x \end{pmatrix},$$

where $u(x, y)$ is harmonic in D. Compute

$$\nabla \times \boldsymbol{w} = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \partial_x & \partial_y & \partial_z \\ -u_y & u_x & 0 \end{vmatrix} = \hat{\boldsymbol{z}}\,(u_{xx} + u_{yy}) = 0,$$

since u is harmonic in D. By Stokes's theorem applied to the simply-connected domain D, there exists a potential function v such that

$$\boldsymbol{w} = \begin{pmatrix} -u_y \\ u_x \end{pmatrix} = \nabla v.$$

Specifically,

$$\begin{aligned} v(\boldsymbol{x}) &= \int_{\boldsymbol{a}}^{\boldsymbol{x}} \boldsymbol{w} \cdot \mathrm{d}\boldsymbol{x}, \\ &= \int_{\boldsymbol{a}}^{\boldsymbol{x}} \boldsymbol{w} \cdot \widehat{\boldsymbol{t}} \mathrm{d}\ell, \\ &= \int_{\boldsymbol{a}}^{\boldsymbol{x}} (-u_y t_x + u_x t_y)\,\mathrm{d}\ell, \\ &= \int_{\boldsymbol{a}}^{\boldsymbol{x}} (u_x, u_y) \cdot (t_y, -t_x)\,\mathrm{d}\ell, \\ &= \int_{\boldsymbol{a}}^{\boldsymbol{x}} \nabla u \cdot \widehat{\boldsymbol{n}} \mathrm{d}\ell, \end{aligned}$$

where $\boldsymbol{a} \in D$ is arbitrary, and where the points $\boldsymbol{a}$ and $\boldsymbol{x}$ are joined by a smooth curve; by path-independence, the function $v(\boldsymbol{x})$ is independent of the details of this curve and depends only on the endpoints. Also, $\widehat{\boldsymbol{t}}$ is the unit tangent vector along the curve, and $\widehat{\boldsymbol{n}}$ is the unit normal vector. Hence

$$v \in C^2(D) \cap C^1(\overline{D}).$$

By construction, $\nabla v = (v_x, v_y)^T = (-u_y, u_x)^T$, and

$$u, v \in C^2(D) \cap C^1(\overline{D}).$$

Thus, u and v are C^1 functions that satisfy the Cauchy–Riemann conditions. Hence,

$$f = u + \mathrm{i}v$$

is analytic in D.

Thus, in a loose sense, and only for simpy-connected domains in $\mathbb{R}^2$, a function is harmonic if and only if it is analytic. This result is of immense importance to fluid mechanics. There is only sufficient time to describe sketchily this importance, which we do in Section 2.5.

Example: Denote the unit disc of radius 1 centred at the origin by D_0. The boundary of D_0 is the unit circle. Consider the following Dirichlet problem:

$$\begin{aligned} \nabla^2\Phi &= 0, \qquad (x,y) \in D_0, \\ \Phi &= \sin\varphi, \qquad (x,y) \in \partial D_0. \end{aligned}$$

Solve for $u(x,y)$.

Consider the function $f(z) = z$. This is an analytic function. Thus, $u = x$ and $v = y$ are both harmonic functions. Rewrite $f(z)$ in polar coordinates as

$$f(z) = u + \mathrm{i}v = r\cos\theta + \mathrm{i}r\sin\varphi.$$

We have $v = r\sin\varphi$, with v harmonic in D_0 and $v = \sin\varphi$ on ∂D_0. Thus,

$$\Phi = v = r\sin\varphi = y$$

is the required solution.

Example: Let $u(x,y) = \log(x^2+y^2)^{1/2}$. Write down the domain D on which $u(x,y)$ is defined. Show that $u(x,y)$ is harmonic D and find its harmonic conjugate. Comment on the smoothness properties of the harmonic conjugate.

Solution: Write $u(x,y) = \log r$ in polar coordinates. Clearly, $u(x,y)$ is well defined for $r \neq 0$. Hence, the domain D is the punctured complex plane with the origin removed. On D,

$$\begin{aligned} \nabla^2 u &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\log r\right), \\ &= 0. \end{aligned}$$

Hence, $u(x,y)$ is harmonic on D. We identify

$$f(z) = \mathrm{Log}z = \underbrace{\log r}_{=u} + \mathrm{i}\underbrace{\mathrm{Arg}(z)}_{=v},$$

where we have taken the principal branch of the complex multivaued log function. Hence, the harmonic conjugate to $u = \log r$ is $v = \operatorname{Arg}(x + \mathrm{i}y)$. Again writing $(x, y) = r\mathrm{e}^{\mathrm{i}\varphi}$, we have

$$v = \operatorname{atan2}(y, x) = \varphi, \qquad 0 \leq \varphi < 2\pi$$

which is a smooth function of φ, except across the nonnegative real axis, where there is a jump discontinuity in v ('international date line'). Thus, the harmonic conjugate of $u(x, y)$ is defined on the set

$$\mathbb{C} - \{x \geq 0\}.$$

2.5 Applications of the theory in two dimensions

Connection to fluid flow in two dimensions

Let $\boldsymbol{u}(x, y)$ be the velocity field describing the flow of a fluid in a container $D \in \mathbb{R}^2$. Further, let D be bounded, open, simply-connected, with a smooth boundary ∂D. Suppose that the flow is incompressible:

$$\nabla \cdot \boldsymbol{u} = 0.$$

Suppose further that the flow is irrotational:

$$\nabla \times \boldsymbol{u} = 0.$$

Then, given the topology of the domain D and the irrotational condition, we can write $\boldsymbol{u}$ as the gradient of a potential function:

$$\boldsymbol{u} = \nabla\phi, \qquad \phi \in C^\infty(D) \cap C^1(\overline{D}).$$

The incompressibility condition is now rewritten as follows:

$$\nabla^2\phi = 0, \qquad \boldsymbol{x} \in D.$$

The pertinent boundary condition is a Neumann no-outflow condition $u_n = 0$ on ∂D, or $\partial\phi/\partial n = 0$ on ∂D, where $\partial/\partial n$ denotes the derivative in a direction normal to the boundary ∂D.

Given the harmonic velocity potential ϕ, we obtain the harmonic conjugate ψ and write down the **complex potential**

$$\chi(z) = \phi(x, y) + \mathrm{i}\psi(x, y).$$

Using the Cauchy–Riemann conditions, we have

$$\begin{aligned} u &= \frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial y}, \\ v &= \frac{\partial \phi}{\partial y} = -\frac{\partial \psi}{\partial x}. \end{aligned}$$

Summarizing,

$$u = \frac{\partial \psi}{\partial y}, \qquad v = -\frac{\partial \psi}{\partial x}.$$

Thus, we identify ψ with the **streamfunction** of the flow. We have the following definitions:

Definition 2.2 *The curves*

$$\psi = \text{Const.}$$

are called the **streamlines** *of the flow; the curves*

$$\phi = \text{Const.}$$

are called the **equipotential curves**. Using results from the worked examples in Section 2.6 below, it can be shown that the equipotential curves are are orthogonal to the streamlines, in the sense that

$$\nabla \phi \cdot \nabla \psi = 0.$$

Hence,

$$\boldsymbol{u} \cdot \nabla \psi = 0,$$

and the normal $\nabla \psi$ to the streamline is orthogonal to $\boldsymbol{u}$. Hence, the tangent to the streamline must align with $\boldsymbol{u}$; from these arguments the following further definition follows:

Definition 2.3 *Tangent vectors to the streamlines are everywhere aligned with the flow.*

In summary, all incompressible irrotational flows (on a pertinent domain) can be reduced to the simpler problem of obtaining a harmonic function. Moreover, the same problem can be reduced further to the problem of computing the real part of a certain analytic function. This will be discussed in more detail in the following chapters, especially Chapter 4, where the theory of conformal mapping is introduced.

Jensen's theorem in Complex Analysis

Theorem 2.6 *Let $f(z) : \mathbb{C} \to \mathbb{C}$ be non-constant and analytic in the entire complex plane. Then $|f(z)|^2$ has no maxima and, moreover, its minima extend down to zero.*

This is a mean-value theorem in disguise. We start with the statement about maxima. Assume for contradiction that $|f(z)|^2$ possesses a maximum, attained at z_0. By analyticity, we make a Taylor-series expansion of $f(z)$ in the neighbourhood of z_0:

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n,$$

with $f(z_0) = a_0$. We compute the mean value of F along a circle of radius r centred at z_0:

$$\begin{aligned} \mathrm{avg}|f|^2 &= \frac{1}{2\pi} \int_0^{2\pi} |f(z_0 + r\mathrm{e}^{\mathrm{i}\theta})|^2 \mathrm{d}\theta, \\ &= \frac{1}{2\pi} \int_0^{2\pi} \left(\sum_{m,n} a_m^* a_n r^{n+m} \mathrm{e}^{\mathrm{i}(m-n)\theta} \right) \mathrm{d}\theta, \\ &= \sum_{m,n} a_m^* a_n r^{n+m} \delta_{m,n}, \end{aligned}$$

Continue thus:

$$\begin{aligned} \mathrm{avg}|f|^2 &= \sum_{n=0}^{\infty} |a_n|^2 r^{2n}, \\ &= |a_0|^2 + \sum_{n=1}^{\infty} |a_n|^2 r^{2n}, \\ &= |f(z_0)|^2 + \sum_{n=1}^{\infty} |a_n|^2 r^{2n}. \end{aligned}$$

Hence,

$$\mathrm{avg}|f|^2 \geq \max|f|^2,$$

which is impossible for a non-constant function $f(z)$. Thus, $|f(z)|$ admits no maxima on $\mathbb{C}$.

We now examine the statement about minima. Suppose that $|f(z)|$ admits a minimum at z_0, and moreover, that

$$0 < |f(z_0)|^2 < |f(z)|^2,$$

for all z in a small open neighbourhood D of z_0. Thus, $f(z)$ has no zeros in D, and $1/f(z)$ is analytic there. Hence, by the first part of the theorem, $1/|f(z)|$ has no maxima in D. However, by assumption, $1/|f(z)|$ has a maximum at z_0. This is a contradiction, hence minima of $|f(z)|$ are exactly zero,

$$|f(z_0)| = 0.$$

2.6 Worked examples

1. Prove the following 'minimum principle' for harmonic functions:

   Let D be an open, bounded, and simply connected subset of $\mathbb{R}^n$ and let $u(\boldsymbol{x})$ be harmonic on D. Then

   $$\min_{\overline{D}} u(\boldsymbol{x}) = \min_{\partial D} u(\boldsymbol{x}).$$

   Hint: Take $v = -u$ and apply the maximum principle to v.

We have

$$u_{\min} \leq u(\boldsymbol{x}) \leq u_{\max}, \qquad \boldsymbol{x} \in \overline{D},$$

hence

$$-u_{\min} \geq -u(\boldsymbol{x}) \geq -u_{\max},$$

and

$$-u(\boldsymbol{x}) \leq -u_{\min},$$

or

$$\max(-u) = -\min(u). \tag{2.7}$$

Now, if $u(\boldsymbol{x})$ is harmonic, so is $-u$, hence

$$\max_{\overline{D}} \left[-u(\boldsymbol{x})\right] = \max_{\partial D} \left[-u(\boldsymbol{x})\right]. \tag{2.8}$$

By Equation (2.7), this is the same as

$$-\min_{\overline{D}} \left[u(\boldsymbol{x})\right] = -\min_{\partial D} \left[u(\boldsymbol{x})\right],$$

or

$$\min_{\overline{D}} \left[u(\boldsymbol{x})\right] = \min_{\partial D} \left[u(\boldsymbol{x})\right].$$

2. Consider the following Dirichlet problem:

$$\begin{aligned} \nabla^2\Phi &= 0, \qquad \boldsymbol{x} \in D, \\ \Phi &= \text{Const.}, \qquad \boldsymbol{x} \in \partial D, \end{aligned}$$

where D is an open, bounded, and simply connected subset of $\mathbb{R}^n$ Show that $\Phi = \text{Const.}$ everywhere in D.

Hint: Use the maximum/minimum principles.

Let $\Phi = M$ on ∂D. By the maximum / minimum principles, we have

$$M = \min_{\partial D}\Phi = \min_{\overline{D}}\Phi \leq \Phi(\boldsymbol{x}) \leq \max_{\overline{D}}\Phi = \max_{\partial D}\Phi = M,$$

for all $\boldsymbol{x} \in \overline{D}$. Hence,

$$M \leq \Phi(\boldsymbol{x}) \leq M, \qquad \boldsymbol{x} \in \overline{D},$$

hence $\Phi(\boldsymbol{x}) = M$.

3. Consider the following Dirichlet problem:

$$\begin{aligned} \nabla^2\Phi &= 0, \qquad (x, y) \in D_0, \\ \Phi &= \cos^2\varphi, \qquad (x, y) \in \partial D_0, \end{aligned}$$

where D_0 is the open unit disc centred at the origin, and φ is the angle going around the unit circle. Solve for $u(x, y)$.

On the boundary, we have

$$\Phi = \cos^2\varphi = \tfrac{1}{2}\left(\cos 2\varphi + 1\right).$$

By inspiration, consider the auxiliary compled-valued function

$$F(z) = \tfrac{1}{2}\left(r^2\mathrm{e}^{2\mathrm{i}\varphi} + 1\right) = \tfrac{1}{2}\left(z^2 + 1\right).$$

The function $F(z)$ is analytic (everywhere). On the unit disc, we have

$$F(z) = \tfrac{1}{2}\left(\cos 2\varphi + 1\right) + \tfrac{1}{2}\mathrm{i}\sin 2\varphi.$$

Thus, $\Phi = \mathrm{Re}(F)$ is the required function; specifically,

$$\Phi = \tfrac{1}{2}\left(x^2 - y^2 + 1\right).$$

4. Let $f(x) = u(x,y) + \mathrm{i}v(x,y)$ be analytic. Show that the contours

$$u = \mathrm{Const.}, \qquad v = \mathrm{Const.}$$

are orthogonal, except at critical points $f'(z) = 0$.

Away from a critical point $f'(z) = 0$, consider the curves

$$u(x,y) = \mathrm{Const.}, \qquad v(x,y) = \mathrm{Const.}$$

Assume moreover, that the point (x,y) is a point of intersection of the two curves. At (x,y), the vectors ∇u and ∇v are normal to the two respective curves. Thus, we have the following respective unit normal vectors:

$$\widehat{\boldsymbol{n}_1} = \frac{(u_x, u_y)}{\sqrt{u_x^2 + u_y^2}}, \tag{2.9a}$$

$$\widehat{\boldsymbol{n}_2} = \frac{(v_x, v_y)}{\sqrt{v_x^2 + v_y^2}}. \tag{2.9b}$$

Thus,

$$\begin{aligned} \widehat{\boldsymbol{n}_1} \cdot \widehat{\boldsymbol{n}_2} &\propto u_x v_x + u_y v_y, \\ &= u_x(-u_y) + u_y(u_x), \\ &= 0, \end{aligned}$$

where we have used the Cauchy–Riemann conditions for $u(x,y)$ and $v(x,y)$. Hence, the curves are orthogonal at their points of intersection.

On the other hand, at points of intersection that are also critical points, by Equation (2.9), such points do not have well-defined unit normal vectors, and in fact correspond to the two curves meeting in a cusp.

5. Show that the following functions are harmonic and find their conjugates, valid on $D = \mathbb{R}^2$:

$$u(x,y) = 2x(1-y), \qquad u(x,y) = \mathrm{e}^{-2x}\sin 2y.$$

For the first example, we have $u(x,y) = 2x - 2xy$. We shall construct the harmonic conjugate first of all by inspection. Consider z^2, where $z = x + \mathrm{i}y$. We have

$$\begin{aligned} z^2 &= x^2 - y^2 + 2\mathrm{i}xy, \\ \mathrm{i}z^2 &= \mathrm{i}(x^2 - y^2) - 2xy, \\ \mathrm{Re}\left(\mathrm{i}z^2\right) &= -2xy. \end{aligned}$$

Hence, take

$$f(z) = 2z + \mathrm{i}z^2,$$

with $\mathrm{Re}[f(z)] = 2x - 2xy$, and $\mathrm{i}[f(z)] = 2y + (x^2 - y^2)$. Hence, $v(x,y) = 2y + (x^2 - y^2)$ is the harmonic conjugate.

Alternatively, we may take

$$v(\boldsymbol{x}) = \int_{\boldsymbol{a}}^{\boldsymbol{x}} \nabla u \cdot \widehat{\boldsymbol{n}}\,\mathrm{d}\ell, \qquad \boldsymbol{x} = (x,y),$$

where the path of integration is any curve starting at $\boldsymbol{a}$ (arbitrary) and ending up at $\boldsymbol{x}$, and where $\widehat{\boldsymbol{n}}$ is normal to the same curve. Also, the points $\boldsymbol{a}$, $\boldsymbol{x}$, and the entirety of the curve must be contained in the set D. Finally, the normal vector needs to be chosen carefully to get the sign of v right. First, the tangent vector $\widehat{\boldsymbol{t}}$ should point from $\boldsymbol{a}$ to $\boldsymbol{x}$, with $\widehat{\boldsymbol{t}} = (t_x, t_y)$. Then, the chosen normal vector should be $(t_y, -t_x)$, in keeping with the construction in the notes of the harmonic conjugate. In the present situation, the choices are obvious, we take $\boldsymbol{a} = 0$, and the curve to be a straight line from the origin to the (fixed) location $\boldsymbol{x}$:

$$\boldsymbol{x}(t) = \boldsymbol{x}t = (x,y)t,$$

with unit tangent vector $\widehat{\boldsymbol{t}} = \dot{\boldsymbol{x}}/|\dot{\boldsymbol{x}}| = (x,y)/|(x,y)$ and unit normal vector

$$\widehat{\boldsymbol{n}} = \frac{(y,-x)}{|\boldsymbol{x}|}, \qquad |\boldsymbol{x}| = |(x,y)| = \sqrt{x^2+y^2};$$

also, $d\ell = |\boldsymbol{x}|\mathrm{d}t$, and $t \in [0,1]$, which takes us from the origin to the point $\boldsymbol{x}$. Thus,

$$\begin{aligned} v(\boldsymbol{x}) &= \int_0^1 \left[(\nabla u)_{\boldsymbol{x}(t)} \cdot (y, -x) \right] \mathrm{d}t, \\ &= \int_0^1 (2(1-yt), -2xt) \cdot (y, -x) \mathrm{d}t, \\ &= \int_0^1 \left(2y - 2y^2 t + 2x^2 t \right) \mathrm{d}t, \\ &= 2y + (x^2 - y^2), \end{aligned}$$

which agrees with the previously-obtained answer. Note finally that had I taken $\boldsymbol{a} \neq 0$, I would have obtained $v(\boldsymbol{x}) = 2y + (x^2 - y^2) + C$, where C is a constant. This is legitimate: the harmonic conjugate is not quite unique but rather is unique up to a constant.

For the second problem, we again construct the harmonic conjugate by eye. We start with $f(z) = \mathrm{i}\mathrm{e}^{-2z}$. Consider then the following string of equalities:

$$\begin{aligned} f(z) &= \mathrm{i}\mathrm{e}^{-2z}, \\ &= \mathrm{i}\mathrm{e}^{-2x}\mathrm{e}^{-2\mathrm{i}y}, \\ &= \mathrm{i}\mathrm{e}^{-2x}\left(\cos 2y - \mathrm{i}\sin 2y\right), \\ &= \mathrm{e}^{-2x}\left[\sin 2y + \mathrm{i}\cos 2y\right]. \end{aligned}$$

Hence, $\mathrm{Re}[f(z)] = \mathrm{e}^{-2x}\sin 2y$, and $\mathrm{Im}[f(z)] = \mathrm{e}^{-2x}\cos 2y$, and

$$v(x,y) = \mathrm{e}^{-2x}\cos 2y$$

is the required harmonic conjugate.

6. Using complex variables or some other method, prove Liouville's theorem for harmonic functions:

   Let u be harmonic in the entire two-dimensional plane. Assume that u is bounded, $|u| \leq M$, for all $(x,y) \in \mathbb{R}^2$. Then u is constant.

Let v denote the harmonic conjugate of u. This certainly exists, because the complex plane is simply connected. Also, $u + \mathrm{i}v$ is analytic in the entire complex plane. Consider

$$f(z) = \mathrm{e}^{u+\mathrm{i}v}.$$

Thus,

$$|f(z)| = \mathrm{e}^{u} \leq \mathrm{e}^{M}.$$

Therefore, $f(z)$ is bounded and analytic in the entire complex plane and by Lioville's theorem, $f(z) = \mathrm{Const.}$. Thus,

$$\mathrm{e}^{u+\mathrm{i}v} = \mathrm{Const.},$$

and it follows that u and v are both constant.

Chapter 3

Laplace's Equation – Green's function

Again, we focus on the following problem:

$$\begin{aligned} \nabla^2 u &= 0, \qquad \boldsymbol{x} \in D, \\ u &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D, \end{aligned} \tag{3.1}$$

where D is a bounded open simply-connected set in $\mathbb{R}^n$. The aim of this Chapter is to describe rigorously the Green's function technique for the Laplace problem, whereby the solution to Equation (3.1) can be written as a convolution,

$$u(\boldsymbol{x}) = \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}S_y, \tag{3.2}$$

where the properties of the **Green's function** $G(\boldsymbol{x}, \boldsymbol{y})$ are discussed in this section.

3.1 Brief review – Green's function for $D = \mathbb{R}^n$

Neglecting boundary conditions, we know the Green's function $G_0(\boldsymbol{x}, \boldsymbol{y})$ for $D = \mathbb{R}^n$: for $n = 2$ we have

$$G_0(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2\pi} \log |\boldsymbol{x} - \boldsymbol{y}|,$$

while for $n = 3$ we have

$$G_0(\boldsymbol{x}, \boldsymbol{y}) = -\frac{1}{4\pi |\boldsymbol{x} - \boldsymbol{y}|}.$$

In this chapter, this basic knowledge will be used to construct the Green's function for bounded domains.

3.2 Green's function for bounded domains – basic idea

For definiteness, in this chapter we work in two dimensions. Let D be a finite domain in $\mathbb{R}^2$, with smooth boundary ∂D. We are interested in solving

$$\begin{aligned} \nabla_x^2 G(\boldsymbol{x};\boldsymbol{y}) &= \delta(\boldsymbol{x}-\boldsymbol{y}), \qquad \boldsymbol{x}\in D, \\ G(\boldsymbol{x};\boldsymbol{y}) &= 0, \qquad \boldsymbol{x}\in \partial D. \end{aligned}$$

- Now the function $G_0(\boldsymbol{x}-\boldsymbol{y})$ will satisfy the first of these criteria.
- To construct a G that satisfies both criteria, simply add a smooth function to G_0:

$$G(\boldsymbol{x};\boldsymbol{y}) = G_0(\boldsymbol{x}-\boldsymbol{y}) + h(\boldsymbol{x};\boldsymbol{y}).$$

- There are some conditions on h:

$$\begin{aligned} \nabla_x^2 h(\boldsymbol{x};\boldsymbol{y}) &= 0, \qquad \boldsymbol{x}\in D, \\ G_0(\boldsymbol{x}-\boldsymbol{y}) + h(\boldsymbol{x};\boldsymbol{y}) &= 0, \qquad \boldsymbol{x}\in \partial D. \end{aligned} \tag{3.3}$$

- The boundary term in Equation (3.3) is a smooth function. Existence theory (a version of which we shall tackle later, at least in two dimensions) therefore guarantees that the **corrector function** $h(\boldsymbol{x};\boldsymbol{y})$ exists. Indeed, having constructed a Green's function on the full space, solving for the Green's function in the bounded domain Ω is (at least superficially) straightforward - just add a function that satisfies $\nabla_x^2 h = 0$, together with some BCs.

In the next section, we prove a vital property of the Green's function for the Laplace operator, namely the symmetry property $G(\boldsymbol{x},\boldsymbol{y}) = G(\boldsymbol{y},\boldsymbol{x})$. This then enables us to check that the proposed convolution (3.2) actually works for all bounded domains (or at least, for the usual 'sensible' ones).

3.3 Symmetry of the Green's function

We prove the following result:

Theorem 3.1 *Let $G(\boldsymbol{x},\boldsymbol{y})$ be the Green's function for the Poisson problem on a bounded open, simply connected domain D with smooth boundary ∂D. Then*

$$G(\boldsymbol{x},\boldsymbol{y}) = G(\boldsymbol{y},\boldsymbol{x}).$$

The proof comes in a series of seemingly irrelevant steps, that gradually converge to a relevant final result. First, we define the following functions:

$$v(\boldsymbol{z}) = G(\boldsymbol{z}, \boldsymbol{x}), \qquad w(\boldsymbol{z}) = G(\boldsymbol{z}, \boldsymbol{y}).$$

We aim to show that $v(\boldsymbol{y}) = w(\boldsymbol{x})$. Consider

$$G(\boldsymbol{z}, \boldsymbol{x}) = G_0(\boldsymbol{z} - \boldsymbol{x}) + h(\boldsymbol{z}; \boldsymbol{x}),$$

where

$$\begin{aligned} \nabla_z^2 h(\boldsymbol{z}; \boldsymbol{x}) &= 0, \qquad \boldsymbol{z} \in D, \\ G_0(\boldsymbol{z} - \boldsymbol{x}) + h(\boldsymbol{z}; \boldsymbol{x}) &= 0, \qquad \boldsymbol{z} \in \partial D. \end{aligned}$$

For $\boldsymbol{z} \in \partial D$ then,

$$v(\boldsymbol{z}) = G(\boldsymbol{z}, \boldsymbol{x}) = G_0(\boldsymbol{z} - \boldsymbol{x}) + h(\boldsymbol{z}; \boldsymbol{x}) = 0.$$

Thus,

$$v(\boldsymbol{z}) = 0, \qquad \boldsymbol{z} \in \partial D.$$

Similarly,

$$w(\boldsymbol{z}) = 0, \qquad \boldsymbol{z} \in \partial D.$$

Now consider the following string of relations, for $\boldsymbol{z} \in D$:

$$\begin{aligned} \nabla_z^2 v &= \nabla_z^2 G(\boldsymbol{z}, \boldsymbol{x}), \\ &= \nabla_z^2 G_0(\boldsymbol{z} - \boldsymbol{x}) + \nabla_z^2 h(\boldsymbol{z}; \boldsymbol{x}), \\ &= \nabla_z^2 G_0(\boldsymbol{z} - \boldsymbol{x}), \\ &= \delta(\boldsymbol{z} - \boldsymbol{x}). \end{aligned}$$

Hence, $\nabla_z^2 v = 0$ unless $\boldsymbol{z} = \boldsymbol{x}$. Indeed, far from $\boldsymbol{z} = \boldsymbol{x}$, $v(\boldsymbol{z})$ will be a smooth function. Similarly, $\nabla_z^2 w = 0$ unless $\boldsymbol{z} = \boldsymbol{y}$, and far from $\boldsymbol{z} = \boldsymbol{y}$, the function $w(\boldsymbol{z})$ will also be smooth.

Consider therefore the following set:

$$\mathcal{V}_\epsilon = \{\boldsymbol{z} \in \mathbb{R}^2 | \boldsymbol{z} \in D - [B(\boldsymbol{x}, \epsilon) \cup B(\boldsymbol{y}, \epsilon)]\}.$$

On this set, the functions $v(\boldsymbol{z})$ and $w(\boldsymbol{z})$ are smooth, so Green's theorem applies:

$$\begin{aligned}\int_{\mathcal{V}_\epsilon} \left[v\nabla_z^2 w - w\nabla_z^2 v\right] \mathrm{d}^2 z &= 0, \\ &= \int_{\partial\mathcal{V}_\epsilon} \left[v\frac{\partial w}{\partial n_z} - w\frac{\partial v}{\partial n_z}\right] \mathrm{d}S_z.\end{aligned}$$

Thus,

$$\int_{\partial\mathcal{V}_\epsilon} \left[v\frac{\partial w}{\partial n_z} - w\frac{\partial v}{\partial n_z}\right] \mathrm{d}S_z = 0.$$

But

$$\int_{\partial\mathcal{V}_\epsilon} = \int_{\partial D} - \left[\int_{\partial B(\boldsymbol{x},\epsilon)} + \int_{\partial B(\boldsymbol{y},\epsilon)}\right],$$

and $v = 0$ and $w = 0$ on ∂D. Hence,

$$\int_{\partial B(\boldsymbol{x},\epsilon)} \left[\frac{\partial w}{\partial n_z}v - \frac{\partial v}{\partial n_z}w\right] \mathrm{d}S_z + \int_{\partial B(\boldsymbol{y},\epsilon)} \left[\frac{\partial w}{\partial n_z}v - \frac{\partial v}{\partial n_z}w\right] \mathrm{d}S_z = 0,$$

or

$$\int_{\partial B(\boldsymbol{x},\epsilon)} \left[\frac{\partial w}{\partial n_z}v - \frac{\partial v}{\partial n_z}w\right] \mathrm{d}S_z = -\int_{\partial B(\boldsymbol{y},\epsilon)} \left[\frac{\partial w}{\partial n_z}v - \frac{\partial v}{\partial n_z}w\right] \mathrm{d}S_z.$$

Multiply both sides by (-1) to obtain the following identity:

$$\int_{\partial B(\boldsymbol{x},\epsilon)} \left[\frac{\partial v}{\partial n_z}w - \frac{\partial w}{\partial n_z}v\right] \mathrm{d}S_z = \int_{\partial B(\boldsymbol{y},\epsilon)} \left[\frac{\partial w}{\partial n_z}v - \frac{\partial v}{\partial n_z}w\right] \mathrm{d}S_z.$$

We show that $LHS = w(\boldsymbol{x})$ and that $RHS = v(\boldsymbol{y})$. Start with the LHS. Consider first the term

$$\int_{\partial B(\boldsymbol{x},\epsilon)} \frac{\partial w}{\partial n_z}v \, \mathrm{d}S_z.$$

The function $w(\boldsymbol{z})$ is smooth near $\boldsymbol{z} = \boldsymbol{x}$ (recall, $\nabla_z^2 w = \delta(\boldsymbol{z} - \boldsymbol{y})$, so $w(\boldsymbol{z})$ will only be problematic near $\boldsymbol{z} = \boldsymbol{y}$). Thus, in the ball $B(\boldsymbol{x}, \epsilon)$, we have

$$\left|\frac{\partial w}{\partial n_z}\right| \leq C(\boldsymbol{x}, \epsilon), \qquad \forall \boldsymbol{z} \in \overline{B(\boldsymbol{x}, \epsilon)},$$

where C is some positive upper bound. Thus,

$$\left|\int_{\partial B(\boldsymbol{x},\epsilon)} \frac{\partial w}{\partial n_z}v \, \mathrm{d}S_z\right| \leq C(\boldsymbol{x}, \epsilon) \left|\int_{\partial B(\boldsymbol{x},\epsilon)} v \, \mathrm{d}S_z\right|.$$

Now, $v = (2\pi)^{-1} \log|\boldsymbol{z} - \boldsymbol{x}| + h(\boldsymbol{z}; \boldsymbol{x})$, where $h(\boldsymbol{z}; \boldsymbol{x})$ is a smooth function. Thus, as $|\boldsymbol{z} - \boldsymbol{x}| \to 0$, we have

$$|v| \sim \frac{1}{2\pi} \left|\log|\boldsymbol{z} - \boldsymbol{x}|\right|.$$

But $|\boldsymbol{z}-\boldsymbol{x}|=\epsilon$ for $\boldsymbol{z}\in\partial B(\boldsymbol{x},\epsilon)$, hence

$$|v|\sim\frac{1}{2\pi}|\log\epsilon|,\qquad \boldsymbol{z}\in\partial B(\boldsymbol{x},\epsilon).$$

Also for $\boldsymbol{z}\in\partial B(\boldsymbol{x},\epsilon)$, $\mathrm{d}S_z=\epsilon\mathrm{d}\theta$, hence

$$\begin{aligned}\left|\int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial w}{\partial n_z}v\,\mathrm{d}S_z\right| &\le C(\boldsymbol{x},\epsilon)\left|\int_{\partial B(\boldsymbol{x},\epsilon)}v\,\mathrm{d}S_z\right|,\\ &\sim C(\boldsymbol{x},\epsilon)\left|\int_{\partial B(\boldsymbol{x},\epsilon)}\left(\frac{1}{2\pi}\log\epsilon\right)\epsilon\,\mathrm{d}\theta\right|,\\ &= C(\boldsymbol{x},\epsilon)\epsilon\log\epsilon,\end{aligned}$$

hence

$$\left|\int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial w}{\partial n_z}v\,\mathrm{d}S_z\right|\to 0,\qquad \text{as } \epsilon\to 0.$$

Thus, in the limit as $\epsilon\to 0$, we are left with

$$LHS=\int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial v}{\partial n_z}w\,\mathrm{d}S_z.$$

But

$$v(\boldsymbol{z})=G_0(\boldsymbol{z}-\boldsymbol{x})+h(\boldsymbol{z};\boldsymbol{x}),$$

and $w(\boldsymbol{z})$ is smooth near $\boldsymbol{z}=\boldsymbol{x}$. Also, $h(\boldsymbol{z},\boldsymbol{x})$ is smooth everywhere for $\boldsymbol{z}\in D$. Thus,

$$\int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial h}{\partial n_z}w\,\mathrm{d}S_z\to 0\qquad\text{as } \epsilon\to 0.$$

Thus, we are left with

$$LHS=\int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial G_0(\boldsymbol{z}-\boldsymbol{x})}{\partial n_z}w(\boldsymbol{z})\,\mathrm{d}S_z.$$

We proceed by direct computation:

$$\begin{aligned}LHS &= \int_{\partial B(\boldsymbol{x},\epsilon)}\frac{\partial G_0(\boldsymbol{z}-\boldsymbol{x})}{\partial n_z}w(\boldsymbol{z})\,\mathrm{d}S_z,\\ &= \frac{1}{2\pi}\left[\int_0^{2\pi}\left(\frac{\partial}{\partial\rho}\log\rho\right)_{\rho=|\boldsymbol{z}-\boldsymbol{x}|}w(\boldsymbol{z})\,\rho\,\mathrm{d}\theta\right]_{|\boldsymbol{z}-\boldsymbol{x}|=\epsilon},\\ &= \left(\frac{1}{2\pi}\int_0^{2\pi}w(\boldsymbol{z})\mathrm{d}\theta\right)_{|\boldsymbol{z}-\boldsymbol{x}|=\epsilon},\\ &\to w(\boldsymbol{x}),\qquad\text{as } \epsilon\to 0.\end{aligned}$$

Similarly, we obtain

$$RHS=v(\boldsymbol{y})\qquad\text{as } \epsilon\to 0,$$

hence $w(\boldsymbol{x}) = v(\boldsymbol{y})$, and the result is shown.

3.4 Checking that the convolution works

We solve the following problem:

$$\begin{aligned} \nabla^2 u(\boldsymbol{x}) &= 0, \qquad \boldsymbol{x} \in D, \\ u(\boldsymbol{x}) &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D, \end{aligned} \tag{3.4}$$

on the domain D. We know that the answer should involve a Green's function, obtained in the following manner:

1. Construct the fundamental solution $G_0(\boldsymbol{x}, \boldsymbol{y})$ on the whole space (e.g. by Fourier transforms);
2. Add a regular solution that solves $\nabla_x^2 h(\boldsymbol{x}, \boldsymbol{y}) = 0$ to soak up the boundary conditions.
3. Call the answer $G(\boldsymbol{x}; \boldsymbol{y})$. Then,

$$\begin{aligned} \nabla_x^2 G(\boldsymbol{x}; \boldsymbol{y}) &= \delta(\boldsymbol{x} - \boldsymbol{y}), \qquad \boldsymbol{x} \in D, \\ G(\boldsymbol{x}; \boldsymbol{y}) &= 0, \qquad \boldsymbol{x} \in \partial D. \end{aligned}$$

To solve Equation (3.4) , we propose the following convolution solution:

$$u(\boldsymbol{x}) = \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) \, \mathrm{d}S_y,$$

$\hat{\boldsymbol{n}}(\boldsymbol{y})$ is the outward-pointing normal on the boundary ∂D, and $\mathrm{d}S_y$ is an element of area. Let's check this ansatz. We work with $\boldsymbol{x} \in D$ first:

$$\begin{aligned} \nabla_x^2 u(\boldsymbol{x}) &= \nabla_x^2 \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) \, \mathrm{d}S_y, \\ &= \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y \left[\nabla_x^2 G(\boldsymbol{x}; \boldsymbol{y}) \right] \, \mathrm{d}S_y, \\ &= \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y \, \delta(\boldsymbol{x} - \boldsymbol{y}) \, \mathrm{d}S_y. \end{aligned}$$

We assume $\boldsymbol{x} \in D$, hence, if $\boldsymbol{y} \in \partial D$ it is impossible for $\boldsymbol{x} - \boldsymbol{y} = 0$, since a boundary point and an interior point cannot coincide. Thus, $\delta(\boldsymbol{x} - \boldsymbol{y}) = 0$ in the second integral, and

$$\nabla_x^2 u(\boldsymbol{x}) = 0.$$

We now work on the boundary condition, taking $\boldsymbol{x} \in \partial D$. On the boundary,

$$u(\boldsymbol{x} \in \partial D) = \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) \, \mathrm{d}S_y.$$

But we have,

$$\begin{aligned}
\int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) \, \mathrm{d}S_y &= \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) \, \mathrm{d}S_y - \underbrace{\int_{\partial D} G(\boldsymbol{x}; \boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y f(\boldsymbol{y}) \, \mathrm{d}S_y}_{=0, \, \boldsymbol{x} \in \partial D}, \\
&= \int_{\partial D} \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \left[f(\boldsymbol{y}) \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) - G(\boldsymbol{x}; \boldsymbol{y}) \nabla_y f(\boldsymbol{y}) \right] \mathrm{d}S_y, \\
&= \int_D \nabla_y \cdot \left[f(\boldsymbol{y}) \nabla_y G(\boldsymbol{x}; \boldsymbol{y}) - G(\boldsymbol{x}; \boldsymbol{y}) \nabla_y f(\boldsymbol{y}) \right] \mathrm{d}^2 y, \\
&\qquad \text{(by Gauss's theorem)} \\
&= \int_D \left[f(\boldsymbol{y}) \nabla_y^2 G(\boldsymbol{x}; \boldsymbol{y}) - G(\boldsymbol{x}; \boldsymbol{y}) \nabla_y^2 f(\boldsymbol{y}) \right] \mathrm{d}^2 y, \\
&\qquad \boldsymbol{x} \in \partial D;\ G(\boldsymbol{x}, \boldsymbol{y}) \text{ vanishes on the boundary} \\
&= \int_D \left[f(\boldsymbol{y}) \nabla_y^2 G(\boldsymbol{x}; \boldsymbol{y}) - 0 \times \nabla_y^2 f(\boldsymbol{y}) \right] \mathrm{d}^2 y, \\
&= \int_D f(\boldsymbol{y}) \left[\nabla_y^2 G(\boldsymbol{x}; \boldsymbol{y}) \right] \mathrm{d}^2 y, \\
&= \int_D f(\boldsymbol{y}) \left[\nabla_y^2 G(\boldsymbol{y}; \boldsymbol{x}) \right] \mathrm{d}^2 y, \qquad \text{(by symmetry)} \\
&= \int_D f(\boldsymbol{y}) \delta(\boldsymbol{x} - \boldsymbol{y}) \, \mathrm{d}^2 y, \\
&= f(\boldsymbol{x}).
\end{aligned}$$

Hence,

$$u(\boldsymbol{x} \in \partial D) = f(\boldsymbol{x}),$$

and the convolution is valid.

3.5 Worked Examples

The aim of this exercise is to compute the so-called **Poisson kernel** for the Poisson problem on the unit disc. Specifically, we seem to solve the following problem:

$$\begin{aligned} \nabla^2 u &= 0, \qquad \boldsymbol{x} \in D, \\ u &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D, \end{aligned} \tag{3.5}$$

where D is the unit disc in $\mathbb{R}^2$ centred at the origin. The proposed approach is a brute-force type effort.

1. Solve Equation (3.5) by completing the following sequence of steps.

> (a) Solve $\nabla^2 u = 0$ on the unit disc by sepration of variables, in polar coordinates, without regard for the boundary conditions.
>
> Hint: For the ODE $r^2 R'' + rR' - n^2 R = 0$, attempt a trial solution $R = r^\alpha$, where α is to be determined.
>
> Answer clue:
>
> $$u(r,\theta) = \sum_{n=-\infty}^{\infty} c_n r^{|n|} \mathrm{e}^{\mathrm{i}n\theta},$$
>
> where the $c_n \in \mathbb{C}$ are arbitrary constants.

Solution: Write $\nabla^2 u = 0$ as

$$u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} = 0,$$

and take $u = R(r)\Theta(\theta)$ to obtain

$$\left(R'' + \frac{1}{r} R' \right) \Theta + \frac{1}{r^2} R \Theta'' = 0.$$

Rearrange:

$$\frac{r^2}{R} \left(R'' + \frac{1}{r} R' \right) + \frac{\Theta''}{\Theta} = 0.$$

Obtain $\Theta = \mathrm{e}^{\mathrm{i}n\theta}$, with $n \in \mathbb{Z}$. Back-substitution:

$$r^2 R'' + rR' - n^2 R = 0.$$

Attempt a solution $R = r^\alpha$. Obtain

$$\alpha(\alpha - 1) + \alpha - n^2 = 0,$$

hence

$$\alpha = \pm n.$$

Choose $\alpha = |n|$ to obtain a bounded solution at $r = 0$. Hence, the general solution is

$$u(r, \theta) = \sum_{n=-\infty}^{\infty} c_n r^{|n|} \mathrm{e}^{\mathrm{i}n\theta},$$

where the $c_n \in \mathbb{C}$ are arbitrary constants.

(b) Write down formulae for the c_n's in terms of the boundary function f. Deduce that

$$u(r, \theta) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} r^{|n|} \mathrm{e}^{\mathrm{i}\theta} \int_0^{2\pi} f(\varphi) \mathrm{e}^{-\mathrm{i}n\varphi} \mathrm{d}\varphi.$$

We have

$$f(\theta) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{\mathrm{i}n\theta},$$

since $r = 1$ at the boundary. But this is a Fourier series, hence

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}n\theta} f(\theta).$$

Hence,

$$u(r, \theta) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} r^{|n|} \mathrm{e}^{\mathrm{i}\theta} \int_0^{2\pi} f(\varphi) \mathrm{e}^{-\mathrm{i}n\varphi} \mathrm{d}\varphi.$$

(c) By reversing the order of the summation in Part (2), as well as other operations, show that

$$u(r,\theta) = \frac{1}{2\pi}\int_0^{2\pi} f(\varphi)\left(\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\right)\mathrm{d}\varphi. \tag{3.6}$$

Take $\Delta = \theta - \varphi$. We have

$$\begin{aligned}
\sum_{n=-\infty}^{\infty} r^{|n|}\mathrm{e}^{\mathrm{i}\Delta n} &= \sum_{n=-\infty}^{0} r^{|n|}\mathrm{e}^{\mathrm{i}\Delta n} + \sum_{n=0}^{\infty} r^{|n|}\mathrm{e}^{\mathrm{i}\Delta n} - 1, \\
&= \sum_{n=0}^{\infty} r^{n}\mathrm{e}^{-\mathrm{i}\Delta n} + \sum_{n=0}^{\infty} r^{n}\mathrm{e}^{\mathrm{i}\Delta n} - 1, \\
&= \frac{1}{1-r\mathrm{e}^{-\mathrm{i}\Delta}} + \frac{1}{1-r\mathrm{e}^{\mathrm{i}\Delta}} - 1, \qquad \ldots \qquad r<1, \\
&= \frac{1-r\mathrm{e}^{\mathrm{i}\Delta n}+1-r\mathrm{e}^{-\mathrm{i}\Delta n}}{1-2r\cos\Delta+r^2} - 1, \\
&= \frac{2-2r\cos\Delta}{1-2r\cos\Delta+r^2} - 1, \\
&= \frac{2-2r\cos\Delta-1+2r\cos\Delta-r^2}{1-2r\cos\Delta+r^2}, \\
&= \frac{1-r^2}{1-2r\cos\Delta+r^2}, \\
&= \frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}.
\end{aligned}$$

Thus,

$$\begin{aligned}
u(r,\theta) &= \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} r^{|n|}\mathrm{e}^{\mathrm{i}\theta}\int_0^{2\pi} f(\varphi)\mathrm{e}^{-\mathrm{i}n\varphi}\mathrm{d}\varphi, \\
&= \frac{1}{2\pi}\int_0^{2\pi} f(\varphi)\sum_{n=-\infty}^{\infty} r^{|n|}\mathrm{e}^{\mathrm{i}(\vartheta-\varphi)n}, \\
&= \frac{1}{2\pi}\int_0^{2\pi} f(\varphi)\left(\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\right)\mathrm{d}\varphi.
\end{aligned}$$

(d) Identify

$$\frac{\partial G(r,\theta;s,\varphi)}{\partial s} := \frac{1}{2\pi}\frac{s^2-r^2}{s^2-2sr\cos(\theta-\varphi)+r^2}.$$

Write $\boldsymbol{x} = r(\cos\theta, \sin\theta)$ and $\boldsymbol{y} = s(\cos\varphi, \sin\varphi)$. Show that

$$\frac{\partial G(\boldsymbol{x},\boldsymbol{y})}{\partial s} = \frac{1}{2\pi}\frac{|\boldsymbol{y}|^2-|\boldsymbol{x}|^2}{|\boldsymbol{x}-\boldsymbol{y}|^2}.$$

Hence, conclude that

$$u(\boldsymbol{x}) = \int_{\partial D} f(\boldsymbol{y})\nabla_y G(\boldsymbol{x},\boldsymbol{y})\cdot \mathrm{d}\boldsymbol{\ell}, \tag{3.7}$$

where D is the unit disc.

For the first part, we have $|\boldsymbol{x}|^2 = r^2$ and $|\boldsymbol{y}|^2 = s^2$. Also,

$$\begin{aligned} |\boldsymbol{x}-\boldsymbol{y}|^2 &= |\boldsymbol{x}|^2 - 2\boldsymbol{x}\cdot\boldsymbol{y} + |\boldsymbol{y}|^2, \\ &= r^2 - 2rs\cos\alpha + s^2, \end{aligned}$$

where α is the angle between $\boldsymbol{x}$ and $\boldsymbol{y}$. But from a sketch of $\boldsymbol{x}$ and $\boldsymbol{y}$ or from experience, $\cos\alpha = \cos(\theta-\varphi)$, hence

$$|\boldsymbol{x}-\boldsymbol{y}|^2 = r^2 - 2rs\cos(\theta-\varphi) + s^2.$$

Hence,

$$\frac{\partial G(r,\theta;s,\varphi)}{\partial s} = \frac{1}{2\pi}\frac{s^2-r^2}{s^2-2sr\cos(\theta-\varphi)+r^2} = \frac{1}{2\pi}\frac{|\boldsymbol{y}|^2-|\boldsymbol{x}|^2}{|\boldsymbol{x}-\boldsymbol{y}|^2}.$$

For the second part, consider

$$\begin{aligned} u(r,\theta) &= \int_0^{2\pi} f(\varphi)\left(\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\right)\mathrm{d}\varphi, \\ &= \int_0^{2\pi} f(\varphi)\left[\frac{\partial G(r,\theta;s,\varphi)}{\partial s}\right]_{s=1}\mathrm{d}\varphi. \end{aligned}$$

On the unit circle $s=1$, and let $\hat{\boldsymbol{n}}$ be the outward-pointing unit normal to the unit circle. We have

$$\begin{aligned} \nabla_y\Phi(s,\varphi)\cdot\mathrm{d}\boldsymbol{\ell} &= \nabla_y\Phi(s,\varphi)\cdot\hat{\boldsymbol{n}}\,\mathrm{d}\varphi, \\ &= \left(\frac{\partial\Phi}{\partial s}\right)_{s=1}\mathrm{d}\varphi. \end{aligned}$$

Hence,

$$u(\boldsymbol{x}) = \int_{\partial D} f(\boldsymbol{y}) \nabla_y G(\boldsymbol{x}, \boldsymbol{y}) \cdot \mathrm{d}\boldsymbol{\ell},$$

where $\boldsymbol{x} = (r\cos\theta, r\sin\theta)$, $\boldsymbol{y} = (s\cos\varphi, s\sin\varphi)$, and where $s = 1$ on ∂D.

The convolution result in Parts (4)–(5) is particular case of the general solution already derived for the Green's function of the Laplace problem. The kernel in Part (4) is called the **Poisson kernel**. Recall, in general, to solve the problem

$$\nabla^2 u = 0, \qquad \boldsymbol{x} \in D, \qquad u(\boldsymbol{x}) = f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D,$$

for a bounded, open, simply-connected domain $D \in \mathbb{R}^n$, one solves the auxiliary problem

$$\begin{aligned} \nabla_x^2 G(\boldsymbol{x}, \boldsymbol{y}) &= \delta(\boldsymbol{x} - \boldsymbol{y}), \qquad \boldsymbol{x} \in D, \\ G(\boldsymbol{x}, \boldsymbol{y}) &= 0, \qquad \boldsymbol{x} \in \partial D. \end{aligned}$$

Then, the solution to the full Poisson problem is available by convolution as follows:

$$u(\boldsymbol{x}) = \int_{\partial D} f(\boldsymbol{y}) \hat{\boldsymbol{n}}(\boldsymbol{y}) \cdot \nabla_y G(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}S_y, \tag{3.8}$$

where $\mathrm{d}S_y$ is an element of surface area on the surface $\partial\Omega$. We have already sketched this more general result in the previous sections of the present Chapter; the particular result of these exercises has been to compute a definite form for Green's function (or equivalently, the Poisson kernel) for the case when the domain D is the unit disc in $\mathbb{R}^2$.

Quantitative example

2. Solve Equation (3.5) with the following quantitative boundary data:

$$u(r=1,\varphi) = h(\varphi) := \begin{cases} 1, & \text{if } 0 < \varphi < \pi, \\ 0, & \text{otherwise.} \end{cases}$$

Using the Poisson kernel results in a horrible integral that is difficult to evaluate. Thus, you might prefer to obtain an equivalent answer by going through the following sequence of steps:

(a) As in Question 1, use Fourier series to show that

$$u(r,\varphi) = \sum_{n=-\infty}^{\infty} c_n r^{|n|} \mathrm{e}^{\mathrm{i}n\varphi},$$

with

$$c_n = \frac{1}{2\pi}\int_0^{\pi} \mathrm{e}^{-\mathrm{i}n\varphi}\mathrm{d}\varphi.$$

Hence, deduce that $c_0 = 1/2$ and that

$$c_n = \begin{cases} \frac{1}{\mathrm{i}\pi n}, & n = \pm 1, \pm 3, \cdots, \\ 0, & n = \pm 2, \pm 4, \cdots. \end{cases}$$

We have

$$\begin{aligned} c_n &= \frac{1}{2\pi}\int_0^{2\pi} f(\varphi)\mathrm{e}^{-\mathrm{i}n\varphi}\mathrm{d}\varphi, \\ &= \frac{1}{2\pi}\int_0^{\pi} \mathrm{e}^{-\mathrm{i}n\varphi}. \end{aligned}$$

For $n = 0$ this is $1/2$. Otherwise, we have

$$c_n = -\frac{1}{2\pi n\mathrm{i}}\left(\mathrm{e}^{-\mathrm{i}n\pi} - 1\right)$$

If n is odd, then $\mathrm{e}^{-\mathrm{i}n\pi} = -1$. If n is even, then $\mathrm{e}^{-\mathrm{i}n\pi} = 1$. Thus,

$$c_n = \begin{cases} \frac{1}{\mathrm{i}\pi n}, & n \text{ odd}, \\ 0, & n \text{ even}, \end{cases}$$

and the result is shown.

(b) Hence, show that

$$u(r,\varphi) = \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\left[\sum_{p=0}^{\infty} \frac{1}{2p+1}\left(r\mathrm{e}^{\mathrm{i}\varphi}\right)^{2p+1} - \mathrm{cc}\right], \qquad r<1.$$

Hence, show that

$$u(r,\varphi) = \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\left[\tanh^{-1}(r\mathrm{e}^{\mathrm{i}\varphi}) - \mathrm{cc}\right].$$

Note that $g(z) = \tanh^{-1}(z)$ has branch cuts emanating from $z = \pm 1$, but $|z| = r < 1$, so the proposed solution is given on an open set on which $g(z)$ is well defined.

From the series solution, we have

$$\begin{aligned}
u(r,\varphi) &= \tfrac{1}{2} + \sum_{n\neq 0} c_n r^{|n|}\mathrm{e}^{\mathrm{i}n\varphi}, \\
&= \tfrac{1}{2} + \sum_{\substack{n\neq 0 \\ n \text{ odd}}} \frac{1}{\mathrm{i}\pi n} r^{|n|}\mathrm{e}^{\mathrm{i}n\varphi}, \\
&= \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\sum_{n=1,3,\cdots} \frac{1}{n} r^{n}\mathrm{e}^{\mathrm{i}n\varphi} + \frac{1}{\mathrm{i}\pi}\sum_{n=-1,-3,\cdots} \frac{1}{n} r^{|n|}\mathrm{e}^{\mathrm{i}n\varphi}, \\
&= \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\sum_{p=0}^{\infty} \frac{1}{2p+1}(r\mathrm{e}^{\mathrm{i}\varphi})^{2p+1} - \frac{1}{\mathrm{i}\pi}\sum_{p=0}^{\infty} \frac{1}{2p+1}(r\mathrm{e}^{-\mathrm{i}\varphi})^{2p+1}, \\
&= \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\left[\sum_{p=0}^{\infty} \frac{1}{2p+1}(r\mathrm{e}^{\mathrm{i}\varphi})^{2p+1} - \mathrm{cc}\right].
\end{aligned}$$

The series should now be obvious. Recall from Leaving Cert.,

$$\begin{aligned}
\frac{1}{1-x^2} &= 1 + x^2 + x^4 + \cdots, \qquad x^2 < 1, \\
\int \frac{1}{1-x^2}\mathrm{d}x &= C + x + \tfrac{1}{3}x^3 + \tfrac{1}{t}x^5 + \cdots, \\
\tanh^{-1} x &= C + x + \tfrac{1}{3}x^3 + \tfrac{1}{5}x^5,
\end{aligned}$$

and the constant is obviously zero because $\tanh^{-1}(0) = 0$. Hence,

$$\tanh^{-1} x = \sum_{p=0}^{\infty} \frac{1}{2p+1} x^{2p+1}, \qquad x^2 < 1.$$

Putting it all together,

$$u(r,\varphi) = \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi}\left(\tanh^{-1}(r\mathrm{e}^{\mathrm{i}\varphi}) - \mathrm{cc}\right), \qquad r<1.$$

(c) Use trigonometric identities (e.g. Abramowitz and Stegun, Chapter 4) and rewrite the solution as

$$u(r,\varphi) = \tfrac{1}{2} + \frac{1}{\pi}\left[\tan^{-1}\left(\frac{2y}{1-r^2}\right) + k\pi\right], \tag{3.9}$$

where $y = r\sin\varphi$ and where k is arbitrary and will be fixed in what follows.

We have (cf. Abramowitz and Stegun, 4.6.28),

$$\tanh^{-1}(z_1) \pm \tanh^{-1}(z_2) = \tanh^{-1}(z)\left(\frac{z_1 \pm z_2}{1 \pm z_1 z_2}\right) + k\pi\mathrm{i}, \qquad k \in \mathbb{Z}.$$

Again using notation from Section 4.6 of Abramowitz and Stegun, we have hence

$$\begin{aligned}
\tanh^{-1}(r\mathrm{e}^{\mathrm{i}\varphi}) - \mathrm{cc} &= \tanh^{-1}\left(\frac{2\mathrm{i}y}{1-r^2}\right) + k\pi\mathrm{i}, \qquad y = r\cos\varphi, \\
&:= \mathrm{Arctanh}(Z), \qquad Z = \frac{2\mathrm{i}y}{1-r^2}, \\
&= -\mathrm{i}\,\mathrm{Arctan}(\mathrm{i}Z), \\
&= +\mathrm{i}\,\mathrm{Arctan}\left(\frac{2y}{1-r^2}\right), \\
&= \mathrm{i}\left[\arctan\left(\frac{2y}{1-r^2}\right) + k\pi\right],
\end{aligned}$$

and finally,

$$u(r,\varphi) = \tfrac{1}{2} + \frac{1}{\pi}\left[\tan^{-1}\left(\frac{2y}{1-r^2}\right) + k\pi\right].$$

(d) Use the following formula for A real:

$$\tan^{-1} A = \begin{cases} -\frac{1}{2}\pi - \tan^{-1}(1/A), & A < 0, \\ \frac{1}{2}\pi + \tan^{-1}(1/A), & A > 0, \end{cases}$$

Use this formula and various values of k in the upper and lower half planes $y > 0$ and $y < 0$ respectively to deduce the following functional form for the solution:

$$u(r,\varphi) = \begin{cases} 1 - \frac{1}{\pi}\tan^{-1}\left(\frac{1-r^2}{2y}\right), & y > 0, \\ \frac{1}{2}, & y = 0, \\ -\frac{1}{\pi}\tan^{-1}\left(\frac{1-r^2}{2y}\right), & y < 0. \end{cases}$$

Plot the solution.

For $y < 0$, we have

$$\begin{aligned} u(r,\varphi) &= \tfrac{1}{2} + \left[-\tfrac{1}{2} - \tfrac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right) + k_1 \right], \\ &= -\tfrac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right) + k_1. \end{aligned}$$

For $y > 0$, we have

$$\begin{aligned} u(r,\varphi) &= \tfrac{1}{2} + \left[\tfrac{1}{2} + \tfrac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right) + k_2 \right], \\ &= -\tfrac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right) + (1 + k_2). \end{aligned}$$

The solution should be continuous across $y = 0$. Also, given $(y = 0 \implies \varphi = 0, \pi)$ and starting with

$$u(r, \varphi = 0, \pi) = \tfrac{1}{2} + \frac{1}{\mathrm{i}\pi} \left[\tanh^{-1}(\pm r) - \mathrm{cc} \right] = 0$$

the solution should be equal to $1/2$ at $y = 0$. With these observations, we take $y \to 0$ through negative values, we get

$$\begin{aligned} u(r,\varphi) &= k_1 - \left[\tfrac{1}{\pi} \lim_{y \to 0^-} \tan\left(\frac{1-r^2}{2y} \right) \right], \\ &= k_1 + \tfrac{1}{2}, \end{aligned}$$

hence $k_1 = 0$. Also, take $y \to 0$ through positive values:

$$\begin{aligned} u(r,\varphi) &= (1 + k_2) - \left[\tfrac{1}{\pi} \lim_{y \to 0^+} \tan\left(\frac{1-r^2}{2y} \right) \right], \\ &= 1 + k_2 - \tfrac{1}{2}, \\ &= \tfrac{1}{2} + k_2. \end{aligned}$$

hence $k_2 = 0$. Put it all together:

$$u(r,\varphi) = \begin{cases} 1 - \frac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right), & y > 0, \\ \frac{1}{2}, & y = 0, \\ -\frac{1}{\pi} \tan^{-1}\left(\frac{1-r^2}{2y} \right), & y < 0. \end{cases}$$

The full two-dimensional solution is plotted in Figure 3.1. The solution is plotted at fixed $x = 1/2$ as a function of y in Figure 3.2. The Matlab codes are also provided.

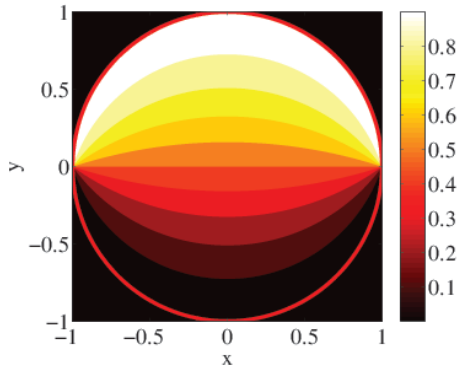


Figure 3.1: Solution of Laplace problem with piecewise boundary conditions.

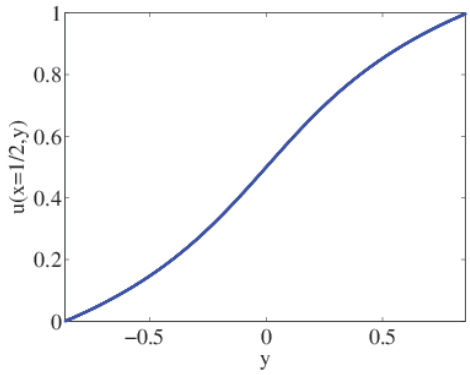


Figure 3.2: Slice of solution of Laplace problem with piecewise boundary conditions through $x = 1/2$. The corresponding y-range is $y \in (-\sqrt{3}/2, \sqrt{3}/2)$.

Matlab functions

```
function [x,y,mysln]=my_laplace(dx)

x=-1:dx:1;
y=-1.1:dx:1.1;

mysln=zeros(length(x),length(y));

for i=1:length(x)
    for j=1:length(y)

        x_val=x(i);
        y_val=y(j);

        r_val=x_val*x_val+y_val*y_val;

        %*****************************************************************

        if(r_val<1)

            if(y_val>0)
                argtan=(1-r_val)/(2*y_val);
                mysln(i,j)=1-(1/pi)*atan(argtan);
            elseif(y_val<0)
                argtan=(1-r_val)/(2*y_val);
                mysln(i,j)=-(1/pi)*atan(argtan);
            else
                mysln(i,j)=1/2;
            end

        end

        %*****************************************************************

    end
end
```

Plot commands

```
[x,y,M]=my_laplace(.001);
[~,hhh]=contourf(x,y,M')
set(hhh,'edgecolor','none')
axis equal
colorbar
colormap hot
yup=sqrt(1-x.^2);
hold on
plot(x,yup,x,-yup,'color','red','linewidth',3)
xlim([-1 1])
ylim([-1 1])
set(gca,'fontsize',18,'fontname','times new roman')
xlabel('x')
ylabel('y')
```

Poisson kernel – further properties

For completeness, we describe further important properties of the **Poisson kernel**

$$P(r,\theta) = \frac{1-r^2}{1-2r\cos\theta + r^2}, \qquad 0 \le r < 1. \tag{3.10}$$

Theorem 3.2 *For $P(r,\theta)$ as given in Equation* (3.10)*, we have*

$$P(r,\theta) = \mathit{Re}\left(\frac{1+re^{i\theta}}{1-re^{i\theta}}\right).$$

The proof is a straightforward computation.

Also:

Theorem 3.3 *For $P(r,\theta)$ as given in Equation* (3.10)*, we have*

$$\int_0^{2\pi} P(r,\theta)\,d\theta = 1, \qquad 0 < r < 1.$$

We compute

$$I = \frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1+re^{i\theta}}{1-re^{i\theta}}\right)d\theta.$$

Let $z = r\mathrm{e}^{\mathrm{i}\theta}$. On the circle $C(r,0)$ of radius r and centre zero, we have

$$\mathrm{d}z = \mathrm{i}r\mathrm{e}^{\mathrm{i}\theta}\mathrm{d}\theta = \mathrm{i}z\mathrm{d}\theta,$$

hence

$$\frac{\mathrm{d}z}{\mathrm{i}z} = \mathrm{d}\theta,$$

and

$$I = \frac{1}{2\pi\mathrm{i}}\oint_{C(0,r)}\left(\frac{1+z}{1-z}\right)\frac{\mathrm{d}z}{z}.$$

The function

$$f(z) = \frac{1}{z}\left(\frac{1+z}{1-z}\right)$$

has simple poles at $z = 0$ and $z = 1$. However, the circle $C(0,r)$ does not enclose the pole located at $z = 1$. Thus, the only pole to consider is at $z = 0$. Near $z = 0$, $f(z)$ has the Laurent expansion

$$f(z) = \frac{1}{z}\left(\frac{1+z}{1-z}\right) = \frac{1}{z}(1+z)\sum_{n=0}^{\infty} z^n = \frac{1}{z} + \text{Taylor series},$$

hence $\mathrm{Res}(f,0) = 1$, hence by Cauchy's theorem,

$$I = 1,$$

and the result is shown.

Crucially, we have the following 'Green's function type result' for the Poisson kernel:

Theorem 3.4 *Let*

$$\begin{aligned} \nabla^2 u &= 0, \qquad (x,y) \in D_0, \\ u &= h(x,y), \qquad (x,y) \in \partial D_0 \end{aligned}$$

have the candidate Poisson-kernel solution

$$u(r,\varphi) = \frac{1}{2\pi}\int_0^{2\pi} h(\theta)\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\mathrm{d}\theta. \tag{3.11}$$

Also, let $h(\varphi)$ be continuous. Then, by direct computation,

$$\lim_{r\to 1} u(r,\varphi) = h(\varphi).$$

Proof: If the denominator in the expression (3.11) is nonzero, then the limit would be vanishing. Thus, the integral in Equation (3.11) has nonzero contributions only for certain ranges of the angle

θ. In detail, the integral has nonzero contributions only in the neighbourhood of that θ-value such that

$$1 - 2\cos(\theta - \varphi) + 1 = 0 \implies \theta = \varphi.$$

Thus,

$$\begin{aligned}
\frac{1}{2\pi}\lim_{r\to 1}\int_0^{2\pi} h(\theta)\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\mathrm{d}\theta = &= \frac{1}{2\pi}\lim_{r\to 1}\int_{\varphi-\epsilon}^{\varphi+\epsilon} h(\theta)\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\mathrm{d}\theta, \\
&= \frac{1}{2\pi}h(\varphi)\lim_{r\to 1}\int_{\varphi-\epsilon}^{\varphi+\epsilon}\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\mathrm{d}\theta, \\
&= \frac{1}{2\pi}h(\varphi)\lim_{r\to 1}\int_0^{2\pi}\frac{1-r^2}{1-2r\cos(\theta-\varphi)+r^2}\mathrm{d}\theta, \\
&= \frac{1}{2\pi}h(\varphi)\lim_{r\to 1}(2\pi), \\
&= h(\varphi).
\end{aligned}$$

Chapter 4

Conformal Mapping

Overview

You may already be familiar with the 'morphisms' for particular mathematical objects. Morphisms are invertible maps between mathematical structures, such that the structure is preserved under the mapping. In linear algebra, (invertible) linear transformations are the relevant morphisms, in group theory, group homomorphisms; in topology, homeomorphpisms, in differential geometry, diffeomorphisms and so on. In complex analysis, the relevant morphisms are called conformal maps. These are invertible, differentiable maps that connect one complex domain to another. These maps will enable us to solve Laplace's equation in arbitrary domains, by conformally mapping the problem to the open unit disc, where the solution is known, via Poisson's kernel.

4.1 Analytic maps

Let

$$g : D \rightarrow D', \tag{4.1}$$

$$z \mapsto g(z) := \zeta \tag{4.2}$$

be an analytic function on the open domain $D \in \mathbb{C}$. We specify further that $g(z)$ should be invertible with an analytic inverse defined on the (open) set D'. (Note: D' is necessarily open – why?). In other words, we specify that $g^{-1}(\zeta)$ exists and is analytic on D'. This requirement means that D cannot contain any critical points of $g(z)$:

Theorem 4.1 *Let $g(z)$ be given as in Equation* (4.2)*. Then the domain D contains no critical points: $g'(z) \neq 0$, for all $z \in D$.*

Proof:

We have

$$g^{-1}(g(z)) = z.$$

Differentiate both sides and use the Chain Rule:

$$1 = \left[\frac{d}{d\zeta}g^{-1}(\zeta)\right]\frac{dg}{dz}.$$

Hence,

$$\frac{d}{d\zeta}g^{-1}(\zeta) = \frac{1}{g'(z)}, \tag{4.3}$$

as in ordinary real-variable calculus. By assumption, $(d/d\zeta)g^{-1}(\zeta)$ exists everywhere in D', hence the R.H.S. of Equation (4.3) exists, hence $g'(z) \neq 0$.

Definition 4.1 *We call a map between domains D and D' of the type* (4.2) *an* **analytic map**.

Examples

1. Consider the following translation:

$$\zeta = z + \beta = (x + a) + \mathrm{i}(y + b), \tag{4.4}$$

   where $\beta = a + \mathrm{i}b$ is a constant complex number. The effect of this map is to translate the entire complex plane by the distance and by the direction specficied by the vector $(a, b)^T$. Also, the map (4.4) maps the disc $|z + \beta| < 1$ of radius 1 and centre $-\beta$ to the unit disc $|\zeta| < 1$.

2. The scaling

$$\zeta = \rho z = \rho(x + \mathrm{i}y), \qquad \rho \in \mathbb{R}^+$$

   maps the disc $|z| < 1/\rho$ to the unit disc $|\zeta| < 1$.

3. The rotation

$$\zeta = \mathrm{e}^{\mathrm{i}\varphi}z, \qquad \varphi \in \mathbb{R},$$

   maps the unit disc to the unit disc, and rotates an arbitrary point z by an angle φ about the origin.

4. The **affine transformation**

$$\zeta = \alpha z + \beta, \qquad \alpha \neq 0 \tag{4.5}$$

is an invertible map analytic on the entire complex plane, with inverse

$$z = \alpha^{-1}(\zeta - \beta),$$

also analytic on the entire complex plane. Note also that the affine transformation is a composition:

- First, a rotation, through an angle $\arg(\alpha)$.
- Next, a scaling, by an amount $\rho = |\alpha|$.
- Finally, a translation, through β.

The affine transformation (4.5) maps the disc $|\alpha z + \beta| < 1$ centred at $-\beta/\alpha$ and of radius $1/|\alpha|$ to the unit disc $|\zeta| < 1$.

5. Consider the following map:

$$\zeta = \frac{1}{z}.$$

Or, writing $\zeta = \xi + \mathrm{i}\eta$ and $z = x + \mathrm{i}y$,

$$\xi = \frac{x}{x^2 + y^2}, \qquad \eta = -\frac{y}{x^2 + y^2}.$$

If we take D to be the punctured complex plane (with the origin removed), then $g(z) = 1/z$ is analytic on D. Also, the inverse exists, with

$$z = \frac{1}{\zeta}.$$

Hence, $g(z) = 1/z$ maps the punctured complex plane to itself. Also,

$$\frac{dg}{dz} = -\frac{1}{z^2} \neq 0, \qquad z \in D,$$

hence the map is analytic on D.

Consider also the set $E = \{|z| > \rho\}$. Then the image of this set under the map $g(z)$ is the set

$$g(E) = \{\zeta \,|\, |\zeta| < \rho\}.$$

Thus, in particular, $g(z)$ maps the exterior of the unit disc to the punctured unit disc and as such, $g(z)$ can be thought of as in 'inversion' of the complex plane.

6. Consider the complex exponential:

$$\zeta = g(z) = \mathrm{e}^z.$$

This function satisfies the condition $g'(z) \neq 0$ everywhere on the complex plane, and moreover, $g(z)$ is itself analytic on the entire complex plane. However, the exponential function is not one-to-one, since

$$\mathrm{e}^{z+2\pi \mathrm{i}n} = \mathrm{e}^z \qquad n \in \mathbb{Z}.$$

Thus, the condition $g'(z) \neq 0$ is necessary but not sufficient for a generic map $g(z)$ to be invertible.

However, if we restrict the domain D to be the horizontal open strip

$$D = \{z = x + \mathrm{i}y \in \mathbb{C} | -\infty < x < \infty, 0 < y < 2\pi\},$$

then $g(z)$ is one-to-one on this (open) domain, hence $g(z)$ is an analytic map on D. Note the strict inequalities here: these are needed to make D into an open domain.

We compute the image of D under $g(z)$. We write $\zeta = \xi + \mathrm{i}\eta$ and $z = x + \mathrm{i}y$. We have

$$\xi = \mathrm{e}^x \cos y, \qquad \eta = \mathrm{e}^x \sin y, \qquad 0 < y < 2\pi.$$

Letting x run over the entire real line and y run between the closed interval $[0, 2\pi]$, all points in $\mathbb{R}^2$ are traced out. However, we are not allowed to do this, as $y = 0, 2\pi$ is excluded. Thus, the line $\xi > 0$ is excluded from D'. Also, the point $(\xi, \eta) = (0, 0)$ is excluded, since this corresponds to $x = -\infty$ in D. Thus, D' is the set

$$D' = \mathbb{C} - \{\xi \geq 0\}.$$

Thus, D' contains a branch cut – precisely the same branch cut that was required to make the complex-valued logarithm into a single-valued function. This is not a coincidence (why?).

Consider now instead the following strip:

$$D = \{z = x + \mathrm{i}y \in \mathbb{C} | -\infty < x < \infty, 0 < y < a\},$$

where $0 < a < 2\pi$. As before, under the exponential map, points in D are given the following ζ-coordinates:

$$\xi = \mathrm{e}^x \cos y, \qquad \eta = \mathrm{e}^x \sin y, \qquad 0 < y < a,$$

where $-\infty < x < \infty$. Thus, D' is a wedge ('pizza slice'). Using polar coordinates (ρ, θ), the wedge D' extends from the origin out to $\rho = \infty$, and extending also from $\theta = 0$ to $\theta = a$.

4.2 Conformal maps

Definition 4.2 *Let $g(z) : D \to D'$ be an analytic map. Then $g(z)$ is called* **conformal** *if it preserves angles.*

Now, we need to clarify what we mean by 'preserving angles'. For, it is not necessary that $g(z)$ be a linear function. Thus, vectors in $\mathbb{R}^2$ will not necessarily be mapped to vectors under $g(z)$. However, the angle between curves is a well-defined quantity both before and after the transformation $g(z)$. We therefore develop the notion of curves in $\mathbb{C}$ and formulate the notion of the angle between two curves, at a point of intersection.

As in real space, a curve γ in $\mathbb{C}$ is a one-parameter smooth map:

$$\begin{aligned} \gamma : I &\to \mathbb{C}, \\ t &\mapsto z = \gamma(t), \end{aligned}$$

where I is a closed interval, $\gamma(t)$ is a differentiable function of the single real variable t, and where $\dot{\gamma}(t) \neq 0$, for all $t \in I$. As usual, we write the parametrized curve as $\gamma(t) \equiv z_\gamma(t) \equiv z(t)$. We identify $z(t)$ with the relevant coordinate pair $(x(t), y(t))$: this is a point on the curve. Similarly, $\dot{z}(t)$ is identified with the pair $(\dot{x}(t), \dot{y}(t))$; this is a tangent vector to the curve at the point $(x(t), y(t))$. The unit tangent vector is

$$\hat{\boldsymbol{t}} = \frac{(\dot{x}(t), \dot{y}(t))}{\sqrt{\dot{x}(t)^2 + \dot{y}(t)^2}} = \frac{(\dot{x}(t), \dot{y}(t))}{|\dot{z}|}.$$

Thus, the curve is degenerate at a point if $|\dot{z}| = 0$ there, since then a unit tangent vector cannot be ascribed to the curve at the same point (e.g. cusps).

Suppose that two curves, written here as $z_1(t)$ and $z_2(t)$ intersect at a point t_0:

$$z_1(t_0) = z_2(t_0) := z_0.$$

The angle between the x-axis and the tangent vector of the z_1-curve at t_0 is

$$\theta_1 = \arg(\dot{z}_1(t_0));$$

similarly,

$$\theta_2 = \arg(\dot{z}_2(t_0)).$$

The angle between the two curves at their point of intersection is thus

$$\theta = \theta_2 - \theta_1 = \arg(\dot{z}_2(t_0)) - \arg(\dot{z}_1(t_0)).$$

Next, consider the effect of an analytic map $\zeta = g(z)$ on the curves z_1 and z_2. The curve z_1 will be mapped two a new curve $\zeta_1(t) = g(z_1(t))$; similarly, we shall obtain a second mapped curve $\zeta_2 = g(z_2(t))$. We compute the velocity vectors of the new curves using the chain rule:

$$\dot{\zeta}_i(t) = g'(z_i(t))\dot{z}_i(t), \qquad i = 1, 2, \qquad g'(z_i(t)) \neq 0. \tag{4.6}$$

Interestingly,

$$|\dot{\zeta}_i| = |g'(z)||\dot{z}_i|, \qquad i = 1, 2.$$

Thus, the speed of the mapped curve is proportional to the speed of the original curve, and the proportionality factor is **totally independent of the details of the particular curve** and depends only on location in space. In other words, all curves passing through a particular point z are sped up or slowed down by the same factor, $|g'(z)|$. Similarly, for from Equation (4.6) applied to arguments,

$$\arg(\dot{\zeta}_i(t)) = \arg(g'(z)) + \arg(\dot{z}_i(t)), \qquad i = 1, 2.$$

Thus, the tangent vectors for all curves passing through a particular point z get rotated by the same amount, $\arg(g'(z))$, independent of the details of the curves themselves! Calling $\psi_i = \arg(\zeta_i(t_0))$, we have

$$\begin{aligned}\psi_2 - \psi_1 &= \arg(\dot{\zeta}_2(t_0)) - \arg(\dot{\zeta}_1(t_0)) \\ &= [\arg(g'(z_0)) + \arg(\dot{z}_2(t))] - [\arg(g'(z_0)) + \arg(\dot{z}_1(t))] = \arg(\dot{z}_2(t_0)) - \arg(\dot{z}_1(t_0)) = \theta,\end{aligned}$$

which is the same as the angle between the two original curves. Thus, we have shown the following result:

Theorem 4.2 *If $\zeta = g(z)$ is an analytic map, then it is a conformal map.*

The converse is also true: all angle-preserving planar transformations can be associated with an analytic map. This is given below in the worked examples.

Finally, conformal mapping is extremely useful, because of the celebrated **Riemann mapping theorem**, which we merely state here:

Theorem 4.3 (Riemann) *Let $D \subset \mathbb{C}$ be a simply-connected open subset of $\mathbb{C}$, with $D \neq \mathbb{C}$. Then, there exists an analytic map that maps D to the open unit disc.*

This is an extremely powerful theorem that states that **any** open simply-connected subset of the complex plane (but not the complex plane itself) can be mapped conformally to the open unit disc. The proof of the theorem is an existence-type proof, and gives no hint of how to construct the conformal map. Also, the analytic map is not unique. For example, suppose I have a conformal map

g between the domain D and the open disc D_0. I could choose first to map D to itself conformally, and then to map D conformally to an intermediate domain D', followed by a further conformal map to D_0. Just for good measure, I could then conformally map D_0 to itself by a further conformal map. The composition of these maps would be another conformal map from D to D_0, different from g. Indeed, there is an infinite variety of such combinations. Thus, conformal maps from a domain D to the unit disc are far from unique. Also, in practice, finding the conformal map is very difficult. But at least we know it is possible.

4.3 Application to Harmonic Functions and Laplace's Equation

We have shown already that conformal mapping preserves both the analytical and the geometrical structures in the complex plane. We now show that conformal mapping also preserves harmonicity. Thus, given an analytic map and a harmonic function on a certain domain, then the mapped function on the mapped domain is also harmonic. This is a very useful result (which we prove below), because instead of solving the Laplace problem in a complicated domain, we can choose instead to map the problem conformally to a relatively simple domain, where the solution is known.

We start with the following theorem:

Theorem 4.4 *Let $\zeta = \xi + \mathrm{i}\eta$ and let $U(\xi, \eta)$ be a harmonic function of ζ, η, and let the following analytic map be given:*

$$\zeta = g(z), \qquad z = x + \mathrm{i}y.$$

Then the composition

$$u(x, y) = U(\xi(x, y), \eta(x, y))$$

is a harmonic function of x and y.

The proof is a straightforward application of the chain rule:

$$\frac{\partial u}{\partial x} = \frac{\partial U}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial U}{\partial \eta}\frac{\partial \eta}{\partial x}, \qquad \frac{\partial u}{\partial y} = \frac{\partial U}{\partial \xi}\frac{\partial \xi}{\partial y} + \frac{\partial U}{\partial \eta}\frac{\partial \eta}{\partial y}.$$

Also,

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2} &= \frac{\partial^2 U}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial^2 U}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2 + 2\frac{\partial^2 U}{\partial \eta \partial \xi}\frac{\partial \eta}{\partial x}\frac{\partial \xi}{\partial x} + \frac{\partial U}{\partial \xi}\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial U}{\partial \eta}\frac{\partial^2 \eta}{\partial x^2}, \\
\frac{\partial^2 u}{\partial y^2} &= \frac{\partial^2 U}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2 + \frac{\partial^2 U}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2 + 2\frac{\partial^2 U}{\partial \eta \partial \xi}\frac{\partial \eta}{\partial y}\frac{\partial \xi}{\partial y} + \frac{\partial U}{\partial \xi}\frac{\partial^2 \xi}{\partial y^2} + \frac{\partial U}{\partial \eta}\frac{\partial^2 \eta}{\partial y^2}.
\end{aligned}$$

Now, $\zeta = \xi + \mathrm{i}\eta = g(z)$ is an analytic function, hence

$$\frac{\partial \xi}{\partial x} = \frac{\partial \eta}{\partial y}, \qquad \frac{\partial \xi}{\partial y} = -\frac{\partial \eta}{\partial x}.$$

Thus, the expressions for u_{xx} and u_{yy} are re-arranged as follows:

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2} &= \frac{\partial^2 U}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial^2 U}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2 + 2\frac{\partial^2 U}{\partial \eta \partial \xi}\frac{\partial \eta}{\partial x}\frac{\partial \xi}{\partial x} + \frac{\partial U}{\partial \xi}\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial U}{\partial \eta}\frac{\partial^2 \eta}{\partial x^2}, \\
\frac{\partial^2 u}{\partial y^2} &= \frac{\partial^2 U}{\partial \xi^2}\left(\frac{\partial \xi}{\partial y}\right)^2 + \frac{\partial^2 U}{\partial \eta^2}\left(\frac{\partial \eta}{\partial y}\right)^2 - 2\frac{\partial^2 U}{\partial \eta \partial \xi}\frac{\partial \eta}{\partial x}\frac{\partial \xi}{\partial x} + \frac{\partial U}{\partial \xi}\frac{\partial^2 \xi}{\partial y^2} + \frac{\partial U}{\partial \eta}\frac{\partial^2 \eta}{\partial y^2}.
\end{aligned}$$

Add them up in an obvious way now:

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 U}{\partial \xi^2}\left[\left(\frac{\partial \xi}{\partial x}\right)^2 + \left(\frac{\partial \xi}{\partial y}\right)^2\right] + \frac{\partial^2 U}{\partial \eta^2}\left[\left(\frac{\partial \eta}{\partial x}\right)^2 + \left(\frac{\partial \eta}{\partial y}\right)^2\right] \\
+ \frac{\partial U}{\partial \xi}\left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2}\right) + \frac{\partial U}{\partial \eta}\left(\frac{\partial^2 \eta}{\partial x^2} + \frac{\partial^2 \eta}{\partial y^2}\right).
\end{aligned}$$

The terms along the bottom line here vanish: $\zeta = \xi + \mathrm{i}\eta = g(z)$ is an analytic function, hence $\xi(x, y)$ and $\eta(x, y)$ are harmonic. Also, by Cauchy–Riemann,

$$\left(\frac{\partial \xi}{\partial x}\right)^2 + \left(\frac{\partial \xi}{\partial y}\right)^2 = \left(\frac{\partial \xi}{\partial x}\right)^2 + \left(\frac{\partial \eta}{\partial x}\right)^2 = \left|\frac{\partial g}{\partial x}\right|^2 = \left|\frac{dg}{dz}\right|^2,$$

where the last result follows because the complex derivative is indendent of approach. Similarly,

$$\left(\frac{\partial \eta}{\partial x}\right)^2 + \left(\frac{\partial \eta}{\partial y}\right)^2 = \left|\frac{dg}{dz}\right|^2,$$

hence

$$\nabla^2 u = |g'(z)|^2 \nabla^2 U.$$

Thus, if U is harmonic in the (ξ, η) variables, then u is harmonic in the (x, y) variables. Conformal mapping preserves harmonicity.

The way forward for solving Laplace's problem is now clear. Suppose we are to solve the following difficult Dirichlet problem:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \qquad (x, y) \in D, \qquad u = h(x, y), \qquad (x, y) \in \partial D,$$

where $D \neq \mathbb{C}$ is an open simply connected (but not necessarily bounded) domain. We endeavour to construct a conformal mapping (which must exist, by the Riemann Mapping Theorem), $\zeta = g(z)$, such that $g(D) = D_0$, where D_0 is the open unit disc. Under the conformal map, we have

$U(\xi,\eta) = u(x(\xi,\eta), y(\xi,\eta))$, and

$$\frac{\partial^2 U}{\partial \xi^2} + \frac{\partial^2 U}{\partial \eta^2} = 0, \qquad (\xi,\eta) \in D_0, \tag{4.7a}$$

with the following boundary data on the unit circle:

$$U = h(x(\xi,\eta), y(\xi,\eta)) := H(\xi,\eta), \qquad (\xi,\eta) \in \partial D_0. \tag{4.7b}$$

Equation (4.7) is relatively easy to solve – we have already done so, using the Poisson kernel. Thus, the strategy is clear:

1. Start with Laplace's equation on a 'difficult' simply-connected domain $D \neq \mathbb{C}$.
2. Find a conformal mapping to map D to the unit disc D_0 (difficult, but it must exist).
3. Solve Laplace's equation on the unit disc using the Poisson kernel.
4. Invert the transformation to find the solution valid on the original domain D.

We consider two examples of this procedure in the remainder of this section.

Example 1 Consider the following Dirchlet problem on the positive half-plane:

$$\nabla^2 u = 0, \qquad x > 0, \qquad u(x=0,y) = h(y).$$

In the worked examples below, it is shown in detail that the map $\zeta = g(z)$, with

$$g(z) = \frac{z-1}{z+1}$$

takes the positive half-plane in xy-space into the open unit disc in $\xi\eta$ space. Thus, we let

$$U(\xi,\eta) = u(x(\xi,\eta), y(\xi,\eta)),$$

with

$$\nabla^2 U = 0, \qquad (\xi,\eta) \in D_0.$$

Polar coordinates in (ξ,η) are appropriate for the boundary of D_0: we let $\xi = \sqrt{\xi^2+\eta^2}\cos\varphi$ and $\eta = \sqrt{\xi^2+\eta^2}\sin\varphi$. Thus, on the boundary,

$$U = H(\varphi), \qquad (\xi,\eta) \in \partial D_0, \qquad 0 \leq \varphi < 2\pi.$$

It is instructive to connect $H(\varphi)$ to the original boundary condition involving the function $h(y)$.

From the worked examples in Section 4.5 below, we have

$$\xi = \frac{x^2 + y^2 - 1}{(x+1)^2 + y^2}, \qquad \eta = \frac{2y}{(x+1)^2 + y^2}.$$

However, the inverse of this relation is more useful here. We have

$$\zeta = \frac{z-1}{z+1} \implies z = \frac{1+\zeta}{1-\zeta} = \frac{(1+\zeta)(1-\overline{\zeta})}{|1-\zeta|^2} = \frac{1+\zeta-\overline{\zeta}-|\zeta|^2}{|1-\zeta|^2}.$$

With $\zeta = \xi + \mathrm{i}\eta$, this becomes

$$z = x + \mathrm{i}y = \frac{1 - \xi^2 - \eta^2 + 2\mathrm{i}\eta}{(\xi-1)^2 + \eta^2}. \tag{4.8}$$

Hence,

$$y = \frac{2\eta}{(\xi-1)^2 + \eta^2}.$$

Now, on the boundary ∂D_0, we have

$$y = \frac{2\sin\varphi}{(\cos\varphi - 1)^2 + \sin\varphi^2} = \frac{2 \cdot 2\sin\varphi/2\cos\varphi/2}{2(1-\cos\varphi)} = \frac{2\sin\varphi/2\cos\varphi/2}{1-\cos\varphi} = \frac{2\sin\varphi/2\cos\varphi/2}{2\sin^2\varphi/2} = \cot\varphi/2.$$

Hence, the boundary data on ∂D_0 are

$$H(\varphi) = h(\cot\varphi/2),$$

and the simple problem to solve is now the following:

$$\nabla^2 U = 0, \qquad (\xi,\eta) \in D_0, \qquad U = h(\cot\varphi/2), \qquad (\xi,\eta) = (\cos\varphi, \sin\varphi) \in \partial D_0.$$

Let us be specific and take the following example of a particular boundary function, with

$$h(y) = \begin{cases} 1, & y > 0, \\ 0, & y < 0. \end{cases}$$

In the transformed coordinates,

$$H(\varphi) = \begin{cases} 1, & 0 < \varphi < \pi, \\ 0, & \pi < \varphi < 2\pi. \end{cases} \tag{4.9}$$

We shudder at applying Poisson's kernel directly to Equation (4.9); instead, we use the results from

the worked examples in Chapter 3

$$U(\xi,\eta) = \tfrac{1}{2} + \frac{1}{\pi}\left[\tan^{-1}\left(\frac{2\eta}{1-\xi^2-\eta^2}\right) + k\pi\right]$$

where $(\xi,\eta) = \rho(\cos\varphi, \sin\varphi)$, and k is our old friend the arbitrary integer. Using Equation (4.8), this simpifies to

$$u(x,y) = \tfrac{1}{2} + \frac{1}{\pi}\left[\tan^{-1}(y/x) + k\pi\right],$$

and the explicit dependence on the variable integer k is removed by rewriting this as

$$u(x,y) = \tfrac{1}{2} + \frac{1}{\pi}\mathrm{Arg}(x+\mathrm{i}y), \tag{4.10}$$

with branch cut placed on the negative real axis (i.e. conveniently located outside of the domain of the PDE); Equation (4.10) is the solution to $\nabla^2 u = 0$ on the half plane $x > 0$ and $-\infty < y < \infty$.

4.4 Mapping to the annulus

The Riemann Mapping Theorem does not apply to non-simply-connected domains: it is impossible to map a non-simply-connected domain to the unit disc in a smooth way. In this section we consider conformal maps from non-simply-connected domains to a two-parameter annulus

$$A_{r,R} = \{r < |\zeta| < R\}, \tag{4.11}$$

assumed to be centred at the origin. The case $r = 0$ corresponds to a punctured disc, while setting $R = \infty$ gives the exterior of a disc of radius r. It can be shown that any other domain with a single hole can be conformally mapped to an annulus. The annular radii r, R are not uniquely specified: in particular, the linear map $\xi = \alpha z$ maps the annulus (4.11) to a rescaled annulus $A_{\rho r,\rho R}$, with $\rho = |\alpha|$, where the inner and outer radii have both been scaled by a factor $\rho = |\alpha|$. Note, however, the ratio r/R of the inner to outer radii is still uncahged. Indeed, this is uniquely specified, and annuli with different ratios **cannot** be mapped to each other by a conformal map. Here, if $r = 0$ or $r = \infty$ (but not both), then $r/R = 0$ by convention. The punctured plane, with $r = 0$ and $R = \infty$ is a separate case.

In the following example a conformal mapping is constructed that takes us from an annulus where the two bounding circles are non-concentric, to a concentric annulus of the form (4.11). Thus, we start with the domain

$$D - \{|z| < 1 \text{ and } |z-c| > c\}$$

with c real and $c < 1/2$ such that the inner, offset circle $|z-c| < c$ stays firmly inside the outer

circle of radius 1, centred at the origin. Note that the centre of the inner circle lies at $x = c, y = 0$, with one extremity of the circle coinciding with the origin. Looking again at the worked examples in Section 4.5 below, we see that the linear fractional mapping

$$\zeta = g(z), \qquad g(z) = \frac{z - \alpha}{\overline{\alpha} z - 1}, \qquad |\alpha| < 1,$$

maps the unit disc to itself, yet shifts the origin by an amount α. This map therefore seems like a good candidate to take the off-centre annulus into a concentric one. In particular, we would like the extremities of the mapped inner circle to lie at $\pm r$ along the x-axis. In other words,

$$z = (0, 0) \to r, \qquad z = (2c, 0) \to -r.$$

Thus,

$$\begin{aligned} r &= g(0), \\ &= \alpha, \end{aligned}$$

and

$$\begin{aligned} -r &= g(2c), \\ &= \frac{2c - \alpha}{2c\alpha - 1}. \end{aligned}$$

One eliminates r to find

$$-\alpha = \frac{2c - \alpha}{2c - 1},$$

or

$$\alpha = \frac{1 \pm \sqrt{1 - 4c^2}}{2c}.$$

Now, the linear fractional map maps the unit disc to itself (see Section 4.5 below, Question 3), hence the extremities of the outer circle at $x = \pm 1$ are preserved. Thus, the mapped inner circle, now centred at the origin, must be of radius $r < 1$. Since $0 < c < 1/2$ is positive, the positive sign is therefore inadmissible here, hence

$$\alpha = \frac{1 - \sqrt{1 - 4c^2}}{2c},$$

and

$$\zeta = g(z), \qquad g(z) = \frac{z - 1 + \sqrt{1 - 4c^2}}{(1 - \sqrt{1 - 4c^2})z - 2c}.$$

Note, the radius of the mapped inner circle is $r = \alpha \neq c$, so that the size of the inner circle is not preserved under the mapping. Note, however, that the outermost circle, being the boundary of the

unit disc, is preserved.

Finally, for the following example, we note that taking $c = 2/5$ gives the conformal map

$$g(z) = \frac{2z-1}{z-2}.$$

We now use this theory to solve the following PDE:

$$\nabla^2 u = 0, \qquad (x,y) \in D,$$

where D is the open annular domain enclosed within the following circles:

$$\begin{aligned} C_{\text{in}} &: \left|z - \tfrac{2}{5}\right| = \tfrac{2}{5}, \\ C_{\text{out}} &: |z| = 1, \end{aligned}$$

and where the following boundary conditions are imposed:

$$\begin{aligned} \text{on } C_{\text{in}} &: u = b, \\ \text{on } C_{\text{out}} &: u = a. \end{aligned}$$

We conformally map the domain D to the annulus D' where the bounding circles are concentric, with

$$\begin{aligned} C'_{\text{in}} &: |\zeta| = r, \\ C'_{\text{out}} &: |\zeta| = 1; \end{aligned}$$

with

$$r = \frac{1-\sqrt{1-4c^2}}{2c}, \qquad c = \tfrac{2}{5} \implies r = \tfrac{1}{2}.$$

For the concentric annulus, the only radially-symmetric solution of Laplace's equation is

$$\begin{aligned} U(\xi,\eta) &= A\log|\zeta| + B, \qquad |\zeta| = \sqrt{\xi^2+\eta^2}, \\ &= \tfrac{1}{2}A\log(\xi^2+\eta^2) + B, \end{aligned}$$

where A and B are complex constants. The boundary conditions are

$$\begin{aligned} \text{on } C'_{\text{in}} &: U = b, \\ \text{on } C'_{\text{out}} &: U = a. \end{aligned}$$

Hence,

$$U(\xi,\eta) = \frac{b-a}{2\log 2}\log(\xi^2+\eta^2) + b.$$

Using the results from the worked examples below in Section 4.5, with $\alpha = r = 1/2$, this becomes

$$u(x,y) = \frac{b-a}{2\log 2}\log\left(\frac{(2x-1)^2+4y^2}{(x-2)^2+y^2}\right) + b.$$

4.5 Worked examples

1. Recall the following problem from the previous work on Laplace's equation:

   Consider the following Dirichlet problem:

   $$\begin{aligned} \nabla^2\Phi &= 0, \qquad (x,y) \in D, \\ \Phi &= \text{Const.}, \qquad (x,y) \in \partial D, \end{aligned}$$

   where $D \subset \mathbb{R}^n$ is open, bounded, simply connected. Show that $\Phi = \text{Const.}$ everywhere in D.

   Specialize to dimension $n = 2$ and extend to all simply-connected domains $D \neq \mathbb{C}$. Use the Riemann Mapping Theorem and the Poisson kernel to construct an equivalent proof of this statement in this particular special case.

By the Riemann mapping theorem there exists an analytic map $\zeta = g(z)$, such that $g(D) = D_0$, the open unit disc. Take $\zeta = \xi + \mathrm{i}\eta$, and let

$$U(\xi,\eta) = \Phi(x(\xi,\eta), y(\xi,\eta)).$$

Thus, U is harmonic on the open unit disc. Take $\Phi = h(x,y)$ on ∂D, with $h = \text{Cont.}$.

$$U(\xi,\eta) = h(x(\xi,\eta), y(\xi,\eta)) = \text{Const.}, \qquad (\xi,\eta) \in \partial D_0.$$

Take $U(\xi,\eta) = C$ on ∂D_0. By the Poisson kernel,

$$U(r,\varphi) = \int_0^{2\pi} C\left[\frac{r^2-1}{r^2-2r\cos(\theta-\varphi)+1}\right]\mathrm{d}\varphi = C, \qquad r<1, \qquad 0 \le \varphi < 2\pi.$$

Hence,

$$U(\xi,\eta) = C, \qquad (\xi,\eta) \in D_0.$$

But

$$\Phi(x(\xi,\eta), y(\xi,\eta)) = U(\xi,\eta) = C,$$

hence $\Phi(x,y) = C$ on D also, and the result is shown.

2. Consider the following map:

$$\zeta = g(z), \qquad g(z) = \frac{z-1}{z+1}.$$

(a) Let $z = x + \mathrm{i}y$ and $\zeta = \xi + \mathrm{i}\eta$. Show that

$$\xi = \frac{x^2+y^2-1}{(x+1)^2+y^2}, \qquad \eta = \frac{2y}{(x+1)^2+y^2}.$$

(b) Obtain the domain D and the image $g(D)$ that make $g(z)$ into an analytic map.

(c) Show that the map $g(z)$ maps the positive half-plane $\{\mathsf{Re}(z) > 0\}$ into the unit disc $|\zeta| < 1$.

(a) We have

$$\begin{aligned}
\xi + \mathrm{i}\eta &= \frac{z-1}{z+1}, \\
&= \frac{(z-1)(\overline{z}+1)}{(z+1)(\overline{z}+1)}, \\
&= \frac{|z|^2 - 1 + z - \overline{z}}{|z|^2 + 1 + z + \overline{z}}, \\
&= \frac{|z|^2 - 1 + 2\mathrm{i}\,\mathsf{Im}(z)}{|z|^2 + 1 + 2\,\mathsf{Re}(z)}, \\
&= \frac{x^2+y^2-1+2y\mathrm{i}}{x^2+y^2+1+2x}, \\
&= \frac{x^2+y^2-1+2y\mathrm{i}}{(x+1)^2+y^2}.
\end{aligned}$$

Equate real and imaginary parts:

$$\xi = \frac{x^2+y^2-1}{(x+1)^2+y^2}, \qquad \eta = \frac{2y}{(x+1)^2+y^2}.$$

(b) The point $z = -1$ must be excluded from the domain. Also,

$$\begin{aligned} g'(z) &= \frac{(z+1)-(z-1)}{(z+1)^2}, \\ &= \frac{2}{(z+1)^2}, \end{aligned}$$

which is never zero. Thus, $D = \mathbb{C} - \{1\}$. By straightforward computation, the inverse is

$$z = \frac{1+\zeta}{1-\zeta},$$

hence $\zeta \neq 1$. Thus, the domain D is mapped to itself, and

$$g(z) : D \to D, \qquad D = \mathbb{C} - \{1\}$$

is an analytic map.

(c) Take $|\zeta| < 1$. Thus, $|z-1| < |z+1|$, hence

$$(x-1)^2 + y^2 < (x+1)^2 + y^2,$$

hence $x^2 - 2x + 1 < x^2 + 2x + 1$, hence $-4x < 0$, hence $x > 0$, with y arbitrary. Thus, $|\zeta| < 1$ is mapped to the right half-plane under the map $g^{-1}(\zeta)$ and by invertibility, the right-half-plane is mapped to the unit disc.

3. Consider

$$\zeta = g(z), \qquad g(z) = \frac{z-\alpha}{\overline{\alpha}z - 1}, \qquad |\alpha| < 1,$$

where α is a complex constant.

(a) Show that $g(z)$ is an analytic map on an appropriate domain.

(b) Show also that $g(z)$ maps the unit disc $|z| < 1$ to itself.

(c) Show that the origin $z = 0$ is moved to the point $\zeta = \alpha$. Explain why this does not contradict (b).

(d) For the particular case where α is real, let $\zeta = \xi + \mathrm{i}\eta$, $z = x + \mathrm{i}y$, and $\eta = g(z)$. Hence, show that

$$\xi^2 + \eta^2 = \frac{\left(\frac{1}{\alpha}x - 1\right)^2 + \frac{1}{\alpha^2}y^2}{\left(x - \frac{1}{\alpha}\right)^2 + y^2}.$$

Hint: An explicit computation of ξ and η is not necessary.

Note that $z = 1/\overline{\alpha}$ is a singularity. Hence,

$$D = \mathbb{C} - \left\{\frac{1}{\overline{\alpha}}\right\}$$

is the relevant domain. Also,

$$\begin{aligned} g'(z) &= \frac{(\overline{\alpha}z - 1) - (z - \alpha)\overline{\alpha}}{(\overline{\alpha}z - 1)^2}, \\ &= \frac{|\alpha|^2 - 1}{(\overline{\alpha}z - 1)^2}, \end{aligned}$$

and this is nonzero because $|\alpha| < 1$. Finally, the inverse map is obtained by straightforward algebraic computations:

$$z = \frac{\zeta - \alpha}{\overline{\alpha}\zeta - 1},$$

hence,

$$g : D \to D,$$

with $g'(z)$ and $(d/d\zeta)g^{-1}(\zeta)$ nowhere zero on D is an analytic map.

For the second part, let $z = r\mathrm{e}^{\mathrm{i}\varphi}$ and let $\alpha = r_0\mathrm{e}^{\mathrm{i}\varphi_0}$. We compute

$$\begin{aligned} \zeta &= \frac{r\mathrm{e}^{\mathrm{i}\varphi} - r_0\mathrm{e}^{\mathrm{i}\varphi_0}}{rr_0\mathrm{e}^{-\mathrm{i}\varphi_0}\mathrm{e}^{\mathrm{i}\varphi} - 1}, \\ &= \mathrm{e}^{\mathrm{i}\varphi_0}\frac{r\mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-\mathrm{i}\varphi} - r_0}{rr_0\mathrm{e}^{-\mathrm{i}\varphi_0}\mathrm{e}^{\mathrm{i}\varphi} - 1}, \qquad (4.12) \\ & \qquad (4.13) \end{aligned}$$

Hence,

$$\begin{aligned} |\mathrm{Num.}|^2 &= r^2 + r_0^2 - 2rr_0\cos(\varphi - \varphi_0), \\ |\mathrm{Den.}|^2 &= r^2r_0^2 + 1 - 2rr_0\cos(\varphi - \varphi_0). \end{aligned}$$

Thus,

$$\begin{aligned} |\mathrm{Num.}|^2 - |\mathrm{Den.}|^2 &= r^2 + r_0^2 - r^2r_0^2 - 1, \\ &= -(1 - r_0^2)(1 - r^2) < 0, \end{aligned}$$

where the strict inequality follows because $0 \leq r < 1$ and $0 \leq r_0 < 1$. Thus,

$$|\mathrm{Num.}| < |\mathrm{Den.}|,$$

hence

$$|\zeta| < 1,$$

and the unit disc in z-space is mapped to the unit disc in ζ-space. Finally, under the conformal map,

$$\begin{aligned} \zeta_0 &= g(0), \\ &= \frac{-\alpha}{-1}, \\ &= \alpha. \end{aligned}$$

The origin is mapped to the point α under the conformal map. This does not contradict the fact that the unit disc is mapped to itself: a further point

$$z_1 = \alpha$$

is mapped to the origin in ζ-space: the conformal map 'twists' the unit disc such that the origin is shifted by an amount α, but a further point z_1 is also shifted and takes its place at the origin in the mapped space. Check:

$$\begin{aligned} g(z_1) &= \frac{\alpha - \alpha}{|\alpha|^2 - 1}, \qquad |\alpha| < 1, \\ &= 0. \end{aligned}$$

For the last part, we have

$$\begin{aligned} \zeta &= \frac{(z-\alpha)(\alpha\overline{z}-1)}{(\overline{\alpha}z-1)(\alpha\overline{z}-1)}, \\ &= \frac{(z-\alpha)(\alpha\overline{z}-1)}{(\alpha z-1)(\alpha\overline{z}-1)}, \\ &= \frac{\alpha|z|^2 - z - \alpha^2\overline{z} + \alpha}{\alpha^2|z|^2 + 1 - \alpha(z+\overline{z})}, \\ &= \frac{\alpha(x^2+y^2) - (x+\mathrm{i}y) - \alpha^2(x-\mathrm{i}y) + \alpha}{\alpha^2(x^2+y^2) + 1 - 2\alpha x}. \end{aligned}$$

Hence,

$$\begin{aligned} \xi &= \frac{\alpha\left[(x^2+y^2)+1\right] - x(1+\alpha^2)}{\alpha^2(x^2+y^2) + 1 - 2\alpha x}, \\ \eta &= \frac{y(1-\alpha^2)}{\alpha^2(x^2+y^2) + 1 - 2\alpha x}. \end{aligned}$$

For the final part, instead of evaulating $\xi^2 + \eta^2$ by direct computation, we start instead from Equation (4.13), such that we obtain the followiong expressions:

$$\begin{aligned}
\xi^2 + \eta^2 &= \frac{r^2 + \alpha^2 - 2\alpha_0 x}{r^2\alpha^2 + 1 - 2x}, \\
&= \frac{(x^2 + y^2) + \alpha^2 - 2\alpha x}{\alpha^2(x^2 + y^2) + 1 - 2\alpha x}, \\
&= \frac{(x - \alpha)^2 + y^2}{(\alpha x - 1)^2 + \alpha^2 y^2}, \\
&= \frac{\left(\frac{1}{\alpha}x - 1\right)^2 + \frac{1}{\alpha^2}y^2}{\left(x - \frac{1}{\alpha}\right)^2 + y^2}.
\end{aligned}$$

4. Show that every planar conformal map comes from a complex analytic function with nonvanishing derivative. You may use any method you like. However, the following method is suggested:

   (a) Prove the following lemma:

   Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be a linear angle-preserving map. Then T is a scalar multiple of an orthogonal matrix.

   Hints:

   - Choose an orthonormal basis $\boldsymbol{e}_i$. Compute the image of the basis under the linear transformation, $\boldsymbol{f}_i = T\boldsymbol{e}_i$. Argue that the $\boldsymbol{f}_i$'s are an orthogonal basis for $\mathbb{R}^n$ (but not necessarily orthonromal).
   - Let $D = T^T T$, and construct the matrix $D_{ij} = \langle \boldsymbol{e}_i, D\boldsymbol{e}_j \rangle$. Show that

   $$D_{ij} = \|\boldsymbol{f}_i\|_2^2 \delta_{ij}, \qquad \text{no sum over } i.$$

   - Define $\theta = \text{angle}(\boldsymbol{e}_1, \boldsymbol{e}_1 + \boldsymbol{e}_k)$, with $k \neq 1$. Show that

   $$\cos\theta = \tfrac{1}{\sqrt{2}}.$$

   - Using the angle-preserving nature of the map T, show that

   $$\cos\theta = \frac{\|\boldsymbol{f}_1\|_2^2}{\|\boldsymbol{f}_1\|_2 \sqrt{\|\boldsymbol{f}_1\|_2^2 + \|\boldsymbol{f}_2\|_2^2}} = \tfrac{1}{\sqrt{2}},$$

   hence deduce that $\|\boldsymbol{f}_1\|_2 = \|\boldsymbol{f}_k\|_2$, for all $k = 1, \cdots, n$, and finally, deduce that $D = \lambda \mathbb{I}$, for some scalar lambda.

   - Conclude that T is a scalar multiple of an orthogonal matrix. Rule out improper

rotations, such that T is a scalar multiple of a rotation matrix.

(b) Using the lemma from part (a), start with two curves $\boldsymbol{x}(t)$ and $\boldsymbol{y}(t)$ in $\mathbb{R}^2$, and let $\boldsymbol{g}(\boldsymbol{x})$ be an angle-preserving map, such that

$$\widetilde{\boldsymbol{x}(t)} = \boldsymbol{g}(\boldsymbol{x}(t)) = (g_1(x(t), y(t)), g_2(x(t), y(t)))\,,$$

and similarly for $\widetilde{\boldsymbol{y}(t)}$. We proceed as follows, where all calculations are performed at a point of intersection of the two curves:

- Show that
$$\frac{d}{dt}\widetilde{\boldsymbol{x}(t)} = J\dot{\boldsymbol{x}}, \qquad J = \begin{pmatrix} \frac{\partial g_1}{\partial x} & \frac{\partial g_1}{\partial y} \\ \frac{\partial g_2}{\partial x} & \frac{\partial g_2}{\partial y} \end{pmatrix}.$$
- Compute
$$\cos\tilde{\theta} = \frac{\langle J\dot{\boldsymbol{x}}, J\dot{\boldsymbol{y}}\rangle}{\|J\dot{\boldsymbol{x}}\|_2\|J\dot{\boldsymbol{y}}\|_2}.$$
Deduce, using the angle-preserving property of the map $\boldsymbol{g}$, that J takes the following form:
$$J = \lambda \begin{pmatrix} \cos\Phi & -\sin\Phi \\ \sin\Phi & \cos\Phi \end{pmatrix},$$
where λ is a scalar.
- Hence, show that the components of the map $\boldsymbol{g}$ satisfy the Cauchy–Riemann conditions, and conclude the proof.

For part (a), choose an orthnormal basis $\boldsymbol{e}_i$, ane let $\boldsymbol{f}_i = T\boldsymbol{e}_i$ Consider

$$\begin{aligned} \boldsymbol{f}_i \cdot \boldsymbol{f}_j &= \|\boldsymbol{f}_i\|\|\boldsymbol{f}_j\|\text{angle}(\boldsymbol{f}_i, \boldsymbol{f}_j), \\ &= \|\boldsymbol{f}_i\|\|\boldsymbol{f}_j\|\text{angle}(\boldsymbol{e}_i, \boldsymbol{e}_j), \\ &= \|\boldsymbol{f}_i\|\|\boldsymbol{f}_j\|\boldsymbol{e}_i \cdot \boldsymbol{e}_j, \\ &= \|\boldsymbol{f}_i\|\|\boldsymbol{f}_j\|\delta_{ij}, \\ &= \|\boldsymbol{f}_i\|^2\delta_{ij}, \end{aligned}$$

Hence, the $\boldsymbol{f}_i$'s are an orthogonal basis for $\mathbb{R}^n$.

Next, consider

$$\begin{aligned} D_{ij} &= (\boldsymbol{e}_i) \cdot (D\boldsymbol{e}_j), \\ &= \boldsymbol{e}_i^T T^T T \boldsymbol{e}_j, \\ &= (T\boldsymbol{e}_i)^T (T\boldsymbol{e}_j), \\ &= \boldsymbol{f}_i \cdot \boldsymbol{f}_j, \\ &= \|\boldsymbol{f}_i\|^2 \delta_{ij}. \end{aligned}$$

Consider

$$\theta = \text{angle}(\boldsymbol{e}_1, \boldsymbol{e}_1 + \boldsymbol{e}_k), \qquad k \neq 1.$$

We have

$$\begin{aligned} \boldsymbol{e}_1 \cdot (\boldsymbol{e}_1 + \boldsymbol{e}_k) &= \boldsymbol{e}_1 \cdot \boldsymbol{e}_1 + \boldsymbol{e}_1 \cdot \boldsymbol{e}_k, \\ &= 1, \\ &= \|\boldsymbol{e}_1\|_2 \|\boldsymbol{e}_1 + \boldsymbol{e}_k\|_2 \cos\theta, \\ &= \sqrt{\boldsymbol{e}_1^2 + 2\boldsymbol{e}_1 \cdot \boldsymbol{e}_k + \boldsymbol{e}_k^2} \cos\theta, \\ &= \sqrt{2} \cos\theta, \end{aligned}$$

hence

$$\cos\theta = \frac{1}{\sqrt{2}}.$$

However, using the angle-preserving map, we also have

$$\theta = \text{angle}(\boldsymbol{f}_1, \boldsymbol{f}_1 + \boldsymbol{f}_k)$$

Also,

$$\begin{aligned} \boldsymbol{f}_1 \cdot (\boldsymbol{f}_1 + \boldsymbol{f}_2) &= \boldsymbol{f}_1^2 = \|\boldsymbol{f}_1\|_2^2, \\ &= \|\boldsymbol{f}_1\| \|\boldsymbol{f}_1 + \boldsymbol{f}_2\|_2 \cos\left[\text{angle}(\boldsymbol{f}_1, \boldsymbol{f}_1 + \boldsymbol{f}_k)\right], \\ &= \|\boldsymbol{f}_1\|_2 \|\boldsymbol{f}_1 + \boldsymbol{f}_k\|_2 \cos\theta, \\ &= \|\boldsymbol{f}_1\|_2 \sqrt{\boldsymbol{f}_1^2 + 2\boldsymbol{f}_1 \cdot \boldsymbol{f}_2 + \boldsymbol{f}_k^2} \cos\theta, \\ &= \|\boldsymbol{f}_1\|_2 \sqrt{\|\boldsymbol{f}_1\|_2^2 + \|\boldsymbol{f}_k\|_2^2} \cos\theta, \end{aligned}$$

hence

$$\cos\theta = \frac{\|\boldsymbol{f}_1\|_2^2}{\|\boldsymbol{f}_1\|_2 \sqrt{\|\boldsymbol{f}_1\|_2^2 + \|\boldsymbol{f}_k\|_2^2}} = \frac{1}{\sqrt{2}}.$$

Tidy up this last result now to obtain

$$\frac{\|\boldsymbol{f}_1\|_2}{\sqrt{\|\boldsymbol{f}_1\|_2^2 + \|\boldsymbol{f}_k\|_2^2}} = \frac{1}{\sqrt{2}}.$$

Square both sides:

$$\frac{\|\boldsymbol{f}_1\|_2^2}{\|\boldsymbol{f}_1\|_2^2 + \|\boldsymbol{f}_k\|_2^2} = \tfrac{1}{2}.$$

Hence,

$$\|\boldsymbol{f}_1\|_2^2 = \tfrac{1}{2}\|\boldsymbol{f}_1\|_2^2 + \tfrac{1}{2}\|\boldsymbol{f}_k\|_2^2,$$

hence

$$\|\boldsymbol{f}_k\|_2^2 = \|\boldsymbol{f}_1\|_2^2, \qquad k = 2, \cdots, n.$$

Hence, each $\boldsymbol{f}_i$-vector has the same length – say $\|\boldsymbol{f}_k\|_2 = \lambda$, for all $k = 1, \cdots, n$, hence

$$D_{ij} = \lambda \delta_{ij}.$$

But $D = T^T T$, hence

$$T^T T = \lambda \mathbb{I},$$

hence T is a constant times an orthogonal matrix. In order to rule out the possibility that vectors are 'flipped' (i.e. $\theta \to \theta' = -\theta$, but with $\cos\theta' = \cos\theta$), we rule out improper rotations, such that T must be a constant times a special orthogonal matrix, i.e. a constant times a rotation matrix. This concludes the proof.

For Part (b), take $\boldsymbol{x}$ and $\widetilde{\boldsymbol{x}}$ to be **column vectors**, and start with

$$\widetilde{\boldsymbol{x}(t)} = \boldsymbol{g}(\boldsymbol{x}(t)) = \begin{pmatrix} g_1(x(t), y(t)) \\ g_2(x(t), y(t)) \end{pmatrix},$$

hence

$$\begin{aligned} \frac{d}{dt}\widetilde{\boldsymbol{x}(t)} &= \begin{pmatrix} \frac{d}{dt} g_1(x(t), y(t)) \\ \frac{d}{dt} g_2(x(t), y(t)) \end{pmatrix}, \\ &= \begin{pmatrix} \frac{\partial g_1}{\partial x}\dot{x} + \frac{\partial g_1}{\partial y}\dot{y} \\ \frac{\partial g_2}{\partial x}\dot{x} + \frac{\partial g_2}{\partial y}\dot{y} \end{pmatrix}, \\ &= \begin{pmatrix} \frac{\partial g_1}{\partial x} & \frac{\partial g_1}{\partial y} \\ \frac{\partial g_2}{\partial x} & \frac{\partial g_2}{\partial y} \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix}, \\ &:= J\dot{\boldsymbol{x}}, \end{aligned}$$

where

$$J = \begin{pmatrix} \frac{\partial g_1}{\partial x} & \frac{\partial g_1}{\partial y} \\ \frac{\partial g_2}{\partial x} & \frac{\partial g_2}{\partial y} \end{pmatrix}, \qquad \dot{\boldsymbol{x}} = \frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix}.$$

Thus, consider the point of intersection of two curves $\boldsymbol{x}(t)$ and $\boldsymbol{y}(t)$, such that

$$\boldsymbol{x}(t_0) = \boldsymbol{y}(t_0).$$

In the mapped space, we have

$$g(\boldsymbol{x}(t_0)) = g(\boldsymbol{y}(t_0)),$$

i.e.

$$\widetilde{\boldsymbol{x}(t_0)} = \widetilde{\boldsymbol{y}(t_0)}.$$

The unit tangent vectors of the mapped curves at the point of intersection are

$$\widetilde{\boldsymbol{t}_1} = \frac{\frac{d\widetilde{\boldsymbol{x}}}{dt}}{\|\frac{d\widetilde{\boldsymbol{x}}}{dt}\|} = \frac{J\dot{\boldsymbol{x}}}{\|J\dot{\boldsymbol{x}}\|}, \qquad t = t_0,$$

and

$$\widetilde{\boldsymbol{t}_2} = \frac{\frac{d\widetilde{\boldsymbol{y}}}{dt}}{\|\frac{d\widetilde{\boldsymbol{y}}}{dt}\|} = \frac{J\dot{\boldsymbol{y}}}{\|J\dot{\boldsymbol{y}}\|}, \qquad t = t_0.$$

hence the angle $\widetilde{\theta}$ between the tangent vectors in the mapped space is

$$\cos\widetilde{\theta} = \widetilde{\boldsymbol{t}_1} \cdot \widetilde{\boldsymbol{t}_2}.$$

Note that we must take $J\dot{\boldsymbol{x}}$ and $J\dot{\boldsymbol{y}} \neq 0$. In addition, to construct tangent vectors to the original curves $\boldsymbol{x}(t)$ and $\boldsymbol{y}(t)$, we must have $\dot{\boldsymbol{x}}$ and $\dot{\boldsymbol{y}} \neq 0$ at the point of intersection. Thus, it is required that the kernel of J should be trivial, in other words J should be an invertible map, hence

$$\frac{\partial g_1}{\partial x}\frac{\partial g_2}{\partial y} - \frac{\partial g_1}{\partial y}\frac{\partial g_2}{\partial x} \neq 0. \tag{4.14}$$

But by the inverse function theorem, the condition for the vector-valued function to be invertible is the non-vanishing of the determinant of the Jacobian. Since invertibility is assumed, condition (4.14) is guaranteed.

In any case, by the angle-preserving property, we have, at $t = t_0$,

$$\begin{aligned}\frac{\langle J\dot{\boldsymbol{x}}, J\dot{\boldsymbol{y}}\rangle}{\|J\dot{\boldsymbol{x}}\|_2\|J\dot{\boldsymbol{y}}\|_2} &= \widetilde{\boldsymbol{t}}_1 \cdot \widetilde{\boldsymbol{t}}_2,\\ &= \cos\widetilde{\theta},\\ &= \cos\theta,\\ &= \boldsymbol{t}_1 \cdot \boldsymbol{t}_2,\\ &= \frac{\langle \dot{\boldsymbol{x}}, \dot{\boldsymbol{y}}\rangle}{\|\dot{\boldsymbol{x}}\|_2\|\dot{\boldsymbol{y}}\|_2}.\end{aligned}$$

Thus, for the general point of intersection,

$$\frac{\langle J\dot{\boldsymbol{x}}, J\dot{\boldsymbol{y}}\rangle}{\|J\dot{\boldsymbol{x}}\|_2\|J\dot{\boldsymbol{y}}\|_2} = \frac{\langle \dot{\boldsymbol{x}}, \dot{\boldsymbol{y}}\rangle}{\|\dot{\boldsymbol{x}}\|_2\|\dot{\boldsymbol{y}}\|_2}.$$

From Part (a) it follows that J is a constant times a rotation matrix:

$$J = \lambda \begin{pmatrix} \cos\Phi & -\sin\Phi \\ \sin\Phi & \cos\Phi \end{pmatrix},$$

hence

$$\begin{aligned}\frac{\partial g_1}{\partial x} &= \lambda\cos\Phi,\\ \frac{\partial g_1}{\partial y} &= -\lambda\sin\Phi,\\ \frac{\partial g_2}{\partial x} &= \lambda\sin\Phi,\\ \frac{\partial g_2}{\partial y} &= \lambda\cos\Phi.\end{aligned}$$

Matching up the terms, we have

$$\frac{\partial g_1}{\partial x} = \frac{\partial g_2}{\partial y}, \qquad \frac{\partial g_1}{\partial y} = -\frac{\partial g_2}{\partial x}.$$

Hence, $(g_1(x,y), g_2(x,y))$ satisfies the Cauchy–Riemann conditions. Also, $(g_1(x,y), g_2(x,y))$ is assumed to be smooth, hence all partial derivatives exist are continuous. Thus, the complex-valued map

$$F(z) = g_1(x,y) + \mathrm{i}g_2(x,y), \qquad z = x + \mathrm{i}y$$

is a holomorphic function. This completes the proof.

As an aside, apply the Cauchy–Riemann conditions to Equation (4.14). Thus,

$$\left(\frac{\partial g_2}{\partial x}\right)^2 + \left(\frac{\partial g_2}{\partial y}\right)^2 \neq 0,$$

and

$$\left(\frac{\partial g_1}{\partial x}\right)^2 + \left(\frac{\partial g_1}{\partial y}\right)^2 \neq 0.$$

In other words, the condition for the angle-preserving map to be invertible boils down to

$$|\nabla g_1|^2 + |\nabla g_2|^2 \neq 0.$$

Chapter 5

Laplace Transforms

We define the Laplace transform and specify the class of functions for which it exists. We demonstrate how Laplace transforms can be inverted. The procedure for computing Laplace-transform and inverse-Laplace-transform pairs is very similar to the analogous procedure in Fourier Analysis. Examples of these calculations are provided. The associated homework assignment show the range of applications in which Laplace transforms can be used to reduce seemingly difficult calculus problems into simple algebraic ones.

Overview

5.1 The Definition

In this Chapter, let

$$\begin{aligned} F : [0, \infty) &\to \mathbb{C}, \\ t &\mapsto F(t) \end{aligned} \tag{5.1}$$

be a complex-valued function of a real variable.

Definition 5.1 *Let The function $F(t)$ is* **at most exponentially diverging** *if there exist real numbers $(\lambda_0, M > 0)$ such that*

$$|\mathrm{e}^{-\lambda_0 t} F(t)| \leq M, \qquad \text{as } t \to \infty;$$

we call λ_0 the **divergence parameter**.

Definition 5.2 *Let $F(t)$ be at most exponentially diverging, with divergence parameter λ_0.* **Laplace-transform** *of $F(t)$ is defined as follows:*

$$\widehat{F}_\lambda \equiv \mathcal{L}(F) := \int_0^\infty \mathrm{e}^{-\lambda t} F(t)\mathrm{d}t, \qquad \mathit{Re}(\lambda) > \lambda_0.$$

Theorem 5.1 *The Laplace transform is linear, in the sense that*

$$\mathcal{L}(\alpha F(t) + \beta G(t)) = \alpha\mathcal{L}(F) + \beta\mathcal{L}(G),$$

where α and β are complex constants and the functions F and G are functions of type (5.1) *whose Laplace transforms exist.*

5.2 Simple examples

1. We compute the Laplace Transform of $F(t) = \mathrm{e}^{kt}$, with $k > 0$ real.

   We have

   $$\begin{aligned} \widehat{F}_\lambda &= \int_0^\infty \mathrm{e}^{(k-\lambda)t}\mathrm{d}t, \\ &= \lim_{L\to\infty}\left[\frac{1}{k-\lambda}\left(\mathrm{e}^{(k-\lambda)L} - 1\right)\right]. \end{aligned} \tag{5.2}$$

   Obviously, we need $\mathrm{Re}(\lambda) > k$ for this integral to exist, hence

   $$\widehat{F}_\lambda = \frac{1}{\lambda - k}, \qquad \mathrm{Re}(\lambda) > k.$$

   The transform has a simple pole at $\lambda = k$, which is connected to the failure of the integral (5.2) to exist for $\mathrm{Re}(\lambda)$ sufficiently small. See Figure 5.1 for a sketch of the λ-domain where $\mathcal{L}(\mathrm{e}^{kt})$ is well-defined.

2. Consider $F(t) = \sinh kt$, with $k > 0$ real. We compute the Laplce transform of $F(t)$ as follows:

   $$\begin{aligned} \mathcal{L}(\mathrm{e}^{kt}) &= \int_0^\infty \mathrm{e}^{(k-\lambda)t}, \\ &= \frac{1}{\lambda - k}, \qquad \mathrm{Re}(\lambda) > k. \end{aligned}$$

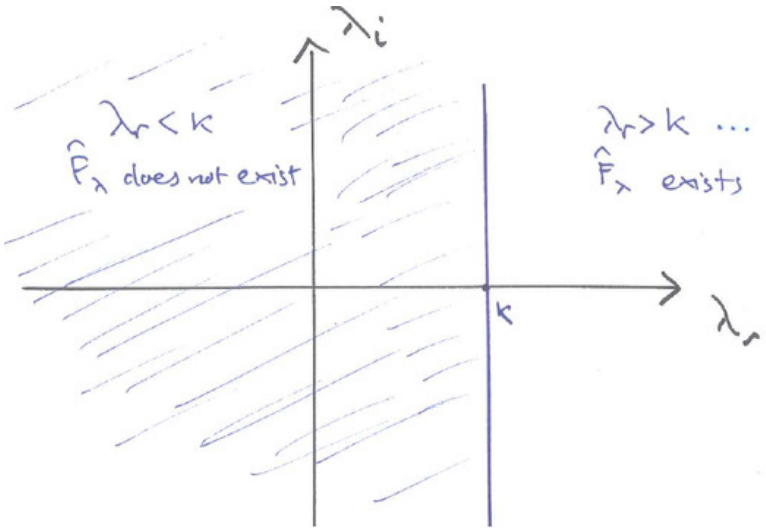


Figure 5.1: Domain of existence of the complex Laplace transform of e^{kt}.

Also,

$$\begin{aligned}\mathcal{L}(\mathrm{e}^{-kt}) &= \int_0^\infty \mathrm{e}^{(-k-\lambda)t}\mathrm{d}t, \\ &= \frac{1}{\lambda+k}, \qquad \mathsf{Re}(\lambda) > -k.\end{aligned}$$

By linearity,

$$\mathcal{L}(\sinh kt) = \tfrac{1}{2}\left(\frac{1}{\lambda-k} - \frac{1}{\lambda+k}\right), \qquad \mathsf{Re}(\lambda) > k,$$

where the first inequality trumps the second one. Finally,

$$\mathcal{L}(\sinh kt) = \frac{k}{\lambda^2-k^2}, \qquad \mathsf{Re}(\lambda) > k.$$

3. Let $F(t) = \sin kt$, with $k > 0$ real. We compute

$$\begin{aligned}\mathcal{L}(\mathrm{e}^{\mathrm{i}kt}) &= \int_0^\infty \mathrm{e}^{(\mathrm{i}k-\lambda)t}\mathrm{d}t, \\ &= \lim_{L\to\infty}\left[\frac{1}{\mathrm{i}k-\lambda}\left(\mathrm{e}^{(\mathrm{i}k-\lambda)L}-1\right)\right], \\ &= \frac{1}{\lambda-\mathrm{i}k}, \qquad \mathsf{Re}(\lambda) > 0.\end{aligned}$$

Similarly,

$$\mathcal{L}(\mathrm{e}^{-\mathrm{i}kt}) = \frac{1}{\lambda+\mathrm{i}k}, \qquad \mathsf{Re}(\lambda) > 0.$$

By linearity,

$$\begin{aligned}\mathcal{L}(\sin kt) &= \tfrac{1}{2\mathrm{i}}\left(\frac{1}{\lambda-\mathrm{i}k}-\frac{1}{\lambda+\mathrm{i}k}\right), \qquad \mathsf{Re}(\lambda)>0,\\ &= \frac{k}{\lambda^2+k^2}, \qquad \mathsf{Re}(\lambda)>0.\end{aligned}$$

Note that

$$\lim_{\lambda\to 0}\widehat{F}_\lambda = 1/k.$$

Thus, we can assign a value to $\int_0^\infty \sin(kt)\,\mathrm{d}t$ as

$$\int_0^\infty \sin(kt)\mathrm{d}t := \frac{1}{k}, \qquad k\neq 0$$

in the sense of a limiting process determined by Laplace transforms.

4. Let $F(t)=t^n$, where $n=0,1,\cdots$ is an integer. We have

$$\begin{aligned}\widehat{F}_\lambda &= \int_0^\infty \mathrm{e}^{-\lambda t}t^n\mathrm{d}t,\\ &= \frac{1}{\lambda^{n+1}}\int_0^\infty \mathrm{e}^{-t}t^n\mathrm{d}t, \qquad \mathsf{Re}(\lambda)>0,\\ &= \frac{n!}{\lambda^{n+1}}.\end{aligned}$$

5. Let $F(t)=\delta(t-t_0)$, with $t_0>0$. We have

$$\widehat{F}_\lambda = \int_0^\infty \mathrm{e}^{\lambda t}\delta(t-t_0)\mathrm{d}t = \mathrm{e}^{\lambda t_0}.$$

We take $t_0\downarrow 0$ and define

$$\mathcal{L}(\delta(t))=1.$$

5.3 Inverting Laplace transforms

Let

$$\begin{aligned}F:[0,\infty) &\to \mathbb{C},\\ t &\mapsto F(t)\end{aligned}$$

be a complex-valued function of a real variable, and moreover, let $F(t)$ be at worst exponentially diverging, with exponential parameter λ_0. We re-write $F(t)$ as

$$F(t) = \mathrm{e}^{\gamma t} G(t),$$

where $\lim_{t\to\infty} G(t) = 0$. Such a G-function exists; we take

$$G(t) = F(t)\mathrm{e}^{-(\lambda_0+\epsilon)t},$$

for ϵ arbitrary and positive (hence, $\gamma = \lambda_0 + \epsilon$). We have

$$\begin{aligned} |G(t)| &= |F(t)|\mathrm{e}^{-\lambda_0 t - \epsilon t}, \\ &\leq M\mathrm{e}^{\lambda_0 t}\mathrm{e}^{-\lambda_0 t - \epsilon t}, \qquad \text{as } t \to \infty, \\ &\leq M\mathrm{e}^{-\epsilon t}, \\ &\to 0, \qquad \text{as } t \to \infty. \end{aligned}$$

Also, define $G(t) = 0$ for $t < 0$. It follows that G is L^2 square integrable. Subject to the usual further conditions on G (i.e. piecewise differentiable for $t \in \mathbb{R}$), G can be written in Fourier transform notation:

$$\begin{aligned} G(t) &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{\mathrm{i}\omega t} \widehat{G}_\omega, \\ &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{\mathrm{i}\omega t} \left[\int_{-\infty}^{\infty} \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}\omega s} G(s) \right] \end{aligned}$$

Multiply across by $\mathrm{e}^{\gamma t}$:

$$\begin{aligned} \mathrm{e}^{\gamma t} G(t) &= \frac{\mathrm{e}^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{\mathrm{i}\omega t} \left[\int_{-\infty}^{\infty} \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}\omega s} G(s) \right], \\ F(t) &= \frac{\mathrm{e}^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{\mathrm{i}\omega t} \left[\int_{0}^{\infty} \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}\omega s} F(s) \mathrm{e}^{-\gamma s} \right], \\ &= \frac{\mathrm{e}^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{\mathrm{i}\omega t} \underbrace{\left[\int_{0}^{\infty} \mathrm{d}s\, \mathrm{e}^{-\lambda s} F(s) \right]}_{=\widehat{F}_\lambda}. \end{aligned}$$

Let $\lambda = \gamma + \mathrm{i}\omega$, hence $\omega = (\lambda - \gamma)/\mathrm{i}$.

$$F(t) = \frac{\mathrm{e}^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} \left(\mathrm{d}\omega\, \mathrm{e}^{\mathrm{i}\omega t} \right)_{\omega = \frac{\lambda-\gamma}{\mathrm{i}}} \widehat{F}_\lambda.$$

Effecting the change of variables, this is

$$\begin{aligned} F(t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\mathrm{d}\omega\,\mathrm{e}^{(\gamma+\mathrm{i}\omega)t}\right)_{\omega=\frac{\lambda-\gamma}{\mathrm{i}}}\widehat{F}_\lambda, \\ &= \frac{1}{2\pi\mathrm{i}}\int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty}\mathrm{d}\lambda\,\mathrm{e}^{\lambda t}\widehat{F}_\lambda. \end{aligned}$$

The contour

$$\mathcal{B} = \{z \in \mathbb{C} | z = \gamma + \mathrm{i}y, y \in \mathbb{R}\}$$

is called the **Bromwich contour**. It is sketched in Figure 5.2.

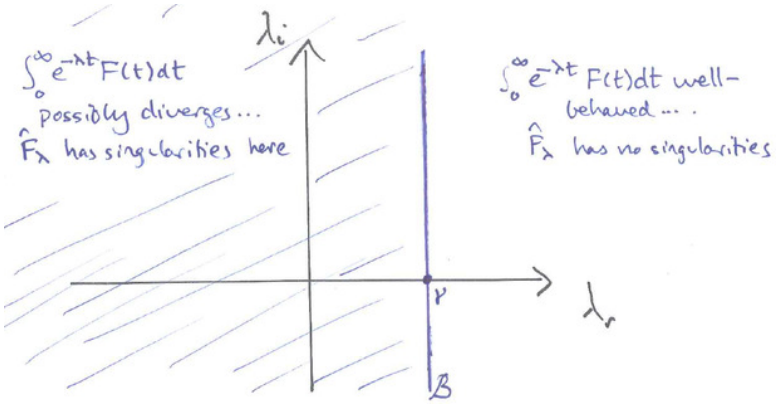


Figure 5.2: Definition sketch – the Bromwich contour

Suppose now that

$$\lim_{\lambda\to\infty}|\mathrm{e}^{\lambda t}\widehat{F}_\lambda| = 0, \qquad t > 0$$

and consider the contour $\mathcal{C}+\mathcal{B}$ in Figure 5.3. For now, we consider the case where the singularities of $\mathrm{e}^{\lambda t}\widehat{F}_\lambda$ are poles; branch-cut singularities are considered on a case-by-case basis in the examples to follow. Also, we use the notation $\mathcal{C}$ to denote the limiting contour associated with a semi-circle of radius R centred at $(\gamma, 0)$, with $R \to \infty$. In this limit, the semi-circle encloses all of the singularities (poles) of $\widehat{F}_\lambda$. Also, $\int_{\mathcal{C}}\mathrm{e}^{\lambda t}\widehat{F}_\lambda\mathrm{d}\lambda = 0$. Hence,

$$\begin{aligned} \frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}+\mathcal{B}}\mathrm{e}^{\lambda t}\widehat{F}_\lambda &= \sum\text{enclosed residues}, \\ &= \frac{1}{2\pi\mathrm{i}}\left(\int_{\mathcal{C}}\mathrm{d}\lambda + \int_{\mathcal{B}}\mathrm{d}\lambda\right)\mathrm{e}^{\lambda t}\widehat{F}_\lambda, \\ &= \frac{1}{2\pi\mathrm{i}}\left(0 + \int_{\mathcal{B}}\mathrm{d}\lambda\right)\mathrm{e}^{\lambda t}\widehat{F}_\lambda. \end{aligned}$$

Hence,

$$F(t) = \sum\text{enclosed residues}, \tag{5.3}$$

where 'residues' refers to the residues of $\mathrm{e}^{\lambda t}\widehat{F}_\lambda$ in the half-plane to the left of the line $\mathrm{Re}(\lambda) = \gamma$.

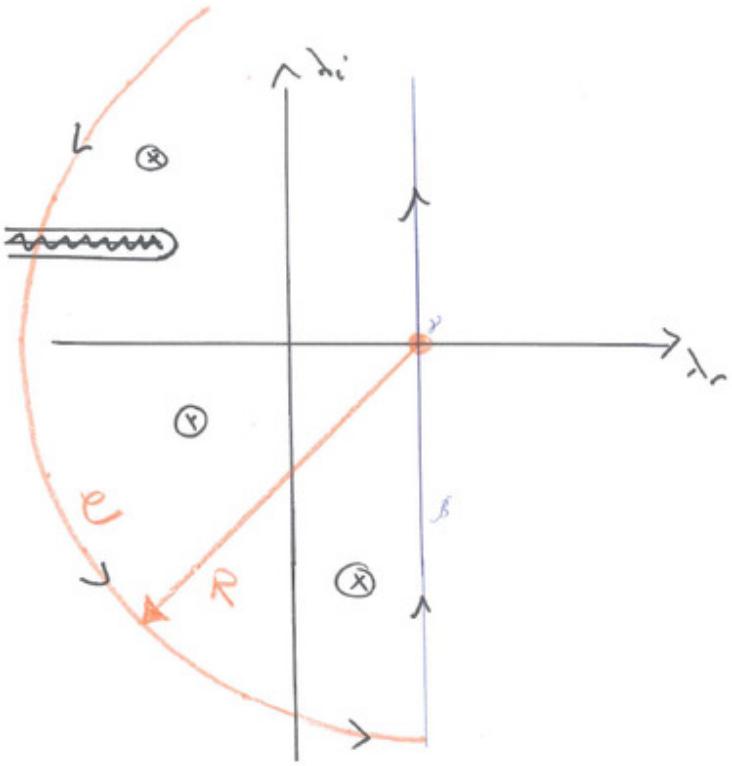


Figure 5.3: Integration along the Bromwich contour using the Residue Theorem

5.4 Examples of Laplace-Transform inversion

1. Let $f(\lambda) = k/(\lambda^2 - k^2)$, with $k > 0$ real. If $f(\lambda)$ is a Laplace transform, compute the generating function of the transform.

   We compute

   $$F(t) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{B}} \frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2} \mathrm{d}\lambda,$$

   where $\mathcal{B}$ is the Bromwich contours: it is a straight line parallel to the imaginary axis to the right of the singularities of the integrand

   $$\frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2}. \tag{5.4}$$

   Since the singularites of Equation (5.4) are $\lambda = \pm k$, the Bromwich contour is

   $$\mathcal{B} = \{z \in \mathcal{C} | z = (k + \epsilon) + \mathrm{i}y,\ y \in \mathbb{R},\ \epsilon > 0\}.$$

Using the residue theorem, we have

$$F(t) = \mathrm{Res}\left(\frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2}, k\right) + \mathrm{Res}\left(\frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2}, -k\right)$$
$$= \lim_{\lambda \to k}\left[(\lambda - k)\frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2}\right] + \lim_{\lambda \to -k}\left[(\lambda + k)\frac{k\mathrm{e}^{\lambda t}}{\lambda^2 - k^2}\right]$$
$$= \tfrac{1}{2}\left(\mathrm{e}^{kt} - \mathrm{e}^{-kt}\right) = \sinh(kt),$$

in agreement with Example 2 in Section 5.1.

2. Let $f(\lambda) = \lambda^{-1/2}$ be the Laplace transform of a function. Find the generating function.

   The function $f(\lambda)$ has a branch cut along the curve

$$\{z = x + 0\mathrm{i}y | x \leq 0\}.$$

   Consider the closed contour $\mathcal{C}$ shown in Figure 5.4. Since $\mathcal{C}$ encloses no singularities, we have

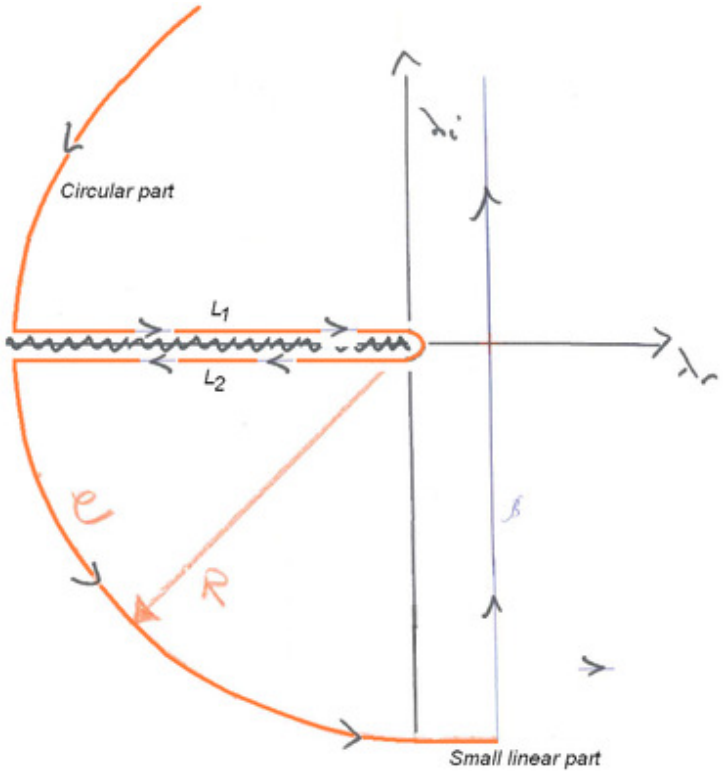


Figure 5.4: Integration along the Bromwich contour for a function with branch cut along the negative real axis

$$\int_{\mathcal{C}} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}} \mathrm{d}\lambda = 0.$$

   Moreover, the contour $\mathcal{C}$ can be regarded as being made up of many parts:

- The Bromwich contour;
- A small semi-circle of radius ϵ centred at zero.
- The lines surrounding the branch cut.
- Semi-circular parts (centred at zero) of radius R, with $R \to \infty$.
- Small linear parts with $z = x \pm \mathrm{i}R$, and $x \in [0, 2\epsilon]$ (say).

We consider these parts separately now, starting with the semi-circle of radius ϵ. This evaluates to

$$\int_{-\pi/2}^{\pi/2} (\epsilon \,\mathrm{i}\, \mathrm{d}\theta) \, \frac{\mathrm{e}^{\epsilon t \cos\theta + \mathrm{i}\epsilon t \sin\theta}}{\epsilon^{1/2} \mathrm{e}^{\mathrm{i}\theta/2}},$$

which vanishes as $\epsilon^{1/2}$ as $\epsilon \to 0$. Also, the semi-circular parts of radius R contain contributions such as

$$\int (R \,\mathrm{i}\, \mathrm{d}\theta) \, \frac{\mathrm{e}^{Rt\cos\theta + \mathrm{i}Rt\sin\theta}}{R^{1/2}\mathrm{e}^{\mathrm{i}\theta/2}}.$$

The limits of integration are unspecified; however, they are in the second and third quadrants where $\cos\theta < 0$. Thus, these contributions vanish as

$$R^{1/2}\mathrm{e}^{-R\alpha}, \qquad \alpha \in \mathbb{R}^+,$$

as $R \to 0$ (we take $t > 0$). The linear parts vanish similarly. It follows then that

$$F(t) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{B}} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}} \mathrm{d}\lambda = -\frac{1}{2\pi\mathrm{i}} \left(\int_{L_1} \mathrm{d}\lambda + \int_{L_2} \mathrm{d}\lambda \right) \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}}, \tag{5.5}$$

where L_1 and L_2 are the contributions from the linear contours surrounding the branch cut.

Consider the integral along L_1. We have

$$\begin{aligned} \lambda &= |\lambda| \mathrm{e}^{+\mathrm{i}\pi}, \\ &= (-x)\mathrm{e}^{+\mathrm{i}\pi}, \\ \lambda^{1/2} &= (-x)^{1/2}\mathrm{e}^{\mathrm{i}\pi/2} = \mathrm{i}(-x)^{1/2} \end{aligned}$$

We also have $\lambda = x$ on L_1, and we use whichever form is convenient in the following string of relations:

$$\begin{aligned} \int_{L_1} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}} \mathrm{d}\lambda &= \int_{-\infty}^{0} \frac{\mathrm{e}^{xt}}{(-x)^{1/2}\mathrm{i}} \mathrm{d}x, \\ &= \frac{1}{\mathrm{i}} \int_0^{\infty} \frac{\mathrm{e}^{-yt}}{y^{1/2}} \mathrm{d}y. \end{aligned}$$

Let $X = (ty)^{1/2}$ to get

$$\begin{aligned}\int_{L_1} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}}\mathrm{d}\lambda &= \frac{2}{\mathrm{i}t^{1/2}}\int_0^\infty \mathrm{e}^{-X^2}\mathrm{d}X,\\ &= \frac{2}{\mathrm{i}}\left(\tfrac{1}{2}\sqrt{\pi/t}\right),\\ &= \frac{1}{\mathrm{i}}\sqrt{\pi/t}.\end{aligned}$$

We make similar arguments for the second linear contour, L_2. We have

$$\begin{aligned}\lambda &= |\lambda|\mathrm{e}^{-\mathrm{i}\pi},\\ &= (-x)\mathrm{e}^{-\mathrm{i}\pi},\\ \lambda^{1/2} &= (-x)^{1/2}\mathrm{e}^{-\mathrm{i}\pi/2}.\end{aligned}$$

We also have $\lambda = x$ on L_2. Hence,

$$\begin{aligned}\int_{L_2} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}}\mathrm{d}\lambda &= \int_0^{-\infty} \frac{\mathrm{e}^{xt}}{(-x)^{1/2}\mathrm{e}^{-\mathrm{i}\pi/2}}\mathrm{d}x,\\ &= \frac{1}{\mathrm{i}}\int_0^\infty \frac{\mathrm{e}^{-yt}}{y^{1/2}}\mathrm{d}y,\\ &= \frac{1}{\mathrm{i}}\sqrt{\pi/t}.\end{aligned}$$

Starting with Equation (5.6), we assemble the results as follows:

$$F(t) = -\frac{1}{2\pi\mathrm{i}}\left(\int_{L_1}\mathrm{d}\lambda + \int_{L_2}\mathrm{d}\lambda\right)\frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}} = -\frac{1}{2\pi\mathrm{i}}\left(\frac{2}{\mathrm{i}}\sqrt{\pi/t}\right) = \frac{1}{\sqrt{\pi t}}.$$

5.5 Laplace transforms – further properties

Throughout this section, let $(F(t), \widehat{F}_\lambda)$ be a valid Laplace-transform pair:

$$\widehat{F}_\lambda = \int_0^\infty F(t)\mathrm{e}^{-\lambda t}\mathrm{d}t, \qquad F(t) = \frac{1}{2\pi\mathrm{i}}\int_{\mathcal{B}} \widehat{F}_\lambda \mathrm{e}^{\lambda t},$$

where $\mathcal{B}$ is the Bromwich contour.

Theorem 5.2 (Substitution) *Let $a \in \mathbb{C}$, and let $f(\lambda) := \widehat{F}_\lambda$ denote the Laplace transform of the function F. Then*

$$f(\lambda - a) = \mathcal{L}\left(\mathrm{e}^{at}F(t)\right).$$

Proof: By direct calculation we have

$$\begin{aligned} f(\lambda - a) &= \widehat{F}_{\lambda - a}, \\ &= \int_0^\infty \mathrm{e}^{-(\lambda - a)t} F(t) \mathrm{d}t, \\ &= \int_0^\infty \mathrm{e}^{-\lambda t} \left[\mathrm{e}^{at} F(t) \right] \mathrm{d}t, \\ &= \mathcal{L}\left(\mathrm{e}^{at} F(t) \right). \end{aligned}$$

Theorem 5.3 (Translation) *Let a be a real positive number and let $f(\lambda) := \widehat{F}_\lambda$. Then*

$$\mathrm{e}^{-b\lambda} f(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} F(t-b) H(t-b) \mathrm{d}t,$$

where $H(\cdot)$ is the unit step function,

$$H(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0. \end{cases}$$

Proof: We have

$$\begin{aligned} \mathrm{e}^{-b\lambda} f(\lambda) &= \int_0^\infty \mathrm{e}^{-b\lambda} \mathrm{e}^{-\lambda t} F(t) \, \mathrm{d}t, \\ &= \int_0^\infty \mathrm{e}^{-(b+t)\lambda} F(t) \, \mathrm{d}t. \end{aligned}$$

Let $\tau = b + t$, with $\tau_{\mathrm{lw}} = b$ and $\tau_{\mathrm{up}} = \infty$. Hence,

$$\mathrm{e}^{-b\lambda} f(\lambda) = \int_b^\infty \mathrm{e}^{-\lambda \tau} F(\tau - b) \, \mathrm{d}\tau.$$

However, consider

$$F(\tau - b) H(\tau - b) = \begin{cases} F(\tau - b), & \tau > b \\ 0, & \tau < b. \end{cases}$$

Hence,

$$\mathrm{e}^{-b\lambda} f(\lambda) = 0 \times \int_0^b \mathrm{e}^{-\lambda \tau} F(\tau - b) \, \mathrm{d}\tau + 1 \times \int_b^\infty \mathrm{e}^{-\lambda \tau} F(\tau - b) \, \mathrm{d}\tau$$
$$= \int_0^\infty \mathrm{e}^{-\lambda \tau} F(\tau - b) H(\tau - b) \, \mathrm{d}\tau.$$

Theorem 5.4 (Differentiation in real space) *$F(t)$ be a C^1 function of t, with F and its deriva-*

tive at worst exponentially diverging. Then $\left(\widehat{dF/dt}\right)_\lambda$ *exists and*

$$\widehat{\left(\frac{dF}{dt}\right)}_\lambda = \int_0^\infty \lambda \mathrm{e}^{-\lambda t} F(t) \mathrm{d}t - F(0).$$

Proof: By assumption, dF/dt is at worst exponentially diverging, and its Laplace transform exists, at least for appropriate λ-values. Also by definition,

$$\begin{aligned}
\widehat{\left(\frac{dF}{dt}\right)}_\lambda &= \int_0^\infty \mathrm{e}^{-\lambda t} \frac{dF}{dt} \mathrm{d}t, \\
&= \int_0^\infty \left[\frac{d}{dt}\left(\mathrm{e}^{-\lambda t} F\right) + \lambda \mathrm{e}^{-\lambda t} F\right] \mathrm{d}t, \\
&= \lim_{L\to\infty} \mathrm{e}^{-\lambda L} F(L) - F(0) + \int_0^\infty \lambda \mathrm{e}^{-\lambda t} F(t) \mathrm{d}t.
\end{aligned}$$

For Re(λ) sufficiently large and positive, the limiting boundary term vanishes, and

$$\widehat{\left(\frac{dF}{dt}\right)}_\lambda = \int_0^\infty \lambda \mathrm{e}^{-\lambda t} F(t) \mathrm{d}t - F(0),$$

as required.

Theorem 5.5 (Differentiation in transform space) $F(t)$ *be piecewise differentiable with respect to* t*. Then* $f(\lambda) := \widehat{F}_\lambda$ *is differentiable with respect to* λ *and, moreover,*

$$f'(\lambda) = \mathcal{L}\left(-tF(t)\right).$$

Proof: For suitable λ, the integral

$$f(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} F(t) \mathrm{d}t$$

is well-defined and is uniformly convergent and may be differentiated under the integral sign with

respect to λ. We compute:

$$\begin{aligned} f'(\lambda) &= \frac{d}{d\lambda}\int_0^\infty \mathrm{e}^{-\lambda t}F(t)\mathrm{d}t, \\ &= \int_0^\infty \left[\frac{\partial}{\partial\lambda}\mathrm{e}^{-\lambda t}\right]F(t)\mathrm{d}\lambda, \\ &= \int_0^\infty \mathrm{e}^{-\lambda t}\left[-tF(t)\right]\mathrm{d}t, \\ &= \mathcal{L}\left(-tF(t)\right). \end{aligned}$$

Definition 5.3 (Convolution) *Let $F(t)$ and $G(t)$ be at-worst exponentially diverging. The convolution of F and G is defined as*

$$(F * G)(t) = \int_0^t F_1(t-\tau)F_2(\tau)\mathrm{d}\tau.$$

Theorem 5.6 (by Faltung) *Let $F(t)$ and $G(t)$ be at-worst exponentially diverging, with Laplace transforms $\widehat{F}_\lambda$ and $\widehat{G}_\lambda$ respectively. Then*

$$\widehat{F}_\lambda\widehat{G}_\lambda = \mathcal{L}\left[(F * G)(t)\right]$$

Proof: By direct computation, we have

$$\widehat{F}_\lambda\widehat{G}_\lambda = \int_0^\infty \mathrm{e}^{-\lambda t}F(t)\,\mathrm{d}t\int_0^\infty \mathrm{e}^{-\lambda s}G(s)\,\mathrm{d}s.$$

We first of all re-write the integral as follows:

$$\widehat{F}_\lambda\widehat{G}_\lambda = \lim_{L\to\infty}\int_0^L \mathrm{e}^{-\lambda t}F(t)\mathrm{d}t\int_0^L \mathrm{e}^{-\lambda s}G(s)\,\mathrm{d}s.$$

The **trick** is to re-write this further as

$$\widehat{F}_\lambda\widehat{G}_\lambda = \lim_{L\to\infty}\int_0^L \mathrm{e}^{-\lambda t}F(t)\,\mathrm{d}t\int_0^{L-t} \mathrm{e}^{-\lambda s}G(s)\,\mathrm{d}s.$$

In fact, we have changed the region of integration from an $L\times L$ square to a triangle with vertices at $(0,0)$, $(0,L)$, and $(L,0)$. However, leaving out half the domain of integration does not matter, as the omitted region is 'filled in' as $L\to\infty$ (e.g. Figure 5.5). Now, we proceed by direct calculation. We want only one free variable in the exponential argument. We do not modify the variable s; instead we define

$$t + s = \tau \implies t = s - \tau$$

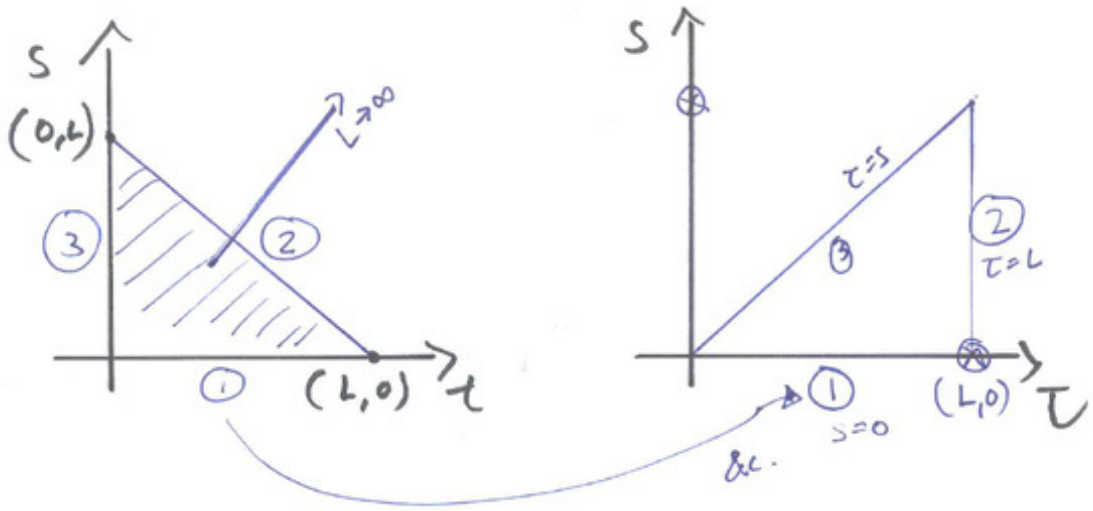


Figure 5.5: Sketch for the change-of-variables in the Convolution Theorem

Again referring to Figure 5.5, we have

- Line Segment 1 ($s = 0$) is mapped to $s = 0$;
- Line Segment 2 ($s = L - t$) implies that $\tau = t + (L - t) = L$ (constant); hence line-segment 2 is mapped to a vertical line segment passing through $\tau = L$.
- The condition on Line Segment 3 ($t = 0$) implies $s = \tau$, hence line segment 3 is mapped to the straight line of slope 45° passing through the origin.

Also, consider the transformation, expressed correctly here as

$$\begin{aligned} \tau &= t + s, \\ s' &= s, \end{aligned}$$

with inverse

$$\begin{aligned} t &= \tau - s', \\ s &= s'. \end{aligned}$$

We have

$$\mathrm{d}t\,\mathrm{d}s = \underbrace{\begin{vmatrix} \frac{\partial t}{\partial \tau} & \frac{\partial t}{\partial s'} \\ \frac{\partial s}{\partial \tau} & \frac{\partial s'}{\partial s} \end{vmatrix}}_{=J} \mathrm{d}\tau\,\mathrm{d}s'.$$

$$J = \begin{vmatrix} 1 & -1 \\ 0 & 1 \end{vmatrix} = 1,$$

hence

$$\mathrm{d}t\,\mathrm{d}s = \mathrm{d}\tau\,\mathrm{d}s'.$$

Putting it all together, we have

$$\begin{aligned}
\widehat{F}_\lambda \widehat{G}_\lambda &= \lim_{L\to\infty} \int_0^L \mathrm{e}^{-\lambda t} F(t)\,\mathrm{d}t \int_0^{L-t} \mathrm{e}^{-\lambda s} G(s)\,\mathrm{d}s, \\
&= \lim_{L\to\infty} \int_0^L \mathrm{d}t \int_0^{L-t} \mathrm{d}s\, \mathrm{e}^{-\lambda t} F(t) \mathrm{e}^{-\lambda s} G(s), \\
&= \lim_{L\to\infty} \int_0^L \mathrm{d}\tau \int_0^{\tau} \mathrm{d}s\, F(\tau - s) \mathrm{e}^{-\lambda(\tau - s)} G(s) \mathrm{e}^{-\lambda s}, \\
&= \lim_{L\to\infty} \int_0^L \mathrm{d}\tau\, \mathrm{e}^{-\lambda\tau} \int_0^{\tau} \mathrm{d}s\, F(\tau - s) G(s), \\
&= \int_0^{\infty} \mathrm{d}\tau\, \mathrm{e}^{-\lambda\tau} \left[\int_0^{\tau} \mathrm{d}s\, F(\tau - s) G(s) \right], \\
&= \int_0^{\infty} \mathrm{d}\tau\, \mathrm{e}^{-\lambda\tau} (F * G)(\tau), \\
&= \mathcal{L}[(F * G)(\tau)].
\end{aligned}$$

Example

Compute the inverse transform of

$$f(\lambda) = \frac{1 - \mathrm{e}^{-a\lambda}}{\lambda}, \qquad a \in \mathbb{R}^+.$$

We break it up into two parts. Consider

$$I_1 = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{B}} \frac{\mathrm{e}^{\lambda t}}{\lambda} \mathrm{d}\lambda.$$

The Bromwich contour is a straight line parallel to the imaginary axis passing through $z = 0 + \mathrm{i}\epsilon$, with $\epsilon \downarrow 0$. The integrand has a single simple pole at $\lambda = 0$, with

$$\mathrm{Res}\left(\frac{\mathrm{e}^{\lambda t}}{\lambda}, 0 \right) = 1.$$

Hence,

$$I_1 = 1, \qquad t > 0.$$

On the other hand, if $t < 0$, to get a convergent integral we would have to close the contour by forming a semi-circle on the **right** of the Bromwich line. However, such a contour encloses no singularities, hence

$$I_1 = 0, \qquad t < 0.$$

We do the second integral by considering

$$I_2 = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{B}} \frac{\mathrm{e}^{(t-a)\lambda}}{\lambda} \mathrm{d}\lambda.$$

The integrand is

$$\frac{\mathrm{e}^{\lambda_\mathrm{r}(t-a)} \mathrm{e}^{\lambda_\mathrm{i}(t-a)}}{\lambda}$$

The Bromiwch contour is the same as before. For the $\mathcal{B}$-contour given there are two possibilities:

1. $t-a>0$ – chose $\lambda_\mathrm{r}<0$ – close the contour on the left. Thus, a contribution to the integral is picked up from the pole at $\lambda=0$.
2. $t-a<0$ – chose $\lambda_\mathrm{r}>0$ – close the contour on the right. Thus, there are no pole-contributions to the integral and the integral vanishes.

In other words,

$$I_2 = \begin{cases} 1, & \text{if } t>a, \\ 0, & \text{if } t<1. \end{cases}$$

Finally, the answer is

$$F(t) = H(t) - H(t-a).$$

However, from a sketch, this can be seen to be a top-hat function:

$$F(t) = \begin{cases} 0, & \text{if } t<0, \\ 1, & \text{if } 0<t<a, \\ 0, & \text{if } t>a. \end{cases}$$

There is another way of getting at the second integral I_2. From the translation theorem, we have

$$\mathrm{e}^{-a\lambda} \widehat{\phi}_\lambda = \int_0^\infty \mathrm{e}^{-\lambda t} \phi(t) H(t-a) \mathrm{d}t,$$

Taking $\phi(t)=H(t)$, with $\widehat{\phi}_\lambda = 1/\lambda$, we have

$$\begin{aligned} \frac{\mathrm{e}^{-a\lambda}}{\lambda} &= \int_0^\infty \mathrm{e}^{-\lambda t} H(t) H(t-a) \mathrm{d}t, \\ &= \int_0^\infty \mathrm{e}^{-\lambda t} H(t-a) \mathrm{d}t. \end{aligned}$$

Hence, the Laplace transform of $H(t-a)$ is $\mathrm{e}^{-a\lambda}/\lambda$, hence

$$\frac{1}{2\pi \mathrm{i}} \int_{\mathcal{B}} \left(\frac{\mathrm{e}^{-a\lambda}}{\lambda} \right) \mathrm{e}^{\lambda t} \mathrm{d}\lambda = H(t-a),$$

as computed already, using a direct approach.

5.6 Worked example

Let $f(\lambda) = \lambda^{-1/p}$ be the Laplace transform of a function, where $p \in \{2, 3, \cdots\}$ is an integer. Find the generating function.

The function $f(\lambda)$ has a branch cut along the curve

$$\{z = x + 0\mathrm{i}y | x \leq 0\}.$$

Consider the closed contour $\mathcal{C}$ shown previously in Figure 5.4. Since $\mathcal{C}$ encloses no singularities, we have

$$\int_{\mathcal{C}} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/p}} \mathrm{d}\lambda = 0.$$

Moreover, the contour $\mathcal{C}$ can be regarded as being made up of many parts:

- The Bromwich contour;
- A small semi-circle of radius ϵ centred at zero.
- The lines surrounding the branch cut.
- Semi-circular parts (centred at zero) of radius R, with $R \to \infty$.
- Small linear parts with $z = x \pm \mathrm{i}R$, and $x \in [0, 2\epsilon]$ (say).

We consider these parts separately now, starting with the semi-circle of radius ϵ. This evaluates to

$$\int_{-\pi/2}^{\pi/2} (\epsilon \, \mathrm{i} \, \mathrm{d}\theta) \, \frac{\mathrm{e}^{\epsilon t \cos\theta + \mathrm{i}\epsilon t \sin\theta}}{\epsilon^{1/p} \mathrm{e}^{\mathrm{i}\theta/p}},$$

which vanishes as $\epsilon^{1-(1/p)} = \epsilon^{(p-1)/p}$ as $\epsilon \to 0$. Also, the semi-circular parts of radius R contain contributions such as

$$\int (R \, \mathrm{i} \, \mathrm{d}\theta) \, \frac{\mathrm{e}^{Rt\cos\theta + \mathrm{i}Rt\sin\theta}}{R^{1/p} \mathrm{e}^{\mathrm{i}\theta/p}}.$$

The limits of integration are unspecified; however, they are in the second and third quadrants where $\cos\theta < 0$. Thus, these contributions vanish as

$$R^{(p-1)/p} \mathrm{e}^{-R\alpha}, \qquad \alpha \in \mathbb{R}^+,$$

as $R \to 0$ (we take $t > 0$). The linear parts vanish similarly. It follows then that

$$F(t) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{B}} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/p}} \mathrm{d}\lambda = -\frac{1}{2\pi \mathrm{i}} \left(\int_{L_1} \mathrm{d}\lambda + \int_{L_2} \mathrm{d}\lambda \right) \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/p}}, \tag{5.6}$$

where L_1 and L_2 are the contributions from the linear contours surrounding the branch cut.

Consider the integral along L_1. We have

$$\begin{aligned} \lambda &= |\lambda| \mathrm{e}^{+\mathrm{i}\pi}, \\ &= (-x) \mathrm{e}^{+\mathrm{i}\pi}, \\ \lambda^{1/p} &= (-x)^{1/p} \mathrm{e}^{\mathrm{i}\pi/p}. \end{aligned}$$

We also have $\lambda = x$ on L_1, and we use whichever form is convenient in the following string of relations:

$$\begin{aligned} \int_{L_1} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/p}} \mathrm{d}\lambda &= \int_{-\infty}^{0} \frac{\mathrm{e}^{xt}}{(-x)^{1/p} \mathrm{e}^{\mathrm{i}\pi/p}} \mathrm{d}x, \\ &= \mathrm{e}^{-\mathrm{i}\pi/p} \int_0^{\infty} \frac{\mathrm{e}^{-yt}}{y^{1/p}} \mathrm{d}y. \end{aligned}$$

Let $y = z^2$, with $\mathrm{d}y = 2z \, \mathrm{d}z$. Then,

$$\begin{aligned} \int_0^{\infty} \frac{\mathrm{e}^{-yt}}{y^{1/p}} \mathrm{d}y &= 2 \int_0^{\infty} \frac{\mathrm{e}^{-z^2 t}}{z^{2/p}} z \, \mathrm{d}z, \\ &= 2 \int_0^{\infty} \mathrm{e}^{-z^2 t} z^{1-2/p} \mathrm{d}z, \\ &= 2 \int_0^{\infty} z^{2n} \mathrm{e}^{-z^2 t} \mathrm{d}z, \qquad n = \tfrac{1}{2} - \tfrac{1}{p}, \\ &= \frac{\Gamma(n + \frac{1}{2})}{t^{n+(1/2)}}, \\ &= \Gamma(1 - \tfrac{1}{p}) t^{-(1-(1/p))}, \\ &= \Gamma(1 - \tfrac{1}{p}) \frac{t^{1/p}}{t}. \end{aligned}$$

Whew!

Next, consider the integral along L_2. We have

$$\begin{aligned} \lambda &= |\lambda| \mathrm{e}^{-\mathrm{i}\pi}, \\ &= (-x) \mathrm{e}^{-\mathrm{i}\pi}, \\ \lambda^{1/p} &= (-x)^{1/p} \mathrm{e}^{-\mathrm{i}\pi/p}. \end{aligned}$$

We also have $\lambda = x$ on L_2. Hence,

$$\begin{aligned}\int_{L_2} \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}} \mathrm{d}\lambda &= \int_0^{-\infty} \frac{\mathrm{e}^{xt}}{(-x)^{1/p}\mathrm{e}^{-\mathrm{i}\pi/p}} \mathrm{d}x, \\ &= -\mathrm{e}^{\mathrm{i}\pi/p} \int_0^{\infty} \frac{\mathrm{e}^{-yt}}{y^{1/p}} \mathrm{d}y.\end{aligned}$$

Putting it all together and using Equation (5.6), we get

$$\begin{aligned}F(t) &= -\frac{1}{2\pi\mathrm{i}} \left(\int_{L_1} \mathrm{d}\lambda + \int_{L_2} \mathrm{d}\lambda \right) \frac{\mathrm{e}^{\lambda t}}{\lambda^{1/2}}, \\ &= -\frac{1}{2\pi\mathrm{i}} \left(\mathrm{e}^{-\mathrm{i}\pi/p} - \mathrm{e}^{\mathrm{i}\pi/p} \right) \Gamma\left(1 - \tfrac{1}{p}\right) \frac{t^{1/p}}{t}, \\ &= \frac{\Gamma\left(1 - \frac{1}{p}\right)}{\pi} \sin(\pi/p) \frac{t^{1/p}}{t}.\end{aligned}$$

But

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x}.$$

Hence,

$$\frac{\sin \pi x}{\pi} = \frac{1}{\Gamma(x)\Gamma(1-x)}$$

Take $x = 1/p$ to obtain

$$\begin{aligned}F(t) &= \Gamma\left(1 - \tfrac{1}{p}\right) \frac{\sin(\pi/p)}{\pi} \frac{t^{1/p}}{t}, \\ &= \Gamma\left(1 - \tfrac{1}{p}\right) \frac{1}{\Gamma(1/p)\Gamma(1-(1/p))} \frac{t^{1/p}}{t}, \\ &= \frac{1}{\Gamma(1/p)} \frac{t^{1/p}}{t}.\end{aligned}$$

Check against standard formula:

$$\begin{aligned}\widehat{t^{1/n}} &= \frac{\Gamma(1+(1/n))}{\lambda^{(1/n)+1}}, \\ \frac{1}{\Gamma(1+(1/n))} \widehat{t^{1/n}} &= \frac{1}{\lambda^{(1/n)+1}},\end{aligned}$$

Take $(1/n) + 1 = 1/p$, hence $1/n = (1/p) - 1$, hence

$$\frac{1}{\Gamma(1/p)} \widehat{t^{(1/n)-1}} = \frac{1}{\lambda^{(1/p)}},$$

and our result is confirmed.

Chapter 6

The steepest-descent method

Overview

The solution to many problems in Applied Mathematics and Mathematical Physics can be written as an integral involving a parameter. Typically, these integrals are difficult if not impossible to evaluate. However, generic techniques exist to evaluate these integrals in the limit of large parameter values. The first such technique is called Laplace's method, and the same method, applied to complex parameters, is called the saddle-point or steepest-descent method. Both techniques are discussed here, with the complex case following naturally from the simpler real case.

6.1 Laplace's asymptotic method for integrals

The idea of this method is to find asymptotic expressions for integrals such as

$$I(\lambda) = \int_a^b F(t)\mathrm{e}^{-\lambda g(t)}\mathrm{d}t, \qquad \text{as } \lambda \to \infty. \tag{6.1}$$

Here, λ is a **real** parameter, and the function g attains a strict **minimum** at c in the interior of $[a, b]$, such that

- $g'(c) = 0$,
- $g''(c) > 0$,
- $F(t)$ is continuous, with $F(t) \neq 0$.

We rewrite Equation (6.1) as

$$I(\lambda) = \mathrm{e}^{-\lambda g(c)} \int_a^b F(t)\mathrm{e}^{-\lambda[g(t)-g(c)]}\mathrm{d}t \tag{6.2}$$

The main idea of Laplace's method is to observe that as $\lambda \to \infty$, the dominant contribution to the integral (6.2) comes from a small neighbourhood of the minimum at $x = c$. Looked at in another way, the argument of the exponential

$$-\lambda[g(t) - g(c)]$$

is negative or zero. At large λ, and for $t \neq c$, the phase is very negative and $\mathrm{e}^{(\mathrm{argument})}$ is small and does not contribute. Thus,

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} F(t)\mathrm{e}^{-\lambda[g(t)-g(c)]}\mathrm{d}t \qquad \text{as } \lambda \to \infty,$$

where ϵ is a small positve number. We compute the integral as follows:

$$\begin{aligned} I(\lambda) &\sim \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} F(t)\mathrm{e}^{-\lambda[g(t)-g(c)]}\mathrm{d}t \qquad \text{as } \lambda \to \infty, \\ &\approx \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} F(t)\mathrm{e}^{-\lambda(1/2)g''(c)(t-c)^2}\mathrm{d}t, \\ &\approx \mathrm{e}^{-\lambda g(c)} F(c) \int_{c-\epsilon}^{c+\epsilon} \mathrm{e}^{-\lambda(1/2)g''(c)(t-c)^2}\mathrm{d}t. \end{aligned}$$

The integrand is now a pure Gaussian integral, whose width is proportional to $\lambda^{-1/2}$. Thus, the Gaussian integrand is approximately zero outside of the small region $[c - \epsilon, c + \epsilon]$, and we can therefore extend the limits of integration, incurring only vanishing errors in the process:

$$\begin{aligned} I(\lambda) &\approx \mathrm{e}^{-\lambda g(c)} F(c) \int_{-\infty}^{\infty} \mathrm{e}^{-\lambda(1/2)g''(c)(t-c)^2}\mathrm{d}t \qquad \text{as } \lambda \to \infty, \\ &= \mathrm{e}^{-\lambda g(c)} F(c) \sqrt{\frac{2\pi}{\lambda g''(c)}} \end{aligned}$$

Thus,

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(c)} F(c) \sqrt{\frac{2\pi}{\lambda g''(c)}} \qquad \text{as } \lambda \to \infty, \tag{6.3}$$

and the leading-order behaviour of Equation (6.1) is captured.

Modification – minimum attained at boundary

Suppose that $g(t)$ attains its minimum at $t = a$ (i.e. $a = c$). We rewrite Equation (6.1) as

$$I(\lambda) = \mathrm{e}^{-\lambda g(a)} \int_{a}^{b} F(t)\mathrm{e}^{-\lambda[g(t)-g(a)]}\mathrm{d}t \tag{6.4}$$

Again by the argument where the 'phase' is minimized, the integral is approximated by

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(a)} \int_a^{a+\epsilon} F(t) \mathrm{e}^{-\lambda[g(t)-g(a)]} \mathrm{d}t$$

Proceeding as before, we have

$$\begin{aligned} I(\lambda) &\sim \mathrm{e}^{-\lambda g(a)} F(a) \int_a^{a+\epsilon} \mathrm{e}^{-\lambda(1/2)g''(a)(t-a)^2} \mathrm{d}t, \\ &= \mathrm{e}^{-\lambda g(a)} F(a) \int_0^{\epsilon} \mathrm{e}^{-\lambda(1/2)g''(a)\tau^2} \mathrm{d}\tau, \\ &\sim \mathrm{e}^{-\lambda g(a)} F(a) \int_0^{\infty} \mathrm{e}^{-\lambda(1/2)g''(a)\tau^2} \mathrm{d}\tau \qquad \text{as } \lambda \to \infty, \\ &= \tfrac{1}{2} \mathrm{e}^{-\lambda g(a)} F(a) \sqrt{\frac{2\pi}{\lambda g''(a)}}, \end{aligned}$$

hence

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(a)} F(a) \sqrt{\frac{\pi}{2\lambda g''(a)}} \qquad \text{as } \lambda \to \infty,$$

Example: Evaulate

$$I(\lambda) = \int_{-1}^{1} \frac{\sin t}{t} \mathrm{e}^{-\lambda \cosh t} \mathrm{d}t,$$

as $t \to \infty$.

We identify $g(t) = \cosh t$. This has a global minimum at $t = c = 0$, contained entirely in the domain of integration. Also, $F(t) := \sin(t)/t$ is continuous, provided we take $F(0) = 1$, consistent with L'Hôpital's Rule. Finally, $g''(t) = \cosh(t)$, hence $g''(0) = 1$. We read off the answer directly from the formula (6.3):

$$I(\lambda) \sim \mathrm{e}^{-\lambda} \sqrt{\frac{2\pi}{\lambda}} \qquad \text{as } \lambda \to \infty.$$

6.2 Stirling's Approximation

We show that

$$n! \sim \sqrt{2\pi} n^{n+1/2} \mathrm{e}^{-n} \qquad \text{as } n \to \infty.$$

We start with the integral definition of the factorial function:

$$\begin{aligned} n! &= \int_0^\infty t^n \mathrm{e}^{-t} \mathrm{d}t \\ &= \int_0^\infty \mathrm{e}^{n \log t} \mathrm{e}^{-t} \mathrm{d}t, \\ &= \int_0^\infty \mathrm{e}^{n \log t - t} \mathrm{d}t, \\ &= \int_0^\infty \mathrm{e}^{n(\log t - t/n)} \mathrm{d}t, \\ &= n \int_0^\infty \mathrm{e}^{n(\log(nz) - z)} \mathrm{d}z, \qquad z = t/n, \\ &= n \mathrm{e}^{n \log n} \int_0^\infty \mathrm{e}^{n(\log z - z)} \mathrm{d}z, \\ &= n^{n+1} \int_0^\infty \mathrm{e}^{n(\log z - z)} \mathrm{d}z. \end{aligned}$$

We now consider the asymptotic integral

$$I(n) = \int_0^\infty \mathrm{e}^{-n(z - \log z)} \mathrm{d}z.$$

We identify $F(z) = 1$ and $g(z) = z - \log z$. The g-function has a minimum at $z = 1$, with $g(1) = 1$ and $g''(1) = 1$. This is clearly a minimum, as $g(z) \to \infty$ as $z \to 0$ and as $z \to \infty$. Thus, Laplace's method applies, and

$$I(n) \sim \mathrm{e}^{-n} \sqrt{\frac{2\pi}{n}} \qquad \text{as } n \to \infty.$$

Putting it all together,

$$n! \sim \sqrt{2\pi} n^{n+1/2} \mathrm{e}^{-n} \qquad \text{as } n \to \infty.$$

6.3 Higher-order approximations

In order for Laplace's method to work, we required that $F(c) \neq 0$ at the location of the (strict) minimum $t = c$. However, this condition can be lifted quite readily, provided $F(c)$ is differentiable.

As before, we start with Equation (6.1) and re-write it as

$$I(\lambda) = \mathrm{e}^{-\lambda g(a)} \int_a^b F(t)\mathrm{e}^{-\lambda[g(t)-g(a)]}\mathrm{d}t \tag{6.5}$$

The dominant contribution to the integral comes from a small neighbourhood of the strict minimum $t = c$ (with $g'(c) = 0$ and $g''(c) > 0$). Thus, the equation is re-written further as

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} F(t)\mathrm{e}^{-\lambda[g(t)-g(c)]}\mathrm{d}t \qquad \text{as } \lambda \to \infty.$$

We exapnd $F(t)$ and $g(t)$ in Taylor series centred at $t = c$:

$$\begin{aligned} I(\lambda) &\sim \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} F(t)\mathrm{e}^{-\lambda[g(t)-g(c)]}\mathrm{d}t \qquad \text{as } \lambda \to \infty, \\ &\approx \mathrm{e}^{-\lambda g(c)} \int_{c-\epsilon}^{c+\epsilon} \left[F(c) + F'(c)(t-c) + \tfrac{1}{2}F''(c)(t-c)^2\right] \mathrm{e}^{-\lambda(1/2)g''(c)(t-c)^2}\mathrm{d}t. \end{aligned}$$

As before, the Gaussian factor $\mathrm{e}^{-\lambda g''(c)(t-c)^2}$ has width proportional to $\lambda^{-1/2}$, and hence contributions to the integral from regions outside of $[c-\epsilon, c+\epsilon]$ are vanishingly small. Thus,

$$I(\lambda) \sim \mathrm{e}^{-\lambda g(c)} \int_{-\infty}^{\infty} \left[F'(c)(t-c) + \tfrac{1}{2}F''(c)(t-c)^2\right] \mathrm{e}^{-\lambda(1/2)g''(c)(t-c)^2}\mathrm{d}t \qquad \text{as } \lambda \to \infty.$$

Change variables: $\tau = t - c$:

$$\begin{aligned} I(\lambda) &\sim \mathrm{e}^{-\lambda g(c)} \int_{-\infty}^{\infty} \left[F'(c)\tau + \tfrac{1}{2}F''(c)\tau^2\right] \mathrm{e}^{-\lambda(1/2)g''(c)\tau^2}\mathrm{d}\tau \qquad \text{as } \lambda \to \infty, \\ &= \mathrm{e}^{-\lambda g(c)}F'(c) \int_{-\infty}^{\infty} \tau\mathrm{e}^{-\lambda(1/2)g''(c)\tau^2}\,\mathrm{d}\tau + \tfrac{1}{2}\mathrm{e}^{-\lambda g(c)}F''(c) \int_{-\infty}^{\infty} \tau^2\mathrm{e}^{-\lambda(1/2)g''(c)\tau^2}\,\mathrm{d}\tau, \\ &= \tfrac{1}{2}\mathrm{e}^{-\lambda g(c)}F''(c) \int_{-\infty}^{\infty} \tau^2\mathrm{e}^{-\lambda(1/2)g''(c)\tau^2}\,\mathrm{d}\tau, \\ &= \tfrac{1}{2}\mathrm{e}^{-\lambda g(c)}F''(c)\left[\lambda g''(c)/2\right]^{-3/2} \int_{-\infty}^{\infty} s^2\mathrm{e}^{-s^2}\mathrm{d}s, \end{aligned}$$

But consider

$$J(\gamma) = \int_{-\infty}^{\infty} \mathrm{e}^{-\gamma s^2}\mathrm{d}s = \sqrt{\pi/\gamma}.$$

Hence,

$$-\frac{dJ}{d\gamma} = \tfrac{1}{2}\sqrt{\pi}\gamma^{-3/2} = \int_{-\infty}^{\infty} s^2\mathrm{e}^{-\gamma s^2}\mathrm{d}s.$$

Set $\gamma = 1$ to obtain

$$\tfrac{1}{2}\sqrt{\pi} = \int_{-\infty}^{\infty} s^2\mathrm{e}^{-s^2}\mathrm{d}s,$$

hence

$$I(\lambda) \sim \tfrac{1}{4}\sqrt{\pi}\mathrm{e}^{-\lambda g(c)}F''(c)\left[\lambda g''(c)/2\right]^{-3/2}.$$

Tidying up, this is

$$I(\lambda) \sim F''(c)\mathrm{e}^{-\lambda g(c)}\sqrt{\frac{\pi/2}{[\lambda g''(c)]^3}} \qquad \text{as } \lambda \to \infty.$$

6.4 The method of steepest descents

In this section, we are interested in integrals of the form

$$I(\lambda) = \int_C f(z)\mathrm{e}^{\lambda g(z)}\,\mathrm{d}z, \tag{6.6a}$$

where $f(z)$ and $g(z)$ are non-constant and analytic for all $z \in \mathbb{C}$, and where C is some contour in the complex plane. Call

$$\begin{aligned} F : \mathbb{C}\times\mathbb{R} &\to \mathbb{C}, \\ (z,\lambda) &\mapsto f(z)\mathrm{e}^{\lambda g(z)}. \end{aligned} \tag{6.6b}$$

Because $F(z,\cdot)$ is analytic, it admits no poles or branch cuts. Hence, Equation (6.6a) admits no contributions from the Residue Theorem, or from other applications of Cauchy's Integral Theorem. Moreover, $|F(z)|$ has no maxima in the complex plane, and therefore the contributions to the integral (6.6a) come neither from singularities nor maxima. Indeed, we have the following result:

Theorem 6.1 (Jensen) *Let $\phi(z) : \mathbb{C} \to \mathbb{C}$ be non-constant and analytic in the entire complex plane. Then $|\phi(z)|^2$ has no maxima and, moreover, its minima extend down to zero.*

We now consider the integral in Equation (6.6a). It turns out that the next feature to provide a dominant contribution to the integral (6.6a) is the **saddle point**. We first of all demonstrate this result for the test case $g(z) = a + (1/2)bz^2$, with $f(0) \neq 0$, and then proceed to the general case where $g(z)$ admits a saddle point at z_0, $g'(z_0) = 0$.

Test case

We start with

$$g(z) = a + \tfrac{1}{2}bz^2, \qquad f(0) \neq 0,$$

where $F(z,\lambda) = f(z)\mathrm{e}^{\lambda g(z)}$. We assume that the contour C is open with endpoints at α and β (the endpoints can be located at infinity). It is a straightforward consequence of Cauchy's integral

theorem that

$$\int_C (\cdots)\mathrm{d}z = \int_{C'} (\cdots)\mathrm{d}z$$

where the contour C' is a deformation of the contour C that leaves the endpoints unchanged. The switch to the new contour is legitimate provided that we do not traverse any singularities of the integrand in doing the deformation. Because $F(z,\lambda)$ is assumed to be analytic, this deformation is always legitimate in the framework in which we work.

We note that $g(z)$ has a regular saddle point at $z = z_0 := 0$: $g'(z_0) = 0$, with $g''(z_0) \neq 0$. We simply **choose** the contour C' such that

- C' passes through z_0;

- The curve C' is defined such that

$$g_{\mathrm{i}}(z) = \mathrm{Const.} = g_{\mathrm{i}}(z_0),$$

  as C' passes through z_0 (curve of constant phase).

But

$$\begin{aligned} g_{\mathrm{r}}(z) &= a_{\mathrm{r}} + \tfrac{1}{2}\left[b_{\mathrm{r}}\left(x^2 - y^2\right) - 2b_{\mathrm{i}}xy\right], \\ g_{\mathrm{i}}(z) &= a_{\mathrm{i}} + \tfrac{1}{2}\left[b_{\mathrm{i}}\left(x^2 - y^2\right) + 2b_{\mathrm{r}}xy\right], \end{aligned}$$

and $z_0 = (x_0, y_0) = 0$, hence $g_{\mathrm{i}}(z_0) = a_{\mathrm{i}}$, which defines at least a portion of the curve C' as

$$b_{\mathrm{i}}\left(x^2 - y^2\right) + 2b_{\mathrm{r}}xy = 0.$$

Hence,

$$y = \frac{xb_{\mathrm{r}} \pm |x||b|}{b_{\mathrm{i}}}.$$

All possibilities for the precise definition of the curve are enumerated by the following two cases:

$$y = \frac{x(|b| + b_{\mathrm{r}})}{b_{\mathrm{i}}}, \qquad y = -\frac{x(|b| - b_{\mathrm{r}})}{b_{\mathrm{i}}}. \tag{6.7}$$

For, consider

$$\begin{aligned}\left[y-\frac{x}{b_{\rm i}}(|b|+b_{\rm r})\right]\left[y+\frac{x}{b_{\rm i}}(|b|-b_{\rm r})\right] &= y^2+\frac{yx}{b_{\rm i}}\left(|b|-b_{\rm r}-|b|-b_{\rm r}\right)-\frac{x^2}{b_{\rm i}^2}\left(|b|+b_{\rm r}\right)\left(|b|-b_{\rm r}\right)\\ &= y^2-2\left(\frac{b_{\rm r}}{b_{\rm i}}\right)xy-\frac{x^2}{b_{\rm i}^2}\left(|b|^2-b_{\rm r}^2\right)\\ &= y^2-2\left(\frac{b_{\rm r}}{b_{\rm i}}\right)xy-x^2\\ &= -\frac{1}{b_{\rm i}}\left[b_{\rm i}(x^2-y^2)+2b_{\rm r}xy\right],\end{aligned}$$

Upon setting the left-hand side to zero, the original definition of the curve is recovered. Furthermore, the two lines in Equation (6.7) are orthogonal. For, consider $y_1=x(|b|+b_{\rm r})/b_{\rm i}$ and $y_2=-x(|b|-b_{\rm r})/b_{\rm i}$, with slopes $m_1=(|b|+b_{\rm r})/b_{\rm i}$ and $m_2=-(|b|-b_{\rm r})/b_{\rm i}$ respectively. Then

$$\begin{aligned}m_1m_2 &= \frac{-(|b|+b_{\rm r})(|b|-b_{\rm r})}{b_{\rm i}^2},\\ &= \frac{-(|b|^2-b_{\rm r}^2)}{b_{\rm i}^2},\\ &= -1.\end{aligned}$$

We shall show that these lines correspond to the so-called lines of steepest descent and ascent (in no particular order) in what follows.

It now remains to choose the appropriate case from Equation (6.7). We have

$$\begin{aligned}g_{\rm r}(z) &= a_{\rm r}+\tfrac{1}{2}\left[b_{\rm r}(x^2-y^2)-2b_{\rm i}xy\right],\\ &= a_{\rm r}+\tfrac{1}{2}\left[-2b_{\rm r}\left(\frac{b_{\rm r}}{b_{\rm i}}\right)xy-2b_{\rm i}xy\right],\\ &= a_{\rm r}-xy\left(\frac{b_{\rm r}^2+b_{\rm i}^2}{b_{\rm i}}\right),\\ &= a_{\rm r}-x^2\left(\frac{b_{\rm r}^2+b_{\rm i}^2}{b_{\rm i}^2}\right)\begin{cases}(|b|+b_{\rm r}),\\ -(|b|-b_{\rm r})\end{cases}.\end{aligned}$$

We have

$$g_{{\rm r},xx}(z_0)=-2\left(\frac{b_{\rm r}^2+b_{\rm i}^2}{b_{\rm i}^2}\right)\begin{cases}(|b|+b_{\rm r}), & \text{case 1}\\ -(|b|-b_{\rm r}), & \text{case 2}\end{cases}.$$

and we choose case 1, such that

$$g_{{\rm r},xx}(z_0)=-2\left(\frac{b_{\rm r}^2+b_{\rm i}^2}{b_{\rm i}^2}\right)(|b|+b_{\rm r}), \tag{6.8}$$

which forces $g_{\rm r}''(z_0)<0$, thereby making $x=0$ into a **maximum**. In more detail then, the contour

C' is chosen such that

- C' passes through z_0;
- The curve C' is defined such that

$$g_{\rm i}(z) = \text{Const.} = g_{\rm i}(z_0),$$

as C' passes through z_0 (curve of constant phase), **and** $g_{\rm r}(z)$ appears to attain a **maximum** along C'.

We note that superficially $g_{\rm r}(z)$ attains a maximum along C'. However, i in the full complex-analytic landscape, this point is a saddle point. The (case 1) path $dy/dx = (|b| + b_{\rm r})/b_{\rm i}$ is called the curve of **steepest descent**: among all possible curves through z_0,the decrease in $g_{\rm r}(z)$ m away from z_0 is the most rapid along the curve of steepst descent.

We now conclude the derivation: C' has been chosen to make the integral

$$\int_{C'} f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z$$

'look like' the integral in Laplace's method. Thus, we now perform straightforward calculations in the spirit of Section 6.1: we set $g_{\rm i}(z) = \text{constant}$ and pick up a contribution to the integral only in the neighbourhood of the C'-maximum, at $z_0 = 0$:

$$\int_{C'} f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z \;\; = \;\; \mathrm{e}^{g_{\rm i}(z)} \int_{z_0-\eta\epsilon}^{z_0+\eta\epsilon} f(z)\mathrm{e}^{\lambda g_{\rm r}(z)}\mathrm{d}z.$$

where η is a constant phase determined from Equation (6.8). We compute:

$$\int_{C'} f(z)\mathrm{e}^{\lambda g(z)\lambda}\mathrm{d}z \;\; \sim \;\; f(z_0)\mathrm{e}^{\mathrm{i}g_{\rm i}(z_0)\lambda} \int_{z_0-\eta\epsilon}^{z_0+\eta\epsilon} \mathrm{e}^{\lambda g_{\rm r}(z)}\mathrm{d}z,$$

where ϵ is a positive constant. We now change over to the real x-variable, thereby enabling us to invoke the arguments in Laplace's method. We have

$$\begin{aligned}
\mathrm{d}z &= \frac{dz}{dx}\mathrm{d}x, \\
&= \left(1 + \mathrm{i}\frac{dy}{dx}\right)\mathrm{d}x, \\
&= \left(1 + \mathrm{i}\frac{|b| + b_{\rm r}}{b_{\rm i}}\right)\mathrm{d}x.
\end{aligned}$$

Hence,

$$\begin{aligned}\int_{C'} f(z)\mathrm{e}^{\lambda g(z)\lambda}\mathrm{d}z &\sim f(z_0)\mathrm{e}^{\mathrm{i}g_{\mathrm{i}}(z_0)\lambda}\int_{z_0-\eta\epsilon}^{z_0+\eta\epsilon}\mathrm{e}^{\lambda g_{\mathrm{r}}(z)}\mathrm{d}z,\\ &= f(z_0)\mathrm{e}^{\mathrm{i}g_{\mathrm{i}}(z_0)\lambda}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{x_0-\delta}^{x_0+\delta}\mathrm{e}^{\lambda g_{\mathrm{r}}(x)}\mathrm{d}x,\end{aligned}$$

where $x_0 = 0$, and where δ is a second positive constant. We also have – by construction, $g_{\mathrm{r},xx}(x_0) < 0$. Hence,

$$\begin{aligned}\int_{C'} f(z)\mathrm{e}^{\lambda g(z)\lambda}\mathrm{d}z &\sim f(z_0)\mathrm{e}^{\mathrm{i}g_{\mathrm{i}}(z_0)\lambda}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{x_0-\delta}^{x_0+\delta}\mathrm{e}^{\lambda g_{\mathrm{r}}(x)}\mathrm{d}x,\\ &= f(z_0)\mathrm{e}^{\mathrm{i}g_{\mathrm{i}}(z_0)\lambda}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{x_0-\delta}^{x_0+\delta}\mathrm{e}^{\lambda\left[g_{\mathrm{r}}(x_0)+g_{\mathrm{r},x}(x_0)(x-x_0)+(1/2)g_{\mathrm{r},xx}(x-x_0)^2\right]}\mathrm{d}x,\\ &= f(z_0)\mathrm{e}^{\mathrm{i}g_{\mathrm{i}}(z_0)\lambda}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\mathrm{e}^{g_{\mathrm{r}}(x_0)\lambda}\int_{x_0-\delta}^{x_0+\delta}\mathrm{e}^{\lambda g_{\mathrm{r},xx}(x-x_0)^2/2}\mathrm{d}x,\\ &= f(z_0)\mathrm{e}^{g(z_0)\lambda}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{x_0-\delta}^{x_0+\delta}\mathrm{e}^{-\lambda|g_{\mathrm{r},xx}|x^2/2}\mathrm{d}x,\end{aligned}$$

The calculation continues as follows:

$$\begin{aligned}\int_{C'} f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z &\sim f(z_0)\mathrm{e}^{\lambda g(z_0)}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{-\delta}^{\delta}\mathrm{e}^{-\lambda|g_{\mathrm{r},xx}(x_0)|x^2/2}\mathrm{d}x,\\ &= \frac{f(z_0)\mathrm{e}^{\lambda g(z_0)}}{\sqrt{\lambda|g_{\mathrm{r},xx}(x_0)|/2}}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{-\delta|g_{\mathrm{r},xx}(x_0)|^{1/2}\lambda^{1/2}/\sqrt{2}}^{+\delta|g_{\mathrm{r},xx}(x_0)|^{1/2}\lambda^{1/2}/\sqrt{2}}\mathrm{e}^{-s^2}\mathrm{d}s,\\ &\sim \frac{f(z_0)\mathrm{e}^{\lambda g(z_0)}}{\sqrt{\lambda|g_{\mathrm{r},xx}(0)|/2}}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right)\int_{-\infty}^{\infty}\mathrm{e}^{-s^2}\mathrm{d}s,\\ &= \sqrt{\frac{2\pi}{|g_{\mathrm{r},xx}(0)|\lambda}}f(z_0)\mathrm{e}^{\lambda g(z_0)}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right).\end{aligned} \tag{6.9}$$

There remains one further calculation:

$$\frac{1}{\sqrt{|g_{\mathrm{r},xx}(0)|}}\left(1+\mathrm{i}\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}}\right) = \frac{1}{\sqrt{|g_{\mathrm{r},xx}(0)|}}\left[2|b|\left(\frac{|b|+b_{\mathrm{r}}}{b_{\mathrm{i}}^2}\right)\right]^{1/2}\mathrm{e}^{\mathrm{i}\theta}$$

where $m_1 = dy_1/dx = (|b|+b_{\mathrm{r}})/b_{\mathrm{i}} = \tan\theta$ and θ is the angle of the line of steepest descent relative

to the x-axis. Thus,

$$\begin{aligned}\frac{1}{\sqrt{|g_{\mathrm{r},xx}(0)|}}\left(1+\mathrm{i}\frac{|b|+b_\mathrm{r}}{b_\mathrm{i}}\right) &= \frac{1}{\left[2\frac{|b|^2}{b_\mathrm{i}^2}(|b|+b_\mathrm{r})\right]^{1/2}}\left[2|b|\left(\frac{|b|+b_\mathrm{r}}{b_\mathrm{i}^2}\right)\right]^{1/2}\mathrm{e}^{\mathrm{i}\theta},\\ &= \frac{1}{\sqrt{|b|}}\mathrm{e}^{\mathrm{i}\theta}=\frac{1}{\sqrt{|g_{zz}(z_0)|}}\mathrm{e}^{\mathrm{i}\theta}.\end{aligned}$$

Thus, Equation (6.9) becomes

$$\int_C f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z=\int_{C'} f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z\sim f(z_0)\mathrm{e}^{\lambda g(z_0)}\mathrm{e}^{\mathrm{i}\theta}\sqrt{\frac{2\pi}{\lambda|g_{zz}(x_0)|}}.$$

This concludes the derivation.

General case

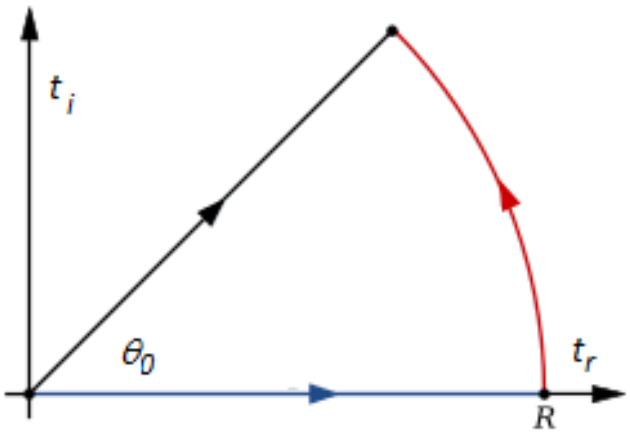
In the general case, where $g(z)$ is some generic analytic function with a saddle point at z_0, the results of the test case carry through directly. We expand $g(z)$ in the neighbourhood of the saddle point, writing

$$g(z)=g(z_0)+\tfrac{1}{2}g_{zz}(z_0)\left(z-z_0\right)^2+O\left(\left(z-z_0\right)^3\right),$$

where $g_z(z_0)=0$. The results of the previous section carry over directly, and the formula

$$\int_C f(z)\mathrm{e}^{\lambda g(z)}\mathrm{d}z\sim f(z_0)\mathrm{e}^{\lambda g(z_0)}\mathrm{e}^{\mathrm{i}\theta}\sqrt{\frac{2\pi}{\lambda|g_{zz}(x_0)|}}. \tag{6.10}$$

is preserved. The curve of steepest descent is still the path $\mathrm{Im}(g(z))=\mathrm{Im}(g(z_0))$, which in the neighbourhood of the saddle point, still resembles the line $dy/dx=\tan\theta$, where $\tan\theta=(|b|+b_\mathrm{r})/b_\mathrm{i}$, and where $b=g_{zz}(z_0)$ as before.



6.5 Worked examples

1. Consider the Fresnel integral

$$F(x) = C(x) + \mathrm{i}S(x) = \int_0^x \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t.$$

Compute the asymptotic ($x \to \infty$) leading-order behaviour in two different ways: first by direct evaluation of

$$\int_0^x \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t$$

using Cauchy's integral theorem and a contour like that in Figure 6.5. In the second way, consider the integral

$$\int_0^1 \mathrm{e}^{\mathrm{i}xt^2}\mathrm{d}t$$

and apply the saddle-point method.

For the first method, we consider the contour C, taken in the anticlockwise sense. This contour encloses no singularities of $\mathrm{e}^{\mathrm{i}t^2}$, hence

$$\int_C \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t = 0.$$

Consider the segment of C consisting of $t = \mathrm{e}^{\mathrm{i}\theta_0}s$, with $s \in [R, 0]$ (direction implied). We have

$$\mathrm{e}^{\mathrm{i}t^2} = \mathrm{e}^{\mathrm{i}(\cos 2\theta_0 + \mathrm{i}\sin 2\theta_0)s^2} = \mathrm{e}^{\mathrm{i}\cos 2\theta_0}\mathrm{e}^{-\sin 2\theta s^2}.$$

Choose $2\theta_0 = \pi/2$, hence $\theta_0 = \pi/4$, hence $\mathrm{e}^{\mathrm{i}t^2} = \mathrm{e}^{-s^2}$. Thus,

$$0 = \int_0^R \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t + \int_0^{\pi/4} \mathrm{e}^{\mathrm{i}z^2}\big|_{z=R\mathrm{e}^{\mathrm{i}\theta}} R\mathrm{i}\mathrm{d}\theta + \int_R^0 \mathrm{e}^{-s^2}\mathrm{d}s\mathrm{e}^{\mathrm{i}\theta_0}. \tag{6.11}$$

Consider

$$\begin{aligned}\int_0^{\pi/4} \mathrm{e}^{\mathrm{i}z^2}\big|_{z=R\mathrm{e}^{\mathrm{i}\theta}} R\mathrm{d}\theta &= \int_0^{\pi/4} \mathrm{e}^{\mathrm{i}R^2(\cos 2\theta+\mathrm{i}\sin 2\theta)} R\mathrm{d}\theta,\\ &= \int_0^{\pi/4} \mathrm{e}^{\mathrm{i}R^2\cos 2\theta}\mathrm{e}^{-R^2\sin 2\theta} R\mathrm{d}\theta.\end{aligned}$$

Since $0 < \sin 2\theta < 1$ on $0 < \theta < \pi/4$, we have $\mathrm{e}^{-R^2\sin 2\theta}R \to 0$ on $0 < \theta < \pi/4$. Thus, Equation (6.11) becomes

$$0 = \int_0^R \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t + \mathrm{e}^{\mathrm{i}\theta_0}\int_R^0 \mathrm{e}^{-s^2}\mathrm{d}s, \qquad \text{as } R\to\infty.$$

Hence,

$$\begin{aligned}\int_0^\infty \mathrm{e}^{\mathrm{i}t^2}\mathrm{d}t &= \mathrm{e}^{\mathrm{i}\pi/4}\int_0^\infty \mathrm{e}^{-s^2}\mathrm{d}s,\\ &= \frac{1+\mathrm{i}}{\sqrt{2}}\frac{\sqrt{\pi}}{2},\\ &= \sqrt{\frac{\pi}{8}}(1+\mathrm{i}).\end{aligned}$$

Thus, $C(x)$, $S(x) \to \sqrt{\pi/8}$ as $x\to\infty$.

For the second approach, consider $I = \int_0^1 \mathrm{e}^{\mathrm{i}xt^2}\mathrm{d}t$ along with the transformation $xt^2 = z^2$, hence

$$I = \frac{1}{x^{1/2}}\int_0^{x^{1/2}} \mathrm{e}^{\mathrm{i}z^2}\mathrm{d}z = \frac{F(x^{1/2})}{x^{1/2}},$$

hence $x^{1/2}I = F(x^{1/2})$.

$$I = \int_0^1 \mathrm{e}^{\mathrm{i}xt^2}\mathrm{d}t = \int_0^1 \mathrm{e}^{g(t)x}\mathrm{d}t,$$

with $g(t) = \mathrm{i}t^2$. This function has a saddle point at $t = 0$. We choose a path $t = \alpha s$ with s real such that

$$\mathrm{i}t^2 = \mathrm{i}\alpha^2 s^2 = -s^2,$$

hence

$$\mathrm{i}\alpha^2 = -1 \implies \alpha^2 = \mathrm{i} \implies \alpha = \mathrm{e}^{\mathrm{i}\pi/4}.$$

Thus,

$$I = \alpha\int \mathrm{e}^{-xs^2}\mathrm{d}s.$$

Care is needed now with the limits because the contour actually starts from the saddle point: taking the limits on the integral to be $\pm\infty$ would mean that the integrand would sample parts

of the complex plane beyond those implied by the original integration path. Hence,

$$\begin{aligned} I &\sim \mathrm{e}^{\mathrm{i}\pi/4}\int_0^\infty \mathrm{e}^{-xs^2}\mathrm{d}s, \qquad \text{as } x\to\infty, \\ &= \tfrac{1}{2}\mathrm{e}^{\mathrm{i}\pi/4}\sqrt{\pi/x}, \end{aligned}$$

So we are left with

$$I \sim \mathrm{e}^{\mathrm{i}\pi/4}\frac{\sqrt{\pi}}{2}\frac{1}{\sqrt{x}}.$$

But $I = F(\sqrt{x})/\sqrt{x}$, hence

$$\mathrm{e}^{\mathrm{i}\pi/4}\frac{\sqrt{\pi}}{2}\frac{1}{\sqrt{x}} \sim F(\sqrt{x})/\sqrt{x} \qquad \text{as } x\to\infty,$$

hence

$$F(\sqrt{x}) \sim \tfrac{1}{2}\mathrm{e}^{\mathrm{i}\pi/4}\sqrt{\pi} \qquad \text{as } x\to\infty,$$

and finally,

$$F(x) \sim \tfrac{1}{2}\mathrm{e}^{\mathrm{i}\pi/4}\sqrt{\pi} \qquad \text{as } x\to\infty,$$

in agreement with the first solution.

2. Recall the factorial integral,

$$s! = \left[\int_0^\infty \mathrm{e}^{s(\log z - z)}\mathrm{d}z\right] s^{s+1},$$

valid for s real. Show that for s complex, a saddle-point-type method can be used to evaluate

$$s! \sim \sqrt{2\pi s}\mathrm{e}^{-s}s^s, \qquad \text{with } \mathrm{Re}(s)\to\infty.$$

Consider

$$J(s) = \int_0^\infty \mathrm{e}^{s(\log z - z)}\mathrm{d}z.$$

Let $g(z) = \log z - z$. There is a saddle point at $g'(z) = 0$, hence $(1/z) - 1 = 0$, hence $z = 1$. Now, let $z = 1 + w$. We have

$$\begin{aligned} g(w) &= \log(1+w) - (1+w), \\ &= w - \tfrac{1}{2}w^2 - (1+1) + O(w^3), \\ &= -1 - \tfrac{1}{2}w^2 + O(w^3). \end{aligned}$$

Hence,

$$J(s) = \mathrm{e}^{-s} \int_{-1}^{\infty} \mathrm{e}^{-sw^2/2+O(w^3)} \mathrm{d}w.$$

The contour looks like the one in Figure 6.1.

Figure 6.1:

Deflect the contour: choose a path $w = \alpha t$ in the neighbourhood of $w = 0$ such that

$$sw^2 = s\alpha^2 t^2 = |s||\alpha|^2 t^2.$$

But

$$s\alpha^2 t^2 = |s||\alpha|^2 \mathrm{e}^{\mathrm{i}\varphi + 2\mathrm{i}\theta} t^2,$$

where $\varphi = \arg(s)$ and $\theta = \arg(\alpha)$, hence

$$\theta = -\varphi/2.$$

Thus,

$$J(s) \sim \mathrm{e}^{-s} \int \mathrm{e}^{-|s||\alpha|^2 t^2/2} \alpha \mathrm{d}t,$$

where the limits of integration are now filled in by selecting the steepest-descent contour, and

by letting $|s| \to \infty$:

$$\begin{aligned} J(s) &\sim \mathrm{e}^{-s}\alpha \int_{-\infty}^{\infty} \mathrm{e}^{-|s||\alpha|^2 t^2/2}\alpha \mathrm{d}t, \qquad |s| \to \infty, \\ &= \frac{\mathrm{e}^{-s}\alpha}{|\alpha|}\sqrt{\frac{2\pi}{|s|}}, \\ &= \frac{\mathrm{e}^{-s}\mathrm{e}^{\mathrm{i}\theta}}{\sqrt{|s|}}\sqrt{2\pi}, \\ &= \frac{\mathrm{e}^{-s}\mathrm{e}^{-\mathrm{i}\varphi/2}}{\sqrt{|s|}}\sqrt{2\pi}, \\ &= \mathrm{e}^{-s}\sqrt{2\pi}\frac{1}{\mathrm{e}^{\mathrm{i}\varphi/2}\sqrt{|s|}}, \\ &= \frac{\mathrm{e}^{-s}\sqrt{2\pi}}{\sqrt{s}}. \end{aligned}$$

Putting it all together,

$$s! = J(s)s^{s+1} \sim \left(\mathrm{e}^{-s}\frac{\sqrt{2\pi}}{s^{1/2}}\right) s^s s, \qquad \text{as } |s| \to \infty,$$

with $\mathrm{Re}(s) > 0$

$$s! \sim \sqrt{2\pi s}\mathrm{e}^{-s}s^s, \qquad \text{as } |s| \to \infty,$$

again, with $\mathrm{Re}(s) > 0$.

3. This question is similar in spirit to Question 3, except that a new special function is considered:

$$\mathrm{Ai}(x) = \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{e}^{(t^3/3)-xt} \mathrm{d}t,$$

where C is the contour shown in Figure 6.2. Evaluate $\mathrm{Ai}(x)$ as $x \to \infty$.

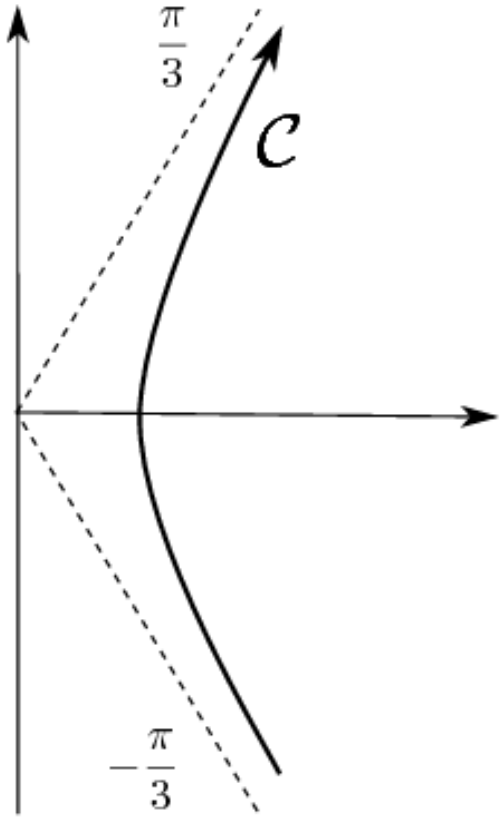


Figure 6.2: Contour for the Airy integral $\mathrm{Ai}(x)$

We write

$$\mathrm{Ai}(x) = \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{e}^{g(t)} \mathrm{d}t,$$

with $g(t) = (t^3/3) - xt$. We seek a saddle point $g'(t) = 0$, hence $t^2 - x = 0$, hence $t = \pm x^{1/2}$. Since x is real and positive, the t-location of the saddle point lies along the real axis. Also, in view of the contour C, the positive sign is to be taken. So take $t = x^{1/2}$ at the pertinent saddle point.

The integral will have a contribution only in the neighbourhood of the saddle point $t_0 = x^{1/2}$.

So let $t = t_0 + w$, with $|w| \ll 1$. We have

$$\begin{aligned} g(w) &= \tfrac{1}{3}(t_0 + w)^3 - x(t_0 + w), \\ &= \tfrac{1}{3}t_0^3 + t_0^2 w + t_0 w^2 + O(w^3) - xt_0 - xw, \\ &= \tfrac{1}{3}x^{3/2} + xw + x61/2w^2 - x^{3/2} - xw, \\ &= -\tfrac{2}{3}x^{3/2} + x^{1/2}w^2. \end{aligned}$$

Hence,

$$\mathrm{Ai}(x) \sim \frac{1}{2\pi\mathrm{i}} \int \mathrm{e}^{-(2/3)x^{3/2}} \mathrm{e}^{x^{1/2}w^2} \mathrm{d}w,$$

as $x \to \infty$, where the limits can be left unspecified for now. Tidying up, we have

$$\mathrm{Ai}(x) \sim \frac{1}{2\pi\mathrm{i}} \mathrm{e}^{-(2/3)x^{3/2}} \int \mathrm{e}^{x^{1/2}w^2} \mathrm{d}w.$$

We choose the path of steepest descent: let $w = \alpha t$, with $w^2 = \alpha^2 t^2 = -t^2$ and t a real parameter. Thus, $\alpha^2 = -1$, hence $\alpha = \pm\mathrm{i}$. In order for th el ine $z = \alpha t$ to deflect smoothly into the curve C, choose $\alpha = +\mathrm{i}$, with t going from negative to positive values. Thus,

$$\mathrm{Ai}(x) \sim \frac{1}{2\pi\mathrm{i}} \mathrm{e}^{-(2/3)x^{3/2}} \mathrm{i} \int_{-\infty}^{\infty} \mathrm{e}^{-(x^{1/2})t^2} \mathrm{d}t,$$

where now the limits have been filled in by taking the steepest-descent contour along with $x \to \infty$.

The remain function evaluation is easy: we obtain

$$\mathrm{Ai}(x) \sim \frac{\mathrm{e}^{-(2/3)x^{3/2}}}{2\pi} \sqrt{\frac{\pi}{x^{1/2}}},$$

hence

$$\mathrm{Ai}(x) \sim \frac{\mathrm{e}^{-(2/3)x^{3/2}}}{2\sqrt{\pi}x^{1/4}} \qquad \text{as } x \to \infty.$$

Chapter 7

The solution of an ODE as a contour integral

Overview

Complex analysis has provided us with methods to solve Ordinary Differential Equations (ODEs) using Laplace Transforms. In this chapter we will extend the concept of transform through a more general use of contour integration.

7.1 Contour integrals depending on a parameter

We have seen the benefits of transforms through the Laplace transform

$$\hat{F}_\lambda = \hat{F}(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} f(t)\,\mathrm{d}t$$

with inversion formula

$$f(t) = \frac{1}{2\pi \mathrm{i}} \int_\gamma \mathrm{e}^{\lambda t} \hat{F}(\lambda)\,\mathrm{d}\lambda$$

where γ is a contour in the complex plane as described in Chapter 5 and, for a slightly different class of functions, the Fourier transform

$$\tilde{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \mathrm{e}^{-\mathrm{i}\omega t} f(t)\,\mathrm{d}t$$

with inversion formula

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_\gamma \mathrm{e}^{\mathrm{i}\omega t} \tilde{f}(\omega)\, \mathrm{d}\omega.$$

In both cases the structure of the term e^{zt}, with $z = \lambda$ for Laplace and $z = -\mathrm{i}\omega$ for Fourier, turns derivatives with respect to t into algebraic multiplication by z inside the integral. In this Chapter, we will extend this idea by considering seeking solutions of ordinary differential equations by introducing the ansatz

$$f(t) = \int_\gamma \mathrm{e}^{tp(z)} q(z)\, \mathrm{d}z \tag{7.1}$$

and making suitable choices for the functions $p(z)$ and $q(z)$ and contour γ. [Note that a change of variable $\bar{z} = p(z)$ so $\mathrm{d}\bar{z} = p'(z)\mathrm{d}z$ can make this look like a Laplace transform but such a change of variable may not be possible or natural.]

Let us consider the general second order linear differential equation

$$\mathcal{L}\big[f(t)\big] = a_2(t)f''(t) + a_1(t)f'(t) + a_0(t)f(t) = 0$$

then with our ansatz (7.1)

$$\mathcal{L}\big[f(t)\big] = \int_\gamma \mathrm{e}^{tp(z)} \left[a_2(t)p(z)^2 + a_1(t)p(z) + a_0(t)\right] q(z)\, \mathrm{d}z. \tag{7.2}$$

Our challenge is that we want the integrand in Equation (7.2) to be such that the integral vanishes by, for example,

1. being a total derivative integrated around a closed contour,

2. being a total derivative integrated along an infinite contour chosen so that the integrated function vanishes at the limits,

3. being a complex analytic function integrated around a contour containing no poles,

while the integrand in Equation (7.1) does not behave in this way and so does not give a trivial solution.

7.2 Constant Coefficient Equation

Start with the simplest example

$$\mathcal{L}\big[f(t)\big] = f''(t) - (\alpha+\beta)f'(t) + \alpha\beta f(t) = 0$$

Taking the simple choice $p(z) = z$ we have

$$f(t) = \int_\gamma \mathrm{e}^{tz} q(z)\,\mathrm{d}z$$

and

$$\mathcal{L}\big[f(t)\big] = \int_\gamma \mathrm{e}^{tz}\left[z^2 - (\alpha+\beta)z + \alpha\beta\right] q(z)\,\mathrm{d}z = \int_\gamma \mathrm{e}^{tz}(z-\alpha)(z-\beta)q(z)\,\mathrm{d}z.$$

The obvious choices for the second integrand to be analytic while the first is not is

$$q_1(z) = \frac{1}{z-\alpha} \qquad q_2(z) = \frac{1}{z-\beta} \qquad \text{if} \quad \alpha \neq \beta$$

and

$$q_1(z) = \frac{1}{z-\alpha} \qquad q_2(z) = \frac{1}{(z-\alpha)^2} \qquad \text{if} \quad \alpha = \beta.$$

The corresponding integrand for $\mathcal{L}\big[f(t)\big]$ is analytic everywhere and so vanishes if we take γ to be any closed contour. On the other hand if the contour encloses α in an anti-clockwise direction we find

$$f_1(t) = \int_\gamma \frac{\mathrm{e}^{tz}}{z-\alpha}\,\mathrm{d}z = 2\pi\mathrm{i}\operatorname*{Res}_{z=\alpha}\frac{\mathrm{e}^{tz}}{z-\alpha} = 2\pi\mathrm{i}\,\mathrm{e}^{\alpha t}$$

and likewise for β, while in the case of repeated roots ($\alpha = \beta$) we have

$$f_2(t) = \int_\gamma \frac{\mathrm{e}^{tz}}{(z-\alpha)^2}\,\mathrm{d}z = 2\pi\mathrm{i}\operatorname*{Res}_{z=\alpha}\frac{\mathrm{e}^{tz}}{(z-\alpha)^2} = 2\pi\mathrm{i}\operatorname*{Res}_{z=\alpha}\frac{\mathrm{e}^{\alpha t}(1+t(z-\alpha)+\dots)}{(z-\alpha)^2} = 2\pi\mathrm{i}\,t\mathrm{e}^{\alpha t}.$$

7.3 Laplace's Linear Equation

As our next example consider the second order version of *Laplace's linear equation*

$$\mathcal{L}\big[f(t)\big] = (a_2t+b_2)f''(t) + (a_1t+b_1)f'(t) + (a_0t+b_0)f(t) = 0.$$

Again taking the choice $p(z) = z$ we have

$$\mathcal{L}\big[f(t)\big] = \int_\gamma \mathrm{e}^{tz} \left[\left(a_2 z^2 + a_1 z + a_0\right) t + \left(b_2 z^2 + b_1 z + b_0\right)\right] q(z)\, \mathrm{d}z.$$

Suppose the integrand is a total derivative $\dfrac{\mathrm{d}}{\mathrm{d}z}\left[\mathrm{e}^{tz} r(z)\right] = \mathrm{e}^{tz}\left[r(z)t + r'(z)\right]$, say, then

$$r'(z) = (b_2 z^2 + b_1 z + b_0) q(z) \qquad r(z) = (a_2 z^2 + a_1 z + a_0) q(z).$$

Hence

$$\frac{r'(z)}{r(z)} = \frac{b_2 z^2 + b_1 z + b_0}{a_2 z^2 + a_1 z + a_0}.$$

Assuming $a_2 z^2 + a_1 z + a_0 = a_2 (z - \alpha)(z - \beta)$ has distinct roots we can split this in partial fractions as

$$\frac{r'(z)}{r(z)} = k_0 + \frac{k_1}{z - \alpha} + \frac{k_2}{z - \beta},$$

and conclude

$$\begin{aligned} \ln r(z) &= k_0 z + k_1 \ln(z - \alpha) + \ln(z - \beta) + c \\ \implies r(z) &= A \mathrm{e}^{k_0 z} (z - \alpha)^{k_1} (z - \beta)^{k_2} \end{aligned}$$

Correspondingly,

$$q(z) = \frac{A}{a_2} \mathrm{e}^{k_0 z} (z - \alpha)^{k_1 - 1} (z - \beta)^{k_2 - 1}.$$

and

$$f(t) = \int_\gamma \mathrm{e}^{(t + k_0) z} (z - \alpha)^{k_1 - 1} (z - \beta)^{k_2 - 1}\, \mathrm{d}z$$

where we have dropped the irrelevant multiplicative constant.

7.3.1 Choice of contour

In general, k_1 and k_2 will not be integers and correspondingly we will need to work in the plane with cuts from α and β which we take to extend to infinity in a direction for which $(t + k_0)z$ is negative. Then we may take the contour to come in from infinity along one side of the cut and return out along the other side as illustrated. We have one such for each root and corresponding generate two

independent solution (or more generally n for the obvious extension to an n^{th}-order equation).

Example

$$\mathcal{L}\big[f(t)\big] = tf''(t) + 2af'(t) - tf(t) = 0 \qquad (a > 0).$$

We have

$$a_2z^2 + a_1z + a_0 = z^2 - 1 = (z+1)(z-1) \qquad b_2z^2 + b_1z + b_0 = 2az$$

so

$$\frac{r'(z)}{r(z)} = \frac{2az}{(z+1)(z-1)} = \frac{a}{z+1} + \frac{a}{z-1},$$

meaning

$$\ln r(z) = a\ln(z+1) + a\ln(z-1) \qquad \Rightarrow \qquad r(z) = (z+1)^a(z-1)^a$$

and then

$$q(z) = \frac{r(z)}{(z+1)(z-1)} = (z+1)^{a-1}(z-1)^{a-1}.$$

Hence our solution will be

$$f(t) = \int_\gamma \mathrm{e}^{tz}(z+1)^{a-1}(z-1)^{a-1}\,\mathrm{d}z \tag{7.3}$$

if we can find suitable contours so that $r(z)$ vanishes at the endpoints.

Since $a > 0$ an obvious choice is the section of the real axis from -1 to 1, that is our first solution is

$$f_1(t) = \int_{-1}^{1} \mathrm{e}^{tz}(1+z)^{a-1}(1-z)^{a-1}\,\mathrm{d}z$$

A second choice is shown in Figure 7.1. We first of all let $z \to -z$ in Equation (7.3) (and neglect the resulting overall minus sign) to obtain

$$f_2(t) = \int_{\gamma_2} \mathrm{e}^{-tz}(z+1)^{a-1}(z-1)^{a-1}\,\mathrm{d}z$$

On γ_2, the small semicircular arc gives 0 contribution in the limit $\epsilon \to 0$ (as $a > 0$), on the upper

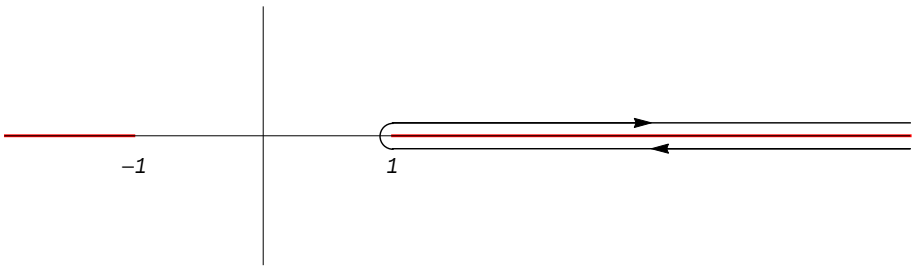


Figure 7.1: The contour defining $f_2(t)$.

section we have $z = 1 + s\mathrm{e}^{\mathrm{i}0}$, where s goes from 0 to ∞ and on the lower section $z = 1 + s\mathrm{e}^{2\pi\mathrm{i}}$ where s goes from ∞ to 0. For $\operatorname{Re} t > 0$ the ends at infinity tend to zero and so our solution is

$$f_2(t) = (1 - \mathrm{e}^{2\pi\mathrm{i}a}) \int_0^\infty \mathrm{e}^{t(1+s)}(2+s)^{a-1}s^{a-1}\,\mathrm{d}s.$$

Note that if we let $f(t) = t^{-a+\frac{1}{2}}g(t)$, then

$$\begin{aligned} f'(t) &= t^{-a-\frac{1}{2}}\left(tg'(t) - (a-\tfrac{1}{2})g(t)\right), \\ f''(t) &= t^{-a-\frac{3}{2}}\left(t^2g''(t) - (2a-1)tg'(t) + (a^2-\tfrac{1}{4})g(t)\right) \end{aligned}$$

so our equation is equivalent to

$$t^2f''(t) + tf'(t) + \left(-t^2 - (a-\tfrac{1}{2})^2\right)f(t) = 0.$$

This is a variation of Bessel's equation

$$\mathcal{L}_B\left[f(t)\right] = t^2f''(t) + tf'(t) + (t^2 - \nu^2)f(t) = 0,$$

(just let $t \to it$).

7.4 Bessel's Equation

An alternative representation of the Bessel function can be given by writing

$$f(t) = \int_\gamma P(\theta)\mathrm{e}^{-\mathrm{i}t\sin\theta}\,\mathrm{d}\theta$$

then

$$\begin{aligned}\mathcal{L}_B\left[f(t)\right] &= \int_\gamma \left(-t^2\sin^2\theta - \mathrm{i}t\sin\theta + (t^2-\nu^2)\right) P(\theta)\mathrm{e}^{-\mathrm{i}t\sin\theta}\,\mathrm{d}\theta \\ &= \int_\gamma \left(t^2\cos^2\theta - \mathrm{i}t\sin\theta - \nu^2\right) P(\theta)\mathrm{e}^{-\mathrm{i}t\sin\theta}\,\mathrm{d}\theta.\end{aligned}$$

We now look for a function $Q(\theta)$ such that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\theta}\left[Q(\theta)e^{-\mathrm{i}t\sin\theta}\right] &= \left(Q'(\theta) - \mathrm{i}t\cos\theta\, Q(\theta)\right)\mathrm{e}^{-\mathrm{i}t\sin\theta} \\ &= \left(t^2\cos^2\theta - \mathrm{i}t\sin\theta - \nu^2\right) P(\theta)\mathrm{e}^{-\mathrm{i}t\sin\theta}.\end{aligned}$$

We can check that

$$Q(\theta) = \left(\mathrm{i}t\cos\theta + \mathrm{i}\nu\right)e^{\mathrm{i}\nu\theta} \qquad \text{with} \qquad P(\theta) = \mathrm{e}^{\mathrm{i}\nu\theta},$$

giving

$$f(t) = \int_\gamma \mathrm{e}^{-\mathrm{i}t\sin\theta + \mathrm{i}\nu\theta}\,\mathrm{d}\theta$$

provided we can choose the contour so that $Q(\theta)\mathrm{e}^{-\mathrm{i}t\sin\theta}$ vanishes at the end-points.

Taking $\mathrm{Re}\, t > 0$ this vanishes along $\mathrm{Re}\,\theta = n\pi$ and

$$\mathrm{Im}\,\theta \to \begin{cases}\infty & n \text{ odd} \\ -\infty & n \text{ even}\end{cases}$$

A natural choice is then to take $n = 0$, so starting at $-\mathrm{i}\infty$ and ending with $n = -1$ or $n = 1$ that is at $-\pi + \mathrm{i}\infty$ or $\pi + \mathrm{i}\infty$ as shown in Figure 7.4.

The corresponding complex solutions $H_\nu^{(1)}(t)$ and $H_\nu^{(2)}(t)$ are called the Hankel functions and represent the combinations $J_\nu(t) \pm \mathrm{i}Y_\nu(t)$. Integral representation of this make the use of the method of steepest descent very natural for determining the asymptotic behaviour of the solutions.

Note that these forms are ideally suited to the use of the method of steepest descent to determine their asymptotic behaviour.

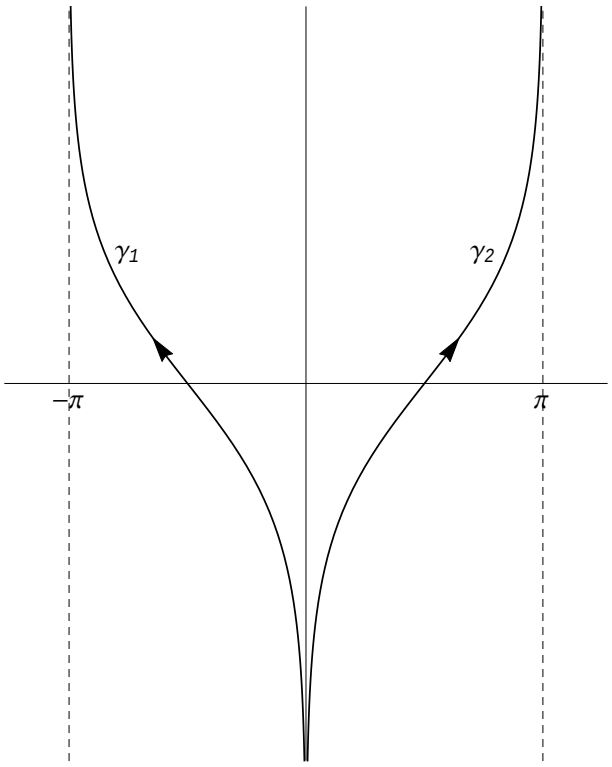


Figure 7.2: The choice of contours for the Hankel functions. The contour γ_1 is used to define $H_\nu^{(1)}(t)$ while the contour γ_2 is used to define $H_\nu^{(2)}(t)$.

7.5 Airy Functions

Airy's equation is given by

$$\mathcal{L}_{\mathrm{Ai}}\big[f(t)\big] = f''(t) - tf(t) = 0.$$

This is a degenerate case of Laplace's linear equation with

$$\frac{r'(z)}{r(z)} = \frac{z^2}{(-1)} \qquad \Rightarrow \qquad \ln r(z) = -\tfrac{1}{3}z^3$$

so

$$f(t) = \int_\gamma \mathrm{e}^{zt-\frac{1}{3}z^3}\,\mathrm{d}z.$$

and clearly

$$\mathcal{L}_{\mathrm{Ai}}\big[f(t)\big] = \left[-\mathrm{e}^{zt-\frac{1}{3}z^3}\right]_\gamma.$$

To have a solution we are then left with the requirement of finding a non-trivial choice of contour such that $\mathrm{e}^{zt-\frac{1}{3}z^3}$ vanishes at the end-points. As the function is entire the only way we can achieve

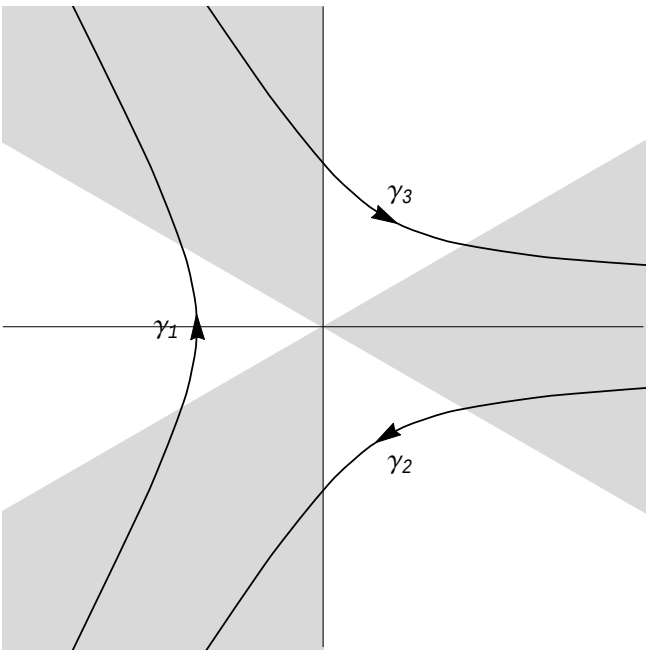


Figure 7.3: The choice of contours for the Airy function.

this is for the contour to end at infinity. For large $|z|$ the cubic term in the exponential dominates and has modulus $\exp(-\frac{1}{3}|z|^3\cos 3\theta)$ where θ is the argument of z. This will then vanish as $|z|\to\infty$ if and only if $\cos 3\theta > 0$ corresponding to $\theta\in(\frac{5}{6}\pi,\frac{1}{2}\pi)$, $\theta\in(-\frac{1}{6}\pi,\frac{1}{6}\pi)$, $\theta\in(\frac{1}{2}\pi,\frac{5}{6}\pi)$ as shown in the figure.

If we go in and out of the same sector we can distort the path to 0 and get the trivial solution but we cannot do that if we leave from a different sector as shown. Thus we have 3 natural contours γ_1, γ_2 and γ_3, and clearly $\gamma_1+\gamma_2+\gamma_3$ can be shrunk to zero so only two are independent. By convention, two combinations are generally taken and called Airy functions:

$$\mathrm{Ai}(t)=\frac{1}{2\pi\mathrm{i}}\int_{\gamma_1}\mathrm{e}^{zt-\frac{1}{3}z^3}\,\mathrm{d}z. \tag{7.4}$$

and

$$\mathrm{Bi}(t)=\frac{1}{2\pi}\int_{\gamma_2}\mathrm{e}^{zt-\frac{1}{3}z^3}\,\mathrm{d}z-\frac{1}{2\pi}\int_{\gamma_3}\mathrm{e}^{zt-\frac{1}{3}z^3}\,\mathrm{d}z.$$

Since we can rotate the contours into one another by a $\frac{2\pi}{3}$ rotation we may show that

$$\mathrm{Bi}(t)=\mathrm{e}^{-\mathrm{i}\pi/6}\mathrm{Ai}(t\mathrm{e}^{-2\pi\mathrm{i}/3})+\mathrm{e}^{\mathrm{i}\pi/6}\mathrm{Ai}\left(t\mathrm{e}^{2\pi\mathrm{i}/3}\right)$$

These forms are ideally suited to the use of the method of steepest descent to determine their

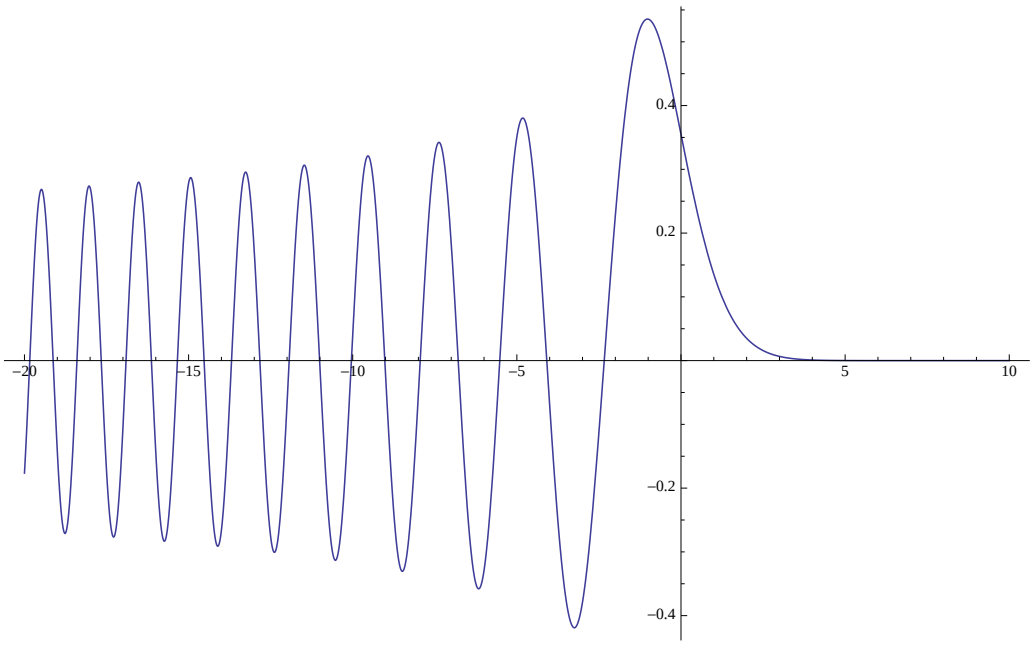


Figure 7.4: The Airy function $\mathrm{Ai}(t)$ showing exponential decay as $t \to \infty$ but oscillatory behaviour for $t < 0$.

asymptotic behaviour although in this case we must first do a change of variable $z = t^{1/2}\bar{z}$ so

$$\mathrm{Ai}(t) = \frac{t^{1/2}}{2\pi \mathrm{i}} \int_{\gamma_1} \mathrm{e}^{t^{3/2}(\bar{z} - \frac{1}{3}\bar{z}^3)} \, \mathrm{d}\bar{z}.$$

so ensure that the saddle point does not move with t. Assuming the saddle point at $\bar{z} = -1$ gives the dominant contribution as $t \to \infty$ we now show that

$$\mathrm{Ai}(t) \sim \frac{1}{2\sqrt{\pi}} t^{-1/4} \mathrm{e}^{-\frac{2}{3}t^{3/2}} \qquad \text{as } t \to \infty.$$

For large *negative* t we first rewrite our solution with $z = (-t)^{1/2}\bar{z}$ as

$$\mathrm{Ai}(t) = \frac{(-t)^{1/2}}{2\pi \mathrm{i}} \int_{\gamma_1} \mathrm{e}^{-(-t)^{3/2}(\bar{z} + \frac{1}{3}\bar{z}^3)} \, \mathrm{d}\bar{z}.$$

In this case the saddle points are at $\mp i$ giving contributions

$$\frac{1}{2\mathrm{i}\sqrt{\pi}} (-t)^{-1/4} \mathrm{e}^{\pm \mathrm{i}(\frac{2}{3}(-t)^{3/2} + \pi/4)},$$

which together give the asymptotic expansion

$$\mathrm{Ai}(t) \sim \frac{1}{\sqrt{\pi}} (-t)^{-1/4} \sin\left(\tfrac{2}{3}(-t)^{3/2} + \tfrac{\pi}{4}\right) \qquad \text{as } t \to -\infty.$$

It can be noted that the definition (7.4) differs superficially from the one previously given in the

worked examples in Chapter 6. However, these two definitions are the same, as $\mathrm{Ai}(t)$ is a real-valued function for t real, and the integral in Equation (7.4) is therefore invariant under the transformation $z = -w^*$, which transforms Equation (7.4) into

$$\mathrm{Ai}(t) = \frac{1}{2\pi \mathrm{i}} \int_{\gamma_1'} \mathrm{e}^{(1/3)w^3 - wt} \mathrm{d}t, \tag{7.5}$$

where γ_1' denotes the contour γ_1 under a reflection through the y axis, and where Equation (7.5) agrees exactly with the definition of $\mathrm{Ai}(t)$ given earlier in Chapter 6. Filling in the details of the outlined calculations is left as an exercise for the reader.

7.6 Worked examples

1. Find all solutions of Legendre's equation

$$(1-t^2)y'' - 2ty' + n(n+1)y = 0 \qquad (n \in \mathbb{N})$$

in the form

$$y(t) = \int_\gamma (z-t)^{\alpha+1} P(z) \mathrm{d}z.$$

Show that one particular solution is

$$y_1(t) = \frac{1}{2^{n+1}\pi \mathrm{i}} \int_\gamma \frac{(z^2-1)^n}{(z-t)^{n+1}} \mathrm{d}z.$$

where γ is any simple closed contour enclosing $z = t$. This is known as *Schläfli's integral form* of $P_n(t)$.

Show that a second linearly independent solution can be given by

$$y_2(t) = Q_n(t) = \frac{1}{2^{n+1}} \int_{-1}^{1} \frac{(1-z^2)^n}{(t-z)^{n+1}} \mathrm{d}z, \qquad (t \in \mathbb{R}, t \notin [-1,1]).$$

Use integration by parts to show that

$$Q_n(t) = \frac{1}{2} \int_{-1}^{1} \frac{P_n(z)}{t-z} \mathrm{d}z.$$

Inserting the trial form into the differential equation we find

$$\mathcal{L}_{\mathsf{Le}}[y] = \int_\gamma (z-t)^{\alpha-1} \left[\alpha(\alpha+1)(1-z^2) + (z-t)2z(1+\alpha)^2 \right.$$
$$\left. + (z-t)^2(n+2+\alpha)(n-1-\alpha) \right] P(z) \mathrm{d}z. \tag{7.6}$$

We want this to be a total derivative with respect to z but the only way we can get the combination $(z-t)^{\alpha-1}$ is for this to be of the form

$$\frac{\mathrm{d}}{\mathrm{d}z} \left[(z-t)^\alpha Q(z) \right] = (z-t)^{\alpha-1} \left[\alpha Q(z) + Q'(z)(z-t) \right].$$

Comparing we see we have no $(z-t)^2$ term and therefore we must choose $\alpha = -n-2$ or $\alpha = n-1$ and correspondingly the integrand in Equation (7.8) becomes

$$\begin{aligned} &(n+1)(z-t)^{\alpha_- -1}\left[\alpha_-(z^2-1)+2(n+1)z(z-t)\right] && \alpha_- = -n-2 \\ &(-n)(z-t)^{\alpha_+ -1}\left[\alpha_+(z^2-1)-2nz(z-t)\right] && \alpha_+ = n-1 \end{aligned}$$

From this we can read off $Q'(z)/Q(z)$ with $(\alpha+1)(1-z^2)P(z) = Q(z)$ and immediately integrate to get of two solutions

$$\begin{aligned} y_-(t) &= \int_{\gamma_-} \frac{(z^2-1)^n}{(z-t)^{n+1}}\mathrm{d}z \qquad \text{with } \mathcal{L}_{\mathsf{Le}}[y_-] = \left[(z-t)^{-n-2}(z^2-1)^{n+1}/(n+1)\right]_{\gamma_-} \\ y_+(t) &= \int_{\gamma_+} \frac{(z-t)^n}{(z^2-1)^{n+1}}\mathrm{d}z \qquad \text{with } \mathcal{L}_{\mathsf{Le}}[y_+] = \left[(z-t)^{n-1}(z^2-1)^{-n}/(-n)\right]_{\gamma_+} \end{aligned}$$

where we most choose the contours either to be closed or to vanish at the limits and ensure that we get a non-trivial solution. Note that since we have specified that $n \in \mathbb{N}$ we do not have to cut the plane for either solution. (We can also consider Legendre's equation for non-integer n and this is the only difference in that case.)

To be specific,

- for $y_-(t)$ we choose any closed contour enclosing the pole at $z = t$. As we have $(z-t)^{n+1}$ in the denominator the corresponding residue is

  $$\frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}z^n}(z^2-1)^n\bigg|_{z=t}$$

  which gives Rodriques's formula for the Legendre polynomials - note the result is clearly a polynomial of degree n in t:

  $$P_n(t) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}z^n}(z^2-1)^n\bigg|_{z=t} = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}t^n}(t^2-1)^n.$$

- we can take contours encircling the poles at $z = \pm 1$ but these clearly give polynomial solutions and we already have found those an alternative is to start at $z = t$ and heading to ∞, these clearly are singular as $t \to \pm 1$ and are the irregular Legendre function $Q_n(t)$.

We may also clearly get a solution using the first class of integral and taking a contour running from $z = -1$ to $z = +1$. In addition, this clearly becomes logarithmically divergent as $t \to \pm 1$ and so is independent of our polynomial solution. The given $y_2(t)$ precisely falls in this class.

Now Rodriques's formula

$$\frac{1}{2}\int_{-1}^{1}\frac{P_n(z)}{t-z}\mathrm{d}z = \frac{1}{2^{n+1}n!}\int_{-1}^{1}\frac{1}{t-z}\frac{\mathrm{d}^n}{\mathrm{d}z^n}(z^2-1)^n\,\mathrm{d}z$$
$$= \frac{1}{2^{n+1}n!}\left(\left[\frac{1}{t-z}\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}(z^2-1)^n\right]_{-1}^{1} - \int_{-1}^{1}\frac{1}{(t-z)^2}\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}(z^2-1)^n\,\mathrm{d}z\right)$$

and the boundary term clearly vanishes at both limits as $(z^2-1)^n = (z-1)^n(z+1)^n$. Continuing we may integrate by parts n times in total to give

$$\frac{1}{2}\int_{-1}^{1}\frac{P_n(z)}{t-z}\mathrm{d}z = \frac{1}{2^{n+1}n!}\left((-1)^n\int_{-1}^{1}\frac{n!}{(t-z)^{n+1}}(z^2-1)^n\,\mathrm{d}z\right) = Q_n(t).$$

2. Consider *Laguerre's equation*

$$ty'' + (1-t)y' + ny = 0 \qquad (n \in \mathbb{N}).$$

Seeking solutions in the form

$$y(t) = \int_\gamma \mathrm{e}^{tz}P(z)\mathrm{d}z.$$

show that a solution is given by

$$y(t) = \int_\gamma \mathrm{e}^{tz}z^{-n-1}(z-1)^n\mathrm{d}z.$$

where γ is any contour such that $\left[\mathrm{e}^{tz}z^{-n}(z-1)^{n+1}\right]_\gamma = 0$

Inserting the trial form into the differential equation we find

$$\mathcal{L}_{\mathsf{La}}[y] = \int_\gamma \left[tz^2 + (1-t)z + n\right]P(z)\mathrm{d}z. \tag{7.7}$$

We want this to be a total derivative with respect to z and to get the combination e^{tz} the simplest form would be

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\mathrm{e}^{tz}Q(z)\right] = \mathrm{e}^{tz}\left[Q'(z) + tQ(z)\right].$$

Comparing we see we would need

$$Q(z) = z(z-1)P(z), \qquad Q'(z) = (z+n)P(z)$$

which implies

$$Q'(z)/Q(z) = \frac{z+n}{z(z-1)} = \frac{n+1}{z-1} - \frac{n}{z} \qquad \Rightarrow \qquad \ln Q(z) = (n+1)\ln(z-1) - n\ln z$$

giving

$$Q(z) = z^{-n}(z-1)^{n+1}, \qquad \text{and} \qquad P(z) = z^{-}n - 1(z-1)^n.$$

So we have a solution provided we choose our contour such that

$$\left[\mathrm{e}^{tz}Q[z)\right]_\gamma = \left[\mathrm{e}^{tz}z^{-n}(z-1)^{n+1}\right]_\gamma = 0.$$

3. Find the solutions of *Hermite's equation*

$$y'' - 2ty' + 2ny = 0 \qquad (n \in \mathbb{N}).$$

in the form $y(t) = \int_\gamma \mathrm{e}^{tz}P(z)\,\mathrm{d}z$.

The function $H_n(t)$ is the solution of Hermite's equation defined by

$$H_n(t) = \frac{n!}{2\pi i}\int_\gamma \frac{\mathrm{e}^{2tz-z^2}}{z^{n+1}}\,\mathrm{d}z$$

where γ is any simple closed contour enclosing the origin. Use the definition to show that

(a) $\displaystyle\sum_{n=0}^{\infty}\frac{1}{n!}u^n H_n(t) = \mathrm{e}^{2tu-u^2} \qquad u \in \mathbb{C}$

(b) $H_n(t) = (-1)^n \mathrm{e}^{t^2}\dfrac{\mathrm{d}^n}{\mathrm{d}t^n}\mathrm{e}^{-t^2}$ Rodriques' definition.

Inserting the trial form $y(t) = \int_\gamma \mathrm{e}^{2tz}P(z)\,\mathrm{d}z$ (with change of variable/apologies) into the differential equation we find

$$\mathcal{L}_{\mathsf{He}}[y] = \int_\gamma \left[4z^2 - 4tz + 2n\right]\mathrm{e}^{2tz}P(z)\mathrm{d}z. \tag{7.8}$$

We want this to be a total derivative with respect to z and to get the combination e^{2tz} the

simplest form would be

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\mathrm{e}^{2tz}Q(z)\right] = \mathrm{e}^{2tz}\left[Q'(z) + 2tQ(z)\right].$$

Comparing we see we would need

$$Q(z) = -2zP(z), \qquad Q'(z) = (4z^2 + 2n)P(z)$$

which implies

$$Q'(z)/Q(z) = -\frac{2z^2+n}{z} = -2z - \frac{n}{z} \qquad \Rightarrow \qquad \ln Q(z) = -z^2 - n\ln z$$

giving

$$Q(z) = \frac{\mathrm{e}^{-z^2}}{z^n}, \qquad \text{and} \qquad P(z) = -\frac{\mathrm{e}^{-z^2}}{2z^{n+1}}.$$

The Hermite function, which is clearly a polynomial, is clearly just this solution taking the contour to encircle the pole at the origin with some appropriate normalization.

(a) Given an $u \in \mathbb{C}$ choose γ to be the circle $|z| = |u| + 1$ say so u lies inside the contour and $|u/z| < 1$ then

$$\begin{aligned}\sum_{n=0}^{\infty}\frac{1}{n!}u^n H_n(t) &= \frac{1}{2\pi i}\sum_{n=0}^{\infty}u^n\int_\gamma \frac{\mathrm{e}^{2tz-z^2}}{z^{n+1}}\,\mathrm{d}z \\ &= \frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{\mathrm{e}^{2tz-z^2}}{z}\sum_{n=0}^{\infty}\left(\frac{u}{z}\right)^n\,\mathrm{d}z \\ &= \frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{\mathrm{e}^{2tz-z^2}}{z-u}\,\mathrm{d}z \\ &= \mathrm{e}^{2tzu-u^2}\end{aligned}$$

where we may interchange the sum and integration as we have absolute convergence within the limit of convergence and the last line is simply an application of Cauchy's residue theorem with the one simple pole at $z = u$ which lies inside the contour.

(b) Because the pole is of order $n+1$ the residue of the integrand is given by

$$\left.\frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}z^n}\mathrm{e}^{2tz-z^2}\right|_{z=0} = \mathrm{e}^{-t^2}\left.\frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}z^n}\mathrm{e}^{(t-z)^2}\right|_{z=0} = \mathrm{e}^{-t^2}\left.\frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\mathrm{e}^{(t-z)^2}\right|_{z=0} = \mathrm{e}^{-t^2}\frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\mathrm{e}^{t^2}.$$

Inserting the normalizations we arrive at Rodriques' formula for Hermite polynomials.

Chapter 8

The WKB (Green-Liouville) approximation

Overview

The WKB approximation is a kind of singular perturbation theory for finding approximate solutions to linear partial differential equations with spatially varying coefficients. In this section we introduce the basic idea behind the method and apply it to solving eigenvalue problems and finding Greens's functions in ordinary differential equations where a certain parameter is very large.

8.1 Solution in amplitude-phase form

Consider differential equations of one of the form:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + \lambda^2 q(t) y = 0$$

where $q(t)$ is some given function and $\lambda \equiv 1/\epsilon$ is a large constant.

Example: The time independent Schrödinger equation is

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x)\psi(x) \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0,$$

where if quantum effects are considered to be small '$\hbar \ll 1$' the the corresponding $\lambda \gg 1$.

If $q(t) = k$ (constant) then solution is $y(t) = A\mathrm{e}^{\mathrm{i}\lambda\sqrt{k}t}$; this suggests in the general case looking for a solution in amplitude-phase form

$$y(t) = A(t)\mathrm{e}^{\mathrm{i}\lambda\psi(t)}.$$

Taking this form we find

$$\begin{aligned} y'(t) &= (\mathrm{i}\lambda\psi' A + A')\mathrm{e}^{\mathrm{i}\lambda\psi} \\ y''(t) &= \left[(\mathrm{i}\lambda\psi')(i\lambda\psi' A + A') + \mathrm{i}\lambda(\psi'' A + \psi' A') + A''\right]\mathrm{e}^{\mathrm{i}\lambda\psi} \end{aligned}$$

so

$$0 = (y'' + \lambda^2 q y)/\mathrm{e}^{\mathrm{i}\lambda\psi} = -\lambda^2(\psi')^2 + \mathrm{i}\lambda(\psi'' A + 2\psi' A') + A'' + \lambda^2 q A$$

We may ask that the 'real' and 'imaginary' parts separately vanish so

$$0 = -\lambda^2(\psi')^2 A + A'' + \lambda^2 q A$$

and

$$0 = \psi'' A + 2\psi' A'.$$

(We use inverted commas here as, in fact, this expansion is equally useful when $q(t)$ is imaginary.)

$$0 = \psi'' A + 2\psi' A' \quad \Longrightarrow \frac{\psi''}{\psi'} = -2\frac{A'}{A} \quad \Longrightarrow \ln|\psi'| = -2\ln A$$

so

$$A = \frac{1}{|\psi'|^{1/2}}$$

Then 'real' part becomes

$$\begin{aligned} 0 &= (\psi')^2 - q - \lambda^{-2} A''/A \\ &= (\psi')^2 - q - \lambda^{-2}\left(-\tfrac{1}{2}\frac{\psi'''}{\psi'} + \tfrac{3}{4}\frac{(\psi'')^2}{(\psi')^2}\right) \end{aligned}$$

To lowest order as $\lambda \to \infty$ we neglect the third term to give $\psi' = \pm\sqrt{q}$:

$$A(t) = \frac{1}{|q(t)|^{1/4}} \qquad \psi(t) = \pm\int^t \sqrt{q(s)}\,\mathrm{d}s$$

and so

$$y(t) \approx \frac{1}{|q(t)|^{1/4}} \exp\left(\pm\mathrm{i}\lambda\int^t \sqrt{q(s)}\,\mathrm{d}s\right).$$

8.2 Comparison with Exact Solutions

So the idea is simple - but how good are the results?

There are many examples from quantum mechanics available (with the WKB nomenclature dating from then) but we want to emphasize the general usefulness of the method (which was actually discovered by Green and Liouville long before the advent of quantum mechanics) and so give different examples here based around the equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + \lambda^2 \mathrm{e}^{2t} y = 0. \tag{8.1}$$

Initial and Boundary Value Problems

Since $q(t) = \mathrm{e}^{2t}$ our two solutions are

$$y_{\mathsf{WKB}}(t) \approx \mathrm{e}^{-t/2} \exp\left(\pm \mathrm{i}\lambda \mathrm{e}^{t}\right),$$

so we can write our general (leading order) WKB solution in real form as

$$y_{\mathsf{WKB}}(t) \approx A\mathrm{e}^{-t/2} \cos\left(\lambda \mathrm{e}^{t}\right) + B\mathrm{e}^{-t/2} \sin\left(\lambda \mathrm{e}^{t}\right).$$

In this case, we can show that the exact solution is

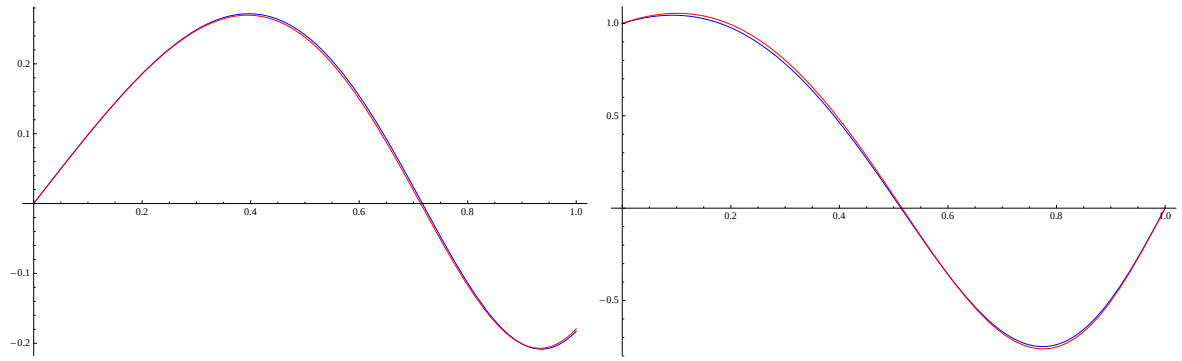
$$y_{\mathsf{WKB}}(t) \approx CJ_0\left(\lambda \mathrm{e}^{t}\right) + DY_0\left(\lambda \mathrm{e}^{t}\right).$$

the Bessel functions of order 0 (`BesselJ[0,t]` and `BesselY[0,t]` in *Mathematica*) so we can compare solutions. For definiteness let us compare the solutions satisfying

1. initial conditions $y(0) = 0$ and $y'(1) = 1$
2. boundary conditions $y(0) = 1$ and $y(1) = 0$

Green functions

Given that we have two independent approximate solution we can also use them to construct a Green function by the method of variation of parameters, for example, if we consider the boundary



(a) (b)

Figure 8.1: The comparison between the WKB solutions (blue) and exact solutions (red) for $\lambda = 3$; the plot in (a) is for the given initial value problem the plot in (b) is for the boundary value problem. Although the solution was only derived under the assumption for $\lambda \gg 1$ if we take λ to be significantly larger that this the lines overlap at this resolution!

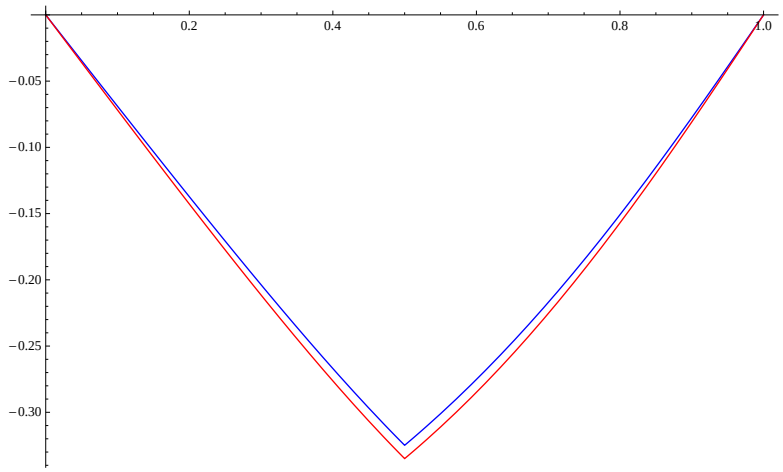


Figure 8.2: The comparison between the WKB Green function (blue) and Green function (red) for $s = \frac{1}{2}$ and $\lambda = 1$.

value problem $y(0) = 0$ and $y(1) = 0$ we have independent approximate homogeneous solutions

$$u_{\mathsf{WKB}}(t) = \mathrm{e}^{-t/2} \sin\left[\lambda(\mathrm{e}^t - 1)\right],$$
$$q_{\mathsf{WKB}}(t) = \mathrm{e}^{-t/2} \sin\left[\lambda(\mathrm{e}^t - e)\right],$$

with Wronskian $W[u_{\mathsf{WKB}}, q_{\mathsf{WKB}}] = \lambda \sin[\lambda(e-1)]$ so the WKB Green function is given by

$$G_{\mathsf{WKB}}(s,t) = \frac{\mathrm{e}^{-(s+t)/2}}{\lambda \sin[\lambda(\mathrm{e}-1)]} \begin{cases} \sin[\lambda(\mathrm{e}^s - 1)] \cos[\lambda(\mathrm{e}^t - \mathrm{e})], & s < t, \\ \sin[\lambda(\mathrm{e}^t - 1)] \cos[\lambda(\mathrm{e}^s - \mathrm{e})], & s > t. \end{cases}$$

Comparison with the exact Green function (in terms of Bessel functions) is shown in Fig. 8.2 (again even for $\lambda = 1$ the agreement is remarkable).

Eigenvalue Problems

It is clear from our plot (and the positive nature of the potential) that our solutions oscillate so we can look for approximate eigenvalues of a Sturm-Liouville problem, for example, values of λ^2 for which we have non-trivial solutions of satisfying $y(0) = 0$ and $y(1) = 0$. In the previous subsection, we constructed the solutions $u_{\mathsf{WKB}}(t)$ and $q_{\mathsf{WKB}}(t)$ that satisfy the boundary condition at $t = 0$ and $t = 1$, respectively. We have an eigenvalue when these two solutions are the same and that is determined by vanishing of the Wronskian

$$W[u_{\mathsf{WKB}}, q_{\mathsf{WKB}}] = \lambda_{\mathsf{WKB}} \sin\left[\lambda_{\mathsf{WKB}}(\mathrm{e} - 1)\right],$$

(in which case the Green function does not exist and we have either no solution or infinitely many solutions differing by a multiple of the eigenfunction corresponding to the *Fredholm alternative*).

Thus our WKB approximations to the eigenvalues here are given by $\lambda = n\pi/(\mathrm{e} - 1)$. The corresponding exact eigenvalues are determined by the transcendental equation

$$2J_0(\lambda)Y_0(\mathrm{e}\lambda) - 2Y_0(\lambda)J_0(\mathrm{e}\lambda) = 0.$$

A comparison of the exact and approximate eigenvalue is given in Figure 8.2. Again it is remarkable how accurate the approximate eigenvalue is even for the lowest possible values of λ_n.

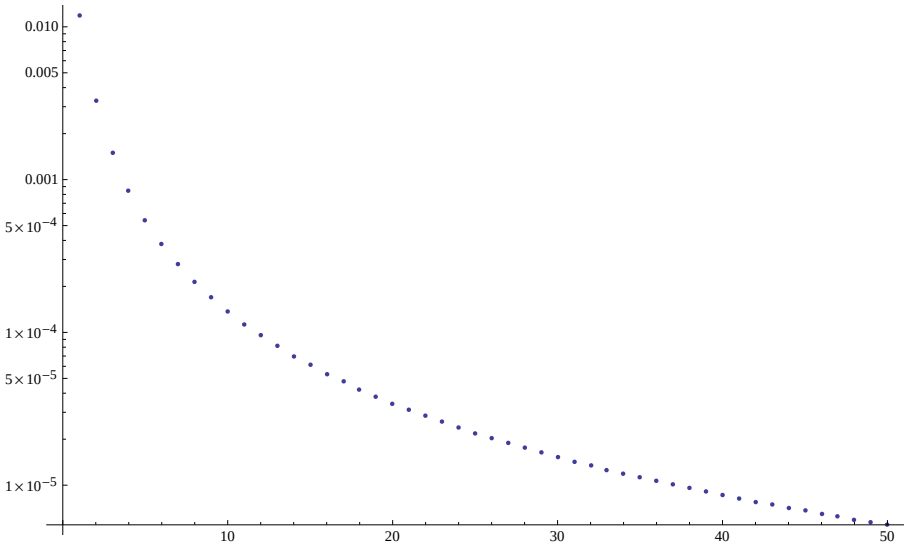


Figure 8.3: The relative error in the eigenvalues λ_{WKB} and the exact eigenvalue λ for mode number $n = 1$ to $n = 50$.

8.3 Higher order terms

To be more systematic we can look for an expansion of the form

$$\exp(\lambda\psi_1(t) + \psi_0(t) + \psi_{-1}(t)/\lambda + \psi_{-2}(t)/\lambda^2 + \cdots)$$

and consider the more general differential equation

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} + \left(\lambda^2 q_2(t) + \lambda q_1(t) + q_0(t)\right) y = 0$$

Since we can write $A(t) = \mathrm{e}^{\ln A(t)}$ we can include $A(t)$ within this expansion, in fact, we will see our ansatz above corresponds to

$$A(t) = \exp\psi_0(t) = \exp\left(-\tfrac{1}{4}\ln|q_2(t)|\right) \qquad \text{when } q_1 = q_0 = 0$$

Differentiating

$$\begin{aligned}
y(t) &\sim \exp\left(\lambda\psi_1(t) + \psi_0(t) + \lambda^{-1}\psi_{-1}(t) + \dots\right)\\
y'(t) &\sim \left(\lambda\psi_1'(t) + \psi_0'(t) + \lambda^{-1}\psi_{-1}'(t) + \dots\right)\exp\left(\lambda\psi_1(t) + \psi_0(t) + \lambda^{-1}\psi_{-1}(t) + \dots\right)\\
y''(t) &\sim \left(\left(\lambda\psi_1''(t) + \psi_0''(t) + \lambda^{-1}\psi_{-1}''(t) + \dots\right) + \left(\lambda\psi_1'(t) + \psi_0'(t) + \lambda^{-1}\psi_{-1}'(t) + \dots\right)^2\right)\times\\
&\qquad \exp\left(\lambda\psi_1(t) + \psi_0(t) + \lambda^{-1}\psi_{-1}(t) + \dots\right)\\
&= \left(\lambda^2\left(\psi_1'(t)\right)^2 + \lambda\left(\psi_1''(t) + 2\psi_1'(t)\psi_0'(t)\right) + \left(\psi_0''(t) + \left(\psi_0'(t)\right)^2 + 2\psi_1'(t)\psi_{-1}'(t)\right) + \dots\right)\times\\
&\qquad \exp\left(\lambda\psi_1(t) + \psi_0(t) + \lambda^{-1}\psi_{-1}(t) + \dots\right)
\end{aligned}$$

So equating order by order

$$\begin{aligned}
&\left(\psi_1'(t)\right)^2 + q_2(t) = 0\\
&\psi_1''(t) + 2\psi_1'(t)\psi_0'(t) + q_1(t) = 0\\
&\qquad\qquad \Rightarrow \psi_0'(t) = -\frac{\psi_1''(t)}{2\psi_1'(t)} - \frac{q_1(t)}{2\psi_1'(t)}\\
&\psi_0''(t) + \left(\psi_0'(t)\right)^2 + 2\psi_1'(t)\psi_{-1}'(t) + q_0(t) = 0
\end{aligned}$$

and solving order by order

$$\begin{aligned}\psi_1(t) &= \pm i \int^t q_2(t')^{1/2}\,\mathrm{d}t' \\ \psi_0(t) &= -\tfrac{1}{2}\ln|\psi_1'(t)| \pm \tfrac{1}{2}\mathrm{i}\int^t \frac{q_1(t')}{q_2(t')^{1/2}}\,\mathrm{d}t' \\ &= -\tfrac{1}{4}\ln|q_2(t)| \pm \tfrac{1}{2}\mathrm{i}\int^t \frac{q_1(t')}{q_2(t')^{1/2}}\,\mathrm{d}t' + \text{const.}\end{aligned}$$

For validity we need $\psi_0(t) \ll \lambda\psi_1(t)$, $\lambda^{-1}\psi_{-1}(t) \ll \psi_0(t)$ as $\lambda \to \infty$.

It is clear that we can continue to any order we wish and that it is

1. horrible by hand!
2. trivial for computer algebra!

8.4 Solution behaviour and Stokes lines

Things start to get interesting if we consider the WKB solution to the Airy equation

$$\frac{\mathrm{d}^2 f}{\mathrm{d}t^2} - \lambda^2 t f = 0, \tag{8.2}$$

where we introduce the parameter λ as a convenience.

Sticking to the lowest order solution we have

$$y_\pm(t) \approx \frac{1}{t^{1/4}}\exp\left(\pm\mathrm{i}\lambda\int^t (-s)^{1/2}\,\mathrm{d}s\right) = t^{-1/4}\exp\left(\mp\mathrm{i}\lambda\tfrac{2}{3}(-t)^{3/2}\right).$$

If we recall that in Chapter 7

$$\mathrm{Ai}(t) \sim \frac{1}{2\sqrt{\pi}}t^{-1/4}\mathrm{e}^{-\frac{2}{3}t^{3/2}} \qquad \text{as } t \to \infty,$$

we see perfect agreement with

$$\mathrm{Ai}(t) \sim \frac{1}{2\sqrt{\pi}}y_-(t) \qquad \text{as } t \to \infty.$$

On the other hand we might equally recall that

$$\mathrm{Ai}(t) \sim \frac{1}{\sqrt{2\pi}}(-t)^{-1/4}\sin\left[\tfrac{2}{3}(-t)^{3/2} + \tfrac{\pi}{4}\right] \qquad \text{as } t \to -\infty,$$

we see perfect agreement with

$$\mathrm{Ai}(t) \sim \frac{1}{2\sqrt{\pi}} \left[\mathrm{e}^{\mathrm{i}\pi/4} y_-(t) - \mathrm{e}^{-i\pi/4} y_+(t) \right] \qquad \text{as } t \to -\infty.$$

Notice that if we write

$$\mathrm{Ai}(t) \sim A_- y_-(t) + A_+ y_+(t),$$

then we need

$$A_- \sim \frac{1}{2\sqrt{\pi}} \qquad A_+ \sim 0, \quad \text{for } t \to \infty$$

and

$$A_- \sim \frac{1}{2\sqrt{\pi}\mathrm{i}} \qquad A_+ \sim -\frac{1}{2\sqrt{\pi}\mathrm{i}}, \qquad \text{for } t \to -\infty.$$

In hindsight we may notice that the WKB solution is singular and can't possibly be right at $t = 0$ and indeed our solution has a cut in the complex plane. In fact, this has saved us as our real solution $\mathrm{Ai}(t)$ must have real coefficients when $y_-(t)$ and $y_+(t)$ are real ($t > 0$) and complex coefficients when $y_-(t)$ and $y_+(t)$ are complex ($t < 0$).

A full understanding of what is going on here was provided by Stokes by considering the behaviour of the solution in the complex t-plane. We start with a simpler example showing the same jump in behaviour. Write

$$\frac{1}{\sinh t} \sim A_- \mathrm{e}^{-t} + A_+ \mathrm{e}^{t},$$

then we need

$$A_- \sim 2 \qquad A_+ \sim 0, \quad \text{for } t \to \infty$$

and

$$A_- \sim 0 \qquad A_+ \sim 2, \qquad \text{for } t \to -\infty.$$

Indeed it is clear that if we consider t in the complex plane e^{t} grows and dominates e^{-t} in the right half plane $\mathrm{Re}(t > 0)$ while e^{-t} grows and dominates e^{t} in the left half plane $\mathrm{Re}(t < 0)$ and as our solution decreases along any radial line excluding the imaginary axis the coefficient of the dominant term must exactly vanish in the corresponding half plane. The transition occurs along the imaginary axis where neither solution $\mathrm{e}^{-\mathrm{i}t}$ and $\mathrm{e}^{\mathrm{i}t}$ dominates. (In this case, there is no particular reason to

consider writing our expansion as a linear sum in this way but clearly for WKB we do.)

Returning to our example of the Airy function $\mathrm{Ai}(t)$ and writing $t = r\mathrm{e}^{\mathrm{i}\theta}$ we have

$$y_{\pm}(t) \approx r^{1/4}\mathrm{e}^{-i\pi/4}\exp\left[\mp\lambda\tfrac{2}{3}r^{3/2}(\cos\tfrac{3}{2}\theta - \mathrm{i}\sin\tfrac{3}{2}\theta)\right].$$

Again we see that one term dominates the other as $r \to \infty$ depending on whether $\cos\frac{3}{2}\theta$ is positive or negative. The dividing lines where the two terms are both of equal magnitude, are called *Stokes' line*, and represent the lines along which the coefficients may jump. In the current case this corresponds to $\cos\frac{3}{2}\theta = 0$, that is the radial lines $\theta = \frac{1}{3}\pi$, π and $\theta = \frac{5}{3}\pi$ with the $\frac{2}{3}\pi$ rotations reflecting the symmetry of Fig. (7.5). In general, for WKB approximations we identify the Stokes lines as being the lines on which the real part of the argument of exponential vanishes.

8.5 Transition points

Returning to our simplest potential

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} + \lambda^2 q(t)y = 0$$

suppose that we have $q(t) > 0$ for $t < a$ and $q(t) < 0$ for $t > a$ then we have WKB approximations

$$y(t) \sim \frac{1}{|q(t)|^{1/4}}\exp\left(\pm i\lambda\int_t^a \sqrt{|q(s)|}\,\mathrm{d}s\right) \qquad t < a,$$
$$y(t) \sim \frac{1}{|q(t)|^{1/4}}\exp\left(\pm\lambda\int_a^t \sqrt{|q(s)|}\,\mathrm{d}s\right) \qquad t > a,$$

where we have chosen a lower limit on our integrals for definiteness. Hence our solution is oscillatory on the right and a combination of real exponentials on the right, of the transition point $t = a$ where $q(a) = 0$. In most (Note that this is reminiscent of our plot of the Airy function.)

The WKB approximation clearly breaks down near points where $x = a$ but in such a region we can approximate our equation by

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} + \lambda^2 q'(a)(t-a)y = 0$$

which with a simple change of variable $x = \alpha(t-a)$, where $\alpha = (\lambda^2 q'(a))^{1/3}$, is precisely Airy's equation. This suggest the hope that we might use the Airy functions and in particular their

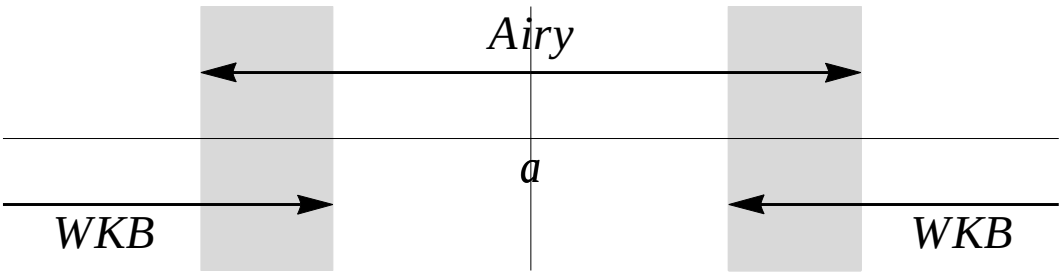


Figure 8.4: The principle of matching asymptotic solutions is to find a range of values in which both solutions are valid.

asymptotics

$$\begin{aligned}
\mathrm{Ai}(x) &\sim \frac{1}{2\sqrt{\pi}} x^{-1/4} \mathrm{e}^{-\frac{2}{3}x^{3/2}} \qquad \text{as } x \to \infty, \\
\mathrm{Ai}(x) &\sim \frac{1}{\sqrt{\pi}} (-x)^{-1/4} \sin\left[\tfrac{2}{3}(-x)^{3/2} + \tfrac{\pi}{4}\right] \qquad \text{as } x \to -\infty, \\
\mathrm{Bi}(x) &\sim \frac{1}{\sqrt{\pi}} x^{-1/4} \mathrm{e}^{\frac{2}{3}x^{3/2}} \qquad \text{as } x \to \infty. \\
\mathrm{Bi}(x) &\sim -\frac{1}{\sqrt{\pi}} (-x)^{-1/4} \cos\left[\tfrac{2}{3}(-x)^{3/2} + \tfrac{\pi}{4}\right] \qquad \text{as } x \to -\infty
\end{aligned}$$

to bridge between our two WKB solutions. If we can get far enough away still using $q(t) = \alpha^3(t-a)$ then $\int_a^t \sqrt{|q(s)|}\,\mathrm{d}s = \frac{2}{3}\alpha^{3/2}|t-a|^{3/2}$ and our WKB forms correspond precisely to those of the Airy functions.

Some fairly hard analysis is required to show that there is indeed a range of parameters for which these expansions are simultaneously valid and is part of the wider theory of matched asymptotic expansions. For the justification of the matching procedure (and much else) the book *Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory* by C.M. Bender and S.A. Orszag (Springer) is highly recommended.

The precise details depend on the problem to be solved - let us take for definiteness the case where we want just the decreasing exponential to the right of the transition point then it is precisely $\mathrm{Ai}(s)$, then to the left we must have the linear WKB combination

$$y(t) \sim \frac{2}{|q(t)|^{1/4}} \sin\left[\lambda \int_t^a \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right]$$

(note the phase).

Example: For a potential with an infinite wall at $t = 0$ and with $q(t) = \frac{1}{2}\omega^2(a^2 - t^2)$, $(t > 0)$. To

match to the decaying exponential we have

$$y(t) \sim \frac{2 \times 2^{1/4}}{[\omega(a^2-t^2)]^{1/2}} \sin\left[\lambda \int_t^a \tfrac{1}{\sqrt{2}}\omega(a^2-s^2)^{1/2}\,\mathrm{d}s + \tfrac{1}{4}\pi\right]$$
$$\sim \frac{2 \times 2^{1/4}}{\left[\omega\left(a^2-t^2\right)\right]^{1/2}} \sin\left\{-\tfrac{1}{2\sqrt{2}}\lambda\omega\left[t\left(a^2-t^2\right)^{1/2} + a^2\left(\sin^{-1}(t/a) - \tfrac{\pi}{2}\right)\right] + \tfrac{1}{4}\pi\right\}$$

This solution vanishes at $t = 0$ as required for an infinite wall if and only if

$$\lambda\omega = \left(n - \tfrac{1}{4}\right)\frac{4\sqrt{2}}{a^2}, \qquad E = \frac{(4n-1)^2}{a^4}.$$

We can extend this idea to match to a decaying exponential to the left of a turning point b of an decreasing potential matches to the linear WKB combination

$$y(t) \sim \frac{2}{|q(t)|^{1/4}} \sin\left(\lambda \int_b^t \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right).$$

This enables us to consider the problem of bound states for a potential increasing at both sides but for consistency these solutions and their derivatives must both match across the range so we require

$$\frac{A}{|q(t)|^{1/4}} \sin\left(\lambda \int_t^a \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right) = \frac{B}{|q(t)|^{1/4}} \sin\left(\lambda \int_b^t \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right),$$

and

$$A|q(t)|^{1/4} \cos\left(\lambda \int_t^a \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right) = B|q(t)|^{1/4} \cos\left(\lambda \int_b^t \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{4}\pi\right).$$

where we have neglected the slow change of the amplitude compared to the phase. For a non-trivial

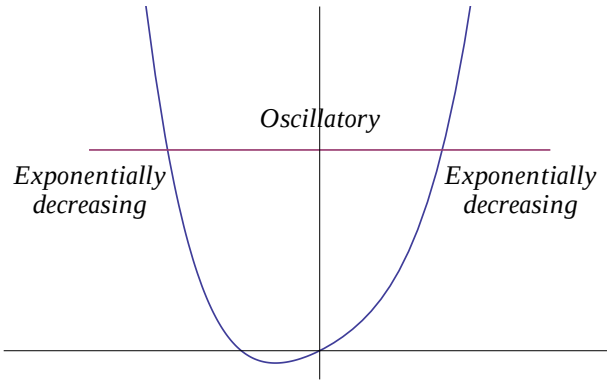


Figure 8.5: Matching left and right gives a quantisation condition.

solution the Wronskian must vanish and this becomes

$$\sin\left(\lambda\int_b^a \sqrt{|q(s)|}\,\mathrm{d}s + \tfrac{1}{2}\pi\right) = 0$$

giving

$$\lambda\int_b^a \sqrt{|q(s)|}\,\mathrm{d}s = (n-\tfrac{1}{2})\pi.$$

8.6 Worked examples

1. (a) Show that the large eigenvalues of

$$y''(t) + \lambda^2 q(t) y = 0, \qquad y(0) = 0, \quad y(1) = 0$$

are given by $\lambda_n = n\pi \left[\int_0^1 \sqrt{q(s)}\,\mathrm{d}s\right]^{-1}$.

(b) Show that the large eigenvalues of

$$y''(t) + \lambda^2 q(t) y = 0, \qquad y(0) = 0, \quad y'(1) = 0$$

are given by $\lambda_n = (n + \frac{1}{2})\pi \left[\int_0^1 \sqrt{q(s)}\,\mathrm{d}s\right]^{-1}$.

We write down the lowest-order WKB approximation of the generic ODE $y''(t) + \lambda^2 q(t) y = 0$, with solution

$$y_{\mathrm{WKB}}(t) = \frac{1}{|q(t)|^{1/4}} \exp\left(\pm \mathrm{i}\lambda \int_0^t \sqrt{q(s)}\mathrm{d}s\right),$$

which more particularly can be taken to be

$$y_{\mathrm{WKB}}(t) = \frac{1}{|q(t)|^{1/4}} \sin\left(\lambda \int_0^t \sqrt{q(s)}\mathrm{d}s + \varphi\right), \tag{8.3}$$

where $\varphi \in \mathbb{R}$ is a phase. Equation (8.3) can also be viewed as the solution of the eigenvalue problem. We need $y_{\mathrm{WKB}}(0) = 0$, hence $\varphi = 0$. Also, for **part (a)**, we need $y_{\mathrm{WKB}}(1) = 0$, hence

$$\lambda \int_0^t \sqrt{q(s)}\mathrm{d}s = n\pi, \qquad n \in \mathbb{N},$$

hence

$$\lambda_n = \frac{n\pi}{\int_0^1 \sqrt{q(s)}\mathrm{d}s}.$$

For **part (b)**, we need $y'_{\mathrm{WKB}}(1) = 0$, hence

$$-\tfrac{1}{4} q'(t) q(t)^{-5/4} \sin\left(\lambda \int_0^1 \sqrt{q(s)}\mathrm{d}s\right) + \lambda q(t)^{-1/4} q(t)^{1/2} \cos\left(\lambda \int_0^1 \sqrt{q(s)}\mathrm{d}s\right) = 0.$$

Here, the second term is proportional to λ and hence dominates in the limit as $\lambda \to \infty$. Hence, to leading order, the boundary condition reads

$$\lambda q(t)^{-1/4} q(t)^{1/2} \cos\left(\lambda \int_0^t \sqrt{q(s)}\mathrm{d}s\right) = 0,$$

hence

$$\cos\left(\lambda\int_0^1\sqrt{q(s)}\mathrm{d}s\right)$$

and thus

$$\lambda_n=\frac{\pi\left(n+\frac{1}{2}\right)}{\int_0^1\sqrt{q(s)}\mathrm{d}s},\qquad n\in\mathbb{N}\cup\{0\}.$$

2. The Weber-Hermite differential equation

$$y''(t)+(\nu+\tfrac{1}{2}-\lambda^2t^2)y(t)=0, \tag{8.4}$$

has solutions known as parabolic cylinder functions. Determine the higher order WKB approximation to terms to order λ^{-1}. Also, identify the Stokes lines for these solutions.

The extended WKB method in Section 8.3 applies directly to Equation (8.4), with

$$\begin{aligned}q_2(t)&=-t^2,\\ q_1(t)&=0,\\ q_0(t)&=\nu+1/2.\end{aligned}$$

From Section 8.3 we have

$$\begin{aligned}\psi_0(t)&=-\tfrac{1}{4}\ln|q_2(t)|\pm\tfrac{1}{2}\mathrm{i}\int^t\frac{q_1(t')}{q_2(t')^{1/2}}\mathrm{d}t'+\text{Const.},\\ &=-\tfrac{1}{4}\ln t^2,\\ &=-\tfrac{1}{2}\ln|t|.\end{aligned}$$

Also,

$$\begin{aligned}\psi_1(t)&=\pm\mathrm{i}\int^t q_2(t')^{1/2}\mathrm{d}t',\\ &=\pm\mathrm{i}\int^t(-t'^2)^{1/2}\mathrm{d}t',\\ &=\pm\int^t t'\mathrm{d}t',\\ &=\pm\tfrac{1}{2}t^2.\end{aligned}$$

The WKB solution is

$$y(t)=\exp\left(\lambda\psi_1(t)+\psi_0(t)+\psi_{-1}(t)/\lambda+\psi_{-2}(t)/\lambda^2+\cdots\right).$$

Including only terms of order λ and λ^0 in the expansion, we are left with

$$\begin{aligned} y(t) &\sim \exp\left(\lambda\psi_1(t) + \psi_0(t)\right), \qquad \lambda \to \infty, \\ &= \exp\left[\pm\tfrac{1}{2}\lambda t^2 - \tfrac{1}{4}\ln t^2\right], \\ &= t^{-1/2}\exp\left(\pm\lambda t^2/2\right). \end{aligned}$$

Stokes lines occur in the complex t-plane where neither of the solutions $t^{-1/2}\exp(\pm\lambda t^2/2)$ dominates the other as $\lambda \to \infty$. This happens when t^2 is purely imaginary, that is on radial lines with argument $\pi/4, 3\pi/4, 5\pi/4, 7\pi/4$.

At next order, we have

$$\psi_0'' + (\psi_0')^2 + 2\psi_1'\psi_{-1}' + q_0 = 0.$$

We have

$$\begin{aligned} \psi_0' &= -\frac{1}{2t}, \\ \psi_0'' &= \frac{1}{2t^2}, \\ \psi_1' &= \pm t, \\ q_0 &= \nu + \tfrac{1}{2}, \end{aligned}$$

hence

$$\frac{1}{2t^2} + \frac{1}{4t^2} \pm 2t\psi_1' + (\nu + 1/2) = 0,$$

and

$$\pm\psi_{-1}' = -\tfrac{1}{2}(\nu + \tfrac{1}{2})\frac{1}{t} - \tfrac{3}{4\cdot 2}\frac{1}{t^2},$$

hence

$$\psi_{-1} = \pm\tfrac{1}{8}\left[-(1+2\nu)\ln t + \tfrac{3}{8}\frac{1}{t^2}\right],$$

and the solution to order λ^{-1} reads

$$y \sim t^{-1/2}\exp\left[\pm\lambda t^2 \pm \frac{1}{8\lambda}\left(-(1+2\nu)\ln t + \tfrac{3}{8}\frac{1}{t^2}\right)\right]$$

The previous discussion about Stokes Lines still applies, as the Stokes lines refer to the dominant term in the solution that is $O(\lambda)$.

3. Find the WKB approximation to the eigenvalues of normalizable functions satisfying

$$y''(t) + (E - t^4)y = 0. \tag{8.5}$$

Also, compute the relative error for E_n given the 'exact' values are given in Table 8.2.

n	0	2	4	6	8	10
E_n	1.060	7.456	16.262	26.528	37.923	50.256

Table 8.1: First few eigenvalues for the equation (8.5)

The theory in Section 8.5 applies here, upon taking $\lambda^2 q(t) = E - t^4$. The turning points are at $E = t^4$, hence $t = \pm E^{1/4}$. We require the following condition

$$\int_{-E^{1/4}}^{E^{1/4}} \sqrt{E - t^4}\mathrm{d}t = \left(n + \tfrac{1}{2}\right)\pi, \qquad n \in \mathbb{N} \cup \{0\}.$$

Let $s = t/E^{1/4}$. The condition now reads

$$\int_{-1}^{1} \sqrt{1 - s^4}\mathrm{d}s = E^{-3/4}\left(n + \tfrac{1}{2}\right)\pi.$$

The integral on the left-hand side can be evaluated in terms of elliptic integrals:

$$\int \sqrt{1 - x^4}\mathrm{d}x = x(1 - x^4)^{1/2} + \tfrac{2}{3}F\left(\sin^{-1}(x)|-1\right),$$

where $F(z|m)$ is an elliptic integral of the first kind. Thus,

$$\begin{aligned} I &= \int_{-1}^{1} \sqrt{1 - x^4}\mathrm{d}x, \\ &= 2\int_{0}^{1} \sqrt{1 - x^4}\mathrm{d}x, \\ &= \tfrac{4}{3}\left[F(\sin^{-1}(1)|-1) - F(\sin^{-1}(0)|-1)\right], \\ &= \tfrac{4}{3}\left[F(\sin^{-1}(1)|-1) - F(0|-1)\right], \\ &= \tfrac{4}{3}F(\sin^{-1}(1)|-1) \end{aligned}$$

where $F(z|m)$ is the complete elliptic integral of the first kind, with $F(0|m) = 0$. Also, using tables,

$$F(\sin^{-1}(z)|-1) = z\,{}_2F_1\left(\tfrac{1}{4}, \tfrac{1}{2}; \tfrac{4}{4}; z^4\right).$$

Thus,

$$I = \tfrac{4}{3}{}_2F_1\left(\tfrac{1}{4}, \tfrac{1}{2}; \tfrac{4}{4}; 1\right).$$

Again using tables (e.g. Abramowitz and Stegun, 15.1.20),

$$\begin{aligned} I &= \tfrac{4}{3}\frac{\Gamma(5/4)\Gamma(1/2)}{\Gamma(3/4)}, \\ &= \frac{\Gamma(5/4)\Gamma(1/2)}{(3/4)\Gamma(3/4)}, \\ &= \frac{\Gamma(5/4)\sqrt{\pi}}{\Gamma(7/4)}, \\ &\approx 1.748038369528080. \end{aligned}$$

where $\Gamma(\cdot)$ is the Gamma function. Thus, the eigenvalues are

$$E = \left[\frac{\left(n+\frac{1}{2}\right)\pi}{I}\right]^{4/3},$$

and in a double-precision approximation this is

$$E = \left[\frac{\left(n+\frac{1}{2}\right)\pi}{1.748038369528080}\right]^{-3/4}.$$

Numerical results are tabulated here:

n	0	2	4	6	8	10
E_n (true)	1.060	7.456	16.262	26.528	37.923	50.256
E_n (WKB)	0.867	7.414	16.233	26.507	37.9055	50.241
True-WKB	0.1928	0.0420	0.0283	0.0215	0.0182	0.0154
(True-WKB)/True	18%	0.56%	0.17%	0.08%	0.05%	0.03%

Table 8.2: First few eigenvalues for the equation (8.5) and comparison with WKB theory

Chapter 9

The model Poisson equation – theoretical background

Overview

We consider analytical solutions to a two-dimensional Poisson problem. The reason for examining this particular problem are manifold: it is a minimal model that nonetheless has a small amount of complexity sufficient to warrant the use of a number of interesting numerical methods. Also, its analytical solution is rather interesting, as it requires plenty of favourite techniques in PDE theory. Finally, analytical solutions in this section will be used as benchmarks for future numerical simulation studies. Throughout the course, the problem considered in this section will be referred to as the **model Poisson equation**.

9.1 The model Poisson equation

We are interested in solving the following elliptic partial differential equation (PDE), given here in non-dimensional form as follows:

$$\nabla^2 u + s(x, y) = 0 \qquad (x, y) \in \Omega, \tag{9.1a}$$

where

$$\Omega = (0, L_x) \times (0, L_y), \tag{9.1b}$$

and $\nabla^2 = \partial_x^2 + \partial_y^2$ is the Laplacian. The partial differential equation is subject to the following **Dirichlet** boundary conditions:

$$u(x = 0, y) = \alpha(y), \qquad u(x = L_x, y) = 0, \tag{9.1c}$$

and

$$u(x, y = 0) = 0, \qquad u(x, y = L_y) = 0. \tag{9.1d}$$

9.2 Decomposition

It is sensible to split the solution into two parts:

$$u(x, y) = u_0(x, y) + u_1(x, y),$$

where

- $u_0(x, y)$ satisfies Laplace's equation $\nabla^2 u_0 = 0$ with inhomogeneous boundary conditions

$$u_0(x = 0, y) = \alpha(y), \qquad u_0(x = L_x, y) = 0, \qquad u_0(x, y = 0) = 0, \qquad u_0(x, y = L_y) = 0.$$

- $u_1(x, y)$ satisfies Poisson's equation $\nabla^2 u_1 = -s(x, y)$ with homogeneous boundary conditions

$$u_1(x = 0, y) = 0, \qquad u_1(x = L_x, y) = 0, \qquad u_1(x, y = 0) = 0, \qquad u_1(x, y = L_y) = 0.$$

By linearity, $u_0 + u_1$ satisfies the full model Poisson equation (10.1a) with the full set of boundary conditions (10.1c)–(10.1d).

9.3 Analytical solution – Laplace part

We solve for $u_0(x, y)$ using separation of variables, writing $u_0(x, y) = X(x)Y(y)$, which gives

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = 0. \tag{9.2}$$

The boundary conditions give $Y(0) = Y(L_y) = 0$ and $X(L_x) = 0$. The boundary condition at $x = 0$ is as yet undetermined, as this amounts to

$$u(x = 0, y) = \alpha(y) = X(0)Y(y).$$

We apply the separation-of-variables argument to Equation (9.2) to get

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -k^2.$$

In view of the y-boundary conditions, we take $k = n\pi/L_y$, with $n \in \{1, 2, \cdots\}$, and $Y(y) = \sin(n\pi y/L_y)$. Then,

$$\frac{1}{X}\frac{d^2X}{dx^2} = k^2.$$

The solution is made up of sinhes and coshes. We take

$$X = \sinh[k(L_x - x)]$$

because this satisfies the boundary condition at $x = L_x$, i.e. $X(L_x) = 0$. Thus, the solution is now

$$u(x,y) = \sum_{n=1}^{\infty} A_n \sinh\left[\frac{n\pi}{L_y}(L_x - x)\right] \sin\left(\frac{n\pi}{L_y}y\right) \qquad \text{(general solution)}.$$

We now work on the boundary condition at $x = 0$. We have

$$u(x=0,y) = \sum_{n=1}^{\infty} A_n \sinh\left[\frac{n\pi L_x}{L_y}\right] \sin\left(\frac{n\pi}{L_y}y\right) = \alpha(y).$$

To back out the A_n's, we multiply both sides of the above equation by $(2/L_y)\sin(n'\pi y/L_y)$ and integrate, to obtain

$$\sum_{n=1}^{\infty} A_n \sinh\left[\frac{n\pi L_x}{L_y}\right] \underbrace{\left[\frac{2}{L_y}\int_0^{L_y} \mathrm{d}y \sin\left(\frac{n\pi}{L_y}y\right)\sin\left(\frac{n'\pi}{L_y}y\right)\right]}_{\delta_{nn'}} = \frac{2}{L_y}\int_0^{L_y} \mathrm{d}y \sin\left(\frac{n'\pi}{L_y}y\right)\alpha(y),$$

hence

$$A_n = \frac{1}{\sinh\left[\frac{n\pi L_x}{L_y}\right]}\frac{2}{L_y}\int_0^{L_y} \mathrm{d}y \sin\left(\frac{n\pi}{L_y}y\right)\alpha(y). \tag{9.3}$$

The solution is therefore

$$u_0(x,y) = \sum_{n=1}^{\infty} A_n \sinh\left[\frac{n\pi}{L_y}(L_x - x)\right] \sin\left(\frac{n\pi}{L_y}y\right),$$

where the A_n's are given by Equation (9.3).

9.3.1 Analytical solution – Poisson part

It is not possible to solve for $u_1(x,y)$ using separation of variables because of the source term $s(x,y)$. However, we can still find a solution using the basis functions

$$\phi_{nm}(x,y) = \sqrt{\frac{2}{L_x}}\sqrt{\frac{2}{L_y}} \sin\left(\frac{n\pi}{L_x}x\right)\sin\left(\frac{m\pi}{L_y}y\right).$$

where n and m are positive integers. We multiply both sides of $\nabla^2 u_1 = -s(x,y)$ by ϕ_{nm} and integrate over the domain to obtain

$$\int_\Omega \phi_{nm} \nabla^2 u_1 \, \mathrm{d}^2x = -\int_\Omega \phi_{nm} s \, \mathrm{d}^2x := -\widehat{s}_{nm}.$$

We focus on the left-hand side:

$$\begin{aligned}
\text{L.H.S.} &= \int_\Omega \phi_{nm} \nabla^2 u_1 \, \mathrm{d}^2x, \\
&= \int_\Omega \left[\nabla \cdot (\phi_{nm} \nabla u_1) - \nabla \phi_{nm} \cdot \nabla u_1 \right] \mathrm{d}x, \\
&= \int_{\partial\Omega} \phi_{nm} \widehat{n} \cdot \nabla u_1 \mathrm{d}\ell - \int_\Omega \nabla \phi_{nm} \cdot \nabla u_1 \, \mathrm{d}x,
\end{aligned}$$

where $\widehat{n}$ is the outward-pointing unit normal to the domain boundary $\partial\Omega$ and $\mathrm{d}\ell$ is an element of length along the domain boundary. In any case, $\phi_{nm} = 0$ on $\partial\Omega$ (because ϕ_{nm} is made up of sine functions that vanish on the boundary), hence

$$\text{L.H.S.} = -\int_\Omega \nabla \phi_{nm} \cdot \nabla u_1 \, \mathrm{d}x.$$

We apply integration by parts again:

$$\begin{aligned}
\text{L.H.S.} &= -\int_\Omega \nabla \phi_{nm} \cdot \nabla u_1 \, \mathrm{d}^2x, \\
&= -\int_\Omega \left[\nabla \cdot (u_1 \nabla \phi_{nm}) - u_1 \nabla^2 \phi_{nm} \right] \mathrm{d}^2x, \\
&= -\int_{\partial\Omega} u_1 \widehat{n} \cdot \nabla \phi_{nm} \, \mathrm{d}\ell + \int_\Omega u_1 \nabla^2 \phi_{nm} \, \mathrm{d}^2x.
\end{aligned}$$

The boundary integral here is zero because $u_1 = 0$ on $\partial\Omega$, which leaves

$$\text{L.H.S.} = \int_\Omega u_1 \nabla^2 \phi_{nm} \, \mathrm{d}^2x.$$

Hence,

$$\begin{aligned}
\text{L.H.S.} &= -k_{nm}^2 \int_\Omega u_1 \phi_{nm} \, \mathrm{d}^2x, \\
&= -k_{nm}^2 \widehat{u}_{1nm},
\end{aligned}$$

where

$$k_{nm}^2 = \left(\frac{n\pi}{L_x} \right) n^2 + \left(\frac{n\pi}{L_y} \right) m^2.$$

Hence,

$$\widehat{u_1}_{nm} = \frac{\widehat{s}_{nm}}{k_{nm}^2}.$$

The proposed solution is

$$u_1(x,y) = \sum_{n,m=1}^{\infty} \widehat{u_1}_{nm}\phi_{nm}(x,y).$$

This makes sense, because the ϕ_{nm}'s are an orthonormal set:

$$\int_\Omega \phi_{nm}\phi_{n'm'}\mathrm{d}^2x = \delta_{nn'}\delta_{mm'}.$$

Hence,

$$u_1(x,y) = \sum_{n,m=1}^{\infty} \frac{\widehat{s}_{nm}}{k_{nm}^2}\phi_{nm}(x,y).$$

Having constructed a solution to Equation (10.1), it is also the case that this is the only such smooth solution:

Theorem 9.1 *The solution $u(x,y) = u_0(x,y) + u_1(x,y)$ is the unique smooth solution of Equation* (10.1)*.*

Exercise 9.1 *Use the maximum principle to prove Theorem* (9.1)*.*

Chapter 10

Model Poisson equation – Numerical setup

Overview

In this chapter we consider numerical solutions of the model Poisson equation. We introduce centred differencing in space as a way of approximating the Laplace operator numerically. After doing this, the PDE problem boils down to a linear-algebra problem wherein a matrix must be inverted. Jacobi iteration is introduced as a method to do this, followed by the slightly more sophisticated SOR method.

10.1 The model

We are interested in solving the PDE from Chapter 9, recalled here to be

$$\nabla^2 u + s(x,y) = 0 \qquad (x,y) \in \Omega, \tag{10.1a}$$

where

$$\Omega = (0, L_x) \times (0, L_y), \tag{10.1b}$$

and $\nabla^2 = \partial_x^2 + \partial_y^2$ is the Laplacian. The partial differential equation is subject to the following **dirichlet** boundary conditions:

$$u(x=0,y) = \alpha(y), \qquad u(x=L_x,y) = 0, \tag{10.1c}$$

and

$$u(x,y=0) = 0, \qquad u(x,y=L_y) = 0. \tag{10.1d}$$

10.2 The discretization

We discretize the PDE and compute its approximate numerical solution on a discrete grid:

$$x_i = (i-1)\Delta x, \qquad i = 1, \cdots, n_x,$$
$$y_j = (j-1)\Delta y, \qquad j = 1, \cdots, n_y,$$

such that

$$(n_x - 1)\Delta x = L_x, \qquad \Delta x = L_x/(n_x - 1),$$

and similarly, $\Delta y = L_y/(n_y - 1)$. The Laplace operator in the PDE (10.1) is approximated by **centred differences**:

$$\left(\nabla^2 u\right)_{ij} \approx \frac{u_{i+1,j} + u_{i-1,j} - 2u_{ij}}{\Delta x^2} + \frac{u_{i,j+1} + u_{i,j-1} - 2u_{ij}}{\Delta y^2} := \mathcal{D}(u_{ij})$$
$$i = 2, 3, \cdots, n_x - 1, \qquad j = 2, 3, \cdots, n_y - 1.$$

Thus, the PDE to solve is reduced to a simpler problem in linear algebra;

$$\frac{u_{i+1,j} + u_{i-1,j} - 2u_{ij}}{\Delta x^2} + \frac{u_{i,j+1} + u_{i,j-1} - 2u_{ij}}{\Delta y^2} = -s_{ij},$$
$$i = 2, 3, \cdots, n_x - 1, \qquad j = 2, 3, \cdots, n_y - 1. \quad (10.2)$$

where $s_{ij} = s(x_i, y_j)$.

10.3 Jacobi method

The focus of this course is on the use of **iterative methods** to solve problems such as Equation (10.2). The idea is to make an initial guess for the solution, plug this into some algorithm for refining the guess, and continue until this iterative procedure converges. The simplest and most naive iterative method is the so-called **Jacobi method**. We re-write Equation (10.2) as

$$u_{ij}\left(\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2}\right) = \frac{u_{i+1,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} + u_{i,j-1}}{\Delta y^2} + s_{ij},$$

or

$$u_{ij} = \frac{\frac{u_{i+1,j}+u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1}+u_{i,j-1}}{\Delta y^2} + s_{ij}}{\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2},} \tag{10.3}$$

all valid for $i = 2, 3, \cdots, n_x - 1$ and $j = 2, 3, \cdots, n_y - 1$. We introduce a sequence of guesses for Equation (10.3), $u^1, u^2, \cdots, u^n, u^{n+1}, \cdots$, such that

$$u_{ij}^{n+1} = \frac{\frac{u_{i+1,j}^n+u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n+u_{i,j-1}^n}{\Delta y^2} + s_{ij}}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2},} \tag{10.4}$$

If this iterative scheme converges, then $\lim_{n\to\infty} u^n = \lim_{n\to\infty} u^{n+1}$, and the approximate solutions u^n and u^{n+1} can be replaced in Equation (10.4) with some identical array u^*, thereby forcing Equation (10.4) to be identical to Equation (10.3).

10.4 Boundary conditions

The idea to solve the PDE (10.2) is to do Jacobi iteration at interior points. However, this approach can only be used at **interior points**

$$i = 2, 3, \cdots, n_x - 1, \qquad j = 2, 3, \cdots, n_y - 1.$$

At boundary points, the boundary conditions are enforced: $u = 0$ at all boundaries except at $x = 0$. Thus,

$$u_{i,1} = u_{i,n_y} = u_{n_x,j} = 0,$$

and

$$u_{1,j} = \alpha(y_j), \qquad y_j = (j-1)\Delta y.$$

10.5 Jacobi Method – the code

A sample code using the Jacobi method is given below and available online. We will work with Matlab first, before moving over to Fortran. The idea of this code is to use simple but still non-trivial source terms (both bulk and surface sources – i.e. $s(x, y)$ and $\alpha(y)$ respectively) that give rise to a particularly simple analytical solution. The numerical and analytical solutions can then be compared. This gives us confidence that the code is working. We can then go off and apply the code to more complicated sources for which the analytical solution is unwieldy.

```
function [xx,yy,u,u_true,res_it]=xtest_poisson_jacobi()

% Numerical method to solve
% [D_{xx}+D_{yy}]C=s(x,y),
% subject to zero boundary conditions except on x=0 where u(0,y)=alpha(y)
% where alpha is a given function.

% ***********************************************************************
% Geometric parameters:

aspect_ratio=2;
Ly=1.d0;
Lx=aspect_ratio*Ly;

% Fundamental wavenumbers:

kx0=pi/Lx;
ky0=pi/Ly;

% Numerical parameters:

Ny=101;
Nx=aspect_ratio*(Ny-1)+1;

% Maximum number of iterations in Jacobi solver:
iteration_max=5000;

dx=Lx/(Nx-1);
dy=Ly/(Ny-1);

dx2=dx*dx;
dy2=dy*dy;

% vectors of x- and y-values

```

```
36 xx=0*(1:Nx);
37 yy=0*(1:Ny);
38
39 % ************************************************************************
40 % Source parameters
41
42 % Bulk source s(x,y) - this is chosen here to be a single mode \phi_{nm},
43 % multiplied by an amplitude As.
44
45 As=10;
46 kx=kx0;
47 ky=3*ky0;
48
49 % Boundary source alpha(y) - this is chosen to be a sine function
50 % sin(n_\alpha\pi y/L_y), multiplied by an ampliutde A_\alpha.
51
52 n_alpha=1;
53 A_alpha=1;
54
55 % ************************************************************************
56 % Initialize sources
57
58 s_source=zeros(Nx,Ny);
59
60 for i=1:Nx
61     for j=1:Ny
62       x_val=(i-1)*dx;
63       y_val=(j-1)*dy;
64       s_source(i,j)=As*sqrt(2/Lx)*sqrt(2/Ly)*sin(kx*x_val)*sin(ky*y_val);
65     end
66 end
67
68 alpha_source=0*(1:Ny);
69
70 for j=1:Ny
71     y_val=(j-1)*dy;
72     alpha_source(j)=A_alpha*sin(n_alpha*pi*y_val/Ly);
73 end
74
75 % ************************************************************************
76 % Compute analytic solution - This is made up of u0 and u1.
77
78
79 u0_true=zeros(Nx,Ny);
80 u1_true=zeros(Nx,Ny);
```

```
81
82 for i=1:Nx
83     for j=1:Ny
84       xx(i)=(i-1)*dx;
85       yy(j)=(j-1)*dy;
86
87       u0_true(i,j)=(A_alpha/sinh(n_alpha*pi*Lx/Ly))*sinh( (n_alpha*pi/Ly)*(Lx-xx
             (i)))*sin(n_alpha*pi*yy(j)/Ly);
88       u1_true(i,j)=(As/(kx*kx+ky*ky))*sqrt(2/Lx)*sqrt(2/Ly)*sin(kx*xx(i))*sin(ky
             *yy(j));
89
90     end
91 end
92
93 u_true=u0_true+u1_true;
94
95 % Iteration step ******************************************************
96 % Initial guess for u:
97 u=zeros(Nx,Ny);
98
99 res_it=0*(1:iteration_max);
100
101 for iteration=1:iteration_max
102
103     u_old=u;
104
105     for i=2:Nx-1
106
107         im1=i-1;
108         ip1=i+1;
109
110         for j=2:Ny-1
111
112             diagonal=(2.d0/dx2)+(2.d0/dy2);
113             tempval=(1.d0/dx2)*(u_old(ip1,j)+u_old(im1,j))+(1.d0/dy2)*(u_old(i,j
                    +1)+u_old(i,j-1))+s_source(i,j);
114             u(i,j)=tempval/diagonal;
115
116         end
117     end
118
119     % Implement Dirichlet conditions
120     u(:,1)=0;
121     u(:,Ny)=0;
122     u(Nx,:)=0;
```

```
123
124     % Special condition at x=0.
125     u(1,:)=alpha_source;
126
127     res_it(iteration)=max(max(abs(u-u_old)));
128
129 end
130
131 end
```

xcodes/poisson_matlab/xtest_poisson_jacobi.m

Results for the presented parameter values / source terms are presented here also.

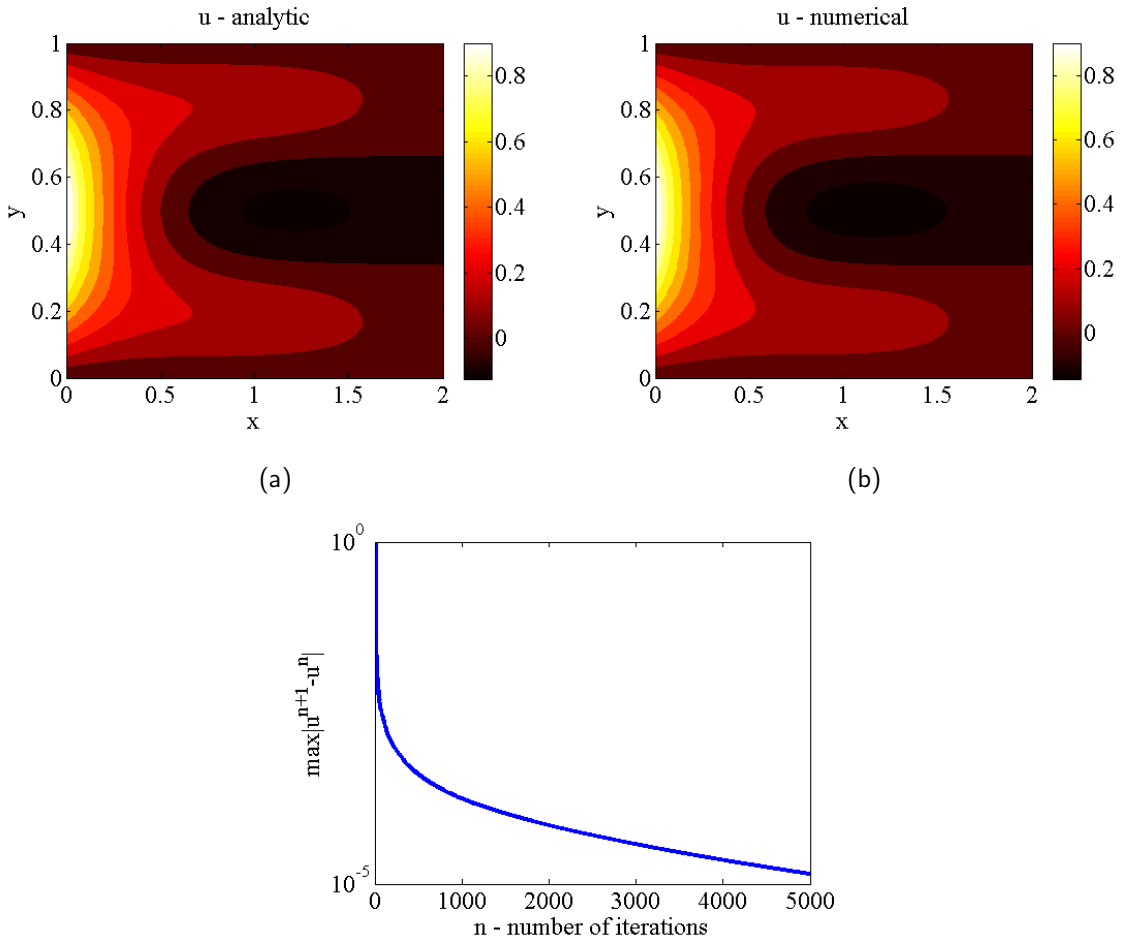


Figure 10.1: Numerical results from the Matlab code

Figures 10.1(a)–(b) show the analytical and numerical results respectively. They are indistinguishable, showing the correctness of the numerical code. Figure 10.1(c) shows the L^∞ norm of the difference between successive iterations, $\max_\Omega |u^{n+1} - u^n|$. Because this is decreasing to zero, the Jacobi iteration scheme is converging.

10.6 Successive over-relaxation – the idea

Start with the generic problem

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}.$$

Recall the Jacobi solution:

$$\mathbf{D}\boldsymbol{v}^{N+1} = -\mathbf{R}\boldsymbol{v}^{N} + \boldsymbol{b}, \qquad \boldsymbol{x} = \lim_{N\to\infty} \boldsymbol{v}^{N}.$$

In index notation, the Jacobi solution reads

$$v_i^{N+1} = -\frac{1}{a_{ii}} \sum_{j=1}^{n} R_{ik} v_k^N + b_i. \tag{10.5}$$

The idea behind SOR is to retrospectively improve the 'old guess' $\boldsymbol{v}^N$ that goes into formulating the 'new guess'. If the 'old guess' can be retrospectively improved, then this makes the new guess even better. To do this, the right-hand side of the Jacobi equation (10.5) is updated with just-recently-created values of $\boldsymbol{v}^{N+1}$. Where this is not possible, the old values of $\boldsymbol{v}^N$ are used. The result is the following iterative scheme:

$$v_i^{N+1} = -\frac{1}{a_{ii}} \sum_{k=1}^{i-1} R_{ik} v_k^{N+1} - \frac{1}{a_{ii}} \sum_{k=i}^{n} R_{ik} v_k^N + \frac{b_i}{a_{ii}}. \tag{10.6}$$

But $R_{ii} = 0$, and $R_{ij} = a_{ij}$ otherwise. Hence, Equation (10.6) can be replaced by

$$v_i^{N+1} = \frac{1}{a_{ii}} \left[b_i - \sum_{k=1}^{i-1} a_{ik} v_k^{N+1} - \sum_{k=i+1}^{n} a_{ik} v_k^N \right]. \tag{10.7}$$

Equation (10.7) is not yet optimal (however, it is already the Gauss–Seidel method for solving a linear system). Instead, we introduce an extra degree of freedom, which allows us to weight how much or how little retrospective improvement of the old guess is implemented in the $(N+1)^{\text{th}}$ iteration step. This is done by a simple modification of Equation (10.7):

$$v_i^{N+1} = (1-\omega)\, v_i^N + \frac{\omega}{a_{ii}} \left[b_i - \sum_{k=1}^{i-1} a_{ik} v_k^{N+1} - \sum_{k=i+1}^{n} a_{ik} v_k^N \right] \tag{10.8a}$$

The factor ω is restricted to the range

$$0 < \omega < 2; \tag{10.8b}$$

this preserves the diagonal-dominance of the system and hence ensures convergence. The exact choice of ω is made by trial-and-error in order to speed up convergence.

Exercise 10.1 *Modify the numerical model Poisson problem above to incorporate the SOR algorithm and vectorization. Do some tests to find out roughly what is the best value of ω to use. An answer clue is given in Figure 10.2.*

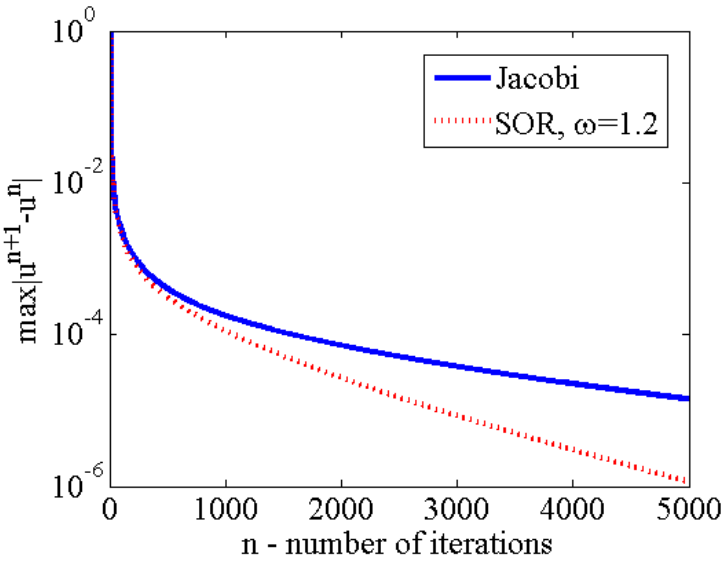


Figure 10.2: Numerical results from the Matlab code – SOR method with $\omega = 1.2$. In Matlab I found that running the SOR code takes much longer than running the Jacobi code. This is all the more reason to go over to Fortran – as in the next chapter.

Chapter 11

Introduction to Fortran

Overview

I am going to try an example-based introduction to Fortran, wherein I provide you with a sample code, and then tell you about it. I will then ask you to some tasks based on the code, and to modify it.

11.1 Preliminaries

A basic Fortran code is written in a single file with a `.f90` file extension. It consists of a **main part** together with **subroutine** definitions. A subroutine is like a subfunction in Matlab or C, with one key difference that I will explain below.

The main part

The main code is enclosed by the following declaration pair:

```
program mainprogram
...
end program mainprogram
```

At the top level, all variables that are to be used must be declared (otherwise compiler errors will ensue). Variables can be declared as integers or as double-precision numbers (other types are possible and will be discussed later on). Before variable declarations are made, a good idea is to type `implicit none`. This means that Fortran will **not** assume that symbols such as `i` have an

(implicit) type. It is best to be honest with the compiler and tell it upfront what you are going to do. Equally, it is not a good idea for the compiler to try to guess what you mean.

An array of double-precision numbers is defined as follows:

```
integer :: Nx,Ny
parameter (Nx = 201, Ny = 101)
double precision, dimension(1:Nx,1:Ny) :: my_array
```

This creates an array of double-precision numbers where the indices go from $i = 1, 2, \cdots, 201$, and $j = 1, 2, \cdots, 101$. there is nothing special in Fortran about starting arrays with $i = 1$: they can start from any integer whatsoever (positive or negative).

After defining all arrays and all other variables operations are performed on them using standard manipulations. These typically include 'do' loops (the Fortran equivalent of 'for' loops), and 'if' and 'if-else' statements. The syntax for these operations is given below in the sample code (Section 11.2).

Column-major ordering

To understand column-major ordering, consider the following array:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

If stored in contiguous memory in a column-major format, this array will take the following form in memory:

$$1\ 4\ 2\ 5\ 3\ 6.$$

Suppose that elements of the array A are denoted by A_{ij} (i for rows, j for columns). When these elements are accessed sequentially in contiguous memory, it is the row index that increases the fastest. Thus, in Fortran, a `do` loop for manipulations on the array A should be written out as follows:

```
do j=1,2
  do i=1,3
    ! manipulations on A(i,j) here
    ...
  end do
end do
```

Subroutines

Subroutines contain discrete tasks that are repeated many times. Instead of having a main code that contains multiple copies of the same piece of code, such code-tasks are relegated to subroutines. The advantages are economy-of-code and computational efficiency. Unlike in C, arrays can be passed to subroutines in a blindly straightforward manner. Examples of such subroutines can be found in the sample code (Section 11.2).

As mentioned previously, a subroutine in Fortran is like a subfunction in C or Matlab. However, there is one key difference: **formally, a subroutine produces no explicit outputs**. Thus, suppose we want to operate on a variable x with an operation f to give a result y (formally, $y = f(x)$). In Fortran, we view x and y as **inputs** to a subroutine wherein y is assigned the value $f(x)$ as part of the subroutine's implementation. This will become clearer in examples.

Output

Finally, the result of these manipulations should be sent to a file, for subsequent reading. The values in an array `my_array` of size $(1, \cdots, N_x) \times (1, \cdots N_y)$ can be written to a file as follows:

```
open(unit=20,file='myfile.dat',status='UNKNOWN')

do j=1,Ny
  do i=1,Nx
    write(20,*) my_array(i,j)
  end do
  end do
close(unit=20, status='KEEP')
```

11.2 The code

The following code solves the model Poisson problem using SOR iteration. If done correctly, it should reproduce exactly the results obtained previously in Matlab. An output file called 'oned.dat' is produced. I cannot remember why I called the output file by this name. However, these things are rather arbitrary.

```
! ************************************************************

program mainprogram
        implicit none

        integer :: Nx,Ny
        parameter (Nx = 201, Ny = 101)

        double precision :: dx,dy,x_val,y_val,Lx,Ly,pi=4.*atan(1.)
        double precision :: ax,ay,diag_val,relax,tempval,err1,err2
        double precision :: As,A_alpha
        double precision, dimension(1:Nx,1:Ny) :: s_source,u,u_old
        double precision, dimension(1:Ny) :: alpha_source

        integer :: i,j,im1,ip1,iteration,max_iteration=5000

        Ly=1.d0
        Lx=2.d0

        As=10.d0
        A_alpha=1.d0

        dx=Lx/dble(Nx-1)
        dy=Ly/dble(Ny-1)

        ax=1.d0/(dx*dx)
        ay=1.d0/(dy*dy)
        diag_val=2.d0*ax+2.d0*ay
        relax=1.5d0

! ************************************************************
! compute source, initialise guess

        s_source=0.d0
        u=0.d0
        u_old=0.d0

        write(*,*) 'getting bulk source'
```

```
39          call get_s_periodic(s_source,Nx,Ny,dx,dy,Lx,Ly,As)
40          write (*,*) 'done'
41
42          write (*,*) 'getting boundary source'
43          call get_alpha_periodic(alpha_source,Nx,Ny,dx,dy,Lx,Ly,A_alpha)
44          write (*,*) 'done'
45
46  ! ************************************************************
47  ! sor steps
48
49          do iteration=1,max_iteration
50            err1 = 0.0
51
52            ! for keeping track of the error
53            u_old=u
54
55            do j=2,Ny-1
56              do i=2,Nx-1
57
58                im1=i-1
59                ip1=i+1
60
61                tempval=ax*(u(ip1,j)+u(im1,j))+ay*(u(i,j+1)+u(i,j-1))+s_source(i,j
                      )
62                u(i,j)=(1-relax)*u(i,j)+relax*tempval/diag_val
63
64              end do
65            end do
66
67            ! Implement Dirichlet conditions
68            u(:,1)=0
69            u(:,Ny)=0
70            u(Nx,:)=0
71
72            ! Special condition at x=0.
73            do j=1,Ny
74              u(1,j)=alpha_source(j)
75            end do
76
77            if(mod(iteration,100)==0)then
78              call get_diff(u,u_old,Nx,Ny,err1)
79              write(*,*) iteration, ' Difference is ', err1
80            end If
81
82          end do
```

```
83
84          write(*,*) ' Difference is ', err1
85
86
87  ! ************************************************************
88  ! write result to file
89
90            write(*,*) 'writing to file'
91            open(unit=20,file='oned.dat',status='UNKNOWN')
92
93            do j=1,Ny
94              do i=1,Nx
95                x_val=(i-1)*dx
96                y_val=(j-1)*dy
97                Write(20,*) x_val, y_val, u(i,j)
98              end do
99            end do
100           close(unit=20, status='KEEP')
101           write(*,*) 'done'
102
103 end program mainprogram
104
105
106 ! ************************************************************
107 ! ************************************************************
108
109   subroutine get_s_periodic(s_src,Nx,Ny,dx,dy,Lx,Ly,As)
110   implicit none
111
112   integer ::i,j,Nx,Ny
113   double precision :: dx,dy,Lx,Ly,x_val,y_val,pi=4.*atan(1.)
114   double precision :: kx0,ky0,kx,ky,As
115   double precision :: s_src(1:Nx,1:Ny)
116
117   kx0=pi/Lx
118   ky0=pi/Ly
119
120   kx=kx0
121   ky=3.d0*ky0
122
123   do j=1,Ny
124     do i=1,Nx
125       x_val=(i-1)*dx
126       y_val=(j-1)*dy
127       s_src(i,j)=As*sqrt(2.d0/Lx)*sqrt(2.d0/Ly)*sin(kx*x_val)*sin(ky*y_val)
```

```
128       end do
129     end do
130
131     return
132     end subroutine get_s_periodic
133
134 ! ************************************************************
135
136     subroutine get_alpha_periodic(alpha_src,Nx,Ny,dx,dy,Lx,Ly,A_alpha)
137     implicit none
138
139     integer ::i,j,Nx,Ny,n_alpha
140     double precision :: dx,dy,Lx,Ly,x_val,y_val,pi=4.*atan(1.)
141     double precision :: A_alpha
142     double precision :: alpha_src(1:Ny)
143
144     n_alpha=1
145
146     do j=1,Ny
147         y_val=(j-1)*dy
148         alpha_src(j)=A_alpha*sin(n_alpha*pi*y_val/Ly)
149     end do
150
151     return
152     end subroutine get_alpha_periodic
153
154 ! ************************************************************
155
156     subroutine get_diff(u,u_old,Nx,Ny,diff)
157     implicit none
158
159     double precision :: diff,sum
160     integer :: Nx,Ny,i,j
161     double precision, dimension(1:Nx,1:Ny) :: u, u_old
162
163     sum = 0.0D0
164     Do j = 1, Ny
165       Do i = 1, Nx
166         sum = sum + (u(i,j)-u_old(i,j))**2
167       End Do
168     End Do
169     diff = sum
170
171     Return
172     End subroutine get_diff
```

```
173
174 !  ************************************************************
175 !  ************************************************************
```

xcodes/poisson_fortran/main_periodic_sor.f90

11.3 Porting Output into Matlab

It can be useful to examine the data in a file such as 'oned.dat' in Matlab. There are many ways of doing this. Below is my favourite way:

```
function [X,Y,C]=open_dat_file()

% We need to specify the size of the computational domain, as this can't be
% inferred from the datafile.

Nx=201;
Ny=101;

% Here I create a character array called "filename". This should
% correspond to the name of the Fortran-generated file.

filename='oned.dat';

% Here is the number of lines in the datafile.
n_lines=Nx*Ny;

% Open the file. Here, fid is a label that labels which line in the file
% is being read. Obviously, upon opening the file, we are at line 1.

fid=fopen(filename);

% Preallocate some arrays for storing the data.

X=0*(1:n_lines);
Y=0*(1:n_lines);
C=0*(1:n_lines);

% Loop over all lines.

for i=1:n_lines
    % Grab the data from the current line. Once the data is grabbed, the
    % label fix automatically moves on to the next line.
    % The data from the current line is grabbed into a string - here called
    % c1.
    c1=fgetl(fid);

    % Next I have to convert the three strings on any given line into three
    % doubles. This is done by scanning the string into an array of
    % doubles, using the "sscanf" command:
    vec_temp=sscanf(c1,'%f');
```

```
41
42      % Now it is simple: just assign each double to a value x, y, or C.
43      x_temp=vec_temp(1);
44      y_temp=vec_temp(2);
45      C_temp=vec_temp(3);
46
47      % Read the x-, y-, and C-values into their own arrays.
48      X(i)=x_temp;
49      Y(i)=y_temp;
50      C(i)=C_temp;
51  end
52
53  % Finally, reshape these arrays into physical, two-dimensional arrays.
54
55  X=reshape(X,Nx,Ny);
56  Y=reshape(Y,Nx,Ny);
57  C=reshape(C,Nx,Ny);
58
59  % Important! Close the file so that it is not left dangling.  Not closing a
60  % file properly means that in future, it will be difficult to manipulate
61  % it.  For example, it is impossible to delete or rename a a currently-open
62  % file.
63
64  fclose(fid);
65
66  end
```

xcodes/poisson_fortran/open_dat_file.m

This file should be stored in the same directory as 'oned.dat'. Then, at the command line, type

```
[X,Y,C]=open_dat_file();
```

The results can be visualized as usual:

```
[h,c]=contourf(X,Y,C);
set(c,'edgecolor','none')
```

Provided the source function and domain size are the same in both cases, this figure should agree exactly with the one generated previously using only Matlab. As before,

$$s(x, y) = A_0 \sin(k_x x) \sin(k_y y), \tag{11.1}$$

with $k_x = k_{x0}$ and $k_y = 3k_{y0}$, and $A_0 = 10$. Further details: $k_{x0} = (\pi/L_x)$ is the fundamental wavenumber in the x-direction, and $k_{y0} = \pi/L_y$ is the fundamental wavenumber in the y-direction.

The domain geometry is chosen to be $L_x = 2$ and $L_y = 1$. As expected, the solution agrees exactly

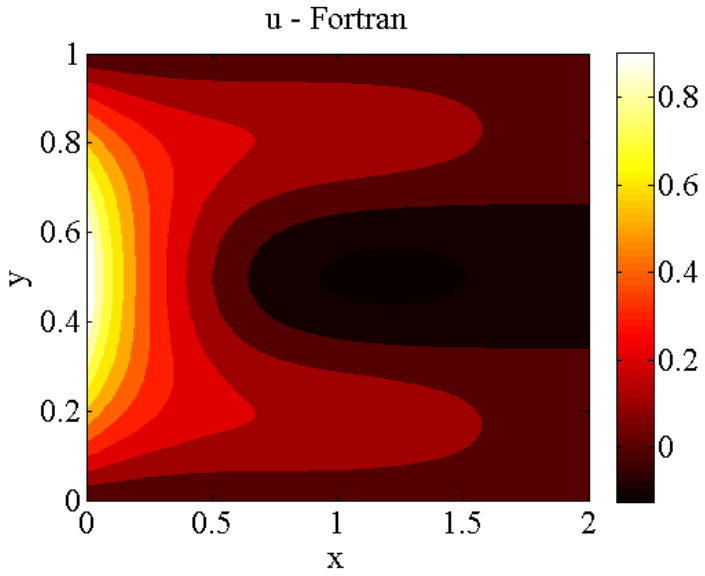


Figure 11.1: Solution of the Poisson problem for the source (11.1). Grid size: $N_x = 201$ and $N_y = 101$.

with the ones calculated previously, both analytically and using the Matlab code. However, the execution time is dramatically reduced when using the Fortran code.

11.4 The challenge problem

Consider the following PDE:

$$\nabla^2 u + s(x, y) = 0 \qquad (x, y) \in \Omega, \tag{11.2a}$$

where

$$\Omega = (0, L_x) \times (0, L_y), \tag{11.2b}$$

and $\nabla^2 = \partial_x^2 + \partial_y^2$ is the Laplacian. The partial differential equation is subject to the following **Dirichlet** boundary conditions:

$$u(x = 0, y) = \alpha(y), \tag{11.2c}$$

$$u(x, y = 0) = \beta(x), \tag{11.2d}$$

$$u(x = L_x, y) = \gamma(y), \tag{11.2e}$$

$$u(x, y = L_y) = \delta(x) \tag{11.2f}$$

Exercise 11.1 *Write a Fortran code to solve Equation* (11.2). *For definiteness, take* $s = 0$, *and*

$$u(x = 0, y) = A_\alpha \sin(\pi y / L_y), \tag{11.3a}$$

$$u(x, y = 0) = A_\beta \sin(\pi x / L_x), \tag{11.3b}$$

$$u(x = L_x, y) = A_\gamma \sin(\pi y / L_y), \tag{11.3c}$$

$$u(x, y = L_y) = A_\delta \sin(\pi x / L_x), \tag{11.3d}$$

where $A_\alpha, \cdots, A_\delta$ *are prescribed constants. Plot the result using Matlab. Also, verify that the solution satisfies the maximum principle.*

Chapter 12

Introduction to shared memory

Overview

Although a modern desktop computer will have a single CPU, they possess possess two (or more) processing units (or cores), which are placed on the same chip. The cores share some cache ('L2 cache'), while some other cache is private to each core ('L1 cache'). This enables the computer to break up a computational task into two (or more) parts, work on each task separately, via the private cache, and communicate necessary shared data via the shared cache. This architecture therefore facilitates a basic form of **parallel computing**, thereby speeding up computation times. High-level programs such as MATLAB take advantage of multiple-core computing without any direction from the user. On the other hand, lower-level programming languages such as Fortran require explicit direction from the user in order to implement multiple-core processing. The aim of this chapter is to do precisely this, usingthe OpenMP standard.

By way of notation, we reserve the word **processor** for the entire chip, which will consist of multiple sub-units called **cores**. Sometimes the cores are referred to as **threads** and this kind of computing is called **multi-threaded**.

12.1 Shared memory – concepts

A useful schematic diagram of shared memory is the following one, obtained on Wikipedia (Figure 12.1):

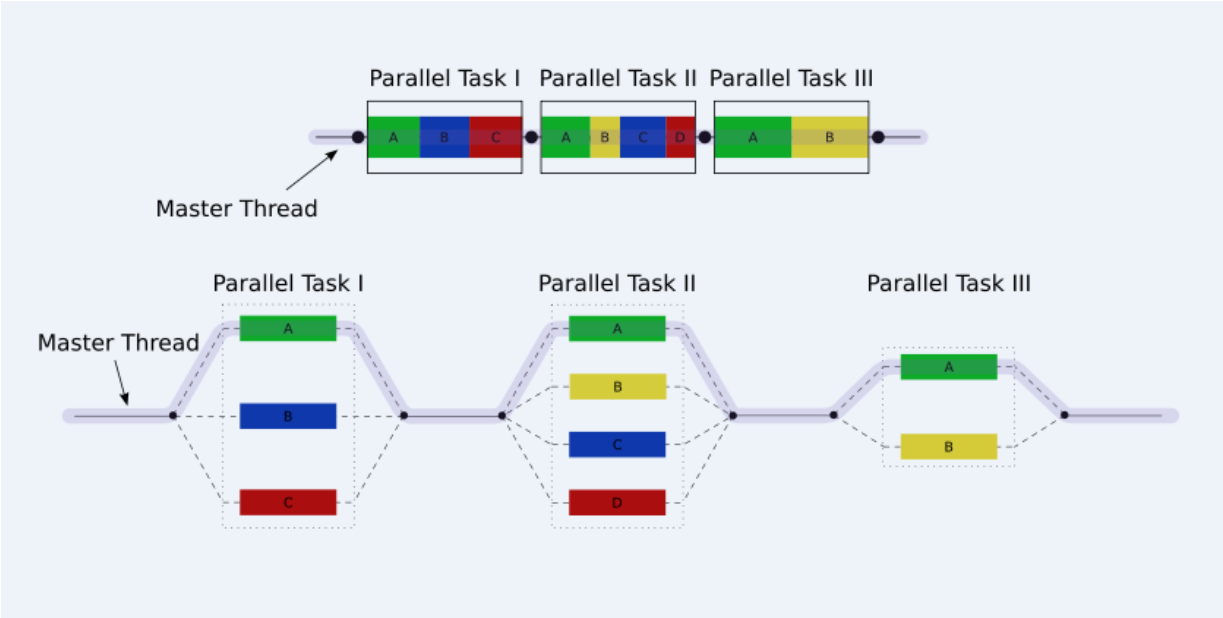


Figure 12.1: Schematic diagram of a multithreaded calculation

The idea is that a code in the absence of multithreading trivially consists of a single thread called the **master**. Then, when a particularly heavy piece of computation needs to be done (such as a large nested 'do' loop), the master breaks the task into many threads. Different parts of the calculation are done on different threads. If the calculation is non-local (also, if the amount of data operated on is small), such that on thread X, data from thread Y is required, then all such data is stored in the L2 cache, to be shared between X and Y and all other threads. On the other hand, data which is strictly local to thread X can be stored in the L1 cache of X. Finally, when all the threads have done their part of the calculation, they rejoin the master. At this end-stage, the master must have access to the necessary data in the L2 cache.

The advantage of such a concept is the existence of a set of simple directives (understandable to a Fortran compiler) to implement multi-threading. The purpose of this chapter is to explain these directives to you. However, a disadvantage of this approach is the limitation imposed by the computer architecture: we can only access as much parallelism as there are cores on the computer. A desktop will have 2 or 4 cores; some machines will have 8 or even 16 cores. Thus, a theoretical speedup of 16 is possible, but no higher. Further limitations:

- The finite bandwidth of the bus that enables communication between the memory of the individual threads (speedup limitation)
- The finite amount of global memory accessible by all the threads (jobsize limitation)

These severe architecture-dependent limitations are overcome by moving to a more sophisticalted parallelism called MPI, beyond the scope of this course.

12.2 OMP directives

To split up a Fortran 'do loop' into threads, it suffices to put a special line before and after the loop, and to decide which variables are thread-private and which variables are shared. Typically,

- Arrays that are operated on are shared.
- Intermediate variables and loop variables (`i`, `j` etc) are private.

Common programming errors:

- Not specifiying which variables are private and which are shared – can lead to catastrophic errors.
- Not initializing private variables. At thread-creation time, all private variables have no value and must be assigned some initial value explicitly in the code.

An example of the relevant OMP directives is shown here. This piece of code assigns the array `f_src` some value.

```
!$omp parallel default(shared), private(i,j,x_val,y_val)
!$omp do
  do j=1,Ny
    do i=1,Nx
      x_val=i*dx-(dx/2.d0)
      y_val=j*dy-(dy/2.d0)
      f_src(i,j)=-A0*cos(kx*x_val)*cos(ky*y_val)
    end do
  end do
!$omp end do
!$omp end parallel
```

The convention here is that all variables are shared – unless indication is given to the contrary. Thus, the private variables are only those intermediate variables that are useed in the construction of the final answer. These private variables are `x_val`, `y_yval`, `i`, and `j`.

12.3 OMP and SOR

It would appear that to do SOR with OMP, it suffices blindly to stick a few lines of code in front of the relevant 'do' loops. However, this could be dangerous, and lead to the failure of the SOR algorithm. Suppose that an array C_{ij} is being obtained by SOR iteration, such that some old value $C_{ij}^{\rm old}$ is being replaced by a new improved value $C_{ij}^{\rm new}$. Assume that for a fixed `j`, a sweep is performed, starting at `i=1`. Thus, symbolically,

$$C_{ij}^{\rm new} = f\left(C_{i-1j}^{\rm new}, C_{i+1j}^{\rm old}\right),$$

where f is some linear function that depends on the particular matrix problem being solved. Now suppose that this job has been split up into threads that share the array C via shared memory. Suppose that C_{ij} is being operated on using thread X. For some `i`, it may be the case that $C_{i-1j}^{\rm new}$ is operated on using thread $Y \neq X$. Thread X may 'race ahead' of thread Y, such that C is replaced by $C^{\rm new}$ slowly on thread Y compared to thread X. Thus, thread Y may use $C_{i-1j}^{\rm old}$ to update C_{ij}, instead of $C_{i-1j}^{\rm new}$, possibly causing the failure of the SOR method and non-convergence. This is an example of a so-called 'race condition' on OMP, and is to be avoided if possible (they can be catastrophic).

Common programming error:

Not noticing a race condition – they are common and not restricted to the SOR algorithm. They typically involve arrays whose elements are being updated with other elements from the same array.

Red-black coloring

The race condition for SOR can be overcome by implementing something called red-black coloring. This works only for problems (such as the Poisson problem) where the discretization uses only nearest neighbours (however, if neighbours other than the nearest neighbours are needed, then a scheme with more colours than just red and black will work). The SOR sweep is split into two half-steps. During the first half-step, and for fixed `j`, grid sites with even `i` are updated. During the next half-step, grid sites with odd `i` are updated.

Alternatively, for fixed `j`, grid sites with even `i` can be thought of as being 'red', while grid sites with odd `i` can be thought of as being 'black'. During the first half-sweep, red sites are updated with the old black values (consistent with the SOR algorithm), and during the second half-seep, the black sites are updated with the just-updated (new) red values.

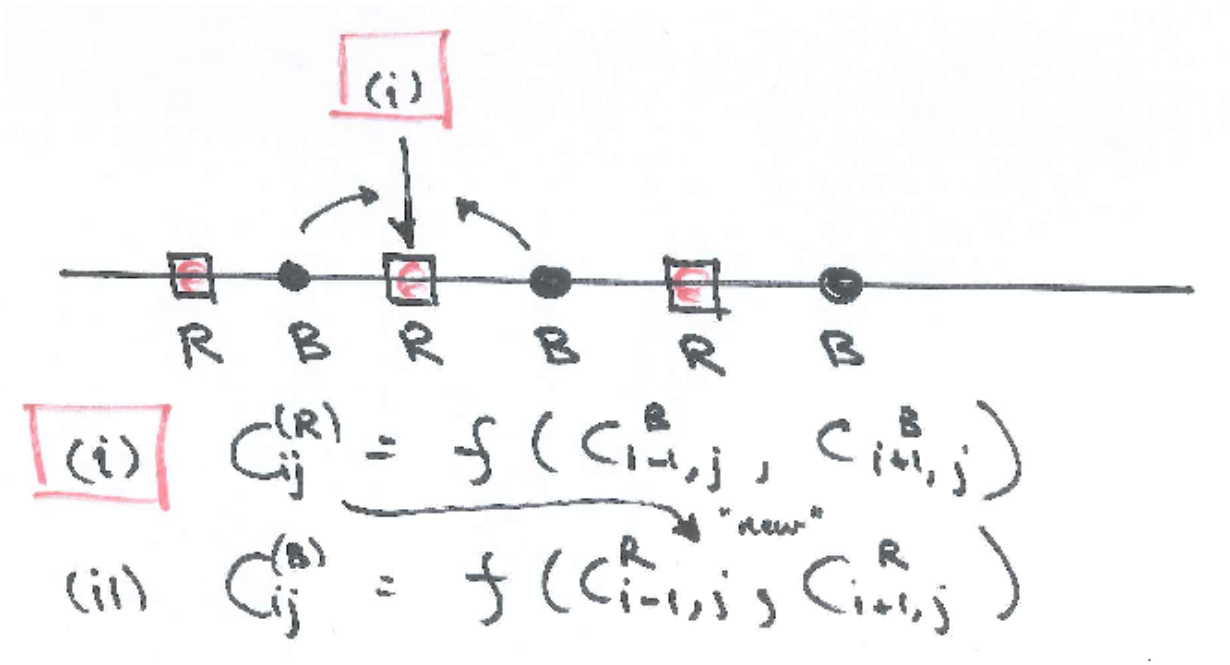


Figure 12.2: Schematic diagram of red-black coloring for the SOR algorithm

The advantage of this approach is synchronization: the second half-sweep does not begin until the first half-sweep has been completed by all threads. The first half-sweep is straightforward: red values are updated with old black values. This sweep is implemented on all threads which then join the master. Then, during the second half-sweep, the threads fork again and the black values are updated with a consistent set of (new) red values.

12.4 Other simple OMP tricks

You may have noticed by now that Fortran (in its '.f90' incarnation) supports vectorization. That is, for a square array C with

$$i = 1, 2, \cdots, n_x, \qquad j = 1, 2, \cdots, n_y, \tag{12.1}$$

the operation

```
do j=1,n_y
  do i=1,n_x
    C(i,j)=1.d0
  end do
end do
```

can be implemented equivalently as

```
  C=1.d0
```

This is still an array operation, whose speed of implementation can be increased with OpenMP. The relevant directive is called a **workshare**:

```
!$omp parallel workshare
  C=1.d0
!$omp end parallel workshare
```

Finally, there are some situations where an array needs to be populated using a very simple formula, with no need for intermediate or temporary variables. Suppose that we wanted to create an array

$$D_{ij} = \frac{1}{\Delta x^2}\left(C_{i+1,j} + C_{i-1,j} - 2C_{ij}\right) + \frac{1}{\Delta z^2}\left(C_{i,j+1} + C_{i,j-1} - 2C_{ij}\right) \tag{12.2}$$

to store a numerical approximation of the Laplacian of C, where C is a square array with the same indices as in Equation (12.1). Of course, it is not possible to compute the Laplacian at boundary points, so we do not even attempt such a thing. The operation in Equation (12.2) can be implemented using a parallel `forall` loop as follows:

```
!$omp parallel workshare
  forall (i = 2:nx-1, j=2:ny-1)
    D(i,j)=(1.d0/dx*dx)*(C(i+1,j)+C(i-1,j)-2.d0*C(i,j)) &
     +(1.d0/dy*dy)*(C(i,j-1)+C(i,j+1)-2.d0*C(i,j))
  end forall
!$omp end parallel workshare
```

Note the use of a **continuation character** to enable a line to be broken, for ease of reading.

12.5 OMP reduction

Sometimes an operation is performed on each thread, with a certain local result, and it is necessary to combine all such local results back into the master thread. Examples of this kind include sums and maxima. For example, suppose that an array C is split up between threads, such that thread i operates only on a chunk of the array, say $C^{(i)}$. Then, suppose that on thread i, the following sum is computed

$$s_i = \sum_{pq} C^{(i)}_{pq}.$$

It might become necessary during the course of an assignment to compute

$$s = \sum_i s_i, \qquad \text{sum over all threads.}$$

This is an example of an OMP **reduction**. The syntax for this operation is given in the following example.

```
  subroutine get_diff(u,u_old,maxl,maxn,diff)
  implicit none

  double precision :: diff,sum
  integer :: maxl,maxn,i,j,tid
  double precision, dimension(0:maxl,0:maxn) :: u, u_old

  sum = 0.0D0
!$omp parallel do default(shared), &
!$omp   private(i,j),  &
!$omp   reduction(+:sum)

  Do j = 1, maxn
    Do i = 1, maxl
      sum = sum + (u(i,j)-u_old(i,j))**2
    End Do
  End Do
!$omp end parallel do
  diff = sum

  Return
  End subroutine get_diff
```

Common programming errors:

Reduction can only be done on shared variables.

Chapter 13

Multithreading for the model Poisson equation

Overview

We solve the model Poisson problem numerically using OpenMP. We test the code's parallel efficiency.

13.1 The code for the model Poisson problem

```
! ************************************************************

program mainprogram
        implicit none

        integer :: Nx,Ny
        parameter (Nx = 201, Ny = 101)

        double precision :: dx,dy,x_val,y_val,Lx,Ly,pi=4.*atan(1.)
        double precision :: ax,ay,diag_val,relax,tempval,err1,err2
        double precision :: As,A_alpha
        double precision, dimension(1:Nx,1:Ny) :: s_source,u,u_old
        double precision, dimension(1:Ny) :: alpha_source

        integer :: i,j,im1,ip1,iteration,max_iteration=5000

        integer :: tid,numthreads,OMP_GET_THREAD_NUM,OMP_GET_NUM_THREADS

        Ly=1.d0
```

```
20          Lx=2.d0
21
22          As=10.d0
23          A_alpha=1.d0
24
25          dx=Lx/dble(Nx-1)
26          dy=Ly/dble(Ny-1)
27
28          ax=1.d0/(dx*dx)
29          ay=1.d0/(dy*dy)
30          diag_val=2.d0*ax+2.d0*ay
31          relax=1.5d0
32
33  ! ************************************************************
34  ! Verify that OMP is working
35
36  !$omp parallel
37          numthreads=OMP_GET_NUM_THREADS()
38  !$omp end parallel
39
40          write(*,*) 'number of threads=',numthreads
41
42  !$omp parallel default(shared), private(tid)
43          tid=OMP_GET_THREAD_NUM()
44          write(*,*) 'hello from thread number ',tid
45  !$omp end parallel
46
47  ! ************************************************************
48  ! compute source, initialise guess
49
50          s_source=0.d0
51          u=0.d0
52          u_old=0.d0
53
54          write (*,*) 'getting bulk source'
55          call get_s_periodic(s_source,Nx,Ny,dx,dy,Lx,Ly,As)
56          write (*,*) 'done'
57
58          write (*,*) 'getting boundary source'
59          call get_alpha_periodic(alpha_source,Nx,Ny,dx,dy,Lx,Ly,A_alpha)
60          write (*,*) 'done'
61
62  ! ************************************************************
63  ! sor steps
64
```

```
65          do iteration=1,max_iteration
66            err1 = 0.0
67
68            ! for keeping track of the error
69 !$omp parallel workshare
70            u_old=u
71 !$omp end parallel workshare
72
73            ! First sweep
74            call do_sor_u(u,s_source,dx,dy,Nx,Ny,0)
75            ! Second sweep
76            call do_sor_u(u,s_source,dx,dy,Nx,Ny,1)
77
78            ! Implement Dirichlet conditions
79            u(:,1)=0
80            u(:,Ny)=0
81            u(Nx,:)=0
82
83            ! Special condition at x=0.
84            do j=1,Ny
85              u(1,j)=alpha_source(j)
86            end do
87
88            if(mod(iteration,100)==0)then
89              call get_diff(u,u_old,Nx,Ny,err1)
90              write(*,*) iteration, ' Difference is ', err1
91            end If
92
93          end do
94
95          write(*,*) ' Difference is ', err1
96
97
98 ! ************************************************************
99 ! write result to file
100
101           write(*,*) 'writing to file'
102           open(unit=20,file='oned.dat',status='UNKNOWN')
103
104           do j=1,Ny
105             do i=1,Nx
106               x_val=(i-1)*dx
107               y_val=(j-1)*dy
108               Write(20,*) x_val, y_val, u(i,j)
109             end do
```

```
110           end do
111           close(unit=20, status='KEEP')
112           write(*,*) 'done'
113
114 end program mainprogram
115
116
117 ! ************************************************************
118 ! ************************************************************
119
120   subroutine get_s_periodic(s_src,Nx,Ny,dx,dy,Lx,Ly,As)
121   implicit none
122
123   integer ::i,j,Nx,Ny
124   double precision :: dx,dy,Lx,Ly,x_val,y_val,pi=4.*atan(1.)
125   double precision :: kx0,ky0,kx,ky,As
126   double precision :: s_src(1:Nx,1:Ny)
127
128   kx0=pi/Lx
129   ky0=pi/Ly
130
131   kx=kx0
132   ky=3.d0*ky0
133
134   do j=1,Ny
135     do i=1,Nx
136       x_val=(i-1)*dx
137       y_val=(j-1)*dy
138       s_src(i,j)=As*sqrt(2.d0/Lx)*sqrt(2.d0/Ly)*sin(kx*x_val)*sin(ky*y_val)
139     end do
140   end do
141
142   return
143   end subroutine get_s_periodic
144
145 ! ************************************************************
146
147   subroutine get_alpha_periodic(alpha_src,Nx,Ny,dx,dy,Lx,Ly,A_alpha)
148   implicit none
149
150   integer ::i,j,Nx,Ny,n_alpha
151   double precision :: dx,dy,Lx,Ly,x_val,y_val,pi=4.*atan(1.)
152   double precision :: A_alpha
153   double precision :: alpha_src(1:Ny)
154
```

```
155   n_alpha=1
156
157   do j=1,Ny
158        y_val=(j-1)*dy
159        alpha_src(j)=A_alpha*sin(n_alpha*pi*y_val/Ly)
160   end do
161
162   return
163   end subroutine get_alpha_periodic
164
165 ! ************************************************************
166
167   subroutine get_diff(u,u_old,Nx,Ny,diff)
168   implicit none
169
170   double precision :: diff,sum
171   integer :: Nx,Ny,i,j
172   double precision, dimension(1:Nx,1:Ny) :: u, u_old
173
174   sum = 0.0D0
175 !$omp parallel do default(shared), &
176 !$omp    private(i,j), &
177 !$omp    reduction(+:sum)
178   Do j = 1, Ny
179     Do i = 1, Nx
180       sum = sum + (u(i,j)-u_old(i,j))**2
181     End Do
182   End Do
183 !$omp end parallel do
184   diff = sum
185
186   Return
187   End subroutine get_diff
188
189 ! ************************************************************
190 ! ************************************************************
191
192        subroutine do_sor_u(u,s_source,dx,dy,Nx,Ny,flag)
193         implicit none
194
195         integer ::i,j,ip1,im1,Nx,Ny,flag
196         double precision :: dx,dy,ax,ay
197         double precision :: s_source(1:Nx,1:Ny),u(1:Nx,1:Ny)
198
199         double precision :: relax,diag_val,tempval
```

```
200
201         ax=1.d0/(dx*dx)
202         ay=1.d0/(dy*dy)
203         diag_val=2.d0*ax+2.d0*ay
204         relax=1.5d0
205
206 !$omp parallel default(shared), private(i,j,im1,ip1,tempval)
207 !$omp do
208         do j=2,Ny-1
209           do i=mod(j+flag,2)+2,Nx-1,2
210
211             im1=i-1
212             ip1=i+1
213
214             tempval=ax*(u(ip1,j)+u(im1,j))+ay*(u(i,j+1)+u(i,j-1))+s_source(i,j)
215             u(i,j)=(1-relax)*u(i,j)+relax*tempval/diag_val
216
217             end do
218           end do
219 !$omp end do
220 !$omp end parallel
221
222         end subroutine do_sor_u
```

xcodes/poisson_fortran/main_periodic_omp.f90

13.2 Execution

On a local machine, compilation is done as follows:

```
gfortran main_periodic_omp.f90 -o poisson.x -fopenmp
```

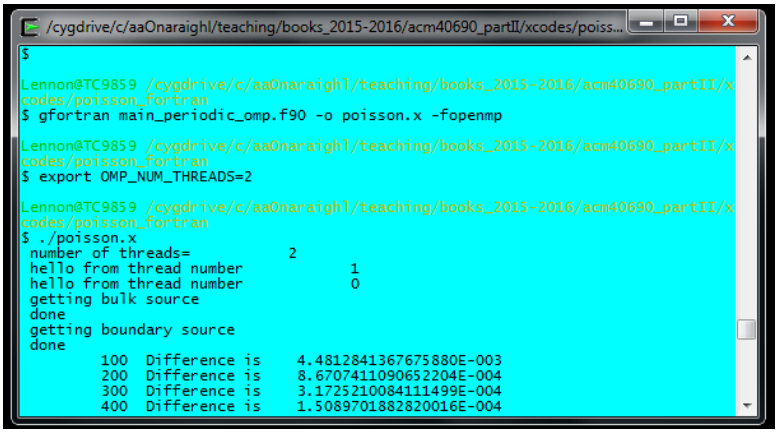
An **environment variable** then needs to be set, as the computer needs to know how many threads to use. This is done as follows:

```
export OMP_NUM_THREADS=2
```

The code is then executed in the usual way, e.g.

```
./poisson.x
```

A nice thing about the code I have written (hehe) is that some diagnostic messages are printed to the standard output at runtime to check that the stated number of threads really is being used. This can be seen here:



In this way we are sure that the code is running on two threads.

13.3 OMP reduction – revsited

Recall in Chapter 12 we examined a method to reduce a sum over all threads. It is instructive to consider an alternative method for doing the OMP reduction in the subroutine get_diff:

```
        subroutine get_diff(C,C_old,Nx,Ny,diff_val)
        implicit none

        integer :: Nx,Ny,i,j
        double precision, dimension(1:Nx,1:Ny) :: C, C_old

        integer :: large,tid,numthreads,OMP_GET_THREAD_NUM,OMP_GET_NUM_THREADS
        parameter (large=100)
        double precision :: diff_vec(0:large),diff_val

!$omp parallel
        numthreads = OMP_GET_NUM_THREADS()
!$omp end parallel

!$omp parallel default(shared), private(i,j,tid,diff_val)
        tid=OMP_GET_THREAD_NUM()
        diff_val=0.d0
!$omp do
        Do j = 1, Ny
          Do i = 1, Nx
            diff_val = diff_val + (C(i,j)-C_old(i,j))**2
          End Do
        End Do
!$omp end do
        diff_vec(tid)=diff_val
        write(*,*) 'tid= ',tid,'diff= ',diff_val, 'num threads= ',numthreads
!$omp end parallel

        diff_val=0.d0
        do tid=0,numthreads-1
          diff_val=diff_val+diff_vec(tid)
        end do
```

```
Return
End subroutine get_diff
```

This subroutine makes use of some new OMP directives – and `OMP_GET_NUM_THREADS`, and `OMP_GET_THREAD_NUM`:

- When called in a parallel region,`OMP_GET_NUM_THREADS` returns an integer N, the number of threads available. It must be called in a parallel region – otherwise the answer returned will be 1.
- When called in a parallel region, `OMP_GET_THREAD_NUM` returns an integer i that labels the current thread, with $i = 0, \cdots, N-1$.

Exercise 13.1 *Implement both kinds of reduction for the model Poisson problem and compare the residuals. Comment on the result.*

Exercise 13.2 *Write a Fortran code from scratch that computes*

$$p(N) = \sum_{n=1}^{N} \frac{1}{n^2}.$$

Parallelize the code using OpenMP, in particular an OMP reduction for the summation.

Now, suppose however that the maximum over all rows and columns of the residual array is required. Here, a similar operation can be performed to obtain the maximum over all threads – either by explicit computation, or by OMP reduction. Notionally, the reduction takes place as follows. Suppose we have an array C, split up between threads, such that thread i operates only on a chunk of the array, say $C^{(i)}$. Then, suppose that on thread i, the following maximum is computed

$$m_i = \max_{pq} |C^{(i)}_{pq}|.$$

Suppose now we are interested in computing

$$m = \max(m_1, m_2, \cdots), \qquad \text{maximum over all threads.}$$

The syntax for this is as follows:

```
  subroutine get_diff(u,u_old,maxl,maxn,diff)
  implicit none

  double precision :: diff,max_val,temp_val
  integer :: maxl,maxn,i,j
  double precision, dimension(0:maxl,0:maxn) :: u, u_old

  max_val=0.d0
!$omp parallel do default(shared), &
!$omp   private(i,j,temp_val), &
!$omp   reduction(max:max_val)

  Do j = 1, maxn
    Do i = 1, maxl
      temp_val=abs(u(i,j)-u_old(i,j))
      if( temp_val .gt. max_val) then
        max_val=temp_val
      end if
    End Do
  End Do
!$omp end parallel do
  diff = max_val

  Return
  End subroutine get_diff
```

13.4 Tasks – timing

OpenMP provides built-in functions to time the execution of a parallel code. In the main code, when variables are declared, one declares three further variables:

```
real(8) :: start_time, end_time, OMP_get_wtime
```

Consider now a given parallel task that is to be performed. Before execution, one measures the wall time:

```
start_time=OMP_get_wtime()
```

Number of threads	Time in seconds
16	3.0292
8	0.8109
4	1.2498
2	1.9827
1	2.7388

Table 13.1: Execution times for the SOR iteration (model Poisson problem)

Then, the parallel segment of code is run and the wall time is measured again:

```
end_time=OMP_get_wtime()
```

The total execution time is the difference of these two snapshots:

```
write(*,*) ' Walltime is ', end_time-start_time
```

I timed the execution of the SOR code on a 201×201 grid, with 1,000 SOR iterations and tabulated the results (Table 13.1). I also plotted the same information in Figure 13.1. The results are okay

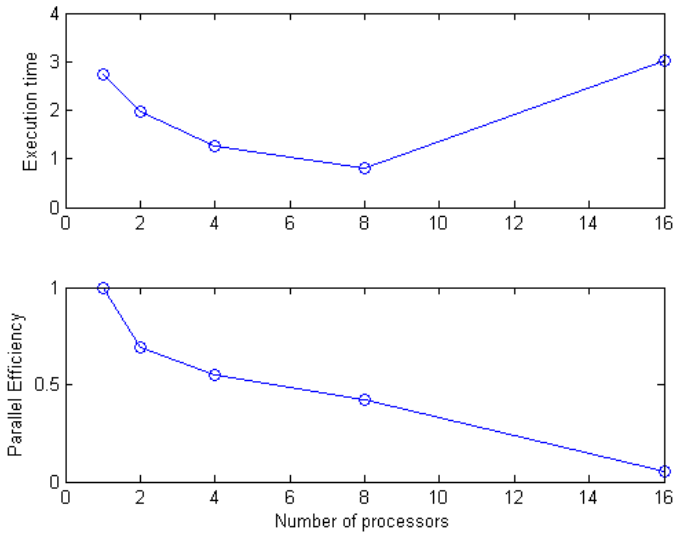


Figure 13.1: Execution times for the SOR iteration (model Poisson problem)

but not brilliant:

- For $N = 1, 2, 4, 8$ the execution time decreases with the increase in thread count. This is good! Our code is running faster because of the multi-threading.
- However, as N increases the gains of the multi-threading become less and less. Indeed, at $N = 16$ something disastrous happens, and the parallel code takes longer to run than the serial code. The reasons for this can be manifold. A possibility is the existence of **communication**

overheads – threads need to share data, not all of which may be in the cache. When threads spend time sharing data, it is wasted time, in other words, time that should be better spent doing the actual calculation. Therefore, we say that our code **scales** out to 8 threads, and we speak of our code's **scalability**.

- The parallel efficiency is defined to be

$$E_N = \frac{T_N}{NT_1},$$

where N is the number of threads, T_N is the time required to run on N threads and T_1 is the time required to run on a single thread. The fall-off in the parallel efficiency as N increases provides evidence that the gains obtained from the multi-threading diminish at higher thread-counts. At $N = 16$ the parallel efficiency is only 6%!

Chapter 14

Memory allocation in Fortran

Overview

We discuss dynamic memory allocation, particularly suitable for large arrays. We extend the model Poisson problem to three dimensions and solve it numerically.

14.1 Dynamic versus static; heap versus stack

So far in Fortran we have declared variables to be of a definite type, for example, integers, doubles, and characters. Additionally, we have created arrays of doubles, where these arrays are of a **fixed size**. The syntax for the array allocation is really quite definite and hints at the immutability of arrays so created:

```
integer :: Nx,Ny
parameter (Nx = 201, Ny = 101)
double precision, dimension(1:Nx,1:Ny) :: C
```

Here, the array C gets a fixed size that cannot be altered. We say that the array C is **static**. Because the amount of memory necessary for the creation of this array is known precisely, the array C can be placed in that highly-structured part of memory known as the **stack**. In contrast, there are situations where static arrays are not desirable:

- If the size of the array C needs to change in the course of a calculation;
- If the size of the array C is simply too large to fit in the stack.

In these situations, it is better to allocate the array C **dynamically**, on the **heap**. The syntax for the dynamic allocation of the array C is shown here:

```
        integer :: Nx,Ny
        parameter (Nx = 201, Ny = 201, Nz=101)
        double precision, allocatable, dimension(:,:) :: C
        ...
        ...

! ************************************************************
! Allocate variables

        allocate(C(1:Nx,1:Ny))
        C=0.d0

! ************************************************************
```

When the array C is no longer needed it needs to be **deallocated**, thereby freeing up space in memory:

```
        deallocate(C)
```

Typically, this is done at the end of the main code, but this is not necessarily the case.

Performance issues

Memory allocation and deallocation is expensive. Allocation on the heap is typically avoided. In particular, dynamic memory allocation in subroutines is a bad idea, because such subroutines tend to be called repeatedly. In a worst-case scenario, one would have a dynamically-allocated array in a subroutine that is called many times, thereby creating successive calls to allocate and free up memory, over and over again. For this reason, dynamic memory allocation tends only to be used in the main part of the code, and the allocation is done on a once-off basis.

Good Programming Practice:

When dealing with large arrays that are passed to subroutines, my practice is to allocate the array dynamically in the main code, and then to allocate copies of the array statically in any subroutines. Then, if I get a segmentation fault due to an excessively large request for memory that does not exist, I can copy the chunk of code for dynamic array allocation into the subroutine.

Of course, having dynamic array allocation in a subroutine that is called repeatedly should be viewed as a last resort.

Chapter 15

Handling data in large files

Overview

We introduce a model Poisson problem in three dimensions and solve it numerically. This gives rise to some very large files. Therefore, we examine new Matlab postprocessing tools to examine such large three-dimensional files. We look at string manipulation to postprocess files in which the data is not structured into neat, ordered columns.

15.1 Example

Consider the following model problem:

$$\nabla^2 C = f(x, y, z), \qquad (x, y, z) \in \Omega \tag{15.1a}$$

where $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$, subject to the following boundary conditions:

- Periodic boundary conditions in the x- and y-directions:

$$C(0, y, z) = C(L_x, y, z), \qquad C(x, 0, z) = C(x, L_x, z), \tag{15.1b}$$

- Neumann boundary conditions in the z-direction:

$$\frac{\partial C}{\partial z} = 0, \qquad \text{on } z = 0 \text{ and } z = L_z. \tag{15.1c}$$

A model multi-threaded code is provided which solves this problem – see `poisson_sor1.f90`.

Exercise 15.1 *Compile and run the model three-dimensional code and benchmark its performance under OMP parallelism.*

Consider the code `poisson_sor1.f90` from Chapter 14, and the resulting output files:

- `poisson.dat`
- `poisson_slice.dat`

The file `poisson_slice.dat` contains a slice of the three-dimensional array $C(x, y, z)$, at $y = L_y/2$, and can be viewed using the two-dimensional Matlab postprocessing tools we have constructed before. As well as viewing this file and plotting the result, it is also instructive to take a look at the data file itself. The first 10 lines of the file can be viewed in Linux by typing

```
head -10 poisson_slice.dat
```

I get this:

```
>> bash-3.2$ head -10 poisson_slice.dat
  0.000000000000000E+000  0.000000000000000E+000  4.668321307964320E-003
  1.000000000000000E-002  0.000000000000000E+000  4.666004491564717E-003
  2.000000000000000E-002  0.000000000000000E+000  4.659109419590812E-003
  3.000000000000000E-002  0.000000000000000E+000  4.647589883399717E-003
  4.000000000000000E-002  0.000000000000000E+000  4.631510159553213E-003
  5.000000000000000E-002  0.000000000000000E+000  4.610833365189051E-003
  6.000000000000000E-002  0.000000000000000E+000  4.585632448160086E-003
  7.000000000000001E-002  0.000000000000000E+000  4.555879996932404E-003
  8.000000000000000E-002  0.000000000000000E+000  4.521657342747652E-003
  9.000000000000000E-002  0.000000000000000E+000  4.482946653571969E-003
```

Obviously, there are three columns containing the various values of X, Y, and C, which are then read into a Matlab file and reshaped into square arrays.

Good programming practice:

Never try opening a large file in its entirety - you will run out of memory and crash your computer. Instead, use tools like 'head', 'tail', 'more', and 'grep' to extract or view relevant information.

Next, we should try to write a Matlab postprocessing program to do the same thing for the full three-dimensional data file. However, before we try anything, we should not assume *a priori* that the data is ordered into columns (why should we?). Long ago, after running the program (I forget where), I typed

```
head -10 poisson.dat
```

and got

```
>> bash-3.2$ head -10 poisson.dat
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 -5.252804656865423E-002
  1.000000000000000E-002  0.000000000000000E+000  0.000000000000000E+000
 -5.250215979901304E-002
  2.000000000000000E-002  0.000000000000000E+000  0.000000000000000E+000
 -5.242439421169698E-002
  3.000000000000000E-002  0.000000000000000E+000  0.000000000000000E+000
 -5.229495753177844E-002
  4.000000000000000E-002  0.000000000000000E+000  0.000000000000000E+000
 -5.211384677229017E-002
```

This is a bit of a disaster: there are of course four columns containing the various values of X, Y, Z, and C, but here C has been pushed on to a second line! In short, in printing to files, unpredictable things can happen, and our Matlab file-reading tools need to be able to take account of these things. I wrote a Matlab file to take account of this line-jumping:

```
function [X,Y,Z,C]=open_single_dat_file_3d()

Nx=201;
Ny=201;
Nz=101;

n_lines=Nx*Ny*Nz;

filename='poisson.dat';
fid=fopen(filename);

X=0*(1:n_lines);
Y=0*(1:n_lines);
Z=0*(1:n_lines);
C=0*(1:n_lines);

```

```
for i=1:n_lines
    c1=fgetl(fid);
    vec_temp=sscanf(c1,'%f');
    x_temp=vec_temp(1);
    y_temp=vec_temp(2);
    z_temp=vec_temp(3);

    X(i)=x_temp;
    Y(i)=y_temp;
    Z(i)=z_temp;

    c1=fgetl(fid);
    vec_temp=sscanf(c1,'%f');
    c_temp=vec_temp(1);

    C(i)=c_temp;

    if(mod(i,100000)==0)
        frac=100*(i/n_lines);
        display(strcat(num2str(frac),'% done'))
    end

end

X=reshape(X,Nx,Ny,Nz);
Y=reshape(Y,Nx,Ny,Nz);
Z=reshape(Z,Nx,Ny,Nz);
C=reshape(C,Nx,Ny,Nz);

fclose(fid);

end
```

xcodes/poisson_threed/open_single_dat_file_3d.m

It is a simple extension to what has been done before, and exploits the fact that variable `fid` labels the current line in the open file, and that upon reading a line, the variable is incremented by one so as to label the next line. On the other hand, if your use of 'head' shows no line-jumping, it is easier (and dramatically faster) do to the following:

```
function [X,Y,Z,C]=open_single_dat_file_3d_no_line_jumping()

Nx=201;
Ny=201;
Nz=101;
```

```
6
7  filename='poisson.dat';
8
9 M=importdata(filename);
10
11 X=M(:,1);
12 Y=M(:,2);
13 Z=M(:,3);
14 C=M(:,4);
15
16 X=reshape(X,Nx,Ny,Nz);
17 Y=reshape(Y,Nx,Ny,Nz);
18 Z=reshape(Z,Nx,Ny,Nz);
19 C=reshape(C,Nx,Ny,Nz);
20
21 end
```

xcodes/poisson_threed/open_single_dat_file_3d_no_line_jumping.m

Having read the data file into Matlab (regardless of which way was used in the end), the challenge is to view it in three dimensions. There is a useful **isosurface** feature in Matlab, which will plot a **level surface** of a three-dimensional function $C(x, y, z)$. Recall, that

$$C(x, y, z) = \text{Const.}$$

is a two-dimensional manifold surface embedded in $\mathbb{R}^3$, and can therefore be plotted. This is precisely the definition of a level surface. A analogue in $\mathbb{R}^2$ is a level line, or, in other words, a contour. There is a tremendous amount of machinery that comes with the isosurface function in Matlab, including how the surface is 'lit', and from what angle it is viewed. The best way to learn about this is to experiment, and use the 'help' pages. As a starting point for this experimentation, one can use the following code which genreates a level surface from the following **four** three-dimensional arrays: (X, Y, Z, C):

```
1  function []=make_iso(X,Y,Z,C,val)
2
3  fv=isosurface(X,Y,Z,C,val);
4
5  h=figure;
6  p=patch(fv);
7  set(p,'FaceColor','red','Edgecolor','none')
8  axis equal
9  view(30,30)
10 axis tight
11 camlight('headlight')
```

```
set(h,'Renderer','zbuffer');
lighting phong
grid on
set(gca,'fontsize',18,'fontname','times new roman')
xlabel('x')
ylabel('y')
zlabel('z')
drawnow

figfilename=strcat('isosurface_val','.fig');
saveas(h,figfilename)

end
```

xcodes/poisson_threed/make_iso.m

Here, 'val' is the level at which the isosurface is to be made. A sample result is shown in Figure 15.1

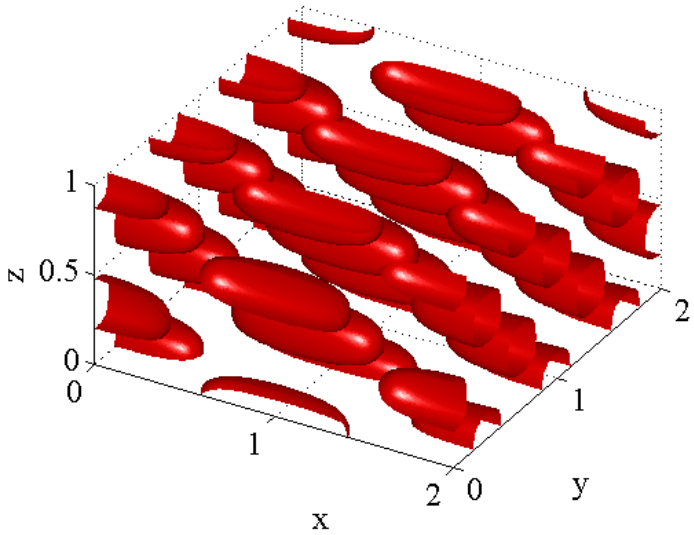


Figure 15.1: Isosurface for the Poisson problem, with $C = 0.015$.

15.2 Challenge problem

Consider the following two files that can be downloaded from the website:

- File A: '3dchannel_ 7000.dat'
- File B: '3dchannel_ 65000.dat'

These files contain outputs from numerical simulations at different points in time. The simulations are from a two-phase Navier–Stokes solver. Ideally, the data should be structured into eight columns: $[X, Y, Z, U, V, W, P, \Phi]$, where X, Y, and Z are coordinates, U, V, and W are velocities, P is a pressure, and Φ is the so-called level-set function, which tracks which phase is which: with $\Phi < 0$ in the more viscous phase of the simulation, and $\Phi > 0$ in the less viscous phase. The numerical grid is of size $304 \times 152 \times 152$, and the files contain two header lines.

Exercise 15.2 *Use appropriate Linux tools to characterize the structure of the data in these files.*

In addition, the number of lines in each file can be estimated as follows:

```
wc -l filename
```

This should be equal to $304 \times 152 \times 152 +$ Number of header lines.

Now, as it turns out, in file A, the data have been output in a straightforward way, in strict column form.

Exercise 15.3 *Write a Matlab code to extract the data from file A, and to generate an isosurface plot, at* $\Phi = 0$.

Hints:

- For this assignment, it is a good idea to create two Matlab functions for the two sub-tasks that appear here. In this way, should the isosurface task fail, you will still have available data from the file-reading part of the task. This means that when you start over writing the isosurface task, you will be starting from a relatively advanced point. This will save a lot of time, given the intensity of the data-reading task to be performed.
- Also, here is a snippet of a 'good' isosurface plot command for this problem:

```
fv = isosurface(X,Y,Z,Phi,0);
    p=patch(fv);
    set(p,'FaceColor','red','Edgecolor','none')
    axis equal
    view(30,30)
```

```
axis tight
zlim([0.1,0.5])
camlight('headlight')
set(h,'Renderer','zbuffer');
lighting phong
```

Now, as it turns out, in file B, the data have been printed to the file in a truly bizarre way (which nevertheless saves some space; file B is smaller than file A):

1. For each gridpoint, the variables $[X, Y, Z, U, V, W, P, \Phi]$ extend over two lines in the output file.
2. Each piece of information is separated by a comma (not a space or a tab).
3. For each gridpoint, if a variable appears twice, it is stored only once. Thus, if at a certain gridpoint, $X = Y$, then instead of printing $[X, Y, Z, U, V, W, P, \Phi]$, $[2 * X, Z, U, V, W, P, \Phi]$ is printed instead.
4. Similarly, if $X = Y = Z$, then $[X, Y, Z, U, V, W, P, \Phi]$ is not printed; instead, $[3*x, U, V, W, P, \Phi]$ is printed.

Obviously, one could at runtime specify explicitly and strictly how the I/O is to be performed. However, I realised after the fact what had taken place, and it is wasteful to perform these large-scale simulations more than once, only to recreate the results a second time in a slightly-different output format. Thus, it is necessary to write a Matlab script to account for all of these variations, and to gather the results into large three-dimensional arrays for isosurface plotting.

Exercise 15.4 *Write a Matlab code to extract the data from file B, and to generate an isosurface plot, at* $\Phi = 0$.

Hint: before doing so investigate the following built-in Matlab commands:

- `fgetl`
- `strrep` – for replacing characters in a string by new characters
- `strcat` – for joining two strings together
- `sscanf` – for reading strings into arrays of a specfied type

The result will be a beautiful picture like Figure 15.2.

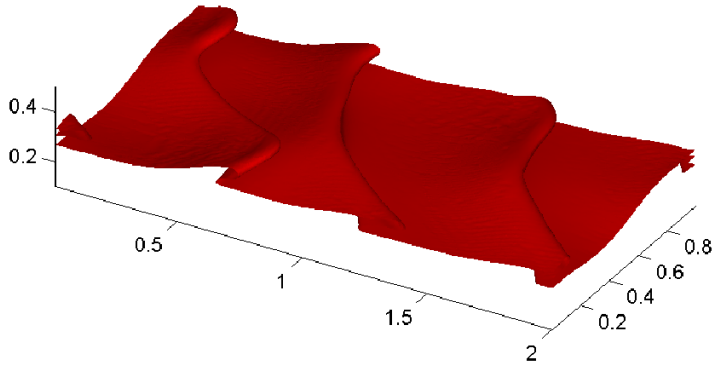


Figure 15.2: Isosurface plot at $\Phi = 0$, for file B