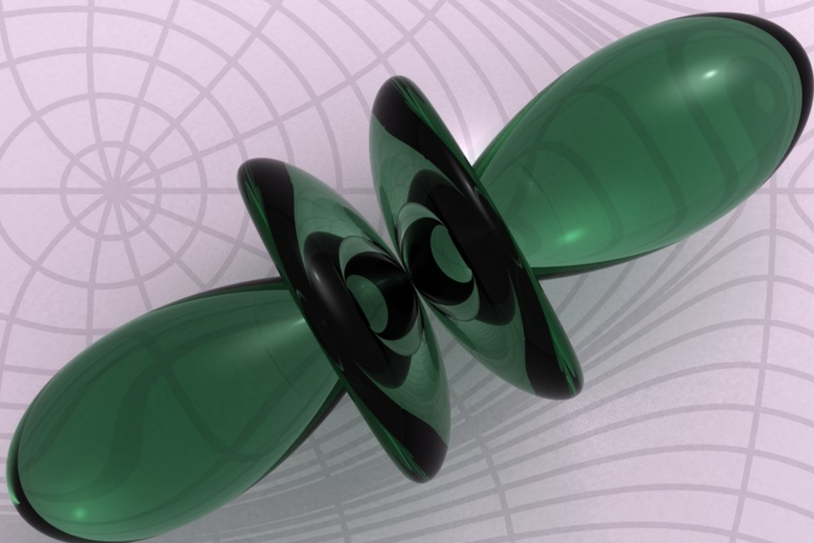
Special Functions of Mathematical Physics



Kyle A. Novak
with Laura J. Fox

Special Functions of Mathematical Physics

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A Tourist's Guidebook

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with LAURA J. FOX

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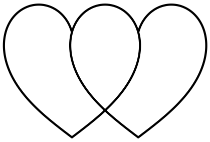
Cover illustration: The spherical harmonic function $F_3^0(\theta, \phi)$ and the equipotentials of the gamma function in the complex plane.

Disclaimer: This book is a work in progress and will be progressively updated. Great efforts have been made to correct typographical and formatting errors. Nonetheless, several errors undoubtedly still lurk within these pages.

Dedicated to my mindblowingly awesome wife

$$\left(\frac{t}{\pi} - \frac{\sin 2t}{1 + \sin^2 t}, \frac{|2\cos t|}{1 + \sin^2 t}\right)$$



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Preface

Strum a guitar. Bang a drum. The sound of one is produced by a series of sine functions and the other a series of Bessel functions. While every scientist and engineer knows the sine function, not as many are familiar with Bessel functions or the broader class of special functions, even though they frequently arise in mathematical physics. A special function is any functions that cannot be represented by combining algebraic functions (polynomials or roots) or elementary transcendental functions (trigonometric functions, exponential functions, and their inverse). They often arise as ways to describe solutions to partial differential equations like Schrödinger, Laplace, Poisson, and Helmholtz equations. In an era when solutions are often numerical, special functions matter because they can be used to validate numerical solutions. More importantly special functions help us better understand the nature of different problems.

This book is an adaptation of lecture notes that I developed for the course "Differential Equations of Mathematical Physics" taught in the Department of Mathematics and Statistics at the Air Force Institute of Technology. The goal of the course was to provide physics and engineering graduate students with the precepts of special functions and a toolbox for working with them. The purpose of the lecture notes was to both guide discussion and provide students a bridge to more rigorous but also more mathematically dense textbooks and resources. The reader of this book should have a good grasp of calculus and differential equations. Some basic understanding of analysis and linear algebra would be helpful.

The book begins with a peek at complex analysis. Real-valued functions are mere slivers of their complex-valued counterparts, and it is helpful to to have know some complex analysis in order to better understand why functions behave the way they do. This chapter provides a foundation for the rest of the book. Because many special functions arise from solutions to differential equations, we will examines the Method of Frobenius as a technique for finding the series solution to second-order linear differential equations. Sturm–Liouville theory and Sturm–Liouville operators provide a theoretical framework for a wide variety of equations that arise in mathematical physics. The solution to these equations in cylindrical and spherical coordinate systems are conveniently expressed using orthogonal polynomials.

We will study the Bessel function in detail, developing different representations and limiting approximations. We also study orthogonal polynomials that frequently arise in mathematical physics such as the Legendre, Hermite, Laguerre, and Chebyshev polynomials. Along the way, Laura will serve as our mathematical tour guide, highlighting important ideas and taking us on a few mathematical detours.

KYLE A. NOVAK
Washington, D.C.
December 2018

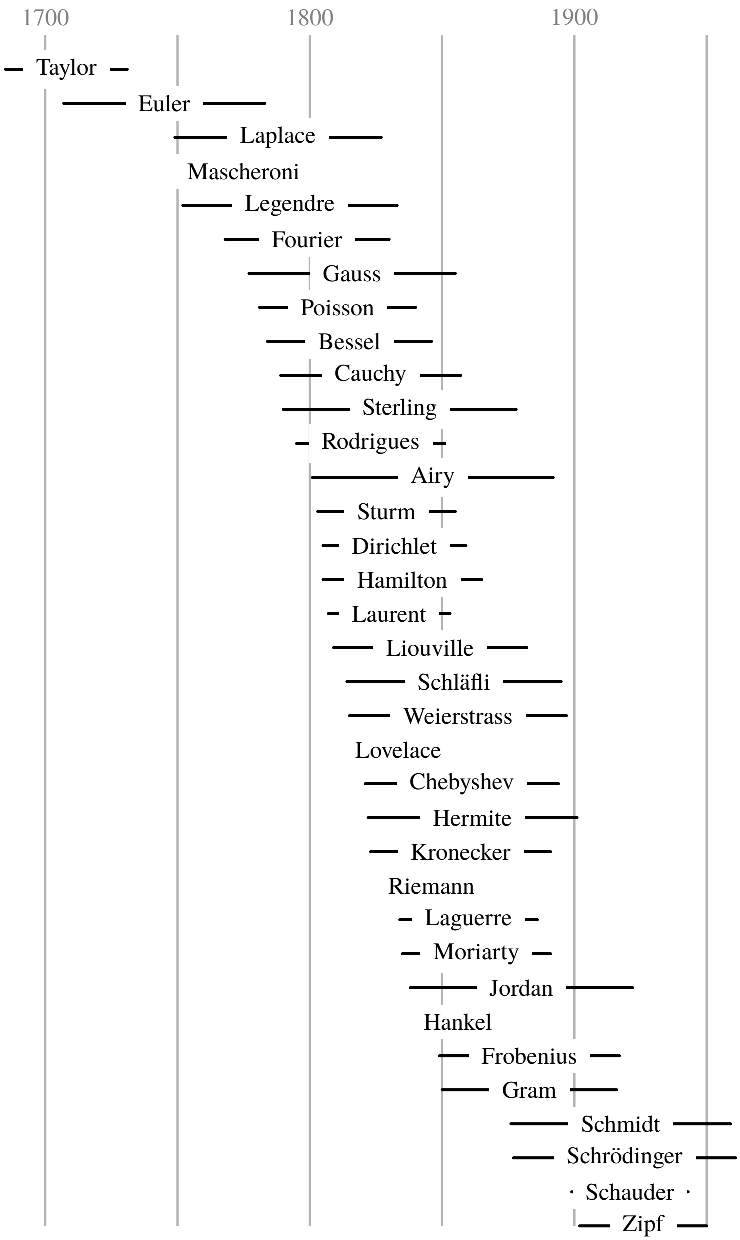
About the author

Kyle Novak has over twenty years of research and analysis experience in modeling, applied mathematics, and scientific computing and visualization including teaching mathematics at the undergraduate and graduate levels. As an Air Force mathematician, he provided decision analysis to senior military leaders in diverse topics such as cryptanalysis, autonomous navigation systems, multiscale networks, and superconducting materials.

About your mathematical tour guide

Laura Fox, Esq. is a special interest attorney with a penchant for mathematical puns. When she is not saving puppies and being awesome, Laura enjoys making minimal surfaces out of soap bubbles. Her favorite number is infinity.

Timeline of Notable Mathematicians and Physicists

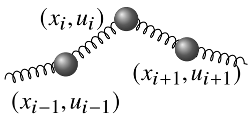


Lives of mathematicians, physicists, and other scientists who have functions, theorems, and other ideas mentioned in this book.

CHAPTER 1

The Guitar and the Drum

Guitar string Suppose that we want to model the motion of a plucked guitar string. The vertical displacement of the string $u(x,t)$ is a function of the horizontal distance x along the string and the time t. We can model the string as a mass-spring system using n small weights of mass m at nodes $(x_i, u(x_i,t))$ connected by massless springs.



We'll make the assumption that the nodes can only move vertically, so $\{x_i\}$ are fixed in time. Also, let's take a uniform horizontal separation δx between the nodes. Using Hooke's law to model the strain F at each node, we have

$$F = m\frac{\mathrm{d}^2u_i}{\mathrm{d}t^2} = \kappa(u_{i+1} - u_i) - \kappa(u_i - u_{i-1}) \tag{1.1}$$

where $u_i = u(x_i,t)$ and κ is the spring stiffness. Take the length of the string $L = n\delta x$, the total mass of the string $M = nm$, and the total stiffness of the string $K = \kappa/n$. Then, we can rewrite (1.1) as

$$\frac{\mathrm{d}^2u_i}{\mathrm{d}t^2} = c^2\frac{u_{i+1} - 2u_i + u_{i-1}}{(\delta x)^2}$$

where $c^2 = KL^2/M$. In the limit as $\delta x \to 0$ (and $n \to \infty$) we have

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2}. \tag{1.2}$$

We call (1.2) the wave equation and the constant c the wave speed. The equation has two time derivatives and two space derivatives, so we need to specify two initial conditions and two boundary conditions in order to ensure a unique solution. For a plucked guitar string, we will consider that the string is clamped at both ends and that it is initially stretched to some initial shape before being released. In this case for a string of length $L = 1$, we have

initial conditions	$u(x,0) = u_0(x)$ and $\frac{\partial}{\partial t}u(x,0) = 0$	
boundary conditions	$u(0,t) = 0$ and $u(1,t) = 0.$	

We can solve this problem using separation of variables. We assume that the solution is of the form

$$u(x,t) = X(x)T(t).$$

By substituting this expression into (1.2), we get

$$XT'' = c^2 T X''$$

or equivalently

$$\frac{T''}{T} = c^2 \frac{X''}{X}.$$

The notation $'$ is used to represent differentiation with respect to the dependent variable. The expression on the left is a function of only t and the expression on the right is a function of only x. The only way that these two expressions can be equal is if both are constant. That is,

$$\frac{1}{c^2}\frac{T''}{T} = \frac{X''}{X} = \lambda$$

for some λ. The constant λ can either be positive or negative. Let's consider both cases in turn by taking $\lambda = \pm k^2$ for some constant k. Starting with positive λ, we have that

$$T'' = c^2 k^2 T \quad \text{and} \quad X'' = k^2 X.$$

The solution to $X'' = k^2 X$ is

$$X(x) = A\,\mathrm{e}^{kx} + B\,\mathrm{e}^{-kx}\,.$$

for some constants A and B. Applying the boundary conditions $X(0) = X(1) = 0$, we have that $A = B = 0$. So, $X(x)$ is identically zero. We'll reject this solution, and instead take λ to be negative. This means that the solution must satisfy

$$T'' = -c^2 k^2 T \quad \text{and} \quad X'' = -k^2 X.$$

The solution to $X'' = -k^2 X$ is

$$X(x) = A\cos kx + B\sin kx$$

for some constants A and B. In order for $X(x)$ to satisfy the boundary conditions $X(0) = X(1) = 0$, we must have that $A \equiv 0$ and $k = n\pi$ for any integer value n. Similarly, the solution to $T'' = -c^2 k^2 T$ is

$$T(t) = C\cos ckt + D\sin ckt$$

for constants C and D. In order for $T(t)$ to satisfy the initial conditions, we must have that $D \equiv 0$. So, for any arbitrary integer n

$$u(x,t) = a_n \sin(n\pi x)\cos(cn\pi t)$$

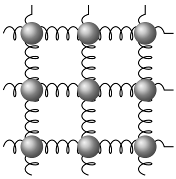
for some constant $a_n = BC$. For each integer n we have an independent solution to the problem. All of these solutions are valid, so we have

$$u(x,t) = \sum_{n=0}^{\infty} a_n \sin(n\pi x)\cos(cn\pi t)$$

for constants a_n that satisfy the initial conditions

$$u(0,t) = \sum_{n=0}^{\infty} a_n \sin(n\pi x) = u_0(x).$$

This representation is called the *Fourier expansion* of $u_0(x)$ and a_n is called a *Fourier coefficient*.



Circular drum Now, instead of a modeling a steel guitar string, let's model a circular drum head. We can again derive the equations of motion from Hooke's law, but this time we consider a network of small weights connected by massless springs in two-dimensions. For a vertical displacement $u_{ij}(t) = u(x_i, y_j, t)$ we have the equation

$$\frac{\mathrm{d}^2 u_{ij}}{\mathrm{d}t^2} = c^2 \left[\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\delta x)^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\delta y)^2} \right]$$

where $c^2 = KL^2/M$. In the limit as $\delta x, \delta y \to 0$ (and $n \to \infty$) this equation becomes

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right].$$

More succinctly

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla^2 u \tag{1.3}$$

where ∇^2 denotes the Laplacian operator. Because of the circular boundary conditions of the drum, it will be easier to solve the problem using polar coordinates (r, θ). In polar coordinates, the Laplacian operator is given by (I'll skip the details of this transformation)

$$\nabla^2 u = \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}.$$

So, we have the equation

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} \tag{1.4}$$

for $u(r,\theta,t)$. In the case where the circular drum head has a radius 1, we have the following initial conditions and boundary conditions[1]

$$\begin{array}{lll} \text{initial conditions} & u(r,\theta,0) = u_0(r,\theta) \quad \text{and} & \dfrac{\partial}{\partial t}u(r,\theta,0) = 0 \\ \text{boundary conditions} & u(1,\theta,t) = 0, & u(0,\theta,t) = 0, \end{array}$$

$$u(r,0,t) = u(r,2\pi,t), \quad \text{and} \quad \frac{\partial}{\partial \theta}u(r,0,t) = \frac{\partial}{\partial \theta}u(r,2\pi,t).$$

As before, let's look for a separable solution

$$u = H(r,\theta)T(t)$$

in which case (1.3) becomes

$$\frac{1}{c^2}HT'' = T\nabla^2 H.$$

or equivalently (after dividing by HT)

$$\frac{1}{c^2}\frac{T''}{T} = \frac{\nabla^2 H}{H}.$$

The left-hand side is only a function of t and the right-hand side is only a function of r and θ. Because these two expressions are functions of different variables, the only way they can be the same for all possible t, r, and θ is if both sides are constant:

$$\frac{1}{c^2}\frac{T''}{T} = \frac{\nabla^2 H}{H} = \lambda$$

where λ can be positive or negative. As before, a positive constant λ leads to an unphysical solution, and we take $\lambda = -k^2$ for some constant k. This gives us two equations

$$T'' = -c^2k^2T \tag{1.5}$$

$$\nabla^2 H = -k^2 H. \tag{1.6}$$

The solution to $T'' = -c^2k^2T$ is

$$T(t) = C\cos ckt + D\sin ckt,$$

[1] It may be more realistic to start with prescribing a non-zero $\frac{\partial}{\partial t}u(r,\theta,0)$ and a zero $u(r,\theta,0)$.

which because of the initial conditions is simply

$$T(t) = A\cos ckt.$$

Now let's examine the solution to

$$\nabla^2 H = -k^2 H.$$

This equation is called the *Helmholtz equation*, commonly written as

$$\nabla^2 H + k^2 H = 0.$$

In polar coordinates we have we have

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial H}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 H}{\partial \theta^2} + k^2 H = 0.$$

Consider a solution of the form $H(r,\theta) = R(r)\Theta(\theta)$. Then

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

Multiplying by r^2 and dividing by ΘR gives us

$$\frac{r(rR)'}{R} + \frac{\Theta''}{\Theta} + k^2 r^2 = 0$$

or equivalently

$$r\frac{(rR')'}{R} + k^2 r^2 = -\frac{\Theta''}{\Theta}.$$

The expression on the left is entirely a function of r and the expression on the right is entirely a function of θ. Hence the two expressions must be constant

$$r\frac{(rR')'}{R} + k^2 r^2 = -\frac{\Theta''}{\Theta} = \mu$$

for some constant μ. Equivalently,

$$\begin{aligned} r\,(rR')' + k^2 r^2 R &= \mu R \\ \Theta'' &= -\mu\Theta \end{aligned}$$

or better still

$$r\,(rR')' + (k^2 r^2 - \mu)R = 0 \tag{1.7}$$
$$\Theta'' + \mu\Theta = 0. \tag{1.8}$$

The angular component $\Theta(\theta)$ must satisfy periodic boundary conditions, therefore μ must be non-negative. We have that

$$\Theta = A\cos\mu\theta + B\sin\mu\theta.$$

for some coefficients A and B. By periodicity of the boundary conditions in the angular θ direction—$\Theta(0) = \Theta(2\pi)$—we must have that $\mu = m$ for some integer m.

We are left to solve the radial component (1.7)

$$r\,(rR')' + (k^2r^2 - m^2)R = 0.$$

Let's scale $r \mapsto r/k$. Then $R' \mapsto kR'$, and we have

$$r\,(rR')' + (r^2 - m^2)R = 0.$$

which when expanded is

$$r^2R'' + rR' + (r^2 - m^2)R = 0. \tag{1.9}$$

This equation is called Bessel's equation. The solution to Bessel's equation cannot be written as a product and sum of elementary functions. Instead, we give the function that solves the problem a name—the Bessel function $\mathrm{J}_m(r)$—so that we can talk about the solution in a closed form. Using the Bessel function, we now have the solution to the equation of the drum

$$y(r,\theta,t) = \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} a_{km}\,\mathrm{J}_m(kr)\sin(m\theta)\cos(k\pi t).$$

If we had considered a rectangular drum head, the solution would be Fourier polynomials (similar to the guitar string). If we had considered an elliptical drum head the solutions would be Mathieu functions. The solutions to many differential equations cannot be expressed in closed form of elementary functions but arise frequently enough to assign them a proper name. The class of such functions are called special functions. The purpose of this course is to examine several important special functions such as the Bessel function, the gamma function and its relatives, and the orthogonal polynomials. In order to comfortably analyze special functions, we will first need to develop some tools of complex analysis.

CHAPTER 2

Complex Analysis

2.1 Taylor series representation

Suppose that we want to find the best local polynomial approximation

$$p(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_n x^n$$

to a smooth function $f(x)$ at $x = 0$. In this case, we want to determine the coefficients $a_0, a_1, a_2, \ldots, a_n$ such that

$$f(0) = p(0), \quad f'(0) = p'(0), \quad f''(0) = p''(0), \quad \ldots, \quad f^{(n)}(0) = p^{(n)}(0).$$

Differentiating $p(x)$ at $x = 0$ gives us

$$\begin{array}{rcl} p(0) = a_0 & \Rightarrow & a_0 = f(0) \\ p'(0) = a_1 & \Rightarrow & a_1 = f'(0) \\ p''(0) = 2a_2 & \Rightarrow & a_2 = \frac{1}{2} f''(0) \\ p^{(3)}(0) = 6a_3 & \Rightarrow & a_3 = \frac{1}{6} f^{(3)}(0) \\ \vdots & \vdots & \vdots \\ p^{(n)}(0) = n! a_n & \Rightarrow & a_n = \frac{1}{n!} f^{(n)}(0.) \end{array}$$

The expression $n!$ reads "n factorial" and represents $n \cdot (n-1) \cdot \cdots \cdot 2 \cdot 1$. We call the polynomial

$$p(x) = f(0) + x f'(0) + \tfrac{1}{2} x^2 f''(0) + \tfrac{1}{3!} x^3 f'''(0) + \cdots + \frac{1}{n!} x^n f^{(n)}(0)$$

a *Taylor polynomial* approximation for $f(x)$ at $x = 0$. By letting the number of terms $n \to \infty$, we get the *Taylor series* (or power series) representation of $f(x)$ about the point $x = 0$

$$f(x) = f(0) + x f'(0) + \tfrac{1}{2} x^2 f''(0) + \tfrac{1}{3!} x^3 f'''(0) + \cdots \tag{2.1}$$

as long as the series converges. For an arbitrary point x_0, we have that

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \tfrac{1}{2}(x - x_0)^2 f''(x_0) + \tfrac{1}{3!}(x - x_0)^3 f'''(x_0) + \cdots$$

Again, this formula is mathematically valid for a given x as long as the series converges. A function that has a Taylor series representation at $x = x_0$ is said to be *analytic* at x_0.

Example. Consider the exponential function e^x. We define the exponential function as the function that equals its own derivative

$$\frac{d}{dx}(e^x) = e^x \tag{2.2}$$

and whose value at zero is one. Using this definition in (2.1), we have that

$$e^x = 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{3!}x^3 + \tfrac{1}{4!}x^4 + \cdots \tag{2.3}$$

because $e^0 = 1$. The factorial $n!$ grows much faster than x^n as $n \to \infty$, so the Taylor series representation is valid for everywhere. Some math texts actually use (2.3) to define the exponential function and prove (2.2) as a result. ◀

> The Taylor series for e^x has a simple pattern:
>
> $$e^x = 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{3!}x^3 + \tfrac{1}{4!}x^4 + \cdots$$
>
> It's a good idea to memorize it, because it's pretty useful.

Example. Consider the cosine function $\cos x$ and the sine function $\sin x$. Recall from calculus that

$$\frac{d}{dx}\cos x = -\sin x \quad \text{and} \quad \frac{d}{dx}\sin x = +\cos x.$$

Also, $\sin 0 = 0$ and $\cos 0 = 1$. From this it follows that the power series for cosine is

$$\cos x = 1 - \tfrac{1}{2}x^2 + \tfrac{1}{4!}x^4 - \cdots \tag{2.4}$$

and the power series for sine is

$$\sin x = x - \tfrac{1}{3!}x^3 + \tfrac{1}{5!}x^5 - \cdots \tag{2.5}$$

Because the factorial grows much faster than a power function, the Taylor series for $\cos x$ and $\sin x$ are valid for all x. ◀

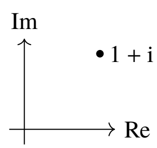
Mathematical detour. We can classify arithmetic operations using a hyperoperation sequence. The simplest arithmetic operation is succession, $x + 1$, which gives us the number that comes after x. Next, addition of two numbers $x + y$, which is the succession of x applied y times. Then, multiplication of two numbers xy, which is x added to itself y times. Followed by exponentiation of two numbers x^y, which is x multiplied by itself y times. The next logical operation is raising x to the x power y times. This operation, called *tetration*, is often denoted as ${}^y x$ or $x \uparrow\uparrow y$. Tetration can create big numbers quickly. For example, computing ${}^x x$ we have ${}^1 3 = 3$, ${}^2 3 = 27$, ${}^3 3 = 7625597484987$, and ${}^4 3 = 1258\ldots9387$ is a number with over three trillion digits. Putting three trillion into perspective, if ${}^4 3$ were to be written out explicitly, then this book's spine would be over 38 miles thick. ◀

2.2 Complex variables

We define the imaginary number i as a number whose square equals -1. That is, $\mathrm{i} = \sqrt{-1}$. Any positive or negative scaling of i is also called an imaginary number. A complex number is any linear combination of real and imaginary numbers. Note that by taking subsequent powers of i we have the sequence

$$\{\mathrm{i}^0, \mathrm{i}^1, \mathrm{i}^2, \mathrm{i}^3, \mathrm{i}^4, \mathrm{i}^5, \ldots\} = \{1, \mathrm{i}, -1, -\mathrm{i}, 1, \mathrm{i}, \ldots\}.$$

We can represent complex numbers either in Cartesian coordinates or in polar coordinates. In Cartesian coordinates, we simply write a complex number as a sum of the scaled real and imaginary components $z = x + \mathrm{i}y$. We call x the real part of z and denote it by $\operatorname{Re} z$ and we call y the imaginary part of x and denote it by $\operatorname{Im} z$.



Let's examine polar coordinates. Start with the power series representation of the exponential function

$$\mathrm{e}^s = 1 + s + \tfrac{1}{2}s^2 + \tfrac{1}{3!}s^3 + \tfrac{1}{4!}s^4 + \tfrac{1}{5!}s^5 + \cdots \tag{2.6}$$

Taking $s = \mathrm{i}\theta$, we have that

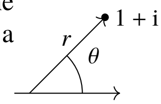
$$\begin{aligned} \mathrm{e}^{\mathrm{i}\theta} &= 1 + \mathrm{i}\theta - \tfrac{1}{2}\theta^2 - \mathrm{i}\tfrac{1}{3!}\theta^3 + \tfrac{1}{4!}\theta^4 + \mathrm{i}\tfrac{1}{5!}\theta^5 + \cdots \\ &= \left(1 - \tfrac{1}{2}\theta^2 + \tfrac{1}{4!}\theta^4 + \cdots\right) + \mathrm{i}\left(\theta - \tfrac{1}{3!}\theta^3 + \tfrac{1}{5!}\theta^5 + \cdots\right) \\ &= (\cos\theta) + \mathrm{i}(\sin\theta) \end{aligned}$$

This identity $\mathrm{e}^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$ is called *Euler's formula* and gives a useful means of relating the polar and Cartesian representations of a complex number. Note that from Euler's formula

$$\cos\theta = \operatorname{Re}\left(\mathrm{e}^{\mathrm{i}\theta}\right) \quad \text{and} \quad \sin\theta = \operatorname{Im}\left(\mathrm{e}^{\mathrm{i}\theta}\right).$$

> Euler's identity $e^{i\pi} + 1 = 0$ contains five important constants e, i, π, 1, and 0. Physicist Richard Feynman called Euler's identity "the most remarkable formula in mathematics."

Euler's formula also gives us a parametric representation for the unit circle in the complex plane. We write the polar form of a complex number z as



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

where r denotes the distance from the origin (the radius) and θ denotes the angle (the arc length along the unit circle). We call r the *modulus* or *magnitude* of z and denote it by $|z|$. We call θ the *argument* or *phase* of z and denote it by $\arg z$. From Cartesian coordinates $x + iy$, we have that $r = \sqrt{x^2 + y^2}$ and $\theta = \arctan(y/x)$

Multiplication using polar form of a complex number $r\,e^{i\theta}$ has a straightforward interpretation: it scales by r and rotates by θ. For example, if

$$z_1 = r_1\,e^{i\theta_1} \quad \text{and} \quad z_2 = r_2\,e^{i\theta_2}$$

then

$$z_1 z_2 = r_1 r_2\,e^{i(\theta_1+\theta_2)}\,.$$

The complex conjugate z^* of a complex number $z = r\,e^{i\theta}$ is given by $z^* = r\,e^{-i\theta}$. That is, if z has the argument θ then z^* has the argument $-\theta$. Taking the complex conjugate is equivalent to reflecting the complex number about the real axis. In Cartesian coordinates $(x + iy)^* = x - iy$. Another common notation for the complex conjugate of z is an overline $\overline{z}$. Furthermore,

$$zz^* = \left(r\,e^{i\theta}\right)\cdot\left(r\,e^{-i\theta}\right) = r^2 = |z|^2.$$

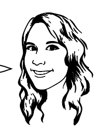
Note that

$$\operatorname{Re} z = \tfrac{1}{2}(z + z^*) \quad \text{and} \quad i\operatorname{Im} z = \tfrac{1}{2}(z - z^*).$$

From $e^{i\theta} = \cos\theta + i\sin\theta$, we have that

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2} \quad \text{and} \quad \sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}.$$

> Remember:
>
> $$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2} \quad \text{and} \quad \sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}.$$
>
> We will use these useful identities throughout the course.



Mathematical detour. To numerically approximate the derivative of a function $f(x)$ we often use a truncated Taylor series representation with a very small step h

$$f(x+h) = f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(x) + \tfrac{1}{6}h^3 f'''(x) + \cdots .$$

Solving this equation for $f'(x)$ give us

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \tfrac{1}{2}hf''(x) + \tfrac{1}{6}h^2 f'''(x) + \cdots .$$

When $h \ll 1$ (h is much smaller than 1) we have that

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}.$$

The truncation error is dominated by $\frac{1}{2}hf''(x)$ when h is small. We denote this with

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

and say that the approximation is first-order or $O(h)$. To get a very accurate approximation we take h very small.

We can improve the numerical approximation by using a centered-difference approach. By taking the Taylor series representations

$$f(x+h) = f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(x) + \tfrac{1}{6}h^3 f'''(x) + \cdots .$$
$$f(x-h) = f(x) - hf'(x) + \tfrac{1}{2}h^2 f''(x) - \tfrac{1}{6}h^3 f'''(x) + \cdots .$$

and subtracting we have

$$f(x+h) - f(x-h) = 2hf'(x) + \tfrac{1}{3}h^3 f'''(x) + \cdots .$$

Solving this equation for $f'(x)$ gives us

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \tfrac{1}{6}h^2 f'''(x) + \cdots .$$

So,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

and the method is second-order.

In a computer's floating-point representation, each number has a limited number of bits associated with a mantissa. Because of this, only a discrete set of numbers can be uniquely represented. For example, the number 1 can be uniquely represented and so can $1+\varepsilon$ where ε is the machine epsilon (about 10^{-16} for double-precision format). All numbers between 1 and $1+\varepsilon$ are either rounded down 1 or up to $1+\varepsilon$. We call this error the round-off error. Due to round-off error $f(x+h)-f(x)$ can only be as accurate as $|f(x)|\varepsilon$. And therefore, the numerical approximation $f'(x)$ is bounded by $f(x)\varepsilon/h$ when h gets small. So,

$$f'(x) = \frac{f(x+h)-f(x)}{h} + \underbrace{O(h)}_{\text{truncation error}} + \underbrace{\frac{|f(x)|\varepsilon}{h}}_{\text{round-off error}}.$$

If $f(x)$ is a real-valued, analytic function, we can use complex arithmetic to derive a second-order method that is not bounded by round-off error. Consider the Taylor series representation of

$$f(x+\mathrm{i}h) = f(x) + \mathrm{i}hf'(x) - \tfrac{1}{2}h^2 f''(x) - \mathrm{i}\tfrac{1}{6}h^3 f'''(x) + \cdots .$$

By taking the imaginary part of this equation we have that

$$\mathrm{Im}[f(x+\mathrm{i}h)] = hf'(x) - \tfrac{1}{6}h^3 f'''(x) + \cdots .$$

Solving for $f'(x)$ give us

$$f'(x) = \mathrm{Im}[f(x+\mathrm{i}h)] + \tfrac{1}{6}h^2 f'''(x) + \cdots$$

or

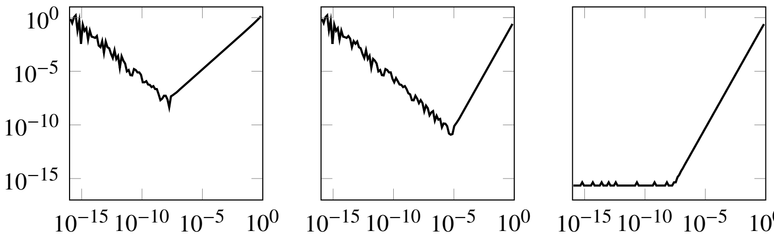
$$f'(x) = \mathrm{Im}[f(x+\mathrm{i}h)] + O(h^2).$$

Numerical error as a function of the step size h for three methods of approximating the derivative of $f(x) = \exp x$.

Let's compare the total error of the three methods

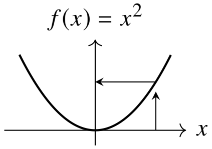
$$\frac{f(x+h)-f(x)}{h}, \quad \frac{f(x+h)-f(x-h)}{2h}, \quad \text{and} \quad \mathrm{Im}[f(x+\mathrm{i}h)]$$

in approximating the derivative of $f(x) = \exp x$. The respective error as a function of step size h for each method:

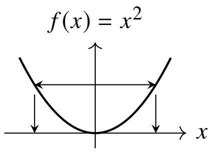


The slopes reflect the order of the error $O(h)$ and $O(h^2)$. When h is relatively large, the total error is dominated by truncation error (the upward sloping segment). When h is sufficiently small, the total error is dominated by round-off error (the downward sloping segment). The third method is not impacted by round-off error, and instead the total error bottoms out due to machine error. ◂

Functions of a complex variable

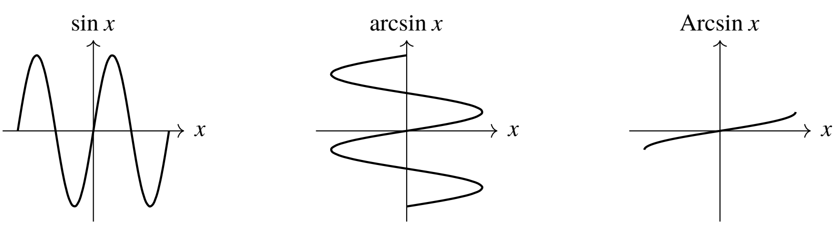


It's easy to visualize the function of a real variable, because we can graph the mapping on a piece of paper. For example, the function $y = x^2$ can be mapped as follows: track any point x on the x-axis vertically to the graph of $f(x)$ and then horizontally to the y-axis to find the value of $f(x)$. The graph gives a simple tool to study any function of one variable. We can easily determine the value $f(x)$ for any value x. And we can see features of the function such as its derivatives and singularities.

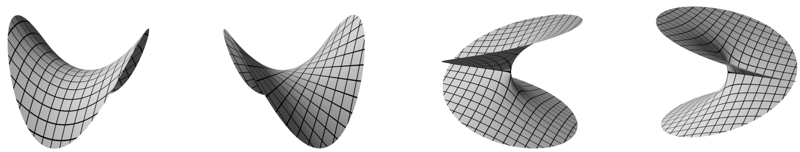


A graph also provides a convenient way of expressing the inverse of a function $f^{-1}(y)$, which tells us the point x from which $f(x)$ came. Starting with a value on the y-axis, track horizontally to the graph and then vertically to the x-axis. The inverse function $f^{-1}(y) = \sqrt{y}$ is multivalued with two branches, one positive and one negative. For example, $\sqrt{9} = 3$ and $\sqrt{9} = -3$. Often, we choose a single-valued principal branch of a multivalued function to avoid ambiguity, such as choosing the single-valued function $|\sqrt{x}|$ for $\sqrt{x}$.

The arcsine (inverse sine) is another example of a multivalued function. Every value $x = \pi \pm 2n\pi$ maps to the same value y for any integer n. For example $\sin n\pi = 0$ for all integers n. Therefore, $\sin^{-1} 0 = n\pi$ for all integer values of n. To avoid ambiguity, we often restrict a multivalued function to its principal branch and take its principal value. The principal branch for arcsine is usually taken to be $x \in [-\pi/2, \pi/2]$.



A function of a complex variable is more difficult to visualize, because there are two input variables (a real and an imaginary) and two output variables (a real and an imaginary). One way to visualize a function of a complex variable is to plot the real and imaginary parts of $f(x, y) = u(x, y) + \mathrm{i}v(x, y)$ separately:



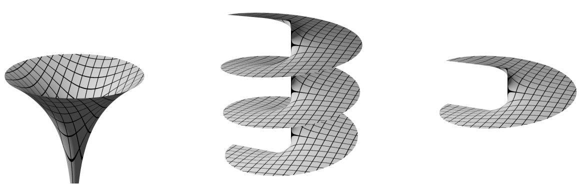
Re z^2 Im z^2 Re $\sqrt{z}$ Im $\sqrt{z}$

To prevent ambiguity in multivalued functions we make a *branch cut* in the complex plane to choose a single-valued branch. A natural branch cut for $\sqrt{z}$ is along the negative real axis, but we can take the branch cut for $\sqrt{z}$ along any simple path from the origin going out to infinity. One will often choose the branch cut to avoid any important regions just as a city planner might choose to district boundaries to go around rather than cut through neighborhoods.

Example. The logarithm is the inverse function of the exponential function. The function $\mathrm{e}^{\mathrm{i}z} = \cos z + \mathrm{i}\sin z$, so we can expect that the logarithm is a multivalued function.

$$\begin{aligned}
\log z &= \log r\,\mathrm{e}^{\mathrm{i}\theta} \\
&= \log r + \log \mathrm{e}^{\mathrm{i}\theta} \\
&= \log r + \log \mathrm{e}^{i\theta}\,\mathrm{e}^{\mathrm{i}2\pi n} \\
&= \log r + \log \mathrm{e}^{\mathrm{i}(\theta + 2\pi n)} \\
&= \log r + \mathrm{i}(\theta + 2\pi n) \\
&= \log |z| + \mathrm{i} \arg z
\end{aligned}$$

where the $\arg z = \theta + 2\pi n$ for any integer value n. To remove ambiguity, we choose the principal branch of $\log z$ by taking $n = 0$ to give $\operatorname{Log} z = \log |z| + \mathrm{i}\operatorname{Arg} z$ where the principal argument $\operatorname{Arg} z = \theta$. It's important to note that $\log z$ is not continuous across a branch cut. Instead, its value jumps by $\mathrm{i}2\pi$. ◂



Re(log z) Im(log z) Arg z

Remember that $\log z$ jumps by $2\pi i$ across a branch cut.

2.3 Derivatives

We define the derivative of a function $f(z)$ as

$$f'(z) = \frac{\mathrm{d}f}{\mathrm{d}z} = \lim_{\delta z \to 0} \frac{f(z+\delta z) - f(z)}{\delta z}$$

as long as the limit exists for all directions δz. If the derivative exists at a point z_0, we say that the function is *analytic* at z_0. If the derivative exists for every point in the complex plane, that is, if the function is analytic for all $z \in \mathbb{C}$, we say that the function is an *entire* function. If the derivative of $f(z)$ fails to exist at some point $z = z_0$, we call z_0 a *singular point* of $f(z)$. Because a limit is a linear operator, we only need to show that the derivative exists and is the same for two directions. Then by linearity it follows that the limit is the same for all directions. Take $z = x + \mathrm{i}y$ and $f(z) = u(x,y) + \mathrm{i}v(x,y)$ for real-valued functions u and v. Then

$$\frac{\delta f}{\delta z} = \frac{\delta u + \mathrm{i}\delta v}{\delta z} = \frac{\delta u}{\delta z} + \mathrm{i}\frac{\delta v}{\delta z}.$$

Letting $\delta x \longrightarrow 0$ while keeping $\delta y = 0$:

$$\frac{\delta f}{\delta z} = \frac{\delta u}{\delta x} + \mathrm{i}\frac{\delta v}{\delta x}.$$

Letting $\delta y \longrightarrow 0$ while keeping $\delta x = 0$:

$$\frac{\delta f}{\delta z} = \frac{\delta u}{\mathrm{i}\delta y} + \mathrm{i}\frac{\delta v}{\mathrm{i}\delta y} = -\mathrm{i}\frac{\delta u}{\delta y} + \frac{\delta v}{\delta y}.$$

In the limit

$$\lim_{\delta x \to 0} \frac{\delta u}{\delta x} + \mathrm{i}\frac{\delta v}{\delta x} = \frac{\partial u}{\partial x} + \mathrm{i}\frac{\partial v}{\partial x}, \quad \text{and}$$

$$\lim_{\delta y \to 0} -\mathrm{i}\frac{\delta u}{\delta y} + \frac{\delta v}{\delta y} = \frac{\partial v}{\partial y} - \mathrm{i}\frac{\partial u}{\partial y}.$$

These two expressions must be the same for $\frac{\mathrm{d}f}{\mathrm{d}z}$ to exist. It follows that $\frac{\mathrm{d}f}{\mathrm{d}z}$ exists if and only if

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \quad \text{and} \quad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}. \tag{2.7}$$

We call these two conditions the *Cauchy–Riemann conditions*. Alternatively, we could write the Cauchy–Riemann conditions as

$$\mathrm{i}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}.$$

A function $f = u + \mathrm{i}v$ is analytic if and only if it satisfies the Cauchy–Riemann conditions..

Example. Determine where z^2, $\sqrt{z}$, $1/z$, and z^* are analytic.

- z^2 is an entire function, because

$$(x+\mathrm{i}y)^2 = x^2 + \mathrm{i}2xy - y^2 = \underbrace{(x^2-y^2)}_{u} + \mathrm{i}\underbrace{2xy}_{v}$$

  and

$$\frac{\partial u}{\partial x} = 2x = \frac{\partial v}{\partial y} \quad \text{and} \quad \frac{\partial u}{\partial y} = 2x = -\frac{\partial v}{\partial x}.$$

- $\sqrt{z}$ is analytic everywhere except along the branch cut, where the function is discontinuous. We can write $\sqrt{z}$ in its Cartesian form $f(x,y) = \log\sqrt{x^2+y^2} + \mathrm{i}\tan^{-1}(y/x)$. Then

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{x}{x^2+y^2} + \mathrm{i}\frac{-y/x^2}{1+(y/x)^2} = \frac{x}{x^2+y^2} + \mathrm{i}\frac{-y}{x^2+y^2} \\
\frac{\partial f}{\partial y} &= \frac{y}{x^2+y^2} + \mathrm{i}\frac{-1/x}{1+(y/x)^2} = \frac{y}{x^2+y^2} + \mathrm{i}\frac{-x}{x^2+y^2}
\end{aligned}$$

  We see from $\mathrm{i}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}$ for every x and y that $\sqrt{z}$ is differentiable everywhere. The function is discontinuous across a branch cut even though the derivatives do match across the branch cut.

- $1/z$ is analytic everywhere except at $z = 0$. Starting with

$$f(z) = \frac{1}{x+\mathrm{i}y}$$

  and differentiating, we have

$$\frac{\partial f}{\partial x} = -\frac{1}{(x+\mathrm{i}y)^2} \quad \text{and} \quad \frac{\partial f}{\partial y} = -\frac{\mathrm{i}}{(x+\mathrm{i}y)^2}.$$

  So, $\mathrm{i}\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}$ everywhere except at the origin $(x,y) = (0,0)$ where the function blows up.

- z^* is not analytic anywhere. Starting with $z^* = x - \mathrm{i}y$ we have that $u = x$ and $v = -y$. Then

$$\frac{\partial u}{\partial x} = \frac{\partial x}{\partial x} = 1 \quad \text{and} \quad \frac{\partial v}{\partial y} = -\frac{\partial y}{\partial y} = -1, \quad \text{so} \quad \frac{\partial u}{\partial x} \neq \frac{\partial v}{\partial y}.$$

The Cauchy–Riemann conditions do not hold for any x or y. ◀

Keep in mind that if a function $f(z)$ is analytic at $z = z_0$, then all of it is infinitely differentiable at z_0. That is, $f'(z_0)$ exists, $f''(z_0)$ exists, $f^{(3)}(z_0)$ exists, ad infinitum. All analytic functions must blow-up at infinity. We say that they have a pole at infinity.

Harmonic functions

Laplace's equation $\nabla^2 u = 0$ is used to model the steady state temperature distribution of heat, charge distribution in a cavity, and the shape of an elastic membrane among other things. The solution to Laplace's equation are called *harmonic functions*. If $f(z) = u(x,y) + \mathrm{i}v(x,y)$ is an analytic function, then u and v are both harmonic functions. We call u the *harmonic conjugate* of v. To verify that u and v are harmonic functions we simply apply the Cauchy–Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \quad \text{and} \quad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}.$$

From this it follows that

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 v}{\partial y \partial x} \quad \text{and} \quad \frac{\partial^2 v}{\partial x \partial y} = -\frac{\partial^2 u}{\partial y^2},$$

and upon combining these equations

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

Similarly, $\nabla^2 v = 0$.

Laplace's equation also says that a harmonic function (the real or imaginary parts of an analytic function) cannot have local minimum or maximum. For example, if $u_{xx} < 0$, then $u_{yy} > 0$. Instead, a harmonic function can have a *saddle point*—a local minimum along one direction and a local maximum along another.

In fluid mechanics and electrostatics, we call the $u(x,y)$ the *complex potential* and $v(x,y)$ the *stream function*. The curves along which u is constant are called the *equipotentials*, and the curves along which v is constant are called the *streamlines* or *field lines*. Note that from the Cauchy–Riemann equations

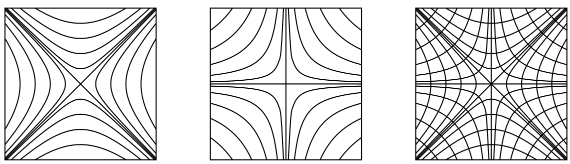
$$\nabla u \cdot \nabla v = \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} = 0,$$

which says that the equipotentials and the streamlines are orthogonal.

Example. Let's find the equipotentials and streamlines of z^2 and $1/z$. We'll start with $f(z) = z^2$ with $z = x + \mathrm{i}y$. Then

$$f = u(x, y) + \mathrm{i}v(x, y) = x^2 - y^2 + \mathrm{i}2xy.$$

So, $u(x, y) = x^2 - y^2$ is the complex potential and $v(x, y) = 2xy$ is the stream function. The equipotentials $x^2 - y^2 = c_1$ are orthogonal to the streamlines $xy = c_2$.



$u(x, y) = c$ $\qquad$ $v(x, y) = c$

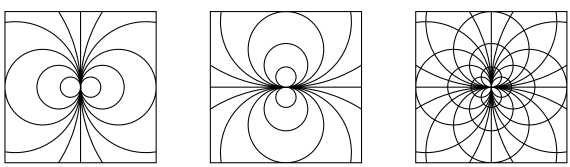
Now take $f(z) = 1/z$ with $z = x + \mathrm{i}y$. Then

$$f(x, y) = \frac{1}{x + \mathrm{i}y} = \frac{x - \mathrm{i}y}{x^2 + y^2}.$$

In polar coordinates ($x = r\cos\theta$ and $y = r\sin\theta$)

$$u(r, \theta) + \mathrm{i}v(r, \theta) = r^{-1}\cos\theta - \mathrm{i}r^{-1}\sin\theta.$$

So, $r^{-1}\cos\theta$ is the complex potential and $r^{-1}\sin\theta$ is the stream function. The equipotentials and streamlines are $r = c_1\cos\theta$ and $r = c_2\sin\theta$.



$u(x, y) = c$ $\qquad$ $v(x, y) = c$

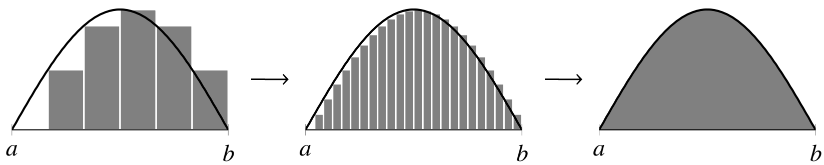
◄

2.4 Path integrals

Along the real axis, the Riemann integral from $x = a$ to $x = b$ is defined

$$\int_a^b f(x)\,\mathrm{d}x = \lim_{n\to\infty} \sum_{j=0}^{n} f(x_i)(x_{i+1} - x_i)$$

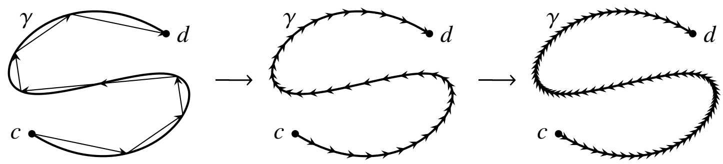
where $x_0 = a$ and $x_n = b$ and the intermediate points $\{x_j\}$ are taken (more or less) uniformly.



Consider a path γ from $z = c$ to $z = d$ in the complex plane. We define the *path integral* or *contour integral* or *line integral* along γ as

$$\int_\gamma f(z)\,\mathrm{d}z = \lim_{n\to\infty} \sum_{j=0}^{n} f(z_i)(z_{i+1} - z_i)$$

where $z_0 = c$ and $z_n = d$ and the intermediate points $\{z_j\}$ are taken (more or less) uniformly along the path γ.



If $c = d$, the path is closed, and the integral sign is denoted by $\oint_\gamma$. Unless stated we will follow convention and integrate all closed paths in the counter-clockwise direction.

Example. Compute the path integral

$$\oint_{|z|=R} z^n\,\mathrm{d}z \quad \text{where } n \text{ is an integer.}$$

On the circle $|z| = R$, $z = R\,\mathrm{e}^{\mathrm{i}\theta}$ and $\mathrm{d}z = \mathrm{i}R\,\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta$, so

$$\begin{aligned}\oint_{|z|=R} z^n\,\mathrm{d}z &= \int_0^{2\pi} \left(R\,\mathrm{e}^{\mathrm{i}\theta}\right)^n \mathrm{i}R\,\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta = \mathrm{i}R^{n+1} \int_0^{2\pi} \mathrm{e}^{\mathrm{i}(n+1)\theta}\,\mathrm{d}\theta \\ &= \begin{cases} R^0\,\mathrm{e}^0\Big|_0^{2\pi} = 2\pi\mathrm{i}, & \text{if } n = -1 \\ R^{n+1}\frac{1}{n+1}\,\mathrm{e}^{\mathrm{i}(n+1)\theta}\Big|_0^{2\pi} = 0, & \text{if } n \neq -1. \end{cases}\end{aligned}$$

In general,

$$\oint_{|z-z_0|=R} (z - z_0)^n\,\mathrm{d}z = \delta_{n,-1}$$

where δ_{ij} is the *Kronecker delta* ($\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$ for integers i and j). ◂

While integrating powers of z over circular contours is not particularly useful in and of itself, it does highlight a rather interesting behavior. Let's generalize the example to an arbitrary path. Take a path γ with starting point $z = a$ and ending point $z = b$. We can parameterize the path γ as $z = \gamma(t)$ where the parameter $t \in [0, 1]$ with $\gamma(0) = a$ and $\gamma(1) = b$. Let $F(z)$ be the anti-derivative of $f(z)$. That is, $F'(z) = f(z)$. Then by the Fundamentral Theorem of Calculus:

$$\int_\gamma f(z)\,\mathrm{d}z = \int_0^1 F'(\gamma(t))\gamma'(t)\,\mathrm{d}t = \int_0^1 \frac{\mathrm{d}F}{\mathrm{d}t}\,\mathrm{d}t = F(b) - F(a).$$

Furthermore, if γ is a closed path ($a = b$) and $F(z)$ is a singled-valued function, then

$$\oint_\gamma f(z)\,\mathrm{d}z = 0.$$

Example. Let's re-work the previous example over an arbitrary simple closed path γ around the origin:

$$\oint_\gamma z^n\,\mathrm{d}z \quad \text{where } n \text{ is an integer.}$$

- When $n \neq -1$
$$\oint_\gamma z^n\,\mathrm{d}z = 0$$
because the anti-derivative of $F(z) = z^{n+1}/(n+1)$ is single-valued.

- When $n = -1$ we have a problem when the closed path goes around the origin. The anti-derivative of z^{-1} is $F(z) = \log z$, which has a branch cut running from the origin to ∞. Without loss of generality let's take $a = b$ on the negative real axis. Choose the branch cut to be the negative real axis. Now, suppose that we shorten the path γ by $\pm\varepsilon$ on either side of the branch cut
$$\int_\gamma \frac{1}{z}\,\mathrm{d}z = \log z\Big|_{\theta=-\pi+\mathrm{i}\varepsilon}^{\theta=\pi+\mathrm{i}\varepsilon} = \log|z| - \mathrm{i}\arg z\Big|_{-\pi+\mathrm{i}\varepsilon)}^{\pi-\mathrm{i}\varepsilon} = 2\pi\mathrm{i} - 2\varepsilon.$$
If we let $\varepsilon \to 0$ we have
$$\oint_\gamma \frac{1}{z}\,\mathrm{d}z = 2\pi\mathrm{i}.$$
◂

The branch cut for $\log z$ must start at the origin but can take any path to ∞. If our closed path γ does not go around the origin, we can move the branch cut to avoid γ. In such a case that the path γ does not include the origin, $\oint_\gamma z^{-n}\,\mathrm{d}z = 0$ for any integer n.

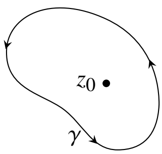
Theorem (Cauchy's Integral Theorem)**.** *If $f(z)$ is analytic in a simply connected region and γ is closed path in that region, then $\oint_\gamma f(z)\,\mathrm{d}z = 0$.*

Proof. The theorem is a direct consequence of Green's Theorem and the Cauchy–Riemann equations. Take $f(z) = u(x,y) + \mathrm{i}v(x,y)$, then

$$\begin{aligned}\oint_\gamma f(z)\,\mathrm{d}z &= \oint_\gamma (u+\mathrm{i}v)(\,\mathrm{d}x + \mathrm{i}\,\mathrm{d}y)\\ &= \oint_\gamma (u\,\mathrm{d}x - v\,\mathrm{d}y) + \mathrm{i}\oint_\gamma (u\,\mathrm{d}x + v\,\mathrm{d}y)\\ &= \iint_D \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\mathrm{d}x\,\mathrm{d}y + \iint_D \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)\mathrm{d}x\,\mathrm{d}y\\ &= \iint_D \left(\frac{\partial u}{\partial y} - \frac{\partial u}{\partial y}\right)\mathrm{d}x\,\mathrm{d}y + \iint_D \left(\frac{\partial v}{\partial y} - \frac{\partial v}{\partial y}\right)\mathrm{d}x\,\mathrm{d}y\\ &= 0.\end{aligned}$$

□

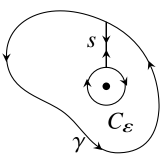
Example. Compute the contour integral



$$\oint_\gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z$$

where $f(z)$ is an analytic function and the contour γ goes around z_0.

We can solve this problem by considering a related contour $\Gamma = \gamma + s + C_\varepsilon - s$ that does not include the $z = z_0$. Because $f(z)/(z - z_0)$ is analytic inside this region bounded by Γ,



$$\oint_\Gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z = 0$$

from Cauchy's integral theorem. Furthermore, the paths s and $-s$ are the same but in opposite directions, so the path integrals along s and $-s$ cancel each other out.

We now have that

$$\oint_\gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z - \oint_{C_\varepsilon} \frac{f(z)}{z - z_0}\,\mathrm{d}z = 0.$$

In other words,

$$\oint_\gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z = \oint_{C_\varepsilon} \frac{f(z)}{z - z_0}\,\mathrm{d}z.$$

Take $z = z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta}$. Then $\mathrm{d}z = \mathrm{i}\varepsilon\,\mathrm{e}^{\theta\mathrm{i}}\,\mathrm{d}\theta$.

$$\begin{aligned}
\oint_{C_\varepsilon} \frac{f(z)}{z - z_0}\,\mathrm{d}z &= \int_0^{2\pi} \frac{f(z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta})}{\varepsilon\,\mathrm{e}^{\mathrm{i}\theta}} \varepsilon\mathrm{i}e^{\mathrm{i}\theta}\,\mathrm{d}\theta \\
&= \int_0^{2\pi} f(z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta})\mathrm{i}\,\mathrm{d}\theta \\
&= \int_0^{2\pi} f(z_0)\mathrm{i}\,\mathrm{d}\theta \qquad \text{by taking } \varepsilon \to 0 \\
&= \mathrm{i}f(z_0)\int_0^{2\pi} \mathrm{d}\theta = 2\pi\mathrm{i}f(z_0).
\end{aligned}$$

So,

$$\oint_\gamma \frac{f(z)}{z - z_0}\,\mathrm{d}z = 2\pi\mathrm{i}f(z_0)$$

along any contour γ that goes around z_0. ◀

Example. The integral

$$\oint_\gamma \frac{z^2}{z-2}\,\mathrm{d}z = \begin{cases} 8\pi\mathrm{i}, & \text{if } \gamma \text{ goes counterclockwise around } z = 2; \\ -8\pi\mathrm{i}, & \text{if } \gamma \text{ goes clockwise around } z = 2; \\ 0, & \text{if } \gamma \text{ doesn't go around around } z = 2. \end{cases}$$ ◀

Example. Compute the value of the contour integral

$$\oint_\gamma \frac{f(z)}{(z - z_0)^n}\,\mathrm{d}z$$

where $f(z)$ is an analytic function, n is any integer, and the contour γ wraps counterclockwise once around $z = z_0$. We will integrate by parts. Because $f(z)$ is analytic (infinitely differentiable), all of its derivatives are continuous along γ. Therefore, the boundary terms from integrating by parts along a closed path will cancel each other.

$$\begin{aligned}\oint_\gamma \frac{f(z)}{(z-z_0)^n}\,\mathrm{d}z &= \frac{1}{n-1}\oint_\gamma \frac{f'(z)}{(z-z_0)^{n-1}}\,\mathrm{d}z\\ &= \frac{1}{(n-1)(n-2)}\oint_\gamma \frac{f''(z)}{(z-z_0)^{n-2}}\,\mathrm{d}z\\ &\quad \text{(repeating in this fashion)}\\ &= \frac{1}{(n-1)!}2\pi\mathrm{i} f^{(n-1)}(z_0).\end{aligned}$$

So, we have that

$$\oint_\gamma \frac{f(z)}{(z-z_0)^n}\,\mathrm{d}z = \frac{1}{(n-1)!}2\pi\mathrm{i} f^{(n-1)}(z_0).$$

From this we also have an expression for the derivative in terms of a contour integral

$$f^{(n)}(z_0) = \frac{n!}{2\pi\mathrm{i}}\oint_\gamma \frac{f(z)}{(z-z_0)^{n+1}}\,\mathrm{d}z.$$

◀

Example. Evaluate $\displaystyle\oint_{|z|=2} \frac{\mathrm{e}^z}{z^2(z-1)}\,\mathrm{d}z.$

By partial fractions we have that

$$\frac{1}{z^2(z-1)} = \frac{az+b}{z^2} + \frac{c}{z-1}$$

for some a, b and c which we find by putting the right-hand side over a common denominator. Then

$$(az+b)(z-1) + cz^2 = 1, \quad \text{so} \quad az^2 + bz - az - b + cz^2 = 1$$

Matching the coefficients of the quadratic

$$\left.\begin{aligned} a + c &= 0\\ b - a &= 0\\ -b &= 1\end{aligned}\right\} \quad \Rightarrow \quad \begin{cases} c = 1\\ a = -1\\ b = 1\end{cases}$$

Hence,

$$\begin{aligned}\oint_{|z|=2} \frac{\mathrm{e}^z}{z^2(z-1)}\,\mathrm{d}z &= \oint_{|z|=2} \frac{\mathrm{e}^z}{z-1} - \frac{(z+1)\,\mathrm{e}^z}{z^2}\,\mathrm{d}z\\ &= \oint_{|z|=2} \frac{\mathrm{e}^z}{z-1}\,\mathrm{d}z - \oint_{|z|=2} \frac{(z+1)\,\mathrm{e}^z}{z^2}\,\mathrm{d}z.\end{aligned}$$

The first integral is $2\pi\mathrm{i}\,\mathrm{e}^1$. To evaluate the second integral, we note that

$$f(z) = (z+1)\,\mathrm{e}^z \quad\Rightarrow\quad f'(z) = (z+1) + (z+1)\,\mathrm{e}^z \quad\Rightarrow\quad f'(0) = 2.$$

So, the second integral is $2\pi\mathrm{i}(2)$. Therefore,

$$\oint_{|z|=2} \frac{\mathrm{e}^z}{z^2(z-1)}\,\mathrm{d}z = 2\pi\mathrm{i}(\mathrm{e} - 2).$$ ◀

2.5 Taylor and Laurent series

We began the chapter by deriving Taylor series using the Taylor polynomial of a function. We can develop a rigorous proof of the existence of Taylor series representation using contour integration.

Theorem (Taylor Series)**.** *A function $f(z)$ that is analytic in a neighborhood about z_0 has the Taylor series representation*

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!}(z-z_0)^n f^{(n)}(z_0).$$

Proof.

$$\begin{aligned}
f(z) &= \frac{1}{2\pi\mathrm{i}} \oint \frac{f(\xi)}{\xi - z}\,\mathrm{d}\xi \\
&= \frac{1}{2\pi\mathrm{i}} \oint \frac{f(\xi)}{\xi - z_0 + z_0 - z}\,\mathrm{d}\xi \\
&= \frac{1}{2\pi\mathrm{i}} \oint \frac{f(\xi)}{\xi - z_0} \frac{1}{1 - \dfrac{z - z_0}{\xi - z_0}}\,\mathrm{d}\xi \\
&= \frac{1}{2\pi\mathrm{i}} \oint \frac{f(\xi)}{\xi - z_0} \sum_{n=0}^{\infty} \left(\frac{z - z_0}{\xi - z_0}\right)^n \mathrm{d}\xi \qquad (\star) \\
&= \frac{1}{2\pi\mathrm{i}} \sum_{n=0}^{\infty} (z - z_0)^n \oint \frac{f(\xi)}{(\xi - z_0)^{n+1}}\,\mathrm{d}\xi \\
&= \frac{1}{2\pi\mathrm{i}} \sum_{n=0}^{\infty} (z - z_0)^n 2\pi\mathrm{i} \frac{1}{n!} f^{(n)}(z_0) \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} (z - z_0)^n f^{(n)}(z_0).
\end{aligned}$$ □

A function $f(z)$ is analytic at a point z_0 if and only if it has a Taylor series representation.

An essential step in the proof above ($\star$) uses the identity that for a geometric series

$$1 + r + r^2 + r^3 + \cdots = \frac{1}{1-r}$$

as long as $|r| < 1$. To see this simply take

$$\begin{aligned}(1-r)(1+r+r^2+r^3+\cdots+r^n) &= 1+r+r^2+\cdots+r^n \\ &\quad -r-r^2-\cdots-r^n-r^{n+1} \\ &= 1-r^{n+1}\end{aligned}$$

which goes to 1 as $n \to \infty$.

An infinite number of mathematicians walk into a bar. The first one orders a beer, the second orders half a beer, the third a quarter, the fourth an eighth at which point the bartender stops them, pours two beers, and says "You guys should know your limits."

Example. Let's derive the binomial expansion

$$(1+z)^m = 1 + mz + \frac{m(m-1)}{1 \cdot 2} z^2 + \cdots = \sum_{n=0}^{\infty} \binom{m}{n} z^n$$

where m is a real number. We can write a Taylor series expansion about $z = 0$ as

$$f(z) = \sum_{n=0}^{\infty} a_n z^n \quad \text{where} \quad a_n = \frac{1}{n!} \frac{\mathrm{d}^n}{\mathrm{d}z^n} f(z)\bigg|_{z=0}$$

For $f(z) = (1+z)^m$, we have that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}z}[(1+z)^m]\Big|_{z=0} &= m(1+z)^{m-1}\Big|_{z=0} = m \\
\frac{\mathrm{d}^2}{\mathrm{d}z^2}[(1+z)^m]\Big|_{z=0} &= m(m-1)(1+z)^{m-2}\Big|_{z=0} = m(m-1) \\
\frac{\mathrm{d}^3}{\mathrm{d}z^3}[(1+z)^m]\Big|_{z=0} &= m(m-1)(m-2)(1+z)^{m-3}\Big|_{z=0} = m(m-1)(m-2) \\
&\vdots \\
\frac{\mathrm{d}^4}{\mathrm{d}z^4}[(1+z)^m]\Big|_{z=0} &= m(m-1)\cdots(m-n+1).
\end{aligned}$$

Hence,

$$(1+z)^m = 1 + mz + \frac{m(m-1)}{1\cdot 2}z^2 + \cdots = \sum_{n=0}^{\infty}\binom{m}{n}z^n.$$

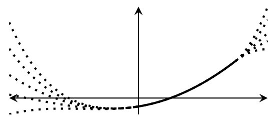
Note that this expansion is good for any real number m and not just integer values. We will return to the general case when we explore the gamma and the beta functions in Chapter 3. If m is an integer value, then the series terminates after $m+1$ terms. However, if m is not an integer, then we have an infinite series. The Taylor series is valid in regions where the function is analytic. Take

$$f(z) = (1+z)^{1/2} = \mathrm{e}^{\frac{1}{2}\log(1+z)}.$$

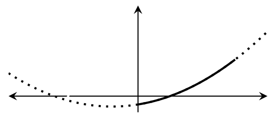
The logarithm function $\log z$ has a branch point at $z = 0$, so the function $\log(1+z)$ has a branch point at $z = -1$. At this branch point, the function fails to be analytic. So the Taylor series expansion only converges in a region that does not include $z = -1$. This means that a Taylor series expansion about $z = 0$ only converges when $|z| < 1$. ◀

Analytic continuation

Suppose that we are given a piece of a smooth (infinitely differentiable) function over the interval $[0,1]$ and then asked to continue the function over the rest of the real axis. For an arbitrary smooth function there is no unique continuation. In fact, there are infinitely many functions that could work. However, if the function happens to be a polynomial $c_0 + c_1x + c_2x^2 + \cdots + c_nx^n$, then there is a unique polynomial extension over the real axis. Just as two points uniquely determine a line and three points uniquely determine a parabola, we only need $n+1$ points sampled from the interval $[0,1]$ to uniquely identify the polynomial.



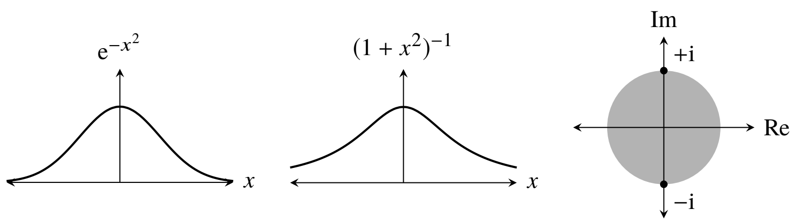
no unique continuation



unique polynomial continuation

The degree of the polynomial can be arbitrarily high, so similarly a Taylor series $c_0 + c_1 x + c_2 x^2 + \cdots$ has a unique Taylor series extension. In the complex plane, an analytic function defined in some domain has a unique analytic continuation over the entire complex plane.

Example. The real-valued function $f(x) = (1+x^2)^{-1}$ has a very similar graph to the real-valued function $g(x) = \mathrm{e}^{-x^2}$. But if we look at the Taylor series representation of each function about the origin, we note that while the Taylor series of $\exp(-x^2)$ is valid for all x, the Taylor series for $(1 + x^2)^{-1}$ blows up as x approaches ± 1. It is easy to understand why these two functions which look similar along the real axis have such different behaviors when we consider their behavior in the complex plane.



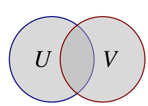
Although we can consider $(1 + x^2)^{-1}$ and $\exp(-x^2)$ both as real-valued functions, what we are seeing are simply thin slices of the complex-valued functions $(1 + z)^{-1}$ and $\exp(-z^2)$. Note that

$$\frac{1}{1+z^2} = \frac{1}{(\mathrm{i}+z)(-\mathrm{i}+z)}$$

has poles at $\pm\mathrm{i}$. A Taylor series fits a function with an infinite polynomial. The polynomial must match the function at every point, so if the function $f(z)$ blows up at ± 1 , the polynomial must also blow up. Taylor series representation is valid in any circle of convergence that does not contain a singularity. The function $\exp(-x^2)$ is an entire function, so the Taylor series is valid everywhere. ◄

We can use the idea of analytic continuation to splice two Taylor series representations together.

Theorem. *Suppose that functions $f_1(z)$ and $f_2(z)$ are analytic in region $U \cup V$. If $f_1(z) = f_2(z)$ in $U \cap V$, then $f_1(z) = f_2(z)$ in $U \cup V$.*



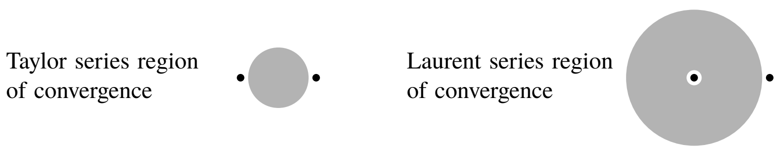
Proof. Let $g(z) = f_1(z) - f_2(z)$. Then $g(z) = 0$ in $U \cap V$. Because $g(z)$ is analytic in $U \cup V$, it has a Taylor series representation which happens to be identically zero. Hence, $g(z) = 0$ in all of $U \cap V$. So, $f_1(z) = f_2(z)$ in $U \cup V$. □

Laurent Series

The Taylor series representation of a function $f(z)$ at z_0 is valid only up to singularities $z_\star$. So, the region of analyticity is a ball centered at z_0 with radius $|z_0 - z_\star|$. Taylor series representation is ideal for entire functions (analytic in the entire complex plane), but they are not so good when $f(z)$ has singularities. Near a singularity, a *Laurent series* representation of $f(z)$ is a better choice. A Laurent series representation decomposes a function into its analytic and singular components $f = f_{\text{analytic}} + f_{\text{singular}}$:

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n = \sum_{n=0}^{\infty} a_n (z - z_0)^n + \sum_{n=-\infty}^{-1} a_n (z - z_0)^n.$$

Such an expression is valid even when z_0 is a singular point of $f(z)$. In this case the region of analyticity of the Laurent series representation is an annulus about the point z_0. Because of this the Laurent series is more versatile than the Taylor series representation.



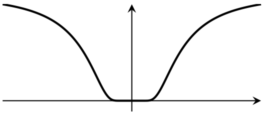
Note that for any closed path γ about z_0 along which $f(z)$ is analytic, we have

$$\oint_\gamma \frac{f(z)}{(z - z_0)^{k+1}} \, \mathrm{d}z = \oint_\gamma \sum_{n=-\infty}^{\infty} a_n (z - z_0)^{n-k-1} \, \mathrm{d}z = 2\pi \mathrm{i} a_k.$$

Hence, the coefficients a_n of the Laurent series can be defined as

$$a_n = \frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{f(z)}{(z - z_0)^{n+1}} \, \mathrm{d}z.$$

Example. Consider the function $f(x) = \mathrm{e}^{-1/x^2}$. The function is infinitely differentiable along the real axis.



$$
\begin{aligned}
f(0) &= \lim_{x\to 0} f(x) = 0 \\
f'(0) &= \lim_{x\to 0} \frac{2}{x^3}\,\mathrm{e}^{-1/x^2} = 0 \\
f''(0) &= \lim_{x\to 0} \left(\frac{4}{x^6} - \frac{6}{x^4}\right)\mathrm{e}^{-1/x^2} = 0 \\
f^{(n)}(0) &= \lim_{x\to 0} p_{3n}\left(\frac{1}{x}\right)\mathrm{e}^{-1/x^2} = 0
\end{aligned}
$$

where $p_{3n}(x)$ is a polynomial of degree $3n$. At $x = 0$, every derivative of $f(x)$ is zero, so the Taylor series representation of $f(x) = 0$. The Taylor series is good only at $x = 0$ and incorrect for every point $x \neq 0$. What went wrong? The function $f(z)$ has a singularity at $z = 0$ in the complex plane—in fact, an essential singularity.

Instead of using a Taylor series representation, we can use a Laurent series representation. Because the exponential function is an entire function, this Laurent series expansion is valid at all points $x \neq 0$. Let's find the Laurent series for $\exp(-1/z^2)$. We know the Taylor series for

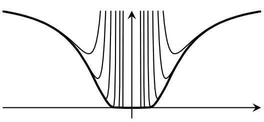
$$\mathrm{e}^z = \sum_{n=0}^{\infty} \frac{1}{n!} z^n$$

is valid for all $z < \infty$. Hence,

$$\mathrm{e}^{-z^2} = \sum_{n=0}^{\infty} \frac{1}{n!}(-z^2)^n = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} z^{2n},$$

and we have

$$\mathrm{e}^{-1/z^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \frac{1}{z}^{2n} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} z^{-2n}.$$



The Laurent series exists, but the series of partial sums slowly converges near $z = 0$. The plot on the left shows the partial sums for $n = 2, 4, 8, 16, 32, 64$. ◀

Example. Find the Laurent series for $\operatorname{sinc} z = \dfrac{\sin z}{z}$.

We know the Taylor series for

$$\sin z = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n+1}.$$

So,

$$\frac{\sin z}{z} = z^{-1}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}z^{2n+1} = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}z^{2n}. \qquad \blacktriangleleft$$

Example. Compute the Laurent series of $\dfrac{1}{\mathrm{e}^z - 1}$ at the origin.

The function $1/(\mathrm{e}^z - 1)$ has a simple pole at the origin. Let's start with a related function

$$f(z) = \frac{\mathrm{e}^z - 1}{z} = \sum_{j=0}^{\infty}\frac{1}{(j+1)!}z^j,$$

and find its reciprocal. The *Cauchy product* of two series is

$$\left(\sum_{i=0}^{\infty} a_i z^i\right)\cdot\left(\sum_{j=0}^{\infty} b_j z^j\right) = \sum_{k=0}^{\infty} c_k z^k \quad \text{where} \quad c_k = \sum_{l=0}^{k} a_l b_{k-l}.$$

That is,

$$\begin{aligned}\left(a_0 + a_1 z + a_2 z^2 + a_3 z^3 + \cdots\right)&\left(b_0 + b_1 z + b_2 z^2 + b_3 z^3 + \cdots\right)\\ &= \underbrace{(a_0 b_0)}_{c_0} + \underbrace{(a_0 b_1 + a_1 b_0)}_{c_1} z + \underbrace{(a_0 b_2 + a_1 b_2 + a_2 b_0)}_{c_2} z^2 + \ldots\end{aligned}$$

Given $\{b_j\}$ and $\{c_k\}$, we can solve for $\{a_n\}$ iteratively

$$a_n = b_0^{-1}\left(c_n - \sum_{l=0}^{n-1} a_l b_{n-l}\right).$$

For our problem, $b_j = 1/(j+1)!$ and $c_0 = 1$ and $c_k = 0$ for $k = 1, 2, 3, \ldots$. The first five coefficients are

$$\begin{aligned}
b_0 &= 1 & a_0 &= 1\\
b_1 &= \tfrac{1}{2!} & a_1 &= -a_0 b_1 = -\tfrac{1}{2}\\
b_2 &= \tfrac{1}{3!} & a_2 &= -(a_0 b_2 + a_1 b_1) = -\left(\tfrac{1}{6} - \tfrac{1}{4}\right) = \tfrac{1}{12}\\
b_3 &= \tfrac{1}{4!} & a_3 &= -(a_0 b_3 + a_1 b_2 + a_2 b_1) = -\left(\tfrac{1}{24} - \tfrac{1}{12} - \tfrac{1}{24}\right) = 0\\
b_4 &= \tfrac{1}{5!} & a_4 &= -\left(\tfrac{1}{120}\cdot 1 + \tfrac{1}{24}\cdot\left(-\tfrac{1}{2}\right) + \tfrac{1}{6}\cdot\tfrac{1}{12} + \tfrac{1}{4}\cdot 0\right) = -\tfrac{1}{720}
\end{aligned}$$

In general, $a_n = B_n/n!$ where B_n are the Bernoulli numbers

$$\{B_0, B_1, B_2 \cdots\} = \{1, -\tfrac{1}{2}, \tfrac{1}{6}, 0, -\tfrac{1}{30}, 0, \tfrac{1}{42}, 0, -\tfrac{1}{30}, 0, \tfrac{5}{66}, 0, -\tfrac{691}{2730}, 0, \tfrac{7}{6}, 0, -\cdots\}.$$

Dividing by z we have

$$\frac{1}{e^z - 1} = z^{-1} - \tfrac{1}{2} + \tfrac{1}{12}z - \tfrac{1}{720}z^3 + \cdots = z^{-1}\sum_{n=0}^{\infty}\frac{B_n}{n!}z^n. \qquad ◂$$

Example. Compute the Laurent series of $\cot z$ at the origin.

$$\cot z = \frac{e^{iz} + e^{-iz}}{e^{iz} - e^{iz}} = \frac{e^{iz}}{e^{iz} - e^{-iz}} - \frac{e^{-iz}}{e^{iz} - e^{-iz}} = \frac{1}{e^{2iz} - 1} + \frac{1}{e^{-2iz} - 1}.$$

Using the Laurent series for $1/(e^z - 1)$ from the previous example we have that

$$\cot z = z^{-1}\sum_{n=0}^{\infty}\frac{B_n}{n!}(2iz)^n + z^{-1}\sum_{n=0}^{\infty}\frac{B_n}{n!}(-2iz)^n = z^{-1}\sum_{n=0}^{\infty}\frac{|B_{2n}|2^{2n}}{(2n)!}z^{2n}. \qquad ◂$$

Mathematical detour. Ada Lovelace is credited as the first computer programmer. In 1843 Lovelace wrote a program to compute the Bernoulli numbers using Charles Babbage's hypothetical Analytical Engine. The Analytic Engine was never built during Babbage's or Lovelace's lifetime, but if it were you could imagine a steampunk mechanical computer the size of a locomotive with gears, lots and lots of gears. Ada Lovelace said of it, "the analytical engine weaves algebraic patterns just as the Jacquard loom weaves flowers and leaves." Check out Sydney Padua's graphic novel *The Thrilling Adventures of Lovelace and Babbage*.

While the modern definition of Bernoulli's numbers are often from the generating function

$$g(z) = \frac{z}{e^z - 1}\sum_{k=0}^{\infty} B_k\frac{z^k}{k!},$$

Bernoulli's numbers originally came about from Faulhaber's formula for the sum of powers

$$\sum_{k=1}^{n} k^p = \sum_{j=0}^{p}\frac{B_j}{j!}\frac{p!}{(p-1+k)!}n^{p+1-k}.$$

We can find Lovelace's program in this formula. Letting $n = 1$, then

$$0 = \sum_{j=0}^{p}\frac{B_j}{j!}\frac{p!}{(p-1+j)!}$$

from which we have a recurrence relation

$$B_p = -\frac{1}{p+1}\sum_{j=0}^{p-1}\frac{B_j}{j!}\frac{p!}{(p+1-j)!} = -\frac{1}{p+1}\sum_{j=0}^{p-1} B_j \binom{p+1}{k}$$

We can compute binomial coefficients with the Pascal triangle recurrence relation

$$\binom{p+1}{k} = \binom{p}{k-1} + \binom{p}{k}.$$

◀

2.6 Singularities

A singularity is a point where a function is not defined. We can classify a singularity as either a removable singularity, an isolated singularity, or an essential singularity.

A function $f(z)$ has a *removable singularity* at a point $z = z_0$ if the function is undefined at z_0 but the function can formally be defined at z_0 to be analytic there. For example, $\operatorname{sinc} z = (\sin z)/z$ is not defined at $z = 0$. But from the Laurent series representation

$$\operatorname{sinc} z = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}z^{2n}$$

we see that $\operatorname{sinc} 0$ can be defined to be 1. In other words, a function $f(z)$ has a removable singularity if the coefficients $a_n = 0$ for all $n < 0$ in its Laurent series representation.

If a function has an *isolated singularity* at z_0, then the function is not analytic at z_0, but it is analytic at all neighboring points. For example, the function $f(z) = \mathrm{e}^z/(1-z)$ has an isolated singularity at $z = 1$. It happens to be a simple pole. The function $f(z) = \mathrm{e}^z/(1-z)^2$ also has an isolated singularity at $z = 1$. This time it's a double pole. If a function has a simple pole, the Laurent series starts at $n = -1$:

$$f(z) = \sum_{n=-1}^{\infty} a_n(z-z_0)^n$$

with $a_{-1} \neq 0$ and $a_n = 0$ for all $n < -1$. If a function has a double pole, the Laurent series starts at $n = -2$:

$$f(z) = \sum_{n=-2}^{\infty} a_n(z-z_0)^n$$

with $a_{-2} \neq 0$ and $a_n = 0$ for all $n < -2$. We say that a function $f(z)$ has a pole of order p if $a_{-p} \neq 0$ and $a_n = 0$ for all $n < p$.

Suppose that the Laurent series for $f(z)$ has no lower N such that the coefficients $a_n = 0$ for all $n < N$. That is, suppose

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

with $a_n \neq 0$ for all or some of the indices n as $n \to -\infty$. In this case we say that $f(z)$ has an *essential singularity* at $z = z_0$. Functions with essential singularities are very pathological. For example,

$$\sin(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} z^{2n+1}$$

is an entire function—it is analytic everywhere in $\mathbb{C}$. As such, it is very well behaved. However,

$$\sin\left(\frac{1}{z}\right) = \sum_{n=-\infty}^{0} \frac{(-1)^n}{(2n+1)!} z^{2n+1}$$

is crazy near the origin.

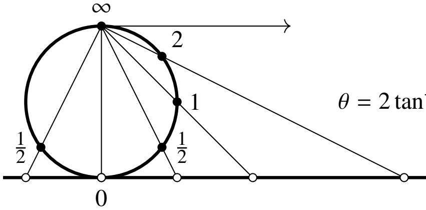
A *meromorphic* function is a function that is analytic everywhere except at isolated singular points. For example,

$$f(z) = \frac{1}{\sin z}$$

is analytic everywhere except at $z = \pm n\pi$ for integer values n.

Mathematical detour. A boundary of a set S is the set of points that can be approached as a limit from both inside S and from outside S. We define an *open set* as any set that does not contain any of its boundary points. A *closed set* is any set that contains all of its boundary points. The set of real numbers $\mathbb{R}$ is open because it does not contain its boundary $\{-\infty, \infty\}$: the limit $\lim_{x\to 0} 1/x$ is not included in the real numbers. We do have to be a bit careful in defining this limit, because from the right $\lim_{x\to 0^+} 1/x = +\infty$ and from the left $\lim_{x\to 0^-} 1/x = -\infty$. By including the boundary points together with the real numbers, we have the *extended real numbers* $\mathbb{R} \cup \{-\infty, +\infty\}$.

One way to visualize the extended real line is by projecting it onto a circle using stereographic projection:



$$\theta = 2\tan^{-1} x \quad \text{or} \quad x = \tan \tfrac{1}{2}\theta$$

where $\theta = 0$ maps to $x = 0$ and $\theta = \pm\pi$ maps to $x = \pm\infty$. Notice that the boundary set $\{-\infty, +\infty\}$ is simply mapped to the same point $\theta = \pi$ on the circle. Points in the interval $(-1, 1)$ are mapped to the bottom semicircle and points outside this interval are mapped to the top semicircle.

We can also use a stereographic projection $z = \tan \frac{1}{2}\theta\, \mathrm{e}^{\mathrm{i}\phi}$ to map the complex plane onto a sphere called the *Riemann sphere*. Stereographic projection has a simple visualization. Imagine a sphere resting on a plane with its south pole kissing the plane. And imagine a lightbulb at the north pole. The shadows cast by points on the sphere onto the plane are the stereographic projections of those points.

This mapping creates a one-to-one mapping of the complex plane to the Riemann sphere. The unit circle is mapped to the the equator of the Riemann sphere. The southern hemisphere is the region inside of the unit circle and the northern hemisphere is the region outside of the unit circle. Circles in the complex plane are simply circles in the Riemann sphere. The boundary points with the set of complex numbers now map to the north pole of the Riemann sphere. In this way, we can define the boundary $\{\infty\}$ and define the *extended complex numbers* $\mathbb{C} \cup \{\infty\}$. Lines in the complex plane are simply circles passing though ∞ in the Riemann sphere. That is, lines are just circles of infinite radius. ◀

My favorite number is infinity, because it can mean "forever and always." Also, the infinity symbol ∞ looks like two circles kissing.

2.7 Residues

Consider the Laurent series

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

We call the coefficient a_{-1} the *residue* of $f(z)$ at z_0. We'll denote the residue of $f(z)$ at z_0 as $\operatorname{Res}[f(z), z_0]$. Recall that for a closed path γ around z_0

$$\oint_\gamma (z - z_0)^n \, \mathrm{d}z = \begin{cases} 2\pi \mathrm{i}, & \text{if } n = -1 \\ 0, & \text{otherwise.} \end{cases}$$

Consider a function $f(z)$ which is analytic everywhere except at a pole z_0. We can compute the contour integral

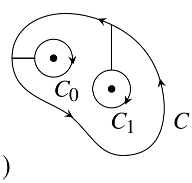
$$\begin{aligned} \oint_\gamma f(z) \, \mathrm{d}z &= \oint_\gamma \left(\sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \right) \mathrm{d}z \\ &= \sum_{n=-\infty}^{\infty} a_n \left(\oint (z - z_0)^n \, \mathrm{d}z \right) \\ &= 2\pi \mathrm{i} a_{-1} \\ &= 2\pi \mathrm{i} \operatorname{Res}[f(z), z_0] \end{aligned}$$

The Laurent series representation is only valid up to the nearest neighboring pole. If $f(z)$ has more than one pole (say at $z = z_0$ and $z = z_1$), we can use analytic continuation. We can choose a contour that excludes the poles. Inside this contour the function is analytic, so the contour integral is zero.

$$\oint_{C_0} f(z) \, \mathrm{d}z = 2\pi \mathrm{i} \operatorname{Res}[f(z), z_0]$$

$$\oint_{C_1} f(z) \, \mathrm{d}z = 2\pi \mathrm{i} \operatorname{Res}[f(z), z_1]$$

$$\oint_{C} f(z) \, \mathrm{d}z = 2\pi \mathrm{i} \left(\operatorname{Res}[f(z), z_0] + \operatorname{Res}[f(z), z_1] \right)$$



$\oint_\gamma f(z) \, \mathrm{d}z$ equals $\left\{ \begin{array}{l} 2\pi \mathrm{i} \text{ times the sum of the residues of all} \\ \text{poles inside the contour } \gamma. \end{array} \right.$

Because residues are so important, let's develop a few techniques for computing the residues of a function $f(z)$.

- If $f(z)$ has a simple pole at $z = z_0$, then

$$\text{Res}\,[f(z), z_0] = \lim_{z\to z_0}(z - z_0)f(z).$$

- If $f(z)$ has a double pole at $z = z_0$, then

$$\text{Res}\,[f(z), z_0] = \lim_{z\to z_0}\frac{\mathrm{d}}{\mathrm{d}z}\left[(z - z_0)^2 f(z)\right].$$

- In general, if $f(z)$ has an nth order pole at $z = z_0$, then

$$\text{Res}\,[f(z), z_0] = \lim_{z\to z_0}\frac{1}{(n-1)!}\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}\left[(z - z_0)^n f(z)\right].$$

- If f and g are both analytic at $z = z_0$ and g has a *simple zero* at z_0, then

$$\text{Res}\left[\frac{f(z)}{g(z)}, z_0\right] = \frac{f(z_0)}{g'(z_0)}.$$

  To prove this statement, we have from above that

$$\begin{aligned}\lim_{z - z_0}(z - z_0)\frac{f(z)}{g(z)} &= \lim_{z\to z_0}(z - z_0)\frac{f(z)}{g(z) - g(z_0)}\\ &= \lim_{z\to z_0}\frac{z - z_0}{g(z) - g(z_0)}f(z) = \frac{f(z_0)}{g'(z_0)}.\end{aligned}$$

  In the case that $f(z) = 1$, we have $\text{Res}\,[1/g(z), z_0] = 1/g'(z_0)$.

- We can extend the discussion above to consider the behavior of the function as $z \longrightarrow \infty$. One way to do this is to simply map ∞ to 0. In this case,

$$\text{Res}\,[f(z), \infty] = \text{Res}\,[f(1/z), 0].$$

Example. Compute the following residues:

$$\begin{aligned}&\text{Res}\left[\frac{1}{z^2+1}, \mathrm{i}\right] = \left.\frac{1}{2z}\right|_{z=\mathrm{i}} = \frac{1}{2\mathrm{i}}\\ &\text{Res}\left[\frac{1}{(z^2+1)^2}, \mathrm{i}\right] = \lim_{z\to \mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{(z+\mathrm{i})^2}\right] = \lim_{z\to i}\left.\frac{-2}{(z+\mathrm{i})^3}\right|_{z=\mathrm{i}} = \frac{1}{4\mathrm{i}}\\ &\text{Res}\left[\frac{\sin z}{z^2}, 0\right] = \lim_{z\to 0}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{\sin z}{z^2}z^2\right) = \cos z\Big|_{z=0} = 1\\ &\text{Res}\,[z+1, \infty] = \text{Res}\left[\frac{1}{z} + 1, 0\right] = 1\end{aligned}$$

◀

Example. Evaluate the following contour integrals:

$$\oint_{|z|=1} \frac{\sin z}{z^2}\,\mathrm{d}z = 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{\sin z}{z^2}, 0\right] = 2\pi\mathrm{i}$$

$$\oint_{|z|=1} \frac{z^2}{\sin z}\,\mathrm{d}z = 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{z^2}{\sin z}, 0\right] = 0$$

◀

Example. Classify the singularities and compute the residues of

$$f(z) = \frac{z^{-k}}{z+1}, \qquad 0 < k < 1.$$

The function has a singularity at $z = -1$ and $z = 0$. Let's start with the easy one, the simple pole at $z = -1$. The residue is

$$\mathrm{Res}\,[f(z), -1] = (-1)^k = (\mathrm{e}^{\mathrm{i}\pi})^k = \mathrm{e}^{\mathrm{i}\pi k}\,.$$

Any function with a logarithm or a noninteger power has a branch point. This function has a branch point at $z = 0$ with a branch cut extending to ∞. Let's take the branch cut along the negative real axis. Because the function is multivalued, the function does not have a Laurent series about $z = 0$. That is, there is no annulus about $z = 0$ in which the function is continuous. So, $f(z)$ has an essential singularity at $z = 0$. To find the residue we will use residue calculus

$$\mathrm{Res}\,[f(z), 0] = \frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{z^{-k}}{z+1}\,\mathrm{d}z$$

where γ is a closed contour encircling the origin. We need to be careful about the branch cut, because now any path will cross the branch cut and we need to consider the contribution from crossing the branch cut. Note that z^{1-k} is continuous near the origin for $0 < k < 1$. This suggests that we should cross near the origin. We can take any path γ, so let's take the simplest—a circle of radius ε. That is, take $z = \varepsilon\,\mathrm{e}^{\mathrm{i}\theta}$. Then $\mathrm{d}z = \varepsilon\,\mathrm{e}^{i\theta}\,\mathrm{i}\,\mathrm{d}\theta$. So,

$$\begin{aligned}\mathrm{Res}\,[f(z), 0] &= \frac{1}{2\pi\mathrm{i}} \int_{-\pi}^{\pi} \frac{\varepsilon^{-k}\,\mathrm{e}^{-\mathrm{i}k\theta}}{\varepsilon\,\mathrm{e}^{i\theta} + 1} \varepsilon\,\mathrm{e}^{i\theta}\,\mathrm{i}\,\mathrm{d}\theta \\ &= \frac{\varepsilon^{1-k}}{2\pi} \int_{-\pi}^{\pi} \frac{\mathrm{e}^{\mathrm{i}(1-k)\theta}}{\varepsilon\,\mathrm{e}^{i\theta} + 1}\,\mathrm{d}\theta.\end{aligned}$$

We can get an upper bound for the integrand by maximizing the numerator and minimizing the denominator to get $1/(1-\varepsilon)$. Then it follows that

$$\begin{aligned}\operatorname{Res}[f(z),0] &\leq \frac{\varepsilon^{1-k}}{2\pi}\int_{-\pi}^{\pi}\frac{1}{1-\varepsilon}\,\mathrm{d}\theta \\ &= \varepsilon^{1-k}\cdot\frac{1}{1-\varepsilon} \\ &\to 0 \text{ as } \varepsilon \to 0.\end{aligned}$$

So, the residue is zero. ◀

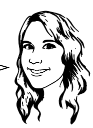
Example. Find the singularities and compute the residues of the function $z^2(\mathrm{e}^z-1)^{-1}$. The function $\mathrm{e}^z = 1$ whenever $z = 2\pi m\mathrm{i}$ for any integer m. So, $z^2(\mathrm{e}^z-1)^{-1}$ has simple poles at $z = 2\pi m\mathrm{i}$. To compute the residue use

$$\operatorname{Res}\left[\frac{f(z)}{g(z)}, z_0\right] = \frac{f(z_0)}{g'(z_0)}$$

where $f(z) = z^2$ and $g(z) = (\mathrm{e}^z-1)$ has a simple zero at $z = 2\pi m\mathrm{i}$. We then have for integer m

$$\operatorname{Res}\left[z^2(\mathrm{e}^z-1)^{-1}, 2\pi m\mathrm{i}\right] = z^2\,\mathrm{e}^{-z}\Big|_{z=2\pi m\mathrm{i}} = (2\pi m\mathrm{i})^2 = -4\pi^2 m^2. \quad ◀$$

Q: Why did the mathematician name his dog Cauchy?
A: Because he left a residue at every pole.



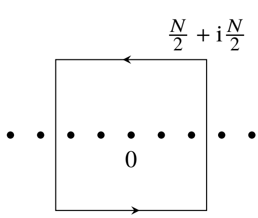
Example. Show that $\displaystyle\sum_{n=1}^{\infty}\frac{1}{n^2} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \cdots = \frac{\pi^2}{6}$.

The function

$$f(z) = \frac{\pi\cot(\pi z)}{z^2}$$

has poles at each integer along the real line and nowhere else in the complex plane. Take

$$\frac{1}{2\pi\mathrm{i}}\oint f(z)\,\mathrm{d}z = \sum_{-\frac{N}{2}<n<\frac{N}{2}} \operatorname{Res}[f(z),n]$$



where the contour is given by a square with sides at $z = \pm\frac{N}{2}$ and $z = \pm\mathrm{i}\frac{N}{2}$ where N is an odd integer.

To compute the residues $f(z)$ we use the Laurent series of $\pi\cot\pi z$ at $z = n$. From page 31:

$$\pi\cot\pi z = \frac{1}{z-n} - \frac{\pi^2(z-n)}{3} - \frac{\pi^4(z-n)^3}{45} - \frac{2\pi^6(z-n)^5}{945} - \cdots \tag{2.8}$$

Then for $n \neq 0$

$$\operatorname{Res}\left[\frac{\pi\cot\pi z}{z^2}, n\right] = \frac{1}{n^2}$$

and for $n = 0$

$$\operatorname{Res}\left[\frac{\pi\cot\pi z}{z^2}, 0\right] = -\frac{\pi^2}{3}.$$

Now let's compute the contour integral in the limit as $N \to \infty$. Note that

$$|\cot\pi z| = \left|\frac{\cos\pi z}{\sin\pi z}\right| = \left|\frac{\mathrm{e}^{\mathrm{i}2\pi z} + \mathrm{e}^{-\mathrm{i}2\pi z}}{\mathrm{e}^{\mathrm{i}2\pi z} - \mathrm{e}^{-\mathrm{i}2\pi z}}\right| = \left|\frac{\mathrm{e}^{\mathrm{i}2\pi x}\, e^{-2\pi y} + 1}{\mathrm{e}^{\mathrm{i}2\pi x}\,\mathrm{e}^{-2\pi y} - 1}\right|$$

and therefore

$$y = N/2: \qquad |\cot\pi z| = \left|\frac{\mathrm{e}^{\mathrm{i}2\pi x}\,\mathrm{e}^{-\pi N} + 1}{\mathrm{e}^{\mathrm{i}2\pi x}\,\mathrm{e}^{-\pi N} - 1}\right| \le \mathrm{e}^{-\pi N} + 1 < 2$$

$$y = -N/2: \qquad |\cot\pi z| = \left|\frac{\mathrm{e}^{\mathrm{i}2\pi x}\,\mathrm{e}^{\pi N} + 1}{\mathrm{e}^{\mathrm{i}2\pi x}\,\mathrm{e}^{\pi N} - 1}\right| \le \frac{e^{\pi N} + 1}{e^{\pi N} - 1} < 2$$

$$x = \pm N/2 \qquad |\cot\pi z| = \left|\frac{\mathrm{e}^{\mathrm{i}\pi N}\,\mathrm{e}^{-\mathrm{i}2\pi y} + 1}{\mathrm{e}^{\pi N}\,\mathrm{e}^{-2\pi y} - 1}\right| = \left|\frac{-\mathrm{e}^{-2\pi y} + 1}{-\mathrm{e}^{-2\pi y} - 1}\right| < 1$$

So $|\cot\pi z| < 2 + 2 + 1 + 1 = 4$ along our square contour. The perimeter of the square is $4N$. Therefore

$$\left|\frac{1}{2\pi\mathrm{i}}\oint f(z)\,\mathrm{d}z\right| \le \frac{1}{2}\left|\frac{\cot\pi z}{z^2}\right| \cdot \left|\oint \mathrm{d}z\right| \le \frac{1}{2}\frac{4}{N^2}\cdot 4N \to 0 \quad \text{as} \quad N \to \infty.$$

Combining all the terms

$$\left(\sum_{n=-\infty}^{-1}\frac{1}{n^2}\right) + \left(-\frac{\pi^2}{3}\right) + \left(\sum_{n=1}^{\infty}\frac{1}{n^2}\right) = 0$$

from which we have that

$$\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}.$$

This series is a type of *Dirichlet series*. With the Laurent series (2.8), we can evaluate the Dirichlet series for any even integer $2s$

$$\sum_{n=1}^{\infty}\frac{1}{n^{2s}} = \frac{(2\pi)^{2s}|B_{2s}|}{2(2s)!}$$

where B_{2s} is the $2s$th Bernoulli number. For example,

$$\sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90} \quad \text{and} \quad \sum_{n=1}^{\infty} \frac{1}{n^6} = \frac{\pi^6}{945}. \qquad \blacktriangleleft$$

Dirichlet's full name was "Johann Peter Gustav Lejeune Dirichlet." Now, that's a mouthful!

Mathematical detour. The Basel problem, posed in 1650, to find the sum of the Dirichlet series $1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \cdots + \frac{1}{n^2} + \cdots$ remained unsolved until 1734 when Leonhard Euler determined it to be $\pi^2/6$. He effectively did this by comparing the coefficients of the x^3 term of the infinte product

$$\sin \pi x = \pi x \left(1 - x^2\right)\left(1 - \frac{x^2}{4}\right)\left(1 - \frac{x^2}{9}\right)\cdots$$

with the Taylor Series

$$\sin \pi x = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots .$$

Rigorous proof of Euler's infinite product sine formulation wouldn't come for another hundred years when in 1876 Karl Weierstrass showed that any entire function can be expressed in terms of product of its zeros. The Weierstrass factorization theorem extends the fundamental theorem of algebra that allows us to express any polynomial as a unique product of its finite zeros $p(x) = c\prod_{i=1}^{n}(z - z_i)$ to an entire function with infinite zeros. ◀

2.8 Residue calculus

We can use *residue calculus* to integrate a real-valued function $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x$ by taking the semicircular contour over the upper (or lower) half-plane:

$$\underbrace{\oint f(z)\,\mathrm{d}z}_{\textcircled{1}} = \underbrace{\lim_{R\to\infty}\int_{-R}^{+R} f(x)\,\mathrm{d}x}_{\textcircled{2}} + \underbrace{\lim_{R\to\infty}\int_{0}^{\pi} f(R\,\mathrm{e}^{\mathrm{i}\theta})R\,\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta}_{\textcircled{3}}$$

Then ② = ① − ③, and hopefully it will be easier to find compute the contour integral ① instead of computing ② directly. For this to work, we must have

③ $\to 0$ as $R \to \infty$. We can put an upper bound on ③ by noting that an integral is bounded by the length of the circumference of the semi-circle times the maximum value of $\max |f(z)|$ along the semi-circle:

$$\int_\gamma f(z)\,\mathrm{d}z \leq ML \quad \text{where} \quad M = \max_{z\in\gamma} |f(z)| \quad \text{and} \quad L = \text{length of } \gamma.$$

We call this the *ML-estimate*. In this case,

$$③ : \qquad \left| \int_0^\pi f(R\,\mathrm{e}^{\mathrm{i}\theta})R\,\mathrm{e}^{\mathrm{i}\theta}\ \mathrm{d}\theta \right| \leq \pi R \cdot \max |f(z)|$$

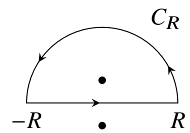
goes to zero as long as $f(z)$ goes to zero faster than R^{-1} as $R \to \infty$. A contour integral equals $2\pi\mathrm{i}$ times the sum of the residues of the poles inside the contour. If the contour is stretched to fill the whole upper half plane, then

$$① : \qquad \oint f(z)\,\mathrm{d}z \text{ equals } \begin{cases} 2\pi\mathrm{i} \text{ times the sum of the residues of all} \\ \text{poles in the upper half plane.} \end{cases}$$

Example. Evaluate $\displaystyle\int_{-\infty}^{\infty} \frac{\cos x}{1+x^2}\,\mathrm{d}x$.

It will be easier if we'll take the real part of $\displaystyle\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z$.

Take the contour integral



$$\oint \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z = \int_{-R}^{+R} \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z + \int_{C_R} \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z.$$

Because $|\,\mathrm{e}^{\mathrm{i}z}\,| \leq 1$ in the upper half plane, we have the ML-estimate

$$\left| \int_{C_R} \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z \right| \leq \frac{1}{R^2-1}\pi R \to 0 \quad \text{as } R \to \infty.$$

Now we just need to evaluate

$$\begin{aligned} \oint \frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}\,\mathrm{d}z &= 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{\mathrm{e}^{\mathrm{i}z}}{1+z^2}, \mathrm{i}\right] \\ &= 2\pi\mathrm{i}\left(\frac{f(z)}{g'(z)}\bigg|_{z=i} \right) = 2\pi\mathrm{i}\frac{\mathrm{e}^{\mathrm{i}z}}{2z}\bigg|_{z=\mathrm{i}} = \pi\,\mathrm{e}^{-1}. \end{aligned}$$

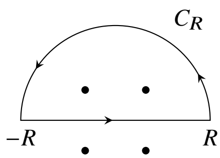
It follows that

$$\int_{-\infty}^{\infty} \frac{\cos x}{1+x^2}\,\mathrm{d}x = \frac{\pi}{\mathrm{e}}.$$

◀

Example. Evaluate $\displaystyle\int_{-\infty}^{\infty} \frac{1}{1+x^4}\,\mathrm{d}x$.

The function $g(z) = 1 + z^4$ has four zeros at $\sqrt[4]{-1}$. From $-1 = \{e^{i\pi}, e^{i3\pi}, e^{-i\pi}, e^{-i3\pi}\}$, we have that $\sqrt[4]{-1} = \{e^{i\pi/4}, e^{i3\pi/4}, e^{-i\pi/4}, e^{-i3\pi/4}\}$. The semicircular contour in the upper half-plane now contains two poles at $z = e^{i\pi/4}$ and $z = e^{i3\pi/4}$.



$$\oint \frac{1}{z^4+1}\,\mathrm{d}z = \int_{-R}^{+R} \frac{1}{1+z^4}\,\mathrm{d}z + \int_{C_R} \frac{1}{1+z^4}\,\mathrm{d}z$$

The path integral

$$\left|\int_{C_R} \frac{1}{1+z^4}\,\mathrm{d}z\right| \le \pi R \cdot \max_{z\in C_R}\left|\frac{1}{1+z^4}\right| \le \pi R\left|\frac{1}{R^4-1}\right| \to 0 \text{ as } R \to \infty$$

The contour integral

$$\begin{aligned}
\oint \frac{1}{z^4+1}\,\mathrm{d}z &= 2\pi i\left(\operatorname{Res}\left[\frac{1}{z^4+1}, e^{i\pi/4}\right] + \operatorname{Res}\left[\frac{1}{z^4+1}, e^{i3\pi/4}\right]\right)\\
&= 2\pi i\left(\left.\frac{1}{4z^3}\right|_{z=e^{i\pi}} + \left.\frac{1}{4z^3}\right|_{z=e^{i3\pi/4}}\right)\\
&= 2\pi i\left(\tfrac{1}{4}\,e^{-i3\pi/4} + \tfrac{1}{4}\,e^{-i9\pi/4}\right)\\
&= 2\pi i \cdot \tfrac{1}{2}\,e^{-i\pi/2} \cdot \left(\frac{e^{-i\pi/4} + e^{i\pi/4}}{2}\right)\\
&= \pi i \cdot e^{-i\pi/2} \cdot (\cos(\pi/4))\\
&= \pi i \cdot (-i) \cdot \left(1/\sqrt{2}\right)\\
&= \pi/\sqrt{2}.
\end{aligned}$$

So,

$$\int_{-\infty}^{\infty} \frac{1}{1+x^4}\,\mathrm{d}x = \pi/\sqrt{2}.$$

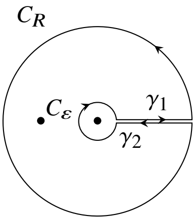
◀

Example. Evaluate $\displaystyle\int_{0}^{\infty} \frac{x^a}{(1+x)^2}\,\mathrm{d}x, \qquad -1 < a < 1.$

The numerator of the integrand x^a is not analytic for $a \ne 0$.

$$z^a = \left(|z|\,e^{i\arg z}\right)^a = |z|^a\,e^{ia\arg z}$$

A branch cut runs from the origin to ∞. We will take the branch cut along the positive real axis. Take the contour C that consists of the following path: γ_1 from ε to R along the real axis above the branch cut; the circular path C_R of radius R running counterclockwise from 0 to 2π; the path γ_2 from R to ε along the real axis below the branch cut; and the circular path C_ε of radius ε running clockwise from 2π to 0.



The contour integral is

$$\oint_C f(z)\,\mathrm{d}z = \int_{C_\varepsilon} f(z)\,\mathrm{d}z + \int_{C_R} f(z)\,\mathrm{d}z + \int_{\gamma_1} f(z)\,\mathrm{d}z + \int_{\gamma_2} f(z)\,\mathrm{d}z.$$

We will need to evaluate each of these integrals in turn. The function $z^a/(1+z)^a$ has a double pole at $z=-1$. Knowing this, we can evaluate

$$\begin{aligned}\oint_C \frac{z^a}{(1+z)^2}\,\mathrm{d}z &= 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{z^a}{(1+z)^2}, -1\right] \\ &= 2\pi\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}\,(z^a)\Big|_{z=-1} \\ &= 2\pi\mathrm{i}az^{a-1}\Big|_{z=-1} \\ &= 2\pi\mathrm{i}a\,\mathrm{e}^{\mathrm{i}\pi a}\,\mathrm{e}^{-\mathrm{i}\pi} \\ &= -2\pi\mathrm{i}a\,\mathrm{e}^{\mathrm{i}\pi a}\end{aligned}$$

Along the outer circular path integral

$$\left|\int_{C_R} \frac{z^a}{(1+z)^2}\,\mathrm{d}z\right| \le 2\pi R \max_{z\in C_R}\left|\frac{z^a}{(1+z)^2}\right| = 2\pi R\frac{R^a}{(R-1)^2} \sim R^{a-1}$$

and $R^{a-1} \to 0$ as $R \to \infty$. Along the inner circular path integral

$$\left|\int_{C_\varepsilon} \frac{z^a}{(1+z)^2}\,\mathrm{d}z\right| \le 2\pi\varepsilon \max_{z\in C_\varepsilon}\left|\frac{z^a}{(1+z)^2}\right| = 2\pi\varepsilon\frac{\varepsilon^a}{(1+\varepsilon)^2} \sim \varepsilon^{a+1}$$

and $\varepsilon^{a+1} \to 0$ as $\varepsilon \to 0$. Now let's consider the two path integrals along the positive real axis. Along the two paths, $\arg z = 0$ above the branch cut and $\arg z = 2\pi$ below the branch cut. That is, $z^a = |z|^a$ along γ_1 and $z^a = |z|^a\,\mathrm{e}^{\mathrm{i}a2\pi}$ along γ_2. So,

$$\int_{\gamma_1} \frac{z^a}{(1+z)^2}\,\mathrm{d}z = \int_\varepsilon^R \frac{x^a}{(1+x)^2}\,\mathrm{d}x$$

and

$$\int_{\gamma_2} \frac{z^a}{(1+z)^2}\,\mathrm{d}z = \int_R^\varepsilon \frac{|z|^a\,\mathrm{e}^{\mathrm{i}a2\pi}}{(1+z)^2}\,\mathrm{d}z = -\,\mathrm{e}^{\mathrm{i}2\pi a}\int_\varepsilon^R \frac{x^a}{(1+x)^2}\,\mathrm{d}x$$

Therefore,

$$\left(\int_{\gamma_1} + \int_{\gamma_2}\right)\frac{z^a}{(1+z)^2}\,\mathrm{d}z = \left(1-\mathrm{e}^{\mathrm{i}2\pi a}\right)\int_\varepsilon^R \frac{x^a}{(1+x)^2}\,\mathrm{d}x$$

Piecing everything back together

$$0+0+\left(1-\mathrm{e}^{\mathrm{i}2\pi}\right)\int_\varepsilon^R \frac{x^a}{(1+x)^2}\,\mathrm{d}x = \oint_C \frac{z^a}{(1+z)^2}\,\mathrm{d}z = -2\pi\mathrm{i}a\,\mathrm{e}^{\mathrm{i}\pi a}$$

in the limit as $R \to \infty$ and $\varepsilon \to 0$. Hence,

$$\int_0^\infty \frac{\mathrm{e}^{ax}}{(1+x)^2}\,\mathrm{d}x = \frac{-2\pi\mathrm{i}a\,\mathrm{e}^{\mathrm{i}\pi a}}{1-\mathrm{e}^{\mathrm{i}2\pi}} = \frac{-2\pi\mathrm{i}a}{\mathrm{e}^{-\mathrm{i}\pi}-\mathrm{e}^{\mathrm{i}\pi}} = \frac{\pi a}{\sin\pi a}.$$ ◀

Cauchy principal value

On occasion it may happen that a pole lies along the path over which we intend to integrate. For example,

$$\int_{-1}^1 \frac{1}{x}\,\mathrm{d}x = \lim_{\varepsilon\to0+}\int_{-1}^{-\varepsilon}\frac{1}{x}\,\mathrm{d}x + \lim_{\varepsilon\to0+}\int_\varepsilon^1 \frac{1}{x}\,\mathrm{d}x$$

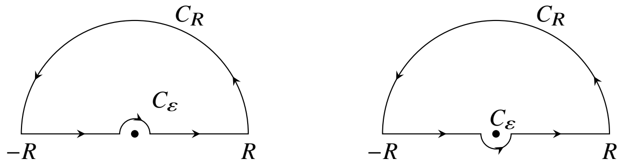
is undefined. Now, the function $1/x$ is an odd function, and we may try to argue that even though both integrals diverge, they diverge at exactly the same rate and cancel each other out. Namely, if we let both sides converge at the same rate we have

$$\int_{-1}^1 \frac{1}{x}\,\mathrm{d}x = \lim_{\varepsilon\to0+}\left(\int_{-1}^{-\varepsilon}\frac{1}{x}\,\mathrm{d}x + \int_\varepsilon^1 \frac{1}{x}\,\mathrm{d}x\right) = 0.$$

This is not true in general if we take the limits independently. For example, if we let the left limit converge twice as fast as the right we get an answer of $\log 2$. The *Cauchy principal value* of $f(x)$ with a pole at x_0 is defined as

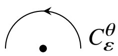
$$\mathrm{PV}\int_a^b f(x)\,\mathrm{d}x = \lim_{\varepsilon\to0+}\left(\int_a^{x_0+\varepsilon} f(x)\,\mathrm{d}x + \int_{x_0+\varepsilon}^b f(x)\,\mathrm{d}x\right).$$

For a contour in the complex plane, the validity of the principal value is a little easier to justify, because we only need to bend the contour slightly to sidestep the pole. We can do this by either excluding the pole or including the pole in our main contour. The results are the same because the first path runs contour clockwise (and excludes the pole) and the second path runs clockwise (and includes the pole).



The contribution of the ε-contour about a simple pole at $z = z_0$ is

$$\int_{C_\varepsilon^\theta} f(z)\,\mathrm{d}z = \mathrm{i}\theta\,\mathrm{Res}\,[f(z), z_0]$$



where θ is the angle that the ε-contour subtends. To see this consider $g(z) = (z - z_0)f(z)$. Note that $g(z)$ is analytic at z_0 because $f(z)$ has a simple pole at z_0. So, $\mathrm{Res}\,[f(z), z_0] = \lim_{z\to z_0} g(z)$. Take $z = z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta}$. Then $\mathrm{d}z = \mathrm{i}\varepsilon\,\mathrm{e}^{\mathrm{i}\theta}\ \mathrm{d}\theta$.

$$\begin{aligned}
\int_{C_\varepsilon^\theta} f(z)\,\mathrm{d}z &= \int_{C_\varepsilon^\theta} \frac{g(z)}{z - z_0}\,\mathrm{d}z \\
&= \int_0^\theta \frac{g(z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta})}{\varepsilon\,\mathrm{e}^{\mathrm{i}\theta}} \mathrm{i}\varepsilon e^{\mathrm{i}\theta}\,\mathrm{d}\theta \\
&= \int_0^\theta g(z_0 + \varepsilon\,\mathrm{e}^{\mathrm{i}\theta})\mathrm{i}\,\mathrm{d}\theta \\
&= \int_0^\theta \mathrm{Res}\,[f(z), z_0]\,\mathrm{i}\,\mathrm{d}\theta \qquad \text{(by taking } \varepsilon \to 0\text{)} \\
&= \mathrm{i}\theta\,\mathrm{Res}\,[f(z), z_0]\,.
\end{aligned}$$

Example. Evaluate $\displaystyle\int_0^\infty \frac{\log x}{x^2 - 1}\,\mathrm{d}x$.

First note that for $z \in (-\infty, 0)$ we have

$$\log(z) = \log|z| + \mathrm{i}\arg(-1) = \log|z| + \mathrm{i}\pi.$$

Therefore,

$$\int_{-\infty}^0 \frac{\log x}{x^2 - 1}\,\mathrm{d}x = \int_0^\infty \frac{\log(-x)}{x^2 - 1}\,\mathrm{d}x = \int_0^\infty \frac{\log x}{x^2 - 1}\,\mathrm{d}x + \mathrm{i}\int_0^\infty \frac{\pi}{x^2 - 1}\,\mathrm{d}x.$$

It follows that

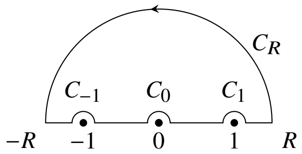
$$\int_{-\infty}^{\infty} \frac{\log x}{x^2-1}\,\mathrm{d}x = 2\int_0^{\infty} \frac{\log x}{x^2-1}\,\mathrm{d}x + \mathrm{i}\int_0^{\infty} \frac{\pi}{x^2-1}\,\mathrm{d}x$$

and so

$$\int_0^{\infty} \frac{\log x}{x^2-1}\,\mathrm{d}x = \tfrac{1}{2}\operatorname{Re}\int_{-\infty}^{\infty} \frac{\log x}{x^2-1}\,\mathrm{d}x.$$

Consider the contour to the right. We avoid the singularities at $z = -1$, 0, and 1 using semicircles of radius ε. The function

$$f(z) = \frac{\log z}{z^2-1}$$



is analytic inside the contour γ, so the integral is zero: $\oint_\gamma f(z)\,\mathrm{d}z = 0$. It follows that

$$\int_{-\infty}^{\infty} \frac{\log z}{z^2-1}\,\mathrm{d}z = -\lim_{\substack{R\to\infty\\ \varepsilon\to 0}} \left(\int_{C_{-1}} + \int_{C_0} + \int_{C_1} + \int_{C_R}\right) \frac{\log z}{z^2-1}\,\mathrm{d}z.$$

We have the ML-estimate along C_R

$$\begin{aligned}\int_{C_R} \frac{\log z}{z^2-1}\,\mathrm{d}z &\le \left(\frac{\log R}{R^2+1}\right)(\pi R)\\ &\approx \frac{\pi \log R}{R} \to 0 \quad \text{as} \quad R\to\infty.\end{aligned}$$

We also have the ML-estimate along C_0.

$$\begin{aligned}\int_{C_\varepsilon} \frac{\log z}{z^2-1}\,\mathrm{d}z &\le \left(\frac{\log \varepsilon}{1-\varepsilon^2}\right)(\pi \varepsilon)\\ &\approx \pi\varepsilon\log\varepsilon \to 0 \quad \text{as} \quad \varepsilon\to 0.\end{aligned}$$

Now let's compute the contributions from the poles at -1 and 1. Each of these contours runs clockwise from π to 0. At $z = -1$

$$\begin{aligned}\int_{C_{-1}} \frac{\log z}{z^2-1}\,\mathrm{d}z &= -\pi\mathrm{i}\operatorname{Res}\left[\frac{\log z}{z^2-1}, -1\right]\\ &= -\pi\mathrm{i}\frac{\log z}{2z}\bigg|_{z=-1} = -\pi\mathrm{i}\frac{\log(-1)}{-2} = -\pi\mathrm{i}\frac{\pi\mathrm{i}}{-2} = -\frac{\pi^2}{2}\end{aligned}$$

Similarly at $z = +1$

$$\int_{C_1} \frac{\log z}{z^2-1}\,\mathrm{d}z = -\pi\mathrm{i}\frac{\log z}{2z}\bigg|_{z=1} = 0.$$

So, we have that

$$\int_{-\infty}^{\infty} \frac{\log z}{z^2 - 1}\, \mathrm{d}z = \frac{\pi^2}{2}.$$

It follows that

$$\int_{0}^{\infty} \frac{\log z}{z^2 - 1}\, \mathrm{d}z = \frac{\pi^2}{4}.$$ ◀

Example. Evaluate $\displaystyle\int_0^\infty \frac{(\log x)^2}{x^2+1}\,\mathrm{d}x$.

Let's first break the integral up

$$\begin{aligned}\int_0^\infty \frac{(\log x)^2}{x^2+1}\,\mathrm{d}x &= \int_{-\infty}^\infty \frac{(\log x)^2}{x^2+1}\,\mathrm{d}x - \int_{-\infty}^0 \frac{(\log x)^2}{x^2+1}\,\mathrm{d}x \\ &= \int_{-\infty}^\infty \frac{(\log x)^2}{x^2+1}\,\mathrm{d}x - \int_0^\infty \frac{(\log(-x))^2}{x^2+1}\,\mathrm{d}x.\end{aligned}$$

Note that

$$\log(-z) = \log z + \log(-1) = \log z + \mathrm{i}\pi,$$

from which it follows that

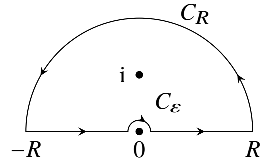
$$(\log(-z))^2 = (\log z)^2 - \pi^2 + 2\mathrm{i}\pi \log z.$$

Therefore, taking the real contributions

$$2\int_0^\infty \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z = \operatorname{Re}\left(\int_{-\infty}^\infty \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z\right) + \int_0^\infty \frac{\pi^2}{z^2+1}\,\mathrm{d}z.$$

For $f(z) = (\log z)^2/(z^2+1)$, the integral

$$\oint_\gamma f(z)\,\mathrm{d}z = \left(\int_{C_\varepsilon} + \int_\varepsilon^R + \int_{C_R} + \int_{-R}^{-\varepsilon}\right) f(z)\,\mathrm{d}z$$



equals

$$\begin{aligned}\oint_\gamma f(z)\,\mathrm{d}z &= 2\pi\mathrm{i}\operatorname{Res}\left[\frac{(\log z)^2}{z^2+1}, \mathrm{i}\right] \\ &= 2\pi\mathrm{i}\frac{(\log \mathrm{i})^2}{2\mathrm{i}} = \pi\left(\frac{\mathrm{i}\pi}{2}\right)^2 = -\frac{\pi^3}{4}\end{aligned}$$

due to the pole at $z = \mathrm{i}$. We have the ML-estimate along C_R

$$\int_{C_R} \frac{\log z}{z^2+1}\,\mathrm{d}z \le \left(\frac{(\log R)^2}{R^2-1}\right)(\pi R)$$
$$\approx \frac{\pi(\log R)^2}{R} \longrightarrow 0 \quad \text{as} \quad R \to \infty.$$

We also have the ML-estimate along C_ε

$$\int_{C_\varepsilon} \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z \le \left(\frac{(\log \varepsilon)^2}{1-\varepsilon^2}\right)(\pi\varepsilon) \approx \pi\varepsilon(\log\varepsilon)^2 \longrightarrow 0 \quad \text{as} \quad \varepsilon \to 0.$$

Therefore,

$$\int_{-\infty}^{\infty} \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z = \lim_{\substack{R\to\infty\\ \varepsilon\to 0}} \int_{\varepsilon}^{R} \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z + \int_{-R}^{-\varepsilon} \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z$$
$$= \oint_\gamma \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z = -\frac{\pi^3}{4}.$$

Note that because the value of this integral real, we also know that

$$\int_0^\infty \frac{\log z}{z^2+1}\,\mathrm{d}z = 0.$$

Finally, the integral

$$\int_0^\infty \frac{\pi^2}{x^2+1}\,\mathrm{d}x = \pi^2 \arctan x\Big|_0^\infty = \pi^2\left(\frac{\pi}{2}\right) = \frac{\pi^3}{2}.$$

So,

$$\int_0^\infty \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z = \frac{1}{2}\int_{-\infty}^{\infty} \frac{(\log z)^2}{z^2+1}\,\mathrm{d}z + \frac{1}{2}\int_0^\infty \frac{\pi^2}{z^2+1}\,\mathrm{d}z$$
$$= -\frac{\pi^3}{8} + \frac{\pi^3}{4} = \frac{\pi^3}{8}.$$

◀

Theorem (Jordan's Lemma)**.** *Suppose that $f(z)$ is analytic in the upper half plane except at finitely many singularities and that $|f(z)| \longrightarrow 0$ as $|z| \longrightarrow \infty$ in the upper half plane. Then*

$$\lim_{R\to\infty} \int_{C_R} f(z)\,\mathrm{e}^{\mathrm{i}az}\,\mathrm{d}z = 0 \quad \textit{for} \quad a > 0.$$

Proof.

$$\left|\int_{C_R} f(z)\,\mathrm{e}^{\mathrm{i}az}\,\mathrm{d}z\right| = \left|\int_0^{\pi} f(R\,\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{e}^{\mathrm{i}aR(\cos\theta+\mathrm{i}\sin\theta)}\,\mathrm{i}R\,\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta\right|$$
$$= \left|\int_0^{\pi} f(R\,\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{e}^{\mathrm{i}aR\cos\theta}\,e^{-aR\sin\theta}\mathrm{i}R\,\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta\right|$$
$$\le \int_0^{\pi} \left|f(R\,\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{e}^{\mathrm{i}aR\cos\theta}\,e^{-aR\sin\theta}\mathrm{i}R\,\mathrm{e}^{\mathrm{i}\theta}\right|\,\mathrm{d}\theta$$
$$= \int_0^{\pi} \left|f(R\,\mathrm{e}^{\mathrm{i}\theta})\right|\mathrm{e}^{-aR\sin\theta}\,R\,\mathrm{d}\theta$$

Taking $M_R = \max_{z\in C_R}|f(z)|$:

$$\le M_R R\int_0^{\pi}\mathrm{e}^{-aR\sin\theta}\,\mathrm{d}\theta$$
$$= 2M_R R\int_0^{\pi/2}\mathrm{e}^{-aR\sin\theta}\,\mathrm{d}\theta$$

Because $\sin\theta \ge 2\theta/\pi$ for $\theta \in [0, \pi/2]$:

$$\le 2M_R R\int_0^{\pi/2}\mathrm{e}^{-2aR\theta/\pi}\,\mathrm{d}\theta$$
$$\le 2M_R R\left(\frac{-\pi}{2aR\mathrm{i}}\right)\mathrm{e}^{-2aR\theta/\pi}\Big|_0^{\pi/2}$$
$$\le M_R\frac{\pi}{a}\left(1-\mathrm{e}^{-aR}\right).$$

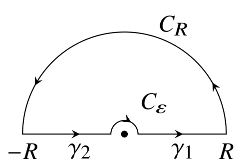
Because $|f(z)| \to 0$ as $|z| \to \infty$, so does $M_R \to 0$. It follows that

$$\lim_{R\to\infty}\int_{C_R} f(z)\,\mathrm{e}^{\mathrm{i}az}\,\mathrm{d}z = 0 \quad \text{for} \quad a > 0.$$ □

Example. Evaluate $\displaystyle\int_{-\infty}^{\infty}\frac{\sin x}{x}\,\mathrm{d}x$.

We'll compute this integral by finding the imaginary part of $\displaystyle\int_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}z}}{z}\,\mathrm{d}z$.

The function $f(z) = \mathrm{e}^{\mathrm{i}z}/z$ has a pole at $z = 0$, so we take the semicircular contour that avoids $z = 0$. The contour C is comprised of path γ_1 from ε to R along the positive real axis; semicircular path C_R of radius R running counterclockwise from 0 to π; the path γ_2 from $-R$ to $-\varepsilon$ along the negative real axis; and the semicircular path C_ε of radius ε running clockwise from π to 0.



Because there are no poles inside the contour, the contour integral is zero:

$$\oint_C f(z)\,\mathrm{d}z = \int_{C_\varepsilon} f(z)\,\mathrm{d}z + \int_{C_R} f(z)\,\mathrm{d}z + \int_{\gamma_1} f(z)\,\mathrm{d}z + \int_{\gamma_2} f(z)\,\mathrm{d}z = 0.$$

By Jordan's lemma

$$\lim_{R\to\infty} \int_{C_R} \frac{\mathrm{e}^{\mathrm{i}z}}{z}\,\mathrm{d}z = 0.$$

The path integral along C_ε in the limit as $r \to \varepsilon$ is

$$\lim_{r\to\varepsilon} \int_{C_\varepsilon} \frac{\mathrm{e}^{\mathrm{i}z}}{z}\,\mathrm{d}z = -\pi\mathrm{i}\,\mathrm{Res}\left[\frac{\mathrm{e}^{\mathrm{i}z}}{z}, 0\right] = -\pi\mathrm{i}\,\mathrm{e}^{\mathrm{i}z}\Big|_{z=0} = -\pi\mathrm{i}.$$

Therefore,

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}z}}{z}\,\mathrm{d}z = \lim_{\substack{R\to\infty \\ \varepsilon\to 0}} \left(\int_{\gamma_1} f(z)\,\mathrm{d}z + \int_{\gamma_2} f(z)\,\mathrm{d}z \right) = \pi\mathrm{i}.$$

So,

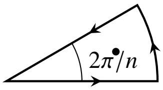
$$\int_{-\infty}^{\infty} \frac{\sin x}{x}\,\mathrm{d}x = \pi.$$

◀

Example. Evaluate $\displaystyle\int_0^\infty \frac{1}{1+x^n}\,\mathrm{d}x.$

The function $1 + z^n$ has n zeros each at

$$z = \sqrt[n]{-1} = \mathrm{e}^{\mathrm{i}(2k+1)\pi/n} \quad \text{for} \quad k = 0, \ldots, n-1.$$



There is one zero at $z = \exp(\mathrm{i}\pi/n)$, so $1/(1 + z^n)$ has a simple pole here. From this pole we will be able to compute a residue and evaluate the integral. We still need to be careful choosing the contour. We take the pie-shaped contour with angle $2\pi/n$. This contour is nice because it contains the pole, the contribution along C_R vanishes as the radius $R \to \infty$, and most importantly it will give us a path integral that we will be able to compute on the return trip. Remember, we need to be able compute the integrals along all paths.

$$\oint_\gamma \frac{1}{1+z^n}\,\mathrm{d}z = \int_{\gamma_1} \frac{1}{1+z^n}\,\mathrm{d}z + \int_{C_R} \frac{1}{1+z^n}\,\mathrm{d}z + \int_{\gamma_2} \frac{1}{1+z^n}\,\mathrm{d}z$$

First, note that

$$\begin{aligned}\oint_\gamma \frac{1}{1+z^n}\,\mathrm{d}z &= 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{1}{1+z^n}, \mathrm{e}^{\mathrm{i}\pi/n}\right]\\ &= 2\pi\mathrm{i}\frac{1}{nz^{n-1}}\bigg|_{z=\mathrm{e}^{\mathrm{i}\pi/n}}\\ &= \frac{2\pi\mathrm{i}}{n}\,\mathrm{e}^{-(n-1)\mathrm{i}\pi/n}\\ &= \frac{2\pi\mathrm{i}}{n}\,\mathrm{e}^{-\mathrm{i}\pi}\,\mathrm{e}^{\mathrm{i}\pi/n} = -\frac{2\pi\mathrm{i}}{n}\,\mathrm{e}^{\mathrm{i}\pi/n}\,.\end{aligned}$$

The ML-estimate gives us

$$\int_{C_R} \frac{1}{1+z^n}\,\mathrm{d}z \le \frac{1}{1+R^n}\left(\frac{2\pi}{n}R\right) \to 0 \text{ as } R \to \infty.$$

Along γ_1 we have

$$\int_{\gamma_1} \frac{1}{1+z^n}\,\mathrm{d}z = \int_0^R \frac{1}{1+r^n}\,\mathrm{d}r.$$

Note that along the return trip γ_2 we have $z = r\,\mathrm{e}^{\mathrm{i}2\pi/n}$, so

$$z^n = \left(r\,\mathrm{e}^{\mathrm{i}2\pi/n}\right)^n = r^n\,\mathrm{e}^{\mathrm{i}2\pi} = r^n \quad \text{and} \quad \mathrm{d}z = \mathrm{e}^{\mathrm{i}2\pi/n}\,\mathrm{d}r.$$

So,

$$\int_{\gamma_2} \frac{1}{1+z^n}\,\mathrm{d}z = \mathrm{e}^{\mathrm{i}2\pi/n}\int_R^0 \frac{1}{1+r^n}\,\mathrm{d}r = -\,\mathrm{e}^{\mathrm{i}2\pi/n}\int_0^R \frac{1}{1+r^n}\,\mathrm{d}r.$$

Therefore,

$$\int_{\gamma_1} \frac{1}{1+z^n}\,\mathrm{d}z + \int_{\gamma_2} \frac{1}{1+z^n}\,\mathrm{d}z = \left(1-\mathrm{e}^{\mathrm{i}2\pi/n}\right)\int_0^R \frac{1}{1+r^n}\,\mathrm{d}r.$$

And so

$$\left(1-\mathrm{e}^{\mathrm{i}2\pi/n}\right)\int_0^\infty \frac{1}{1+r^n}\,\mathrm{d}r = -\frac{2\pi\mathrm{i}}{n}\,\mathrm{e}^{\mathrm{i}\pi/n}$$

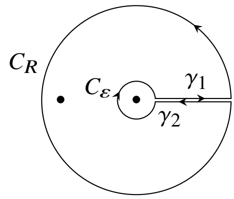
by the residue calculus above. We then have that

$$\begin{aligned}\int_0^\infty \frac{1}{1+r^n}\,\mathrm{d}r &= -\frac{2\pi\mathrm{i}}{n}\,\mathrm{e}^{\mathrm{i}\pi/n}\,\frac{1}{1-\mathrm{e}^{\mathrm{i}2\pi/n}}\\ &= -\frac{\pi}{n}\frac{2\mathrm{i}}{\mathrm{e}^{-\mathrm{i}\pi/n}-\mathrm{e}^{\mathrm{i}\pi/n}}\\ &= \frac{\pi/n}{\sin(\pi/n)}.\end{aligned}$$

◄

Example. Evaluate $\displaystyle\int_0^\infty \frac{x^{-a}}{1+x}\,\mathrm{d}x$ where $0 < a < 1$.

We know that $z^{-a} = \mathrm{e}^{-a\log z}$, so there is a branch point at $z = 0$. Because we are integrating along the positive real axis, we take the branch cut along the positive real axis. In this case, we have the keyhole contour which avoids the branch cut. The function has a pole at $z = -1$, so



$$\begin{aligned}\oint_C f(z)\,\mathrm{d}z &= \left(\int_{C_\varepsilon} + \int_{C_R} + \int_{\gamma_1} + \int_{\gamma_2}\right) f(z)\,\mathrm{d}z \\ &= 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{\mathrm{e}^{-a\log z}}{z+1}, -1\right] \\ &= 2\pi\mathrm{i}\,\mathrm{e}^{-a\log(-1)} = 2\pi\mathrm{i}\,\mathrm{e}^{-a\mathrm{i}\pi}\,.\end{aligned}$$

The ML-estimate gives us

$$\begin{aligned}\int_{C_R} \frac{z^{-a}}{1+z}\,\mathrm{d}z &\le \left(\frac{R^{-a}}{R-1}\right)\pi R \\ &= \frac{\pi R^{1-a}}{R-1} \approx \pi R^{-a} \to 0 \quad \text{as} \quad R \to \infty\end{aligned}$$

and

$$\begin{aligned}\int_{C_\varepsilon} \frac{z^{-a}}{1+z}\,\mathrm{d}z &\le \left(\frac{\varepsilon^{-a}}{1-\varepsilon}\right)\pi\varepsilon \\ &= \frac{\pi\varepsilon^{1-a}}{1-\varepsilon} \approx \pi\varepsilon^{1-a} \to 0 \quad \text{as} \quad \varepsilon \to 0.\end{aligned}$$

Along γ_1 we have

$$\int_{\gamma_1} \frac{\mathrm{e}^{-a\log z}}{z+1}\,\mathrm{d}z = \int_0^R \frac{\mathrm{e}^{-a\log r}}{r+1}\,\mathrm{d}r.$$

Along γ_2 we have $z = r\,\mathrm{e}^{\mathrm{i}2\pi}$, so

$$\begin{aligned}\int_{\gamma_2} \frac{\mathrm{e}^{-a\log z}}{z+1}\,\mathrm{d}z &= \int_R^0 \frac{\mathrm{e}^{-a(\log r+\mathrm{i}2\pi)}}{r+1}\,\mathrm{d}r \\ &= -\int_0^R \frac{\mathrm{e}^{-a\log r}\,\mathrm{e}^{-a\mathrm{i}2\pi}}{r+1}\,\mathrm{d}r \\ &= -\,\mathrm{e}^{-a\mathrm{i}2\pi}\int_0^R \frac{\mathrm{e}^{-a\log r}}{r+1}\,\mathrm{d}r.\end{aligned}$$

Therefore,

$$\left(1 - e^{ai2\pi}\right) \int_0^R \frac{r^{-a}}{r+1}\, dr = 2\pi i\, e^{-ai\pi}$$

from which it follows that

$$\int_0^R \frac{r^{-a}}{r+1}\, dr = \frac{2\pi i\, e^{-ai\pi}}{1 - e^{-ai2\pi}} = \frac{\pi}{\sin a\pi}.$$

◀

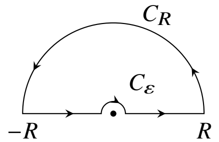
Example. Compute the Fourier transform of the sinc function

$$\int_{-\infty}^{\infty} \frac{\sin t}{t}\, e^{i\xi t}\, dt \quad \text{for real } \xi.$$

By using the Euler identity we have that

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\sin t}{t}\, e^{i\xi t}\, dt &= \int_{-\infty}^{\infty} \frac{e^{it} - e^{-it}}{2ti}\, e^{i\xi t}\, dt \\ &= \int_{-\infty}^{\infty} \frac{e^{i(\xi+1)t} - e^{i(\xi-1)t}}{2ti}\, dt \\ &= \int_{-\infty}^{\infty} \frac{e^{i(\xi+1)t}}{2ti}\, dt - \int_{-\infty}^{\infty} \frac{e^{i(\xi-1)t}}{2ti}\, dt.\end{aligned}$$

The functions $e^{i(\xi+1)z}/2zi$ and $e^{i(\xi-1)z}/2zi$ both have poles at $t = 0$. We can find the integral using a semicircular contour integral. Take $f(z) = e^{i(\xi+1)z}/2zi$. Then



$$\oint_C f(z)\, dz = \int_{C_\varepsilon} f(z)\, dz + \int_{C_R} f(z)\, dz + \int_{\gamma_1} f(z)\, dz + \int_{\gamma_2} f(z)\, dz = 0.$$

If $\xi > -1$, then $\xi + 1 > 0$, and by Jordan's lemma

$$\lim_{R\to\infty} \int_{C_R} \frac{e^{i(\xi+1)z}}{2i}\, dz = 0.$$

Note that Jordan's lemma does not hold when $\xi < -1$. We will have to treat that case separately. The path integral along C_ε in the limit is

$$\lim_{r\to\varepsilon} \int_{C_\varepsilon} \frac{e^{i(\xi+1)z}}{2zi}\, dz = -\pi i \operatorname{Res}\left[\frac{e^{i(\xi+1)z}}{2zi}, 0\right] = -\pi i \frac{e^{i(\xi+1)z}}{2zi}\bigg|_{z=0} = -\frac{\pi}{2}.$$

Therefore,

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi+1)z}}{2z\mathrm{i}}\,\mathrm{d}z = \lim_{\substack{R\to\infty \\ \varepsilon\to 0}} \left(\int_{\gamma_1} f(z)\,\mathrm{d}z + \int_{\gamma_2} f(z)\,\mathrm{d}z \right) = \frac{\pi}{2}$$

as long as $\xi > -1$.

If $\xi < -1$, we can either take a contour that goes through the lower half plane or make the change of variable $z \mapsto -z$. Both will allow us to use Jordan's lemma. The later approach is easier, so let's use that one. Let $z \mapsto -z$ and $\mathrm{d}z \mapsto -\mathrm{d}z$. Then we have

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi+1)z}}{2z\mathrm{i}}\,\mathrm{d}z = \int_{\infty}^{-\infty} \frac{\mathrm{e}^{-\mathrm{i}(\xi+1)z}}{-2z\mathrm{i}}\,(-\,\mathrm{d}z) = -\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(\xi+1)z}}{2z\mathrm{i}}\,\mathrm{d}z.$$

Now $-(\xi + 1) > 0$ and we can use Jordan's lemma as part of a contour integral almost identical to the one above. We have that

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi+1)z}}{2z\mathrm{i}}\,\mathrm{d}z = -\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(\xi+1)z}}{2z\mathrm{i}}\,\mathrm{d}z = -\frac{\pi}{2}$$

when $\xi < -1$.

We can compute the integral for $f(z) = \mathrm{e}^{\mathrm{i}(\xi-1)z}/2z\mathrm{i}$ almost identically as we did above. If $\xi > 1$, then we have

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(\xi-1)z}}{2z\mathrm{i}}\,\mathrm{d}z = \frac{\pi}{2}.$$

When $\xi < 1$, we must take $z \mapsto -z$ so that we can apply Jordan's lemma. In this case, we have that

$$\int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi-1)z}}{2z\mathrm{i}}\,\mathrm{d}z = -\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}(\xi-1)z}}{2z\mathrm{i}}\,\mathrm{d}z = -\frac{\pi}{2}.$$

Therefore,

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{\sin t}{t}\,\mathrm{e}^{\mathrm{i}\xi t}\,\mathrm{d}t &= \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi+1)t}}{2t\mathrm{i}}\,\mathrm{d}t - \int_{-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(\xi-1)t}}{2t\mathrm{i}}\,\mathrm{d}t \\
&= \begin{cases} (-\pi/2) - (-\pi/2) = 0, & \xi < -1 \\ \pi/2 - (-\pi/2) = \pi, & 1 < \xi < -1 \\ \pi/2 - \pi/2 = 0, & 1 < \xi \end{cases} \\
&= \begin{cases} 0, & |\xi| > 1 \\ \pi, & |\xi| < 1 \end{cases}
\end{aligned}$$

Finally, let's see what happens if $|\xi| = 1$. When $\xi = -1$, we have that

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\sin t}{t}\, e^{i\xi t}\, dt &= \int_{-\infty}^{\infty} \frac{1}{2ti}\, dt - \int_{-\infty}^{\infty} \frac{e^{-2it}}{2ti}\, dt \\ &= \int_{-\infty}^{\infty} \frac{1}{2ti}\, dt + \int_{-\infty}^{\infty} \frac{e^{2it}}{2ti}\, dt \\ &= 0 + \pi/2\end{aligned}$$

where the Cauchy principal value of the first integral is simply 0 and the second integral equals $\pi/2$ by the calculus of residues computed above. Similarly, we have that for $\xi = 1$ the integral is $\pi/2$. ◀

Example. Compute the Gaussian integral

$$\int_{-\infty}^{\infty} e^{-mx^2}\, dx \quad \text{for} \quad m > 0. \tag{2.9}$$

Sometimes you don't need complex analysis. Note that

$$\begin{aligned}\left(\int_{-\infty}^{\infty} e^{-x^2}\, dx\right)^2 &= \int_{-\infty}^{\infty} e^{-x^2}\, dx \int_{-\infty}^{\infty} e^{-y^2}\, dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-x^2} e^{-y^2}\, dx\, dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\, dx\, dy.\end{aligned}$$

Changing from Cartesian to polar coordinates:

$$\begin{aligned}&= \int_{0}^{2\pi}\int_{0}^{\infty} e^{-(r^2)}\, r\, dr\, d\theta \\ &= 2\pi \int_{0}^{\infty} e^{-r^2}\, r\, dr \\ &= 2\pi \left(-\tfrac{1}{2}\, e^{-r^2}\right)\Big|_0^{\infty} = \pi.\end{aligned}$$

Therefore,

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}.$$

By making a change of variables $x \longrightarrow x/\sqrt{m}$, we have

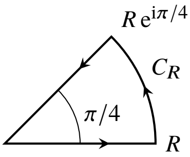
$$\int_{-\infty}^{\infty} e^{-mx^2}\, dx = \frac{1}{\sqrt{m}} \int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi/m}.$$ ◀

Example. Compute the Fresnel integrals

$$\int_0^\infty \cos(x^2)\,\mathrm{d}x \quad \text{and} \quad \int_0^\infty \sin(x^2)\,\mathrm{d}x.$$

We can compute both at once by taking the real and imaginary parts of $\int_0^\infty \exp(\mathrm{i}z^2)\,\mathrm{d}z$. We will try to rewrite this integral in terms of a Gaussian integral. We can integrate along a different path from 0 to ∞ as long as the contribution at ∞ is zero. Taking a path from the origin at angle $\theta = \pi/4$ should do the trick, because if $z = s\,\mathrm{e}^{\mathrm{i}\pi/4}$, then $\mathrm{i}z^2 = -s^2$.

Consider the pie-shaped contour on the right. The function $f(z) = \exp(\mathrm{i}z^2)$ is an entire function, so its integral is zero along the contour. And we have



$$\int_0^R f(z)\,\mathrm{d}z = \int_0^{R\,\mathrm{e}^{\mathrm{i}\pi/4}} f(z)\,\mathrm{d}z - \int_{C_R} f(z)\,\mathrm{d}z.$$

We'll start by showing that the contribution from the outer path vanishes. Take $u = z^2$, and let C_R^* be a the mapping of C_R under z^2, i.e., a quarter circle of radius R^2. Then Then $\mathrm{d}u = 2z\,\mathrm{d}z$ or equivalently $\mathrm{d}z = \mathrm{d}u/\sqrt{2u}$. Then

$$\int_{C_R} \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \int_{C_R^*} \frac{\mathrm{e}^{\mathrm{i}u}}{\sqrt{2u}}\,\mathrm{d}u \to 0 \quad \text{as} \quad R \to \infty$$

by Jordan's Lemma. We are left with

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \int_0^{\infty\,\mathrm{e}^{\mathrm{i}\pi/4}} \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z.$$

Taking $z = \mathrm{e}^{\mathrm{i}\pi/4}\,s$ and $\mathrm{d}z = \mathrm{e}^{\mathrm{i}\pi/4}\,\mathrm{d}s$:

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \mathrm{e}^{\mathrm{i}\pi/4} \int_0^\infty \mathrm{e}^{-s^2}\,\mathrm{d}s.$$

We can now evaluate the Gaussian integral to get

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \mathrm{e}^{\mathrm{i}\pi/4}\,\frac{\sqrt{\pi}}{2} = \frac{\sqrt{\pi}}{2}\left(\frac{1}{\sqrt{2}} + \frac{\mathrm{i}}{\sqrt{2}}\right)$$

So,

$$\int_0^\infty \cos(x^2)\,\mathrm{d}x = \operatorname{Re}\int_0^\infty \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \frac{\sqrt{\pi}}{2\sqrt{2}}$$

and

$$\int_0^\infty \sin(x^2)\,\mathrm{d}x = \operatorname{Im}\int_0^\infty \mathrm{e}^{\mathrm{i}z^2}\,\mathrm{d}z = \frac{\sqrt{\pi}}{2\sqrt{2}}.$$

◀

2.9 Method of steepest descent

Suppose that we want to estimate

$$I(s) = \int_a^b g(z)\, \mathrm{e}^{sf(z)}\, \mathrm{d}z, \quad \text{where} \quad s \gg 1$$

and $f(z)$ and $g(z)$ are analytic functions. Because the integrand is analytic, we can take any contour from a to b as long as the contour doesn't pass though a singularity. Of course, we should choose a contour that makes the integration easier.

Because $f(z) = u(z) + \mathrm{i}v(z)$ with $z = x + \mathrm{i}y$ is analytic, it cannot have a relative maximum or minimum—only a saddlepoint at which

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} = 0; \quad \text{and} \quad \frac{\partial^2 u}{\partial x^2} > 0, \ \frac{\partial^2 v}{\partial y^2} < 0 \quad \text{or} \quad \frac{\partial^2 u}{\partial x^2} < 0, \ \frac{\partial^2 v}{\partial y^2} > 0.$$

We'll assume that $f(z)$ has only one saddle point $z = z_0$. The case of more than one saddle point is a straight-forward generalization. We will choose a contour that passes through z_0 in some direction ϕ. In the neighborhood of z_0 we can approximate

$$f(z) \approx f(z_0) + \tfrac{1}{2} f''(z_0)(z - z_0)$$

because $f'(z_0) = 0$ at the saddle point. Our integral becomes

$$I(s) \approx \mathrm{e}^{sf(z_0)} \int_a^b g(z)\, \mathrm{e}^{\frac{1}{2} s f''(z_0)(z-z_0)^2}\, \mathrm{d}z.$$

In polar coordinates

$$f''(z_0) = |f''(z_0)|\, \mathrm{e}^{\mathrm{i}\theta} \quad \text{where} \quad \theta = \arg f''(z_0).$$

In the neighborhood of z_0, we can take the path $z = z_0 + r\, \mathrm{e}^{\mathrm{i}\phi}$. The integrand can now be written as

$$g(z)\, \mathrm{e}^{\frac{1}{2} s f''(z_0)(z-z_0)^2} = g(z)\, \mathrm{e}^{\frac{1}{2} s |f''(z_0)|\, \mathrm{e}^{\mathrm{i}\theta}\, r^2\, \mathrm{e}^{\mathrm{i}2\phi}}.$$

If we choose $\phi = \frac{1}{2}(\pi - \theta)$, the exponential term simplifies to the Gaussian function

$$\mathrm{e}^{-\frac{1}{2} s |f''(z_0)| r^2}.$$

This direction for ϕ happens to be the direction of steepest descent off the saddle point, giving the method its name. When $s \gg 1$, the integrand decays very rapidly once we have left the saddle-point. This means that it is a good approximation to only consider the contribution near the saddle point and throw out the very small contribution away from the saddle point. In this case, we can approximate $g(z) \approx g(z_0)$. We can also simply integrate along the entire straight line in the direction $\phi = \frac{1}{2}(\pi - \theta)$ through z_0 from infinity to infinity. Taking $z = z_0 + r\,\mathrm{e}^{\mathrm{i}\phi}$ we have that $\mathrm{d}z = \mathrm{e}^{\mathrm{i}\phi}\,\mathrm{d}r = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2}\,\mathrm{d}r$. Now we have the approximation

$$I(s) \approx g(z_0)\,\mathrm{e}^{sf(z_0)}\,\mathrm{i}\,\mathrm{e}^{\mathrm{i}\theta/2} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}s|f''(z_0)|r^2}\,\mathrm{d}r.$$

The integral is a Gaussian integral (2.9), so

$$I(s) \approx g(z_0)\,\mathrm{e}^{sf(z_0)}\,\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2} \left(\frac{2\pi}{s|f''(z_0)|}\right)^{1/2}. \tag{2.10}$$

Method of steepest descent (for $s \gg 1$):

$$\int_C g(z)\,\mathrm{e}^{sf(z)}\,\mathrm{d}z \approx \frac{\sqrt{2\pi}g(z_0)\,\mathrm{e}^{sf(z_0)}\,\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2}}{\sqrt{|sf''(z_0)|}}$$

where $\theta = \arg f''(z_0)$ and z_0 is a saddle point.

Example. Approximate the binomial coefficient

$$\binom{n}{m} = \frac{n!}{m!(n-m)!}$$

when n is large. The binomial coefficient tells us the number of ways that m objects can be chosen out of n objects. It also appears in the binomial expansion

$$(1+z)^n = 1 + nz^2 + \cdots + \binom{n}{m} z^m + \cdots + z^n. \tag{2.11}$$

By taking the contour integral of $(1+z)^n/z^{m+1}$, we have

$$\begin{aligned}\binom{n}{m} &= \frac{1}{2\pi\mathrm{i}} \oint \frac{(1+z)^n}{z^{m+1}}\,\mathrm{d}z \\ &= \frac{1}{2\pi\mathrm{i}} \oint \frac{1}{z} \left(\frac{1+z}{z^{m/n}}\right)^n \mathrm{d}z.\end{aligned}$$

Let $t = m/n$ for $0 < t < 1$, then

$$\binom{n}{m} = \frac{1}{2\pi\mathrm{i}} \oint \frac{1}{z}\,\mathrm{e}^{n(\log(1+z) - t\log z)}\,\mathrm{d}z.$$

Now we apply the method of steepest descent. We find the saddle point of the function $f(z) = \log(1+z) - t\log z$ by first computing its first two derivatives:

$$f'(z) = \frac{1}{1+z} - \frac{t}{z}$$
$$f''(z) = -\frac{1}{(1+z)^2} + \frac{t}{z^2}$$

The location of the saddle point z_0 is the solution to $f'(z_0) = 0$. That is, $z_0 = t/(1-t)$. We'll deform the contour to pass through the saddle point at z_0. So,

$$f(z_0) = -t\log t - (1-t)\log(1-t),$$
$$\theta = \arg f(z_0) = 0, \quad \text{and}$$
$$f''(z_0) = \frac{(1-t)^3}{t}.$$

Note that the saddle point $z_0 = m/(n-m)$ is real. Because $\theta = 0$, this saddle point is a minimum for $f(z)$ along the real axis. Taking $\phi = \frac{1}{2}(\pi - \theta) = \frac{1}{2}\pi$ means we are sending the contour through z_0 in the imaginary direction, along which $f(z)$ is a maximum. Finally, from (2.10) we have that

$$\begin{aligned}\binom{n}{m} &\approx \frac{1}{2\pi \mathrm{i}}\frac{1}{z_0}\,\mathrm{e}^{\mathrm{i}\pi}\,\mathrm{e}^{nf(z_0)}\left(\frac{2\pi}{nf''(z_0)}\right)^{1/2} \\ &= \frac{\exp\left[-n\left(t\log t + (1-t)\log(1-t)\right)\right]}{\sqrt{2\pi n t(1-t)}} \end{aligned} \tag{2.12}$$

where $t = m/n$. We can rewrite expression (2.12) explicitly as

$$\binom{n}{m} = \frac{n!}{m!(n-m)!} \approx \frac{1}{\sqrt{2\pi}}\frac{n^{n+\frac{1}{2}}}{m^{m+\frac{1}{2}}(n-m)^{n-m+\frac{1}{2}}}.$$

Let's check how good our approximation actually is. Taking $n = 88$ and $m = 18$,

$$\binom{88}{18} = 241856196073986978.$$

Our approximation using (2.12) is 2.4304×10^{18}, getting us to within half of one percent error. ◀

CHAPTER 3

Gamma Beta Zeta

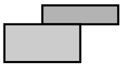
One of the underlying themes in the previous chapter was that real-valued functions are mere slices of complex-valued functions and that by understanding how a function behaves in the complex domain, we can better understand why the function behaves as it does along the real axis. In this chapter, we explore continuous function extensions of discrete functions and examine their analogues in the complex plane.

Mathematical detour. One of the philosophical questions of mathematics is whether mathematical ideas are discoveries or whether they are human inventions. Take numbers. In the physical universe numbers are adjectives that measure quantity of objects. We can talk about three kittens, three bicycles, three hydrogen atoms, and so forth. In the mathematical universe the number three is the object. We can talk about three threes. By abstracting the adjective "three" to a noun "three" we're able to be a bit more clever. Here's where the mathematics becomes really powerful. Cardinal numbers $\{1,2,3,4,\dots\}$ let us count and order objects. Natural numbers $\mathbb{N} = \{1,2,3,4,\dots\}$ let us add. If we add two numbers together $3+4=7$, we can undo the addition with subtraction $7-4=3$. But natural numbers are incomplete under subtraction $3-4 \notin \mathbb{N}$. We can complete the natural numbers under subtraction, by expanding them to integers $\mathbb{Z} = \{\dots,-3,-2,-1,0,1,2,\dots\}$. Multiplication $3\times 3 = 9$ ("three threes") has its inverse operation division $9/3 = 3$. Because integers are incomplete under division, we further need to expand them to the rational numbers $\mathbb{Q} = \{p/q \text{ where } p,q \in \mathbb{Z} \text{ and } q \neq 0\}$. We can also close the set by formally adding in ∞. Polynomials underpin algebra and geometry—take the Pythagorean formula $a^2+b^2=c^2$. Finding solutions to polynomial equations requires us to expand our universe to the algebraic numbers $\mathbb{A}$. Algebraic numbers include the irrational numbers like $\sqrt{3}$, $\sqrt{3+\sqrt{2}}$ and $\sqrt[5]{7}$. Of course, looking for roots of polynomials like x^2+1 requires us to also include complex algebraic numbers. Algebraic numbers are no longer sufficient when we include more novel functions and infinite series. The function $\sin x$ can't be expressed as a polynomial. We need a new set of numbers to fill in the gaps. These number are called transcendental numbers and include π and e. The transcendental numbers along with the algebraic numbers gives us real numbers $\mathbb{R}$ and complex numbers $\mathbb{C}$. Almost all real numbers are transcendental numbers. ◀

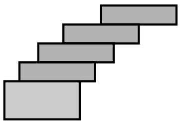
3.1 Harmonic numbers

Example. **Block stacking puzzle.** How can we stack n identical blocks on a table edge to maximize overhang?

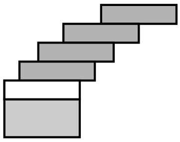
Suppose the blocks are two units in length with unit mass. With just one block, we could balance it half on, half off the table so that its center of mass is at the very edge of the table $x = 0$. The overhang for this one block is $H_1 = 1$.



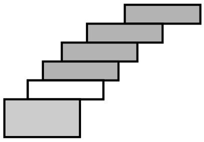
Now, suppose that we have $n - 1$ stacked, overlapping blocks positioned again so that the center of mass of the $n - 1$ blocks is at the very edge of the table. Let H_{n-1} be the total overhang for this set of blocks.



If we were to slip an additional block beneath the stack with its center at -1 so that its end lines up with the edge of the table, then the new center of mass for all n blocks is $nx = (n - 1) \cdot 0 - 1 \cdot 1$. That is, $x = -1/n$.



We can now shift the whole set of n stacked, overlapping blocks by $1/n$ so position its new center of mass is at the very edge of the table. The overhang for the stack is now $H_n = H_{n-1} + 1/n$. By induction, with $H_0 = 1$ we have that



$$H_n = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots + \frac{1}{n} = \sum_{k=1}^{n} \frac{1}{k}. \qquad ◀$$

The series $1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots$ is called the *harmonic series*. The partial sums of the harmonic series are the *harmonic numbers*. The sequence of harmonic numbers $\{1, \frac{3}{2}, \frac{11}{6}, \frac{25}{12}, \cdots\}$ diverges, but it diverges very slowly. We'd need 10^{43} terms before $H_n > 100$. The harmonic series is itself a special case of p-series or hyperharmonic series $\sum_{k=1}^{\infty} k^{-p}$ which we'll come back to at the end of this chapter.

> An infinite number of mathematicians walk into a bar. The first one orders a beer, the second orders half a beer, the third a third, the fourth a fourth at which point the bartender stops them and says "Get the hell out of here! Are you trying to ruin me?!"

Let's examine a couple of questions about harmonic numbers. What continuous function is a natural extension of the discrete sequence of harmonic numbers? How slowly does the sequence harmonic of harmonic numbers diverge?

The first question can be formulated as the problem

$$\text{Find } f(x) \text{ such that } f(n) = H_n = \sum_{k=1}^{n} \frac{1}{k}.$$

Leonard Euler solved this problem in the 1700s. If n is a positive integer,

$$\frac{1-x^n}{1-x} = 1 + x + x^2 + \cdots + x^{n-1}.$$

Integrating this rational gives us

$$\begin{aligned}\int_0^1 \frac{1-x^n}{1-x}\,\mathrm{d}x &= \int_0^1 (1 + x + x^2 + \cdots + x^{n-1})\,\mathrm{d}x \\ &= \left(x + \tfrac{1}{2}x^2 + \tfrac{1}{3}x^3 + \cdots + \tfrac{1}{n}x^n\right)\Big|_0^1 \\ &= 1 + \tfrac{1}{2} + \tfrac{1}{3} + \cdots + \tfrac{1}{n}.\end{aligned}$$

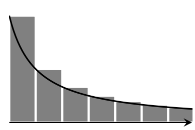
So, the continuous function

$$f(s) = \int_0^1 \frac{1-x^s}{1-x}\,\mathrm{d}x$$

interpolates the partial sums of the harmonic series.

Let's move to the other question of how slowly the sequence diverges. We can use an integral again—this time as an approximation:

$$\sum_{k=1}^{n} \frac{1}{k} \approx \int_1^n \frac{1}{x}\,\mathrm{d}x = \log x$$



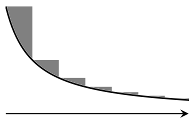
Of course, there is some error in this approximation. Even though both

$$\int_1^\infty \frac{1}{x}\,\mathrm{d}x \quad \text{and} \quad \sum_{n=1}^{\infty} \frac{1}{n}$$

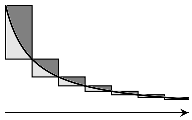
diverge, their differences converge:

$$\gamma = \lim_{n\to\infty}\left[\sum_{k=1}^{n}\frac{1}{k} - \int_1^n \frac{1}{x}\,\mathrm{d}x\right] = \lim_{n\to\infty}\left[\sum_{k=1}^{n}\frac{1}{k} - \log n\right].$$

The constant γ, equal to the shaded area in the plots to the right, is called the *Euler–Mascheroni constant*.

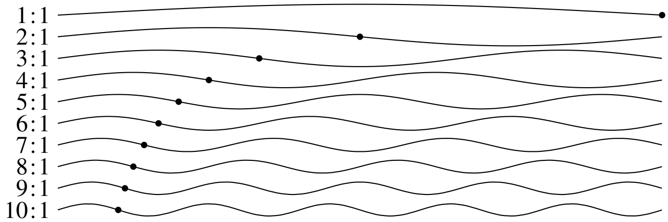


The total (light and dark) shaded area for all rectangles equals one when $n \to \infty$.

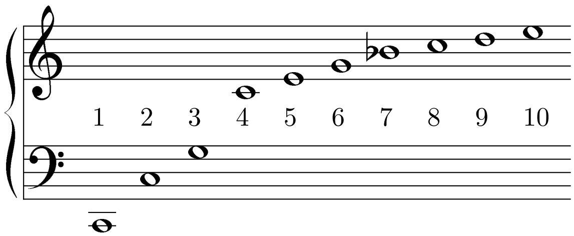


The curve $1/x$ almost evenly divides the rectangles, and it is convex so we can make a rough geometric estimate that γ is slightly larger that 0.5. The actual value is $\gamma = 0.5772156649\ldots$.

Mathematical detour. The harmonic series gets its name from harmonics in music. When a guitar or piano is played, the tone produced is the sum of both the fundamental tone and several diminishing overtones or harmonics. That is to say, every time a string vibrates, it resonates at all the harmonics frequencies (the fundamental tone and the overtones) with higher frequencies having diminishing amplitudes. The fundamental harmonic wavelength is twice the length of the guitar or piano string. The wavelength of the second harmonic is half that of the fundamental harmonic, and its tone is twice the frequency of the fundamental frequency. The wavelength of the third harmonic is one-third that of the first harmonic; its tone is three times the fundamental frequency. And so on. Below we see harmonics of a string along with nodes, positions where the wave is stationary.



Harmonics form the basis of tonal music. Take a piano's C_2 string. It resonates not only at its fundamental frequency, but every integer multiple of the fundamental frequency. The second harmonic frequency C_3, double that of the harmonic, is an octave higher. The third harmonic G_3, with three times the frequency of C_2, is a perfect twelfth (twelve tones) above C_2. The fourth harmonic C_4 is a two octaves up. The fifth harmonic E_4 is a perfect nineteenth with five times the frequency of C_2.



We can build the chromatic scale using these harmonics. Starting with G_3 (3 : 1) and dropping by an octave we get G_2 (3 : 2), a perfect fifth above C_2. Dropping two octaves from E_4 (5:1) we get E_2 (5:4). Dropping from E_4 (4:1) by twelve tones we get E_2 (4 : 3). We can continue like these to build a just diatonic scale:

C	D	E	F	G	A	B	C
1:1	9:8	5:4	4:3	3:2	5:3	15:8	2:1

The smaller the lowest common multiple between two harmonics, the more consonance in those two tones. The perfect octave (2:1) and perfect fifth (3:2) intervals are consonant. The greater the lowest common multiple between two harmonics, the more dissonance in those two tones.

A tritone, an interval of three whole tones such as F to B, is rather dissonant. The tritone is so dissonant that it's often called the devil's interval because of its sinister sound. The scaling from an F and a B is

$$(4:3) : (15:8) = 32:45$$

with a lowest common mulitple $32 \times 45 = 1440$. Play an F and B together or listen to Erik Satie's "Vexations"[1], Jimi Hendrix's "Purple Haze," or *The Twilight Zone* theme music, and you'll get the idea. Dissonance creates tension in music by making our brains feel unsettled and uncomfortable.

Usually we want the sweeter sounding consonance in music. The seventh harmonic is a prime number 7, and its lowest common multiple with respect to other harmonics will be high especially with the sixth (7×6) and fifth harmonics (7×5). The overtones from the seventh harmonic can contribute to harsh dissonance in a note. For this reason, the seventh harmonic is often suppressed in a piano by positioning the hammer one-seventh the distance along

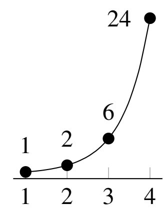
[1] No need to listen to the entire piece, which can last up to 30 hours, depending on the pianist's tempo.

the length of string to prevent a stationary node there. By the time we get to the next prime harmonic up, the eleventh harmonic, its contribution to the amplitude is sufficiently small.

Tuning isn't unique. Just intonation, which builds tones using harmonics 1 through 5, is not agnostic to key changes. Transposing from one key to another produces a very different tonality in the music. Modern tuning uses a twelve tone equal temperament tuning where the frequencies are scaled by $\sqrt[12]{2}$ with each semitone. In modern tuning a tritone is $\sqrt{2}:1$. The frequency of each note in modern tuning is within one-percent high-or-lower of just intonation. ◀

3.2 Gamma function

Like the question Euler asked about harmonic numbers H_n, there is also a natural question we can ask about factorials $n!$:"what continuous function is a natural extension of factorials?" We can in fact extend extend the factorial to an analytic function over the complex plane. This analytic extension is called the *gamma function*.



We start by defining the gamma function as

$$\Gamma(z) = \int_0^\infty e^{-t}\, t^{z-1}\, dt, \qquad \operatorname{Re}(z) > 0. \tag{3.1}$$

This integral is also called the *Euler integral of the second kind*. We'll come back to the Euler integral of the first kind later. Note that

$$\begin{aligned}\Gamma(z+1) &= \int_0^\infty e^{-t}\, t^{z}\, dt \\ &= -t^2\, e^{-t}\Big|_0^\infty + z\int_0^\infty e^{-t}\, t^{z-1}\, dt \\ &= z\Gamma(z),\end{aligned}$$

which provides us with the recursion $\Gamma(z+1) = z\Gamma(z)$. Furthermore, from (3.1) we have that

$$\Gamma(1) = \int_0^\infty e^{-t}\, t^0\, dt = 1.$$

From the recursion formula it follows that

$$\begin{aligned}\Gamma(2) &= 1,\\ \Gamma(3) &= 2\cdot 1,\\ \Gamma(4) &= 3\cdot 2\cdot 1,\\ \Gamma(5) &= 4\cdot 3\cdot 2\cdot 1, \ \ldots,\\ \Gamma(n+1) &= n!\end{aligned}$$

for integer values $n > 0$. Note that $\Gamma(n+1) = n!$—not $\Gamma(n) = n!$ as one might expect. The definition of the gamma function is a bit unfortunate, because it can easily lead to a mistake. The gamma function has a sibling special function, the *pi function* that conforms with the factorial as one might hope—$\Pi(z) = \Gamma(z+1)$ and so $\Pi(n) = n!$.

By making the change of variables $t = s^2$ so that $\mathrm{d}t = 2s\,\mathrm{d}s$, we have an alternate form of the gamma function

$$\Gamma(z) = \int_0^\infty \mathrm{e}^{-t}\, t^{z-1}\,\mathrm{d}t = 2\int_0^\infty \mathrm{e}^{-s^2}\, s^{2z-1}\,\mathrm{d}s, \qquad \mathrm{Re}(z) > 0. \tag{3.2}$$

By using this form of the gamma function we can evaluate the gamma function at half-integer values.

Example. Compute $\Gamma(\frac{1}{2})$.

$$\Gamma(\tfrac{1}{2}) = 2\int_0^\infty e^{-s^2}\,\mathrm{d}s = \int_{-\infty}^\infty e^{-s^2}\,\mathrm{d}s = \sqrt{\pi}$$ ◄

Example. Compute $\Gamma(\frac{3}{2})$.

$$\Gamma(\tfrac{3}{2}) = \tfrac{1}{2}\Gamma(\tfrac{1}{2}) = \tfrac{1}{2}\sqrt{\pi}$$ ◄

Because the integral (3.1) does not converge when $\operatorname{Re} z \le 0$, the integral definition of the gamma function is only valid in the right half-plane. But we can extend the gamma function to $\operatorname{Re} z \le 0$ using analytic continuation. To do this we will use the recursion formula $\Gamma(z+1) = z\Gamma(z)$. If $z > -1$ and $z \ne 0$, we have

$$\Gamma(z) = \frac{1}{z}\Gamma(z+1) = \frac{1}{z}\int_0^\infty \mathrm{e}^{-t}\, t^z\,\mathrm{d}t.$$

We see that the gamma function has a pole at $z = 0$. We can continue

$$\Gamma(z+2) = (z+1)\Gamma(z+1) = (z+1)z\Gamma(z),$$

and for an arbitrary m we have

$$\Gamma(z+m) = (z+m-1)\cdots(z+1)z\Gamma(z).$$

And so,

$$\Gamma(z) = \frac{\Gamma(z+m)}{(z+m-1)\cdots(z+1)z} \tag{3.3}$$

as long as z is not a negative integer at which points $\Gamma(z)$ has a simple pole.

Using (3.3) to compute the gamma function in the negative half plane can sometimes be cumbersome. A better approach may be to use Euler's reflection formula.

Theorem (Euler's reflection formula)**.** $\Gamma(z)\Gamma(1-z) = \dfrac{\pi}{\sin(\pi z)}$.

Proof. By analytic continuation we only need to show this identity when $z = a$ for $0 < \operatorname{Re} a < 1$.

$$\begin{aligned}
\Gamma(a)\Gamma(1-a) &= \int_0^\infty s^{-a}\,\mathrm{e}^{-s}\,\mathrm{d}s \int_0^\infty t^{a-1}\,\mathrm{e}^{-t}\,\mathrm{d}t \\
&= \int_0^\infty \int_0^\infty s^{-a} t^{a-1}\,\mathrm{e}^{-(s+t)}\,\mathrm{d}t\,\mathrm{d}s \\
&= \int_0^\infty \int_0^\infty (t/s)^{a-1}\,\mathrm{e}^{-s(1+t/s)}\,s^{-1}\,\mathrm{d}s\,\mathrm{d}t.
\end{aligned}$$

Making the change of variable $t = su$ and $\mathrm{d}t = s\,\mathrm{d}u$ we have

$$\begin{aligned}
&= \int_0^\infty \int_0^\infty u^{a-1}\,\mathrm{e}^{-s(1+u)}\,\mathrm{d}s\,\mathrm{d}u \\
&= \int_0^\infty u^{a-1}\left(\int_0^\infty \mathrm{e}^{-s(1+u)}\,\mathrm{d}s\right)\mathrm{d}u \\
&= \int_0^\infty u^{a-1}\left(\frac{1}{-(1+u)}\,\mathrm{e}^{-s(1+u)}\Big|_{s=0}^{\infty}\right)\mathrm{d}u \\
&= \int_0^\infty \frac{u^{a-1}}{(1+u)}\,\mathrm{d}u \\
&= \frac{\pi}{\sin \pi a}
\end{aligned}$$

where we evaluated the the last integral as a contour integral in the example on page 52. ◻

We can now compute the gamma function in the negative half plane

$$\Gamma(-z) = -\frac{\pi}{\Gamma(z+1)\sin(\pi z)}.$$

Note that $\Gamma(z)$ has poles at $z = 0, -1, -2, \ldots$. See the figure on the facing page.

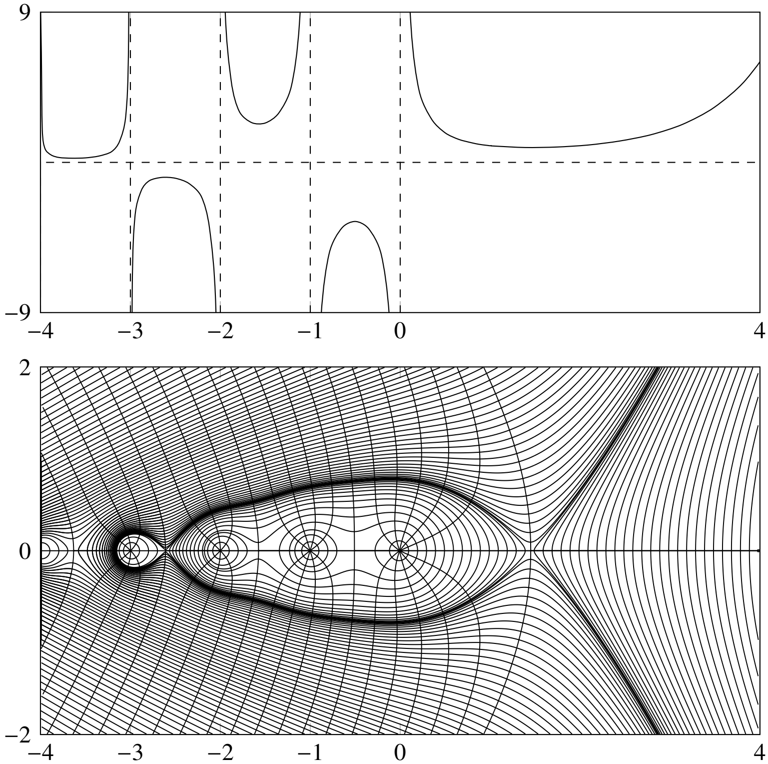


Figure : $\Gamma(z)$ is real for real z (top). Curves of constant phase and constant magnitude of $\Gamma(z)$ in the complex plane (bottom).

Euler's representation

Consider the function

$$F(z,n) = \int_0^n \left(1 - \frac{t}{n}\right)^n t^{z-1}\, \mathrm{d}t. \tag{3.4}$$

Note that

$$\left(1 - \frac{t}{n}\right)^n = \mathrm{e}^{n \log(1-t/n)} = \mathrm{e}^{n\left(-\frac{t}{n} + \frac{t^2}{n^2} - \cdots\right)}$$

which limits e^{-t} as $n \to \infty$. Hence,

$$\Gamma(z) = \int_0^\infty \mathrm{e}^{-t}\, t^{z-1}\, \mathrm{d}t = \lim_{n\to\infty} F(n,z).$$

By making the change of variables $t = nu$ in (3.4) we have

$$F(z,n) = n^z \int_0^1 (1-u)^n u^{z-1}\,\mathrm{d}u$$

and by integrating by parts we have that

$$\begin{aligned} F(z,n) &= n^z \left(\frac{n}{z} \int_0^1 (1-u)^{n-1} u^z \,\mathrm{d}u \right) \\ &= n^z \left(\frac{n(n-1)}{z(z+1)} \int_0^1 (1-u)^{n-2} u^{z+1} \,\mathrm{d}u \right) \\ &= \cdots \\ &= n^z \left(\frac{n(n-1)\cdots 1}{z(z+1)\cdots(z+n-1)} \int_0^1 u^{z+n-1} \,\mathrm{d}u \right) \\ &= n^z \left(\frac{n!}{z(z+1)\cdots(z+n)} \right). \end{aligned}$$

Therefore,

$$\Gamma(z) = \lim_{n\to\infty} \frac{n^z n!}{z\cdots(z+n)}.$$

Here's a summary of useful gamma function formulas:

$$\begin{aligned} (z-1)! = \Gamma(z) &= \int_0^\infty \mathrm{e}^{-t}\, t^{z-1}\,\mathrm{d}t, \qquad \mathrm{Re}(z) > 0 \\ \Gamma(z+1) &= z\Gamma(z) \\ \Gamma(\tfrac{1}{2}) &= \sqrt{\pi} \\ \Gamma(z)\Gamma(1-z) &= \frac{\pi}{\sin(\pi z)} \\ \Gamma(z) &= \lim_{n\to\infty} \frac{n^z n!}{z\cdots(z+n)} \end{aligned}$$

Example. Compute $\displaystyle\int_0^\infty \mathrm{e}^{-x^p}\,\mathrm{d}x,$ for $p > 0$.

For $t = x^p$ we have that $x = t^{1/p}$ from which $\mathrm{d}x = (1/p)t^{(1/p)-1}\,\mathrm{d}t$. Then

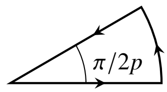
$$\int_0^\infty \mathrm{e}^{-x^p}\,\mathrm{d}x = \frac{1}{p}\int_0^\infty \mathrm{e}^{-t}\, x^{(1/p)-1}\,\mathrm{d}t = \frac{1}{p}\Gamma\left(\frac{1}{p}\right) = \Gamma\left(1+\frac{1}{p}\right).$$ ◀

Example. Compute $\displaystyle\int_0^\infty \cos(x^p)\,\mathrm{d}x$, with $p > 1$.

Note that the integral does not converge if $p \le 1$. Namely, if $p = 1$, then we are computing $\int_0^\infty \cos x\,\mathrm{d}x$ which is clearly divergent.

Let's find the real part of

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z$$



by examining the integral around the wedge γ. The function is analytic inside the contour so the contour integral is zero.

$$\int_0^R \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z + \int_{C_R} \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z - \int_0^{R\,\mathrm{e}^{i\pi/2p}} \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = 0.$$

First note that by making the change of variable $t = z^p$ with $\mathrm{d}z = p^{-1}t^{1-1/p}\,\mathrm{d}t$

$$\lim_{R\to\infty} \int_{C_R} \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = \lim_{R\to\infty} \int_{C'_R} \frac{1}{p}\,\mathrm{e}^{\mathrm{i}t}\,t^{1-1/p}\,\mathrm{d}t = 0$$

by Jordan's Lemma. So,

$$\int_0^R \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = \int_0^{R\,\mathrm{e}^{i\pi/p}} \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z.$$

Take $r = z\,\mathrm{e}^{\mathrm{i}\pi/2p}$. Then

$$z^p = \mathrm{e}^{-\mathrm{i}\pi/2}\,r^p = \mathrm{i}r^p \quad \text{and} \quad \mathrm{d}z = \mathrm{d}r\,\mathrm{e}^{-\mathrm{i}\pi/2p}\,.$$

And we have

$$\int_0^{R\,\mathrm{e}^{i\pi/2p}} \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = \int_0^R \mathrm{e}^{-r^p}\;\mathrm{e}^{\mathrm{i}\pi/2p}\;\mathrm{d}r = \mathrm{e}^{\mathrm{i}\pi/2p}\int_0^R \mathrm{e}^{-r^p}\;\mathrm{d}r$$

So,

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = \mathrm{e}^{-\mathrm{i}\pi/p}\int_0^\infty \mathrm{e}^{-r^p}\;\mathrm{d}r = \mathrm{e}^{\mathrm{i}\pi/2p}\,\Gamma\left(1+\frac{1}{p}\right).$$

Then taking the real part we have

$$\int_0^\infty \mathrm{e}^{\mathrm{i}z^p}\;\mathrm{d}z = \left(\cos\frac{\pi}{2p}\right)\Gamma\left(1+\frac{1}{p}\right).$$

◀

Example. **Stirling's approximation.** Often in mathematics and physics—both statistics and statistical mechanics—we need to use $n!$ when n is large. Taking the factorial of an number greater than 170 will typically cause overflow in computers. One approach is to use Stirling's approximation $n! \approx \sqrt{2\pi} n^{n+\frac{1}{2}} \mathrm{e}^{-n}$. We can derive Stirling's approximation using the method of steepest descent

$$\int_C g(z)\,\mathrm{e}^{sf(z)}\,\mathrm{d}z \approx \frac{\sqrt{2\pi}g(z_0)\,\mathrm{e}^{sf(z_0)}\,\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2}}{\sqrt{|sf''(z_0)|}} \tag{3.5}$$

with $\theta = \arg f''(z_0)$ where z_0 is a saddle point. Start with

$$n! = \Gamma(1+n) = \int_0^\infty t^n\,\mathrm{e}^{-t}\,\mathrm{d}t = n^{n+1}\int_0^\infty \mathrm{e}^{n(\log z - z)}\,\mathrm{d}z$$

where we made the substitution $t = nz$ and $\mathrm{d}t = n\,\mathrm{d}z$ to put the integral in the form (3.5). Then

$$f(z) = \log z - z, \quad f'(z) = \frac{1}{z} - 1, \quad \text{and} \quad f''(z) = -\frac{1}{z^2}.$$

We see that $f(z)$ has a saddle point at $z = 1$ and

$$\theta = \arg f''(1) = \arg(-1) = \pi.$$

So,

$$n! = \Gamma(n+1) \approx \frac{\sqrt{2\pi} n^{n+1}\,\mathrm{e}^{-n}}{\sqrt{n(-1)^{-2}}} = \sqrt{2\pi} n^{n+1/2}\,\mathrm{e}^{-n}.$$

Note that using Stirling's approximation for $n!$ and $m!$ in the binomial coefficient $\binom{m}{n} = n!/m!(n-m)!$ gives the same approximation that we found on page **??**. Another alternative to $\Gamma(n)$ when n is large is the log-gamma function $\log\Gamma(n)$. ◄

Example. **Fractional calculus.** Just as we can extend the factorial from integer values to noninteger values (including complex values) with the gamma function, we can also extend integer derivatives and antiderivatives to noninteger and complex values. The derivative of x^n is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}x^n &= nx^{n-1},\\ \frac{\mathrm{d}^2}{\mathrm{d}x^2}x^n &= n(n-1)x^{n-2}, \dots,\\ \frac{\mathrm{d}^k}{\mathrm{d}x^k}x^n &= n(n-1)\cdots(n+1-k)x^{n-k}\end{aligned}$$

which we can write as

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} x^n = \frac{n!}{(n-k)!} x^{n-k}.$$

Now we can formally define the kth derivative

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} x^n = \frac{\Gamma(n+1)}{\Gamma(n+1-k)} x^{n-k}.$$

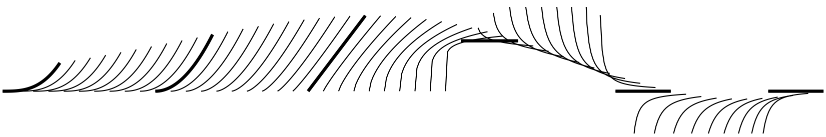
For example, the half-derivative of x^2 is

$$\frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}} x^2 = \frac{\Gamma(3)}{\Gamma(\frac{3}{2})} x^{1/2} = \frac{4}{\sqrt{\pi}} x^{3/2}.$$

Taking another half-derivative gives us a full derivative

$$\frac{\mathrm{d}}{\mathrm{d}x} x^2 = \frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}} \frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}} x = \frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}} \left(\frac{4}{\sqrt{\pi}} x^{1/2} \right) = \frac{4}{\sqrt{\pi}} \frac{\Gamma(\frac{5}{2})}{\Gamma(2)} x = 2x.$$

The following figure shows the zeroth through fifth fractional derivatives of $f(x) = x^3$ of the segment $x \in [0, \frac{3}{2}]$. Curves are offset for clarity, and integer derivatives $\{f^{(0)}, f^{(1)}, \dots, f^{(5)}\} = \{x^3, 3x^2, 6x, 6, 0, 0\}$ are bolded.



We can apply fractional derivatives to analytic functions. For example, the exponential function

$$\mathrm{e}^x = 1 + x + \tfrac{1}{2}x^2 + \tfrac{1}{3!}x^3 + \cdots = \sum_{n=1}^{\infty} \frac{x^n}{\Gamma(n+1)}$$

has the pth derivative

$$\frac{\mathrm{d}^p}{\mathrm{d}x^p} \mathrm{e}^x = \sum_{n=1}^{\infty} \frac{\Gamma(n+1)}{\Gamma(n+1-p)} \frac{x^n}{\Gamma(n+1)} x^{n-p} = \sum_{n=1}^{\infty} \frac{x^{n-p}}{\Gamma(n+1-p)}.$$

We can also compute an antiderivative by taking $k = -1$:

$$\frac{\mathrm{d}^{-1}}{\mathrm{d}x^{-1}} x^n = \frac{\Gamma(n+1)}{\Gamma(n+2)} x^{n+1}.$$

◀

Digamma function

The *logarithmic derivative* of a function f is given by $(\log f)' \equiv f'/f$ and tells us the relative change in f. The logarithmic derivative of the gamma function is called the digamma function:

$$\psi_0(z) = \frac{\mathrm{d}}{\mathrm{d}z} \log \Gamma(z).$$

Let's derive another expression for $\psi_0(z)$. Start with the following definition for the gamma function

$$\Gamma(z+1) = \lim_{n\to\infty} \frac{n!}{(z+1)\cdots(z+n)} n^z$$

and take the logarithm

$$\log \Gamma(z+1) = \lim_{n\to\infty} [\log n! + z \log n - \log(z+1) - \cdots - \log(z+n)].$$

Then

$$\begin{aligned}
\psi_0(z+1) &= \frac{\mathrm{d}}{\mathrm{d}z} [\log \Gamma(z+1)] \\
&= \lim_{n\to\infty} \left(\log n - \sum_{k=1}^{n} \frac{1}{z+k} \right) \\
&= \lim_{n\to\infty} \left(-\gamma + \sum_{k=1}^{n} \frac{1}{k} - \sum_{k=1}^{n} \frac{1}{z+k} \right) \\
&= -\gamma + \sum_{k=1}^{\infty} \left(\frac{1}{k} - \frac{1}{z+k} \right) = -\gamma + \sum_{k=1}^{\infty} \frac{z}{k(k+z)}.
\end{aligned}$$

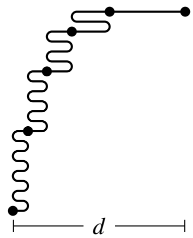
Note that $\gamma = \psi_0(1)$. When $z = m$ is an integer we have

$$\begin{aligned}
\psi_0(m+1) &= -\gamma + \left(\sum_{k=1}^{\infty} \frac{1}{k} - \sum_{k=1}^{\infty} \frac{1}{m+k} \right) \\
&= -\gamma + \left(\sum_{k=1}^{\infty} \frac{1}{k} - \sum_{k=m+1}^{\infty} \frac{1}{k} \right) \\
&= -\gamma + \sum_{k=1}^{m} \frac{1}{k} \\
&= -\gamma + H_m
\end{aligned}$$

where H_m is the mth harmonic number.

Example. **The Jeep problem.** Suppose a Jeep can travel one unit of distance on one drum of fuel and can carry at most one drum of fuel (in its tank). The Jeep can drive forward, drop off some of its fuel, and return to base to refuel and set out again. By storing the fuel in containers along the way, the Jeep progressively moves the base deeper into the desert. How far is the Jeep able to explore on n drums of fuel?

The Jeep can carry $n-1$ drums into the desert by making a total of $n-1$ forward trips and $n-2$ return trips, consuming one drum of fuel and moving the base camp forward a distance of $1/(2n-3)$. From this new base camp the Jeep carries $n-2$ drums of fuel a distance of $1/(2n-5)$ units to the next camp. All-in-all the base camp moves forward n times. For the last one the Jeep simply drives one unit on the remaining barrel of fuel. The total distance d is



$$\sum_{k=1}^{n} \frac{1}{2k-1} = \sum_{k=1}^{2n-1} \frac{1}{k} - \sum_{k=1}^{n-1} \frac{1}{2k}$$
$$= H_{2n-1} - \frac{1}{2} H_{n-1} = \psi_0(2n) - \frac{1}{2}\psi_0(n) + \frac{1}{2}\gamma. \qquad ◀$$

3.3 Beta function

The Euler beta function, a close relative of the gamma function, extends the binomial coefficient $\binom{p}{q}$ to non-integer values p and q. We define the beta function as

$$\mathrm{B}(p,q) = \int_0^1 t^{p-1}(1-t)^{q-1}\,\mathrm{d}t. \tag{3.6}$$

By making the change of variables $t = \sin^2\theta$, so that $\mathrm{d}t = 2\cos\theta\sin\theta\,\mathrm{d}\theta$, we have an alternative representation for the beta function

$$\mathrm{B}(p,q) = \int_0^{\pi/2} \sin^{2p-2}\theta \left(1 - \sin^{2q-2}\theta\right)(2\cos\theta\sin\theta)\,\mathrm{d}\theta$$
$$= 2\int_0^{\pi/2} \cos^{2p-1}\theta\,\sin^{2q-1}\theta\,\mathrm{d}\theta \tag{3.7}$$

Theorem. $\mathrm{B}(p,q) = \dfrac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}.$

Proof. By making the substitution $t = s^2$ with $\mathrm{d}t = 2s\,\mathrm{d}s$ in

$$\Gamma(p) = \int_0^\infty \mathrm{e}^{-t}\, t^{p-1}\,\mathrm{d}t$$

we have

$$\Gamma(p) = 2\int_0^\infty \mathrm{e}^{-s^2}\, s^{2p-1}\,\mathrm{d}s.$$

It follows that

$$\begin{aligned}\Gamma(p)\Gamma(q) &= 4\int_0^\infty \mathrm{e}^{-x^2}\, x^{2p-1}\,\mathrm{d}x \int_0^\infty \mathrm{e}^{-y^2}\, y^{2q-1}\,\mathrm{d}y \\ &= 4\int_0^\infty\int_0^\infty \mathrm{e}^{-(x+y)^2}\, x^{2p-1} y^{2q-1}\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

and switching from Cartesian to polar coordinates gives

$$\begin{aligned}&= 4\int_0^\infty\int_0^{\pi/2} \mathrm{e}^{-r^2}\, r^{2p-1}\cos^{2p-1}\theta r^{2p-1}\sin^{2q-1} r\,\mathrm{d}r\,\mathrm{d}\theta \\ &= 4\int_0^\infty \mathrm{e}^{-r^2}\, r^{2(p+q)-1}\,\mathrm{d}r \int_0^{\pi/2} \cos^{2p-1}\theta\,\sin^{2q-1}\,\mathrm{d}\theta \\ &= \Gamma(p+q)\,\mathrm{B}(p,q).\end{aligned}$$

□

Here's a summary of useful beta function formulas:

$$\mathrm{B}(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}$$

$$\binom{p}{q} = \mathrm{B}(p+1, q+1)$$

$$\mathrm{B}(p,q) = \int_0^1 t^{p-1}(1-t)^{q-1}\,\mathrm{d}t.$$

$$\mathrm{B}(p,q) = 2\int_0^{\pi/2} \cos^{2p-1}\theta\,\sin^{2q-1}\theta\,\mathrm{d}\theta$$

Example. Compute $\displaystyle\int_0^1 \frac{1}{\sqrt{1-x^4}}\,\mathrm{d}x$.

Take $u = x^4$. Then $u^{1/4} = x$ and $\frac{1}{4}u^{-3/4}\,\mathrm{d}u = \mathrm{d}x$.

$$\int_0^1 (1-x^4)^{-1/2}\,\mathrm{d}x = \int_0^1 u^{-1/2}\tfrac{1}{4}u^{-3/4}\,\mathrm{d}u = \mathrm{B}\left(\tfrac{1}{2}, \tfrac{1}{4}\right)$$

◀

Example. Compute $\int_0^\pi \sin^n x \, \mathrm{d}x$.

$$\begin{aligned}\int_0^\pi \sin^n x \, \mathrm{d}x &= 2\int_0^{\pi/2} \sin^n x \, \mathrm{d}x \\ &= 2\,\mathrm{B}\left(\frac{n+1}{2}, \frac{1}{2}\right) \\ &= 2\frac{\Gamma\left(\frac{n+1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{n}{2}+1\right)} = 2\sqrt{2}\frac{\Gamma\left(\frac{n}{2}+\frac{1}{2}\right)}{\Gamma\left(\frac{n}{2}+1\right)}.\end{aligned}$$

◀

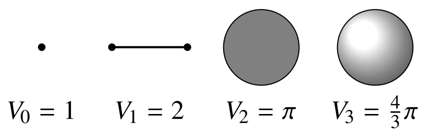
Example. The volume $V_n(r)$ of an n-dimensional ball of radius r can be defined recursively by $V_n(r) = rV_{n-1}\int_{-1}^1 \left(\sqrt{1-x^2}\right)^{n-1} \mathrm{d}x$. Let's find the explicit formula. Making the change of variables $u = x^2$ and $\mathrm{d}u = 2x\,\mathrm{d}x$ (so $\frac{1}{2}u^{-1/2}\,\mathrm{d}u = \mathrm{d}x$) we have that

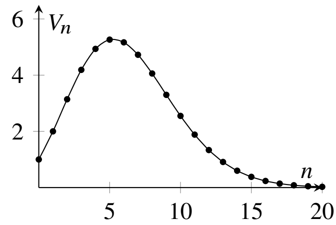
$$\begin{aligned}\int_{-1}^1 (1-x^2)^{(n-1)/2}\,\mathrm{d}x &= 2\int_0^1 (1-x^2)^{(n-1)/2}\,\mathrm{d}x \\ &= \int_0^1 (1-u)^{(n-1)/2}u^{-1/2}\,\mathrm{d}x \\ &= \mathrm{B}\left(\frac{1}{2}, \frac{n}{2}-1\right).\end{aligned}$$

So,

$$\begin{aligned}V_n(r) &= r\,\mathrm{B}\left(\frac{1}{2}, \frac{n}{2}+\frac{1}{2}\right)V_{n-1}(r) \\ &= r\frac{\Gamma(\frac{n}{2}+\frac{1}{2})\Gamma(\frac{1}{2})}{\Gamma(\frac{n}{2}+1)} \cdot V_{n-1}(r) \\ &= r^2\frac{\Gamma(\frac{n}{2}+\frac{1}{2})\Gamma(\frac{1}{2})}{\Gamma(\frac{n}{2}+1)} \cdot \frac{\Gamma(\frac{n}{2})\Gamma(\frac{1}{2})}{\Gamma(\frac{n}{2}+\frac{1}{2})} \cdot V_{n-2}(r) \\ &= r^n\frac{\cancel{\Gamma(\frac{n}{2}+\frac{1}{2})}\Gamma(\frac{1}{2})}{\Gamma(\frac{n}{2}+1)} \cdot \frac{\cancel{\Gamma(\frac{n}{2})}\Gamma(\frac{1}{2})}{\cancel{\Gamma(\frac{n}{2}+\frac{1}{2})}} \cdot \cdots \cdot \frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2})}{\cancel{\Gamma(\frac{3}{2})}} \cdot V_0(r) \\ &= \frac{\Gamma(\frac{1}{2})^n}{\Gamma(\frac{n}{2}+1)}r^n \\ &= \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}r^n\end{aligned}$$

This formula gives the volumes for $n = 1$, $n = 2$, and $n = 3$ that we already know, but we can also use it to consider the volumes of fractional dimensional spheres. ◀





3.4 Riemann zeta function

One way we to generalize the harmonic series $\sum_{k=1}^{\infty} k^{-1}$ is with a hyperharmonic or p-series $\sum_{k=1}^{\infty} k^{-p}$ where p is a real number. The partial sums of the p-series are *generalized harmonic numbers* $H_{n,p} = \sum_{k=1}^{n} k^{-p}$. When $p > 1$, the p-series converges. We evaluated the p-series for even integers p in the example on page 38. Specifically, we solved the Basel problem ($p = 2$) using contour integrals to get $H_{\infty,2} = \pi^2/6$.

The Riemann zeta function is the further generalization of the p-series to complex values:

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} \quad \text{for} \quad \operatorname{Re} s > 1.$$

When s is complex with real part strictly greater than one, we can define the Riemann zeta function using the equivalent integral representation

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{t^{s-1}}{\mathrm{e}^t - 1}\,\mathrm{d}t, \quad \operatorname{Re} s > 1. \tag{3.8}$$

To see this equivalency

$$\begin{aligned}
\int_0^{\infty} \frac{t^{s-1}}{\mathrm{e}^t - 1}\,\mathrm{d}t &= \int_0^{\infty} \mathrm{e}^{-t} \frac{t^{s-1}}{1 - \mathrm{e}^{-t}}\,\mathrm{d}t \\
&= \int_0^{\infty} \mathrm{e}^{-t}\, t^{s-1} \left(\sum_{n=0}^{\infty} (\mathrm{e}^{-t})^n \right) \mathrm{d}t \\
&= \int_0^{\infty} t^{s-1} \sum_{n=1}^{\infty} \mathrm{e}^{-nt}\,\mathrm{d}t \\
&= \sum_{n=1}^{\infty} \int_0^{\infty} t^{s-1}\,\mathrm{e}^{-nt}\,\mathrm{d}t
\end{aligned}$$

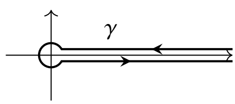
Making the substitution $t \longrightarrow t/n$ and $\mathrm{d}t \longrightarrow \mathrm{d}t/n$:

$$= \sum_{n=1}^{\infty} n^{-s} \int_0^{\infty} t^{s-1}\,\mathrm{e}^{-t}\,\mathrm{d}t = \zeta(z)\Gamma(z).$$

So,

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{t^{s-1}}{\mathrm{e}^t - 1}\,\mathrm{d}t.$$

To find an expression for $\zeta(s)$ when $\mathrm{Re}(s) < 1$ we can use analytic continuation. We'll do this using a *Hankel contour*: a contour γ that runs from infinity just above the positive real axis, circles around the origin, and then back to infinity below the positive real axis.



As before take $\mathrm{Re}\, s > 1$ as before, and define

$$\phi(s) = \int_{\gamma} \frac{(-z)^{s-1}}{\mathrm{e}^z - 1}\,\mathrm{d}z = \left(\int_R^{\varepsilon} + \int_{C_\varepsilon} + \int_{\varepsilon}^{R} \right) \frac{(-z)^{s-1}}{\mathrm{e}^z - 1}\,\mathrm{d}z.$$

Note that when $\mathrm{Re}\, s > 1$, the contribution from C_ε vanishes when $\varepsilon \longrightarrow 0$ by applying the ML-estimate. So, we can consider the integral in the limit as $\varepsilon \longrightarrow 0$ and $R \longrightarrow \infty$. Note that $(-z)^{s-1} = \mathrm{e}^{(s-1)(\log z - \mathrm{i}\pi)}$ has a branch cut running from the origin to infinity, which we'll take along the positive real axis. Across a branch cut, the logarithm jumps by $\mathrm{i}2\pi$. Along the upper portion of the contour $\log(-z) = \log r - \mathrm{i}\pi$ and along the lower portion of the contour $\log z = \log r + \mathrm{i}\pi$ where $r = |z|$. So

$$\begin{aligned}
\phi(s) &= \int_{\infty}^{0} \frac{\mathrm{e}^{(s-1)(\log r - \mathrm{i}\pi)}}{\mathrm{e}^r - 1}\,\mathrm{d}r + \int_0^{\infty} \frac{\mathrm{e}^{(s-1)(\log r + \mathrm{i}\pi)}}{\mathrm{e}^r - 1}\,\mathrm{d}r \\
&= -\mathrm{e}^{-\mathrm{i}\pi(s-1)} \int_0^{\infty} \frac{\mathrm{e}^{(s-1)\log r}}{\mathrm{e}^r - 1}\,\mathrm{d}r + \mathrm{e}^{\mathrm{i}\pi(s-1)} \int_0^{\infty} \frac{\mathrm{e}^{(s-1)\log r}}{\mathrm{e}^r - 1}\,\mathrm{d}r \\
&= \left(-\mathrm{e}^{-\mathrm{i}\pi(s-1)} + \mathrm{e}^{\mathrm{i}\pi(s-1)}\right) \int_0^{\infty} \frac{\mathrm{e}^{(s-1)\log r}}{\mathrm{e}^r - 1}\,\mathrm{d}r \\
&= \left(\mathrm{e}^{-\mathrm{i}\pi s} - \mathrm{e}^{\mathrm{i}\pi s}\right) \int_0^{\infty} \frac{\mathrm{e}^{(s-1)\log r}}{\mathrm{e}^r - 1}\,\mathrm{d}r \\
&= -2\mathrm{i}\sin(\pi s) \int_0^{\infty} \frac{r^{s-1}}{\mathrm{e}^r - 1}\,\mathrm{d}r \\
&= -2\mathrm{i}\sin(\pi s)\Gamma(s)\zeta(s) = -2\mathrm{i}\pi \frac{\zeta(z)}{\Gamma(1-z)}
\end{aligned}$$

And we have that

$$\zeta(s) = \frac{-1}{2\mathrm{i}\sin(\pi s)\Gamma(s)}\phi(s) = \frac{-1}{2\mathrm{i}\sin(\pi s)\Gamma(s)}\int_\gamma \frac{(-z)^{s-1}}{\mathrm{e}^z - 1}\,\mathrm{d}z.$$

Finally, by using Euler's reflection formula, we have that

$$\zeta(s) = \frac{\mathrm{i}\Gamma(1-s)}{2\pi}\phi(s) = \frac{\mathrm{i}\Gamma(1-s)}{2\pi}\int_\gamma \frac{(-z)^{s-1}}{\mathrm{e}^z - 1}\,\mathrm{d}z. \tag{3.9}$$

By analytic continuation this expression defines the Riemann zeta function for all complex numbers.

Example. Compute $\zeta(-n)$ for $n = 0, 1, 2, 3, \ldots$.

We'll use (3.9) to compute $\zeta(-n)$. From the example on page 30, the Laurent series

$$\frac{(-z)^{-(n+1)}}{\mathrm{e}^z - 1} = (-1)^{n+1}\sum_{m=0}^{\infty}\frac{B_m}{m!}z^{m-(n+1)}$$

where the Bernoulli numbers $\{B_0, B_1, B_2, \ldots\} = \{1, -\frac{1}{2}, \frac{1}{6}, 0, -\frac{1}{30}, 0, \frac{1}{42}, 0\ldots\}$. For negative integers n

$$\int_\gamma \frac{(-z)^{n-1}}{\mathrm{e}^z - 1}\,\mathrm{d}z = 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{(-z)^{n-1}}{\mathrm{e}^z - 1}, 0\right] = 2\pi\mathrm{i}(-1)^{n+1}\frac{B_{n+1}}{(n+1)!}.$$

So,

$$\zeta(-n) = (-1)^{n+1}\frac{B_{n+1}}{n+1} \quad \text{for} \quad n = 0, 1, 2, 3, \ldots$$

That is,

$$\{\zeta(0), \zeta(-1), \zeta(-2), \ldots\} = \left\{-\tfrac{1}{2}, \tfrac{1}{12}, 0, \tfrac{1}{120}, 0, -\tfrac{1}{252}, 0, \tfrac{1}{240}, 0, \ldots\right\}. \quad ◀$$

If $\zeta(s)$ is the analytic continuation of the Dirichlet series then does

$$1 + 1 + 1 + 1 + \cdots = -\tfrac{1}{2}$$

$$1 + 2 + 3 + 4 + \cdots = \tfrac{1}{12}$$

How peculiar.*

*There appears to be some mathematical slight of hand. How can a clearly divergent sequence of partial sums actually have a finite or defined limit? It can't. We computed zeta function $\zeta(0) = -\frac{1}{2}$ and $\zeta(-1) = \frac{1}{12}$. And, the zeta function is indeed the analytic continuation of the Dirichlet series $\sum_{n=1}^{\infty} n^{-s}$. But, the Dirichlet series is only defined for $\operatorname{Re} s > 1$. This means that series representation of the zeta function isn't quite valid for $s = 0$ or $s = -1$. Your faith in mathematics can be restored.

Mathematical detour. From the example on the preceding page, we know that the Riemann zeta function has zeros at negative even integers. Where are the other zeros of the Riemann zeta function? They are conjectured to all lie along the line $z = \frac{1}{2} + \mathrm{i}y$. At least this is the million dollar question—quite literally. The Riemann Hypothesis, that the real part of all non-trivial zeros of the Riemann zeta function is $\frac{1}{2}$, is one of Clay Institute's Millennium Prize Problems, and proving it will land you a cool million dollars. This problem has remained unsolved since Bernhard Riemann first proposed it in 1859, and many of the world's top mathematicians have taken their crack at it. Part of the reason why this problem is important is that the Riemann zeta function links two areas of mathematics together: complex analysis and number theory together.

The Riemann zeta function plays an important role in the Prime Number Theorem (PNT) which describes the distribution of prime numbers as $\pi(N) \sim N/\log N$, where the prime counting function $\pi(N)$ is the number of prime numbers less than the integer N. Digging deeper into the PNT would take us on too far of a detour, but we can take a shorter detour to examine another of the ways the Riemann zeta function touches on prime numbers.

Take the following question. If we choose n integers at random, what is the probability that all of these integers have a common factor? For example, the four integers 1625, 4030, 6032, and 923 are all divisible by 13. If p is a prime, then the probability any randomly chosen integer is divisible by p is $1/p$. The probability that all n random numbers are divisible by p is p^{-n}. Alternatively, the probability that any one of these n integers is not divisible by p is $1 - p^{-n}$. So, the probability that there is no factor that divides all n integers is the product of all primes

$$\prod_{p \text{ prime}} (1 - p^{-n})$$

This product, called an *Euler product*, is simply the reciprocal of the zeta function $1/\zeta(n)$. To see this we expand the Dirichlet series

$$\zeta(n) = 1 + 2^{-n} + 3^{-n} + 4^{-n} + \cdots . \tag{3.10}$$

First, by multiplying by 2^{-n} and subtracting this new expression from the original one (3.10) removes terms that have a factor 2^{-n}:

$$(1 - 2^{-n})\,\zeta(n) = 1 + 3^{-n} + 5^{-n} + 7^{-n} + \cdots . \tag{3.11}$$

Next, by multiplying (3.11) by 3^{-n} and subtracting this expression from (3.11) removes terms that have a factor 3^{-n}:

$$(1 - 3^{-n})(1 - 2^{-n})\,\zeta(s) = 1 + 5^{-n} + 7^{-n} + 11^{-n} + 13^{-n} + \cdots . \tag{3.12}$$

By continuing this way, we successively remove terms that have remaining prime factors 5^{-n}, 7^{-n}, 11^{-n}, ... leaving 1 on the right hand side:

$$\cdots(1-7^{-n})(1-5^{-n})(1-3^{-n})(1-2^{-n})\,\zeta(n) = 1.$$

Therefore,

$$\zeta(n) = \prod_{p \text{ prime}} \frac{1}{1-p^{-n}}.$$

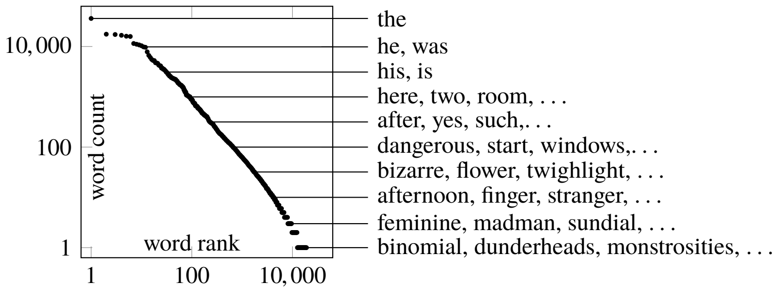
Using the values of $\zeta(2)$ and $\zeta(4)$ in the example on page 38, we find that there is roughly a 40% chance that any two numbers chosen at random have a factor in common. For four numbers, the likelihood of a common factor drops to 8%. ◄

Mathematical detour. George Zipf was a linguist who noticed that a few words, like "the," "is," "of," and "and," are used quite frequently while most words, like "anhydride," "embryogenesis," and "jackscrew," are rarely used at all. By examining word frequency rankings across several corpa, Zipf made a statistical observation, now called Zipf's law. The empirical law states that in any natural language corpus the frequency of any word is inversely proportional to its rank in a frequency table. That is, the most common word is twice as likely to appear as the second most common word, three times as common to appear as the third most common word, and n times as likely as the nth most common word. In other words, Zipf's law describes a harmonic distribution. Succinctly, $f_k = k^{-1}/H_n$ where H_n is the nth harmonic number. With roughly $n = 170{,}000$ unique words English language, $H_n \approx \log n + \gamma \approx 12.62$. By Zipf's law we should expect the top ranking word "the" to appear once in roughly every thirteen words. The Corpus of Contemporary American English (COCA) includes 22 million "the"s out of 450 million words, roughly one in every twenty words. Zipf's law isn't too far off, but it gets better. The word "word" ranks 245, so by Zipf's law we should expect "word" once out of every 3087 words. In COCA, it is one out of every 2940 words. The word "forever" ranks 2099, and by Zipf's law it should appear once out of every 26 thousand words. This frequency matches COCA to within 0.5 percent.

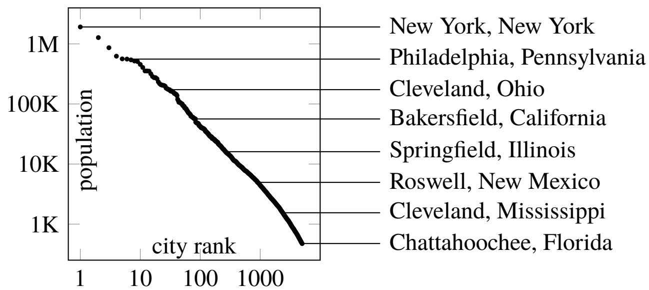
By summing over the top k-ranking words, we have the cumulative distribution function H_k/H_n. With a thousand words ($H_k = 7.48$) we can account for roughly 60 percent ($H_k/H_n = 0.59$) of all words used. The xkcd book *Thing Explainer* takes up a self-imposed challenge of using only the thousand most common words to describe complicated things, calling for example organs "bags of stuff inside you," the heart the "blood pusher," and saliva "mouth water."

The zeta distribution, which generalizes Zipf's law to a power series with $f_k = k^{-s}/\zeta(s)$ or $f_k = k^{-s}/H_{n,s}$, can provide a more accurate empirical law. Let's look at the canon of Sherlock Holmes by Sir Arthur Conan Doyle. Of the

662,817 words that appear in the cannon 18,951 are unique. The word “the” appears 36,125 times. “Holmes” appears 3051 times, “Watson” 1038 times, and “Moriarty”[†] appears 54 times. And there are 6610 words like “binomial,” “dunderheads,” “monstrosities,” “sunburnt,” “vandetta” that appear only once. Fitting the distribution, we can find that power $s = 1.1$.



Zipf’s law applies to more than just words. We can use it to model the size of cities, magnitude of earthquakes, and even distances between galaxies. The log-log plot below shows the population of US cities against their associated ranks. The power $s = 1.16$.



By extending the simple discrete ranking k into a continuous variable x, the zeta distribution $f_k = k^{-s}/\zeta(s)$ becomes a *Pareto distribution* $f(x) = \alpha x^{-(\alpha+1)}$ for a scaled $x \in [1, \infty)$ and the Pareto index $\alpha = s - 1$. Note that the Pareto cumulative distribution function $F(x) = \int_1^x f(t)\,\mathrm{d}t = 1 - x^{-\alpha}$.

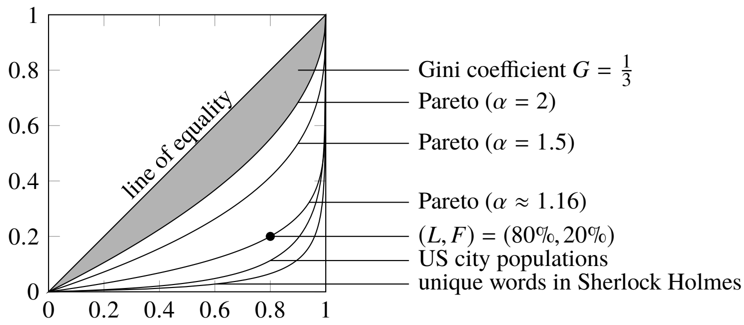
Because the zeta distribution and Pareto distribution measure magnitude against ranking, they often appear in context of the Lorenz curve. The Lorenz curve is a graphical representation of disparity created by plotting the cumulative

[†]Professor James Moriarty—criminal mastermind and archenemy of Sherlock Holmes—was a brilliant mathematician who at age of twenty-one wrote a treatise on the binomial theorem winning him the mathematical chair at a small university. His book on asteroid dynamics is described as one “which ascends to such rarefied heights of pure mathematics that it is said that there was no man in the scientific press capable of criticizing it.”

percentage of an event—such as word count, city size, or income—against cumulative percentage of counted items—number of unique words, number of unique cities, or number of people in a population. In the Lorenz curve, the events are ordered in non-decreasing order. For a discrete distribution $(F_k, L_k) = (k/n, S_k/S_n)$ where $S_k = \sum_{i=1}^{k} f_i$. For the zeta distribution $L_k = H_{k,s}/H_{n,s}$. For a continuous distribution, the Lorenz curve $(F, L(F)) = (F, S(F)/S(1))$ with $S(F) = \int_0^F F^{-1}(t)\,\mathrm{d}t$, where $F^{-1}(t)$ is the inverse cummulative distribution and $F \in [0, 1]$. The curve $L = F$ is called the line of equility. Along this curve events are equally dispersed.

Take the Pareto cumulative distribution $F(x) = 1 - x^{-\alpha}$. By inverting this relationship, we have that $x(F) = (1 - F)^{-1/\alpha}$. Then, the Lorenz curve for the Pareto distribution is

$$L(F) = S(F)/S(1) = 1 - (1 - F)^{1-1/\alpha}. \tag{3.13}$$



The Gini coefficient G—twice the area between the Lorenz curve and line of equality—is a measures of the degree of inequality. The coefficient $G = 0$ for perfect equality when the Lorenz curve agrees completely with the line of equality, and the coefficient $G = 1$ for perfect inequality. For the Pareto distribution, $G = (2\alpha - 1)^{-1}$

There is a maxim of management called the Pareto principle or the 80/20 rule, that says roughly 80 percent of effects are the result of 20 percent of causes. For example, 80 percent of the worlds' wealth is owned by the richest 20 percent of the world's people. Or 80 percent of software failures are caused by 20 percent of the bugs. We can also look to the Lorenz curve and the Pareto distribution to find the 80/20 rule at the point $(F, L) = (0.8, 0.2)$. To find the specifc Pareto distribution that passes through this point, we first solve for α in (3.13) to get

$$\alpha = \left(1 - \frac{\log(1 - L)}{\log(1 - F)}\right)^{-1}$$

For $L = 0.8$ and $F = 0.2$, we find that $\alpha \approx 1.16$.The Gini coefficient $G \approx 0.76$. ◀

CHAPTER 4

Method of Frobenius

We started this book with a guitar string and a drumhead. We had used separation of variables to isolate the components to get linear second-order homogeneous ordinary differential equations. For the guitar string we derived the harmonic oscillator equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + k^2 y = 0,$$

and for the drum we derived Bessel's equation

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + x \frac{\mathrm{d}y}{\mathrm{d}x} + (k^2 x^2 - m^2) y = 0.$$

In this chapter, we develop a general method to solve linear second-order homogeneous ordinary differential equations

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + P(x) \frac{\mathrm{d}y}{\mathrm{d}x} + Q(x) y = 0.$$

Second-order means that the we have a second derivative of y in the equation. Linear means that P and Q are functions only of x and not of y. Homogeneous means that the right-hand side of the equation is zero. Such equations arise frequently as a result of separation of variables of partial differential equations. Just as we could express analytic and meromorphic functions using Taylor and Laurent series representation, we can express solutions to linear ordinary differential equations using series representations. The method of using series representation to solve differential equations is called the Method of Frobenius.

4.1 The guitar string and the drum head

Guitar string: harmonic oscillator

Let's solve the harmonic oscillator equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + y = 0, \quad \text{with} \quad y(0) = 0,\ y(\pi) = 0. \tag{4.1}$$

where we have rescaled $kx \mapsto x$. If the solution is analytic, then it has a Taylor series representation

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

for some values $a_0, a_1, \ldots$. We simply need to find these coefficients. We can do this by substituting the Taylor series into the harmonic oscillator equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\sum_{n=0}^{\infty} a_n x^n\right) + \left(\sum_{n=0}^{\infty} a_n x^n\right) = 0.$$

Applying the second derivative to the first series gives us

$$\left(\sum_{n=2}^{\infty} n(n-1) a_n x^{n-2}\right) + \left(\sum_{n=0}^{\infty} a_n x^n\right) = 0.$$

Notice that the first sum starts at $n = 2$ because the constant term a_0 and linear term $a_1 x$ are annihilated by the second derivative. Because we have an infinite series, we can shift the indices on this series to start at $n = 0$. This will help us line up both series so that we can combine them. To do this we replace n with $n + 2$

$$\left(\sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} x^n\right) + \left(\sum_{n=0}^{\infty} a_n x^n\right) = 0$$

The upper bound of the sum is ∞ and isn't changed when shifting by $+2$. Now, we can combine the two series by matching equal powers of x

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1) a_{n+2} + a_n\right] x^n = 0.$$

This equation must be true for all values of x in our domain. The only way for it to be true is if the coefficients are identically zero:

$$(n+2)(n+1) a_{n+2} + a_n = 0.$$

From this it follows that

$$a_{n+2} = -\frac{1}{(n+1)(n+2)} a_n.$$

Note that the recurrence equation skips every other term. So, starting with a_0 we can find $a_2, a_4, \ldots$, and starting with a_1 we can find $a_3, a_5, \ldots$. To complete the problem we will need to express all the coefficients in terms of either a_0 or a_1. We have that

$$\begin{aligned} a_2 &= -\frac{1}{2} a_0 \\ a_4 &= -\frac{1}{4 \cdot 3} a_2 = -\frac{1}{4 \cdot 3}\left(-\frac{1}{2} a_0\right) = \frac{1}{4!} a_0 \\ a_{2n} &= (-1)^n \frac{1}{(2n)!} a_0 \end{aligned}$$

Similarly,

$$\begin{aligned} a_3 &= -\frac{1}{3 \cdot 2} a_1 \\ a_5 &= -\frac{1}{5 \cdot 4} a_2 = \frac{1}{5 \cdot 4}\left(-\frac{1}{3 \cdot 2} a_1\right) = \frac{1}{5!} a_1 \\ a_{2n+1} &= (-1)^n \frac{1}{(2n+1)!} a_1 \end{aligned}$$

So, the general solution to the harmonic oscillator equation (4.1) is

$$y(x) = a_0 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n)!} x^{2n} + a_1 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n+1)!} x^{2n+1}.$$

Hopefully, you recognize these two Taylor series as $\cos x$ and $\sin x$.

$$y(x) = a_0 \cos x + a_1 \sin x.$$

Finally, from the boundary conditions, $y(0) = 0$ and $y(\pi) = 0$, we note that $a_0 = 0$. So, the solution is of the form $y(x) = a_1 \sin x$.

Drum: Bessel's equation

Let's find the solution to Bessel's equation

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + x \frac{\mathrm{d}y}{\mathrm{d}x} + (x^2 - m^2) y = 0. \tag{4.2}$$

For the drum m needs to be an integer to satisfy the periodic boundary conditions for the angular component, but we can also solve the Bessel equation for arbitrary m. In general, we can't assume that the solution has a Taylor series representation because it may have a singularity at $x = 0$. Instead, we will look for a solution that may include a singularity

$$y(x) = x^r \sum_{k=0}^{\infty} a_k x^k = \sum_{k=0}^{\infty} a_k x^{k+r} \tag{4.3}$$

for some value r with $a_0 \neq 0$. Substituting this series into Bessel's equation (4.2) gives us

$$x^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\sum_{k=0}^{\infty} a_k x^{k+r}\right) + x\frac{\mathrm{d}}{\mathrm{d}x}\left(\sum_{k=0}^{\infty} a_k x^{k+r}\right) + (x^2 - m^2)\left(\sum_{k=0}^{\infty} a_k x^{k+r}\right) = 0.$$

Applying the derivatives across the first two series

$$x^2\left(\sum_{k=0}^{\infty} a_k (k+r)(k+r-1)x^{k+r-2}\right) + x\left(\sum_{k=0}^{\infty} a_k (k+r)x^{k+r-1}\right) + (x^2 - m^2)\left(\sum_{k=0}^{\infty} a_k x^{k+r}\right) = 0.$$

Because we don't know the value of r, we don't know whether or not any of the terms are annihilated by taking derivatives. For now, to be safe we've kept all the sums starting at $k = 0$, and we'll sort the problem out later. Distributing x^2, x, and $(x^2 - m^2)$ gives us

$$\left(\sum_{k=0}^{\infty} a_k (k+r)(k+r-1)x^{k+r}\right) + \left(\sum_{k=0}^{\infty} a_k (k+r)x^{k+r}\right) + \left(\sum_{k=0}^{\infty} a_k x^{k+r+2}\right) - \left(\sum_{k=0}^{\infty} a_k m^2 x^{k+r}\right) = 0.$$

We'll replace the index $k \to k+2$ in the third series, so that we can directly combine the series:

$$\left(\sum_{k=0}^{\infty} a_k (k+r)(k+r-1)x^{k+r}\right) + \left(\sum_{k=0}^{\infty} a_k (k+r)x^{k+r}\right) + \left(\sum_{k=0}^{\infty} a_{k-2} x^{k+r}\right) - \left(\sum_{k=0}^{\infty} a_k m^2 x^{k+r}\right) = 0.$$

Keeping in mind that $a_{-2} = 0$, $a_{-1} = 0$, and $a_0 \neq 0$, we can combine the terms

$$\sum_{k=0}^{\infty} \left(a_k(k+r)(k+r-1) + a_k(k+r) + a_{k-2} - a_k m^2 \right) x^{k+r} = 0,$$

or equivalently

$$\sum_{k=0}^{\infty} \left([(k+r)(k+r-1) + (k+r) - m^2]a_k + a_{k-2} \right) x^{k+r} = 0.$$

For the equation to hold for all possible x, we must have that

$$[(k+r)(k+r-1) + (k+r) - m^2]a_k + a_{k-2} = 0,$$

which we can simplify to

$$[(k+r)^2 - m^2]a_k + a_{k-2} = 0.$$

We start at $k = 0$:

$$[r^2 - m^2]a_0 = 0.$$

Because $a_0 \neq 0$ it follows that

$$r^2 - m^2 = 0.$$

We call this the *indicial equation*, and we will use this equation to determine r. So, $r = \pm m$. For now let's take $r = +m$ with $m \geq 0$ so that we don't have any singularities in our solution. It now follows that

$$[(k+m)^2 - m^2]a_k + a_{k-2} = k(k+2m)a_k + a_{k-2} = 0.$$

Equivalently,

$$k(k+2m)a_k = -a_{k-2}. \tag{4.4}$$

For $k = 1$, because $a_{-1} = 0$, we have that

$$(1+2m)a_1 = 0 \tag{4.5}$$

Either $m = -\frac{1}{2}$ or $a_1 = 0$. For right now we are considering m to be non-negative. (We will come back to the $m = -\frac{1}{2}$ case later.) So, $a_1 = 0$. From (4.4) we have that

$$a_k = \frac{-1}{k(k+2m)} a_{k-2}.$$

From this it follows that

$$
\begin{aligned}
a_2 &= \frac{-1}{2(2+2m)}a_0 = \frac{-1}{4(1+m)}a_0 \\
a_3 &= \frac{-1}{2(2+2m)}a_1 = 0 \\
a_4 &= \frac{-1}{4(4+2m)}a_2 = \frac{1}{8\cdot 4\cdot (2+m)\cdot(1+m)}a_0 \\
a_5 &= 0 \\
a_6 &= -\frac{1}{4^3\cdot 3!\cdot (m+3)(m+2)(m+1)}a_0
\end{aligned}
$$

In general, we see

$$a_{2j} = (-1)^j \frac{1}{2^{2j+m} j!(m+j)!}a_0 \quad \text{and} \quad a_{2j+1} = 0.$$

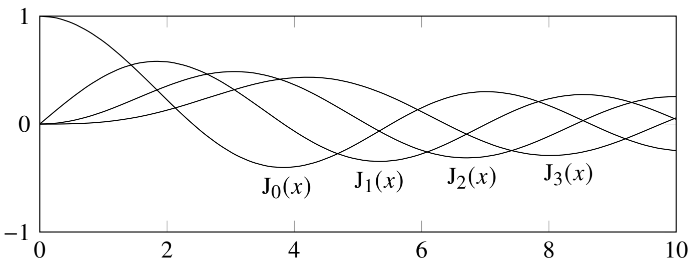
Therefore, the solution (4.3) is given by

$$y(x) = a_0 x^m \sum_{k=0}^{\infty} \frac{(-1)^k}{4^k k!(m+k)!} x^{2k}.$$

By defining the Bessel function of the first kind as

$$\mathrm{J}_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{4^k k!(m+k)!} \left(\frac{x}{2,}\right)^{2k+m} \tag{4.6}$$

then $y(x) = a_0\,\mathrm{J}_m(x)$.



In general, for integer values $-m$ the method of Frobenius does not provide a solution for the Bessel equation because the recurrence

$$a_k = \frac{-1}{k\cdot(k-2m)}a_{k-2}$$

eventually blows up at $k = 2m$.

The method of Frobenius does not always get every solution. The method of Frobenius gave us one solution to Bessel's equation, but just like the harmonic oscillator equation we should expect two linearly independent solutions.

To solve $p_0(x)y'' + p_1(x)y' + p_2(x)y = 0$:

1. Substitute $y(x) = \sum_{k=0}^{\infty} a_k x^{k+r}$
2. Shift the index k so all powers of x are the same.
3. Combine the matching coefficients together.
4. Solve the indicial equation ($k = 0$) to determine r.
5. Develop a recusion formula starting with a_0.

Example. Airy's equation

$$y'' - xy = 0$$

arises in the solution to Schrödinger's equation for a particle in a constant force field (linear potential) and in modelling the diffraction of light. Looking at the equation we can already guess the behavior of the solution. When $x < 0$ Airy's equation looks like $y'' + \lambda^2 y = 0$, which has oscillating solutions of $\sin \lambda x$ and $\cos \lambda x$, and when $x > 0$ Airy's equation looks like $y'' - \lambda^2 y = 0$, which has exponential solutions of $e^{+\lambda x}$ and $e^{-\lambda x}$. Let's find the series solution to Airy's equation. Take

$$y(x) = \sum_{k=0}^{\infty} a_k x^{k+r}.$$

Then

$$y(x) = \sum_{k=0}^{\infty} a_k (k+r)(k+r-1) x^{k+r-2}$$

and $y'' - xy = 0$ becomes

$$\sum_{k=0}^{\infty} a_k (k+r)(k+r-1) x^{k+r-2} - \sum_{k=0}^{\infty} a_k x^{k+r+1} = 0.$$

We have that

$$\sum_{k=0}^{\infty} a_k (k+r)(k+r-1) x^{k+r-2} - \sum_{k=0}^{\infty} a_{k-3} x^{k+r-2} = 0$$

from which it follows that

$$\sum_{k=0}^{\infty}\left(a_k(k+r)(k+r-1)-a_{k-3}\right)x^{k+r-2}=0.$$

For this equation to be true for all x, we must have that

$$a_k(k+r)(k+r-1)-a_{k-3}=0.$$

When $k=0$, we have the indicial equation

$$r(r-1)=0$$

and $r=0$ or $r=1$—it doesn't matter. We have that

$$k(k-1)a_k-a_{k-3}=0$$

or

$$a_{k+3}=\frac{1}{(k+3)(k+2)}a_k$$

from which

$$\begin{aligned}
a_3 &= \frac{1}{3\cdot 2}a_0\\
a_6 &= \frac{1}{6\cdot 5}a_3 = \frac{1}{6\cdot 5\cdot 3\cdot 2}a_0\\
a_9 &= \frac{1}{(9\cdot 8)(6\cdot 5)(3\cdot 2)}a_0\\
a_{3k} &= \frac{1}{[(3k)(3k-1)][(3k-3)(3k-4)]\cdots[6\cdot 5][3\cdot 2]}a_0
\end{aligned}$$

Note that we can write a_{3k} as

$$a_{3k}=\frac{(3k-2)\cdot(3k-5)\cdot 1}{(3k)!}a_0.$$

We can can simplify the expression by introducing the notation $n!^{(j)}$ as an extension to the factorial $n!$. We define the *multifactorial* recursively as $n!^{(j)} = n\cdot(n-j)!^{(j)}$ and $n!^{(j)}=1$ if $-j<n\leq 0$ for a positive integer j. Common multifactorials include the double factorial $n!!=n!^{(2)}$ and triple factorial $n!!!=n!^{(3)}$. Using multifactorial notation

$$a_{3k}=\frac{(3k-2)!!!}{(3k)!}a_0.$$

Similarly,

$$
\begin{aligned}
a_4 &= \frac{1}{4 \cdot 3} a_1 \\
a_7 &= \frac{1}{7 \cdot 6} a_3 = \frac{1}{7 \cdot 6 \cdot 4 \cdot 3} a_1 \\
a_{10} &= \frac{8!!!}{10!} a_1 \\
a_{3k+1} &= \frac{(3k-1)!!!}{(3k+1)!} a_1
\end{aligned}
$$

and

$$a_{3k+2} = 0.$$

So, we have

$$y(x) = a_0 \sum_{k=0}^{\infty} \frac{(3k-2)!!!}{(3k)!} x^{3k} + a_1 \sum_{k=0}^{\infty} \frac{(3k-1)!!!}{(3k+1)!} x^{3k+1}. \qquad \blacktriangleleft$$

Mathematical detour. Airy's equation $y'' - xy = 0$ can also be solved using Fourier transforms. The Fourier transform and inverse Fourier transform mapping a function $y(x)$ to a function $\hat{y}(t)$ can be defined

$$
\begin{aligned}
\hat{y}(t) &= \mathrm{F}\{y(x)\}(t) = \int_{-\infty}^{\infty} y(x)\, \mathrm{e}^{-\mathrm{i}tx}\, \mathrm{d}x \\
y(x) &= \mathrm{F}^{-1}\{\hat{y(t)}\}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{y}(t)\, \mathrm{e}^{\mathrm{i}tx}\, \mathrm{d}t.
\end{aligned}
$$

The Fourier transform of a derivative of a function can be computed using integration by parts

$$\mathrm{F}\{y'\} = \int_{-\infty}^{\infty} y'(x)\, \mathrm{e}^{-\mathrm{i}tx}\, \mathrm{d}x = \mathrm{i}t \int_{-\infty}^{\infty} y(x)\, \mathrm{e}^{-\mathrm{i}tx}\, \mathrm{d}x = \mathrm{i}t\, \mathrm{F}\{y\}$$

Repeating this one more step, we also have $\mathrm{F}\{y''\} = -t^2\, \mathrm{F}\{y\}$. Similarly, $\mathrm{F}\{xy\} = -\mathrm{i}(\mathrm{F}\{y\})'$. Then

$$\mathrm{F}\{y'' - xy\} = \mathrm{F}\{y''\} - \mathrm{F}\{xy\} = -t^2 \hat{y} + \mathrm{i}\hat{y}'.$$

The differential equation $\hat{y}' - \mathrm{i}t^2 \hat{y} = 0$ is separable

$$\frac{\hat{y}'}{\hat{y}} = \mathrm{i}t^2$$

with the solution

$$\hat{y} = c\,\mathrm{e}^{\mathrm{i}t^3/3}$$

for a constant of integration c. Taking the inverse Fourier transform

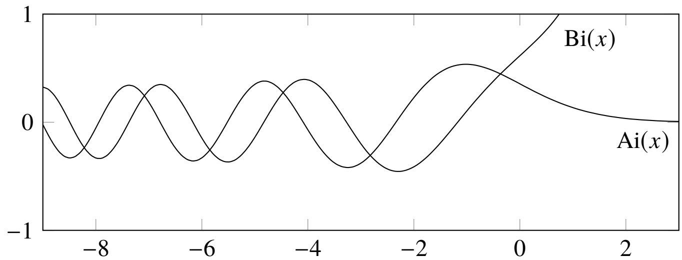
$$\begin{aligned} y(x) = \mathrm{F}\{\hat{y}\} &= c\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}t^3/3}\,\mathrm{e}^{\mathrm{i}tx}\;\mathrm{d}t \\ &= c\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(t^3/3+tx)}\;\mathrm{d}t \\ &= c\frac{1}{\pi}\int_{0}^{\infty} \cos(t^3/3+tx)\,\mathrm{d}t. \end{aligned}$$

We call

$$\mathrm{Ai}(x) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3}+xt\right)\,\mathrm{d}t$$

the Airy function of the first kind. The Airy function of the second kind

$$\mathrm{Bi}(x) = \frac{1}{\pi}\int_0^\infty \exp\left(-\frac{t^3}{3}+xt\right) + \sin\left(\frac{t^3}{3}+xt\right)\,\mathrm{d}t.$$



From the example on on page 71 we also see that $\mathrm{Ai}(0) = \left(3^{2/3}\Gamma(2/3)\right)^{-1}$. ◂

4.2 When will the method of Frobenius work?

Consider the differential equation $y''(x)+P(x)y'(x)+Q(x)y(x) = 0$ with solution $y(x)$. We say that x_0 is an *ordinary point* if $y(x)$ is analytic at x_0. We say that x_0 is a *regular singular point* if $\lim_{x\to x_0}(x-x_0)^p|y(x)| = 0$ for some positive number p. That is, $y(x)$ has a pole of order at most p at x_0. Otherwise, if $y(x)$ has an essential singularity at x_0, we say that x_0 is a *essential singular point*.

1. If both $P(x)$ and $Q(x)$ are analytic in the neighborhood of x_0 (that is, if $P(x)$ and $Q(x)$ remain finite at x_0), then x_0 is an *ordinary point*. The differential equation has two distinct series solutions. The radius of convergence of the solution is at least as large as the minimum of the radii of convergence of $P(x)$ and $Q(x)$.

2. (Fuchs' theorem) If $P(x)$ has at most a simple pole and $Q(x)$ has at most a double pole at x_0, then x_0 is a *regular singular point*. That is, if either $P(x)$ or $Q(x)$ is singular at x_0, but $(x-x_0)P(x)$ and $(x-x_0)^2Q(x)$ are finite at x_0, then x_0 is a regular singular point. The differential equation has at least one distinct series solutions
$$y = \sum_{k=0}^{\infty} a_k (x - x_0)^{k+r}.$$
Namely, if the two roots of the indicial equation differ by a noninteger number, we have two independent solutions. If the two roots of differ by an integer, the larger of the two roots will yield a solution.

3. Otherwise, x_0 is an *essential singular point*. The differential equation may not have any series solutions.

Example. Let's look at possible series solutions at $x = 0$ of a few equations.

- $y'' - xy = 0$. This is Airy's equation again. First, note that the point $x = 0$ is a regular point, because $P(x) = 0$ and $Q(x) = x$ are both analytic functions at $x = 0$. Therefore, the solution will be a combination of Taylor series representations.
- $x^4y'' + 2x^3y' + y = 0$. The function $P(x) = 2/x^3$ has a pole of order 3 at $x = 0$ and $Q(x) = 1/x^4$ has a third order pole of order 4 at $x = 0$. So, the solution $y(x)$ has an essential singularity at the origin. We cannot expect a series solution at $x = 0$. The solution is in fact
$$y(x) = c_1 \cos\left(\frac{1}{x}\right) + c_2 \sin\left(\frac{1}{x}\right).$$
- $x^2y'' - 6y = 0$. In this case, we have $P(x) = 1$ and $Q(x) = -6/x^2$. The function $P(x)$ is analytic at every point and $Q(x)$ is analytic everywhere but at $x = 0$. At this point, $Q(x)$ has a second-order pole. Because $x^2Q(x)$ is finite at $x = 0$, this point is a regular singular point. By Fuch's theorem, we will get at least one solution using the method of Frobenius. To determine how many solutions, we will look at the indicial equation. Substituting $y = \sum_{k=0}^{\infty} a_k x^{k+r}$ into $x^2y'' - 6y = 0$ gives us
$$x^2 \sum_{k=0}^{\infty} (k+r)(k+r-1)a_k x^{k+r-2} - 6 \sum_{k=0}^{\infty} a_k x^{k+r} = 0$$
which we can rewrite as
$$\sum_{k=0}^{\infty} (k+r)(k+r-1)a_k x^{k+r} - 6 \sum_{k=0}^{\infty} a_k x^{k+r} = 0.$$

We combine the two sums to get

$$\sum_{k=0}^{\infty}\big((k+r)(k+r-1)-6\big)a_k x^{k+r} = 0$$

This equation must hold for all x in our domain, so it follows that

$$\big((k+r)(k+r-1)-6\big)a_k = 0 \tag{4.7}$$

for all $k \geq 0$. Since $a_0 \neq 0$, we have the indicial equation ($k = 0$)

$$(r)(r-1)-6 = 0$$

which has solutions $r = 3$ and $r = -2$. Note that (4.7) is not a recurrence. That means, given a_0 we can't use it to get a_1 or a_2 and so on. But we do have two solutions from the indicial equation, $y = x^3$ and $y = x^{-2}$. The solution to the differential equation is

$$y(x) = c_1 x^3 + \frac{c_2}{x^2}.$$

- $x^3 y'' - 6y = 0$. Now we have $Q(x) = -6/x^3$ which has a third-order pole at $x = 0$. We should not have expect any solutions. The indicial equation is found by first substituting $y = \sum_{k=0}^{\infty} a_k x^{k+r}$ into $x^3 y'' - 6y = 0$ to get

$$\sum_{k=0}^{\infty}(k+r)(k+r-1)a_k x^{k+r+1} - 6\sum_{k=0}^{\infty} a_k x^{k+r} = 0$$

  The indicial equation is $-6a_0 = 0$ but since $a_0 \neq 0$, it follows that there are no series solutions.

- $x^2 y'' + xy' + (x^2 - m^2)y = 0$. Bessel's equation can be written as

$$y'' + \frac{1}{x}y' + \left(1 - \frac{m^2}{x^2}\right) y = 0.$$

  We see that $P(x)$ has a simple pole at $x = 0$ and $Q(x)$ has a double pole at $x = 0$. Therefore by Fuchs's theorem, we should only expect one series solution. ◄

The method of Frobenius gives us two analytic solutions centered at x_0 to $y'' + P(x)y' + Q(x)y = 0$ if $P(x)$ and $Q(x)$ are analytic at x_0, and it gives at least one solution if $P(x)$ has at most a simple pole and $Q(x)$ has at most a double pole. Otherwise, the method of Frobenius doesn't work.

4.3 Second solutions

We found only one solution to Bessel's equation. But because Bessel's equation is second order we should have two independent solutions, just as $y'' - y = 0$ has a solution $a_0 \cos x$ and a solution $a_1 \sin x$. Let's find the second solution.

We can find a second solution of a general differential equation

$$y''(x) + P(x)y'(x) + Q(x)y(x) = 0.$$

Suppose $y(x)$ and $v(x)$ are independent solutions:

$$\begin{aligned} &① & y'' + Py' + Qy = 0, \\ &② & v'' + Pv' + Qv = 0. \end{aligned}$$

Taking $v \cdot ① - y \cdot ②$:

$$(vy'' - yv'') + P \cdot (vy' - yv') = 0.$$

Notice that $(vy' - yv')' = (vy'' - yv'')$. Hence

$$(vy' - yv')' + P \cdot (vy' - yv') = 0.$$

Multiply both sides by the integrating factor $\exp(\int_a^x P(t)\,\mathrm{d}t)$ for some constant a:

$$\exp\left(\int_a^x P(t)\,\mathrm{d}t\right)(vy' - yv')' + \exp\left(\int_a^x P(t)\,\mathrm{d}t\right)P(x)(vy' - yv') = 0.$$

We can simplify this expression as

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\exp\left(\int_a^x P(t)\,\mathrm{d}t\right)(vy' - yv')\right] = 0.$$

Hence,

$$\exp\left(\int_a^x P(t)\,\mathrm{d}t\right)(vy' - yv')] = B$$

for some constant B. Therefore, we have

$$\frac{(vy' - yv')}{v^2} = \frac{B\exp(-\int_a^x P(t)\,\mathrm{d}t)}{v^2}.$$

The expression on the left can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y}{v}\right) = \frac{B\exp(-\int_a^x P(t)\,\mathrm{d}t)}{v^2}.$$

Integrating this equation gives us the second solution

$$y(x) = Bv(x)\int \frac{\exp(-\int_a^x P(t)\,\mathrm{d}t)}{v^2(x)}\,\mathrm{d}x. \tag{4.8}$$

where $v(x)$ is the first solution.

Example. We already know that the two independent solutions to the harmonic oscillator equation $y'' + y = 0$ are $\cos x$ and $\sin x$. But, let's use (4.8) to show that $\sin x$ is the second solution to $\cos x$. In this case, $P(x) = 0$ and $v(x) = \cos x$. Then,

$$y(x) = B\cos x \int_0^x \frac{1}{\cos^2 s}\, \mathrm{d}s = B\cos x \tan x = B\sin x.$$ ◀

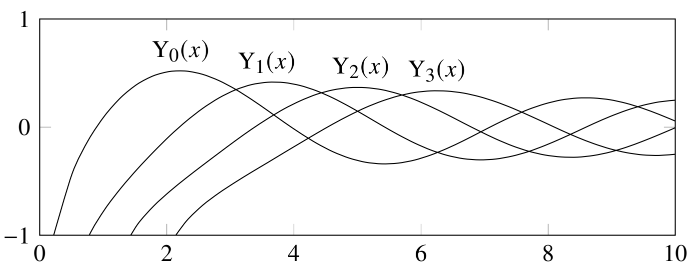
Example. Now let's find the second solution to Bessel's equation

$$x^2 y'' + xy' + (x^2 - m^2)y = 0.$$

$P(x) = 1/x$ and $v(x) = \mathrm{J}_m(x)$. Then, $\exp(\int_1^x t^{-1}\, \mathrm{d}t) = s^{-1}$ and

$$y(x) = B\,\mathrm{J}_m(x) \int_0^s \frac{1}{x\,\mathrm{J}_m^2(s)}\, \mathrm{d}s$$

is the Bessel function of the second kind and is denoted it by $\mathrm{Y}_m(x)$.



Now there is a singularity at zero. ◀

CHAPTER 5

Sturm–Liouville Theory

In the last chapter we used the method of Frobenius to find series solutions to linear homogeneous second-order differential equations. Now, we'll dig into the theory of these types of equations to better understand their solutions. This short chapter looks the class of second-order linear differential equations

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right) + q(x)u(x) = -\lambda w(x)u(x),$$

called Sturm–Liouville equations, which frequently arise from separation of variables for a number of common partial differential equations. We start with a review of function spaces and then apply those concepts to Sturm–Liouville equations.

5.1 Review of linear algebra

Vector spaces

A *vector space* is a collection of objects (called vectors) that is closed under addition and scalar multiplication. Choose any vectors from the collection, then any linear combination of those vectors must also be in the collection. There are many of objects that can be vectors, but we will primarily be interested functions as vectors. So, if $u(x)$ and $v(x)$ are both vectors in a given vector space, then $au(x) + bv(x)$ is also in that vector space for any scalars a and b. One simple example of a vector space is the space of quadratic functions $a_0 + a_1x + a_2x^2$. Take any quadratic function and scale it or add it to another one, and you get another quadratic function. Another vector space is the set of smooth functions over the domain $[0, 1]$ that vanish at end points. Any linear combinations of these functions are still smooth functions that vanish at the end points of $[0, 1]$.

A *basis* for vector space is a smallest collection of vectors that can be used to build all other vectors in the vector space. For the space of quadratic polynomials, the set $\{1, x, x^2\}$ is a basis. We can build any quadratic polynomial using a unique combination of these basis functions. For example,

$$1 + 2x + 3x^2 = 1 \cdot 1 + 2 \cdot x + 3 \cdot x^2.$$

The set $\{1, 2x - 1, 6x^2 - 6x + 1\}$ is another basis for the space of quadratic polynomials. We can similarly use this basis to build the same quadratic polynomial:

$$1 + 2x + 3x^2 = 3 \cdot 1 + \tfrac{1}{2} \cdot (2x - 1) + \tfrac{5}{2} \cdot (6x^2 - 6x + 1).$$

There are, in fact, infinitely many collections of basis functions for quaddratics. The number of vectors that make up a basis is called the *dimension* of the vector space. The space of quadratic polynomials has a dimension of three. Some vector spaces don't have a finite basis. A *Schauder basis* is a basis for an infinite-dimensional vector space. For example, the set $\{\sin \pi x, \sin 2\pi x, \sin 3\pi x, \dots\}$ is a basis for the infinite-dimensional vector space of smooth functions on $[0, 1]$ that vanish at endpoints. We can represent a function in this vector space as

$$f(x) = \sum_{n=1}^{\infty} a_n \sin n\pi x$$

for appropriate coefficients a_n.

Inner product spaces

A *inner product*, denoted by $(\cdot, \cdot)$, is any mapping from a vector space to a complex number with the properties linearity, Hermiticity (conjugate symmetry), and positive-definiteness:

1. $(au + bv, w) = a\,(u, w) + b\,(v, w)$
2. $(u, v) = (v, u)^*$
3. $(u, u) \geq 0$ and $(u, u) = 0$ if and only if $u = 0$

where u, v, and w are vectors in the vector space and a and b are scalar vales. From conjugate symmetry and linearity, it also follows that $(u, av) = a^*\,(u, v)$. A common inner product is the L^2-inner product

$$(u, v) = \int_a^b u(x)v(x)^*\,\mathrm{d}x$$

where v^* is the complex conjugate of v and a and b are boundary points, possibly at $\pm\infty$. As a generalization of the L^2-inner product, we can also define a weighted inner product

$$(u, v)_w = \int_a^b u(x)v(x)^*w(x)\,\mathrm{d}x$$

for some weighting function $w(x)$. A vector space on which an inner product has been defined is called an *inner product space*.

A norm of a vector u is any real-valued function $\|\cdot\|$ with the properties of positive definiteness, absolutely homogeneity, and subadditivity (the triangle inequality):

1. $\|u\| \geq 0$ and $\|u\| = 0$ if and only if $u(x) \equiv 0$,
2. $\|au\| = |a|\|u\|$ for any scalar a,
3. $\|u + v\| \leq \|u\| + \|v\|$.

If a vector space is an inner product space, we can define a natural norm associated with the inner product $\|u\| = \sqrt{(u,u)}$. Similarly, we can define a weighted norm $\|u\|_w = \sqrt{(u,u)_w}$. We normalize a function u by dividing it by its norm.

Two functions u and v are *orthogonal* if their inner product is zero: $(u,v) = 0$. When selecting a basis for a vector space out of the infinite possibilities, it is often beneficial to choose an orthonormal basis. That is, a basis $\{u_1, u_2, \ldots, u_n\}$ with elements that are all mutually orthogonal and have unit norm

$$\left(u_i, u_j\right) = \delta_{ij}$$

where the Kronecker delta $\delta_{ii} = 1$ and $\delta_{ij} = 0$ if $i \neq j$. A huge benefit of orthonormal bases is that they allow functions to be represented as an orthogonal decomposition: $f(x) = \sum_{i=1}^{n} a_i u_i(x)$ where $\{u_1, u_2, \ldots, u_n\}$ is an orthonormal basis. To get a coefficients a_j we simply apply the inner product

$$\left(f(x), u_j\right) = \left(\sum_{i=1}^{n} a_i u_i, u_j\right) = \sum_{i=1}^{n} a_i \left(u_i, u_j\right) = \sum_{i=1}^{n} a_i \delta_{ij} = a_j.$$

So, $a_j = \left(f(x), u_j\right)$.

Example. Show that the functions $\sin m\pi x$ and $\sin n\pi x$ for integers m and n are orthogonal in the L^2-inner product over the interval $[0,1]$. First, note that that we have the identity

$$\begin{aligned}
\sin mx \sin nx &= \operatorname{Im}\left(\mathrm{e}^{\mathrm{i}mx} \sin nx\right) \\
&= \operatorname{Im}\left(\mathrm{e}^{\mathrm{i}mx} \frac{\mathrm{e}^{\mathrm{i}nx} - \mathrm{e}^{-\mathrm{i}nx}}{2\mathrm{i}}\right) \\
&= \operatorname{Im}\left(\frac{\mathrm{e}^{\mathrm{i}(m+n)x} - \mathrm{e}^{\mathrm{i}(m-n)x}}{2\mathrm{i}}\right) \\
&= \tfrac{1}{2} \operatorname{Re}\left(\mathrm{e}^{\mathrm{i}(m+n)x} - \mathrm{e}^{\mathrm{i}(m-n)x}\right) \\
&= \tfrac{1}{2} \left(\cos(m+n)x - \cos(m-n)x\right).
\end{aligned}$$

Therefore, when $m \neq n$ the integral

$$\int_0^1 \sin m\pi x \sin n\pi x \, \mathrm{d}x = \frac{\sin(m+n)\pi x}{2(m+n)\pi} - \frac{\sin(m-n)\pi x}{2(m-n)\pi}\bigg|_0^1 = 0$$

and when $m = n$ the integral

$$\int_0^1 \sin^2 m\pi x \, \mathrm{d}x = \frac{\sin 2m\pi x}{4m\pi} - \frac{x}{2}\bigg|_0^1 = \frac{1}{2}.$$

So, $(\sin m\pi x, \sin n\pi x) = \frac{1}{2}\delta_{mn}$. ◀

Example. We saw that initial conditions $f(x)$ for the guitar string can be represented by a sine series over $[0, 1]$:

$$f(x) = \sum_{n=1}^{\infty} a_n \sin n\pi x.$$

Because $\{u_1, u_2, u_3, \dots\} = \{\sin \pi x, \sin 2\pi x, \sin 3\pi x, \dots\}$ is an orthogonal basis we can determine the coefficients a_n as

$$a_n = \frac{(f(x), u_n)}{\|u_n\|^2} = 2\int_0^1 f(x) \sin n\pi x.$$

This is the sine transform of $f(x)$. ◀

Linear operators

A linear operator L is an operator such that $\mathrm{L}(au(x)) = a\,\mathrm{L}\,u(x)$ for any scalar a and $\mathrm{L}(u(x) + v(x)) = \mathrm{L}\,u(x) + \mathrm{L}\,v(x)$. For example, the derivative operator $\frac{\mathrm{d}}{\mathrm{d}x}$ is a linear operator. So, are $(x^2+1)\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ and the anti-derivative. Given two linear operators L and $\tilde{\mathrm{L}}$ in an inner product space, we say that $\tilde{\mathrm{L}}$ is the *adjoint* of L if $\left(u, \tilde{\mathrm{L}}v\right) = (\mathrm{L}\,u, v)$ for all vectors u and v. For example, take $\mathrm{L} = \frac{\mathrm{d}}{\mathrm{d}x}$ and the space of all smooth functions that vanish at 0 and 1.

$$(u, \mathrm{L}\,v) = \int_0^1 u\frac{\mathrm{d}v}{\mathrm{d}x}\,\mathrm{d}x = -\int_0^1 \frac{\mathrm{d}u}{\mathrm{d}x} v \,\mathrm{d}x = (-\mathrm{L}\,u, v)\,.$$

The $\frac{\mathrm{d}}{\mathrm{d}x}$ is the adjoint of $-\frac{\mathrm{d}}{\mathrm{d}x}$ in this inner product space.

When $(u, \mathrm{L}\,v) = (\mathrm{L}\,u, v)$ for all functions u and v, we say that the operator L is *self-adjoint* or *Hermitian*. The operator $\frac{\mathrm{d}}{\mathrm{d}x}$ is not self-adjoint but the operator $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is self-adjoint in the space of smooth functions that vanish at 0 and 1

Eigenfunctions

The eigenvectors or eigenfunctions of an operator L are vectors or functions that are scaled but otherwise unchanged when the operator L is applied to them. The scalar multiplier is called the eigenvalue. The eigenvalue problem $\mathrm{L}\,u(x) = \lambda u(x)$ asks us to find the eigenvectors $u(x)$ and eigenvalues λ for a given linear operator L. The generalized eigenvalue problem $\mathrm{L}\,u(x) = \lambda w(x)u(x)$ asks to find a function $u(x)$ and associated scalar λ for a linear operator L and weighting function $w(x)$.

> The prefix "eigen" gets a lot of attention: eigenvalue, eigenvector, eigenfunction, eigenbasis, eigenspace, etc. In German "eigen" means "own" as in one's own. In mathematics "eigen" means "characteristic."

Example. The derivative operator $\frac{\mathrm{d}}{\mathrm{d}x}$ has eigenfunctions of the form $\mathrm{e}^{\lambda x}$ with eigenvalue λ. Differentiating $\mathrm{e}^{\lambda x}$ is the same as multiplying it by λ. The real-valued functions $\cos mx$ and $\sin mx$ are eigenfunctions of $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with eigenvalues $-m^2$. Sometimes operators may only have trivial zero eigenfunctions, such as the derivative operator $\frac{\mathrm{d}}{\mathrm{d}x}$ over the space of quadratic polynomials. ◀

Theorem. *The eigenvalues of a self-adjoint operator are real and the eigenfunctions are orthogonal.*

Proof. Suppose that $u_i(x)$ and $u_j(x)$ are eigenfunctions of L with respective eigenvalues λ_i and λ_j. We'll assume that the eigenvalues are nondegenerate, that is, that $\lambda_i \neq \lambda_j$. The theorem still holds for degenerate eigenvalues, but the proof is more complicated. Because L is self-adjoint

$$\left(\mathrm{L}\,u_i, u_j\right) = \left(u_i, \mathrm{L}\,u_j\right)$$

from which it follows that

$$\begin{aligned} 0 &= \left(\mathrm{L}\,u_i, u_j\right) - \left(u_i, \mathrm{L}\,u_j\right) \\ &= \left(\lambda_i u_i, u_j\right) - \left(u_i, \lambda_j u_j\right) \\ &= (\lambda_i - \lambda_j{}^*)\left(u_i, u_j\right) \end{aligned}$$

For $i = j$, we have $\lambda_i = \lambda_i{}^*$, and so the eigenvalues are real. For $i \neq j$, we have $\left(u_i, u_j\right) = 0$, and so the eigenfunctions are orthogonal. □

The harmonic oscillator equation $\frac{d^2}{dx^2} + (m\pi)^2 u = 0$ can be written as $\mathrm{L}\, u = -(m\pi)^2 u$ with $\mathrm{L} = \frac{d^2}{dx^2}$. The operator L is self-adjoint in the L^2-inner product space over $[0, 1]$. Using the above theorem, we know that its eigenfunctions $\sin m\pi x$ are mutually orthogonal. This theorem could have saved us quite a bit of work in the exercise on page 101, where we showed the orthgonality of these eigenfunctions.

5.2 Sturm–Liouville operators

Let's determine the conditions under which a linear second-order differential operator is self-adjoint, and hence when its eigenvectors are orthogonal. Consider any linear second-order differential operator

$$\mathrm{L}\, u = p_0 \frac{d^2}{dx^2} u + p_1 \frac{d}{dx} u + p_2 u$$

where u, p_0, p_1, and p_2 are functions of x in the L^2-inner product space of smooth functions that vanish at $x = a$ and $x = b$. Take the inner product

$$\begin{aligned}(v, \mathrm{L}\, u) &= \int_a^b v(p_0 u'' + p_1 u' + p_2 u)\, dx \\ &= \int_a^b (v p_0) u'' + (v p_1) u' + (v p_2) u \, dx.\end{aligned}$$

We'll firsts find the adjoint of L. After integrating by parts (twice on the first term and once on the second term) we have

$$-(v p_0)' u + (v p_0) u' + (v p_1) u \Big|_a^b + \int_a^b (v p_0)'' u - (v p_1)' u + (v p_2) u \, dx. \tag{5.1}$$

Because functions in the inner product space are zero at $x = a$ and $x = b$, the boundary terms vanish, and we have simply

$$\int_a^b (v p_0)'' u - (v p_1)' u + (v p_2) u \, dx = (\mathrm{L}^* v, u)\,.$$

So, the adjoint is

$$\mathrm{L}^* u = \frac{d^2}{dx^2}(p_0 u) - \frac{d}{dx}(p_1 u) + p_2 u.$$

The adjoint operator is self-adjoint when $\mathrm{L} = \mathrm{L}^*$? We can check by direct computation

$$\begin{aligned}p_0 u'' + p_1 u' + p_2 u &= (p_0 u)'' - (p_1 u)' + p_2 u \\ &= p_0'' u + 2 p_0' u' + p_0 u'' - p_1' u - p_1 u' + p_2 u.\end{aligned}$$

After canceling and rearranging terms, we are left with

$$p_0''u - p_0'u' - p_0'u' + p_1'u = 0.$$

This expression is true when $p_0' = p_1$. In this case

$$\mathrm{L}\,u = \frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right) + q(x)u$$

where we've relabled $p(x) = p_0(x)$ and $q(x) = p_2(x)$. This operator is called a *Sturm–Liouville operator*. Note also that when $p_0' = p_1$, the boundary terms of (5.1) simplify to

$$p_0(vu' - v'u)\Big|_a^b,$$

which vanishes when either

1. $p(a) = p(b) = 0$;
2. $u(a) = u(b) = v(a) = v(b) = 0$;
3. $u'(a) = u'(b) = v'(a) = v'(b) = 0$; or
4. $u(a) = u(b)$, $u'(a) = u'(b)$, $v(a) = v(b)$, and $v'(a) = v'(b)$

This says that the Sturm–Liouville operator is self-adjoint when either 1. the function $p(x)$ is zero on the boundaries, 2. the inner product space consists of functions that vanish on the boundary (Dirichlet boundary conditions), 3. functions whose derivatives vanish on the boundary (Neumann boundary conditions), or 4. functions whose values and derivatives are equal across the boundary (periodic boundary conditions).

Had we instead used a weighted L^2-inner product with weight $w(x)$, the boundary term would also have vanished when $w(a) = 0$ and $w(b) = 0$. So, the Sturm–Liouville operator is also self-adjoint in inner product spaces with weights that vanish at the boundary, such as $w(x) = \mathrm{e}^{-x^2}$ over the domain $(-\infty, \infty)$.

When L is a Sturm–Lioville operator, the generalized eigenvalue equation $\mathrm{L}\,u(x) = \lambda w(x)u(x)$ is called the Sturm–Liouville equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right) + q(x)u(x) = -\lambda w(x)u(x)$$

and the eigenfunctions $u(x)$ are orthogonal.

Example. Put the Legendre equation $(1-x^2)y'' - 2xy' + m(m+1)y = 0$ in self-adjoint form. Note that $-2x$ is the derivative of $(1-x^2)$. So, we can rewrite this equation as

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)\frac{\mathrm{d}y}{\mathrm{d}x}\right) = -m(m+1)y.$$

The eigenvalues are $\lambda = -m(m+1)$ and the weight is $w(x) = 1$. ◀

Example. When we solved the circular drum equation by separation of variables, we got Bessel equation in the radial component. Suppose that the drum has unit radius. The Bessel function $\mathrm{J}_m(x)$ solves the equation

$$x^2y'' + xy' + (x^2 - m^2)y = 0.$$

Take $x = \alpha s$. Then

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}s}\frac{\mathrm{d}s}{\mathrm{d}x} = \frac{1}{\alpha}\frac{\mathrm{d}y}{\mathrm{d}s} \quad \text{and} \quad \frac{\mathrm{d}^2y}{\mathrm{d}x^2} = \frac{1}{\alpha}\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}y}{\mathrm{d}s} = \frac{1}{\alpha^2}\frac{\mathrm{d}^2y}{\mathrm{d}s^2}.$$

In this new basis, Bessel's equation becomes

$$s^2\frac{\mathrm{d}^2y}{\mathrm{d}s^2} + s\frac{\mathrm{d}y}{\mathrm{d}s} + (\alpha^2s^2 - m^2)y = 0,$$

which when put in Sturm–Liouville form is

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(s\frac{\mathrm{d}y}{\mathrm{d}s}\right) - \frac{m^2}{s}y = \alpha^2 sy.$$

For a fixed m, consider eigenfunctions $\mathrm{J}_m(\alpha_i s)$. Orthogonality for the Sturm–Liouville operator requires that $\mathrm{J}_m(\alpha_i s) = 0$ or $\mathrm{J}'_m(\alpha_i s) = 0$ at $s = 1$. We don't need to worry that the boundary at $s = 0$, because $p(s) = s$ vanishes at $s = 0$. Take $\mathrm{J}_m(\alpha_i) = 0$. That is, choose α_i to be zeroes of $\mathrm{J}_m(x)$. Then $\mathrm{J}_m(\alpha_i s)$ are mutually orthogonal:

$$\int_0^1 \mathrm{J}_m(\alpha_i s)\,\mathrm{J}_m(\alpha_j s)s\,\mathrm{d}s = 0 \quad \text{when} \quad i \neq j.$$ ◀

We can always put a second-order linear differential operator into Sturm–Liouville form. Take

$$p_0(x)\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + p_1(x)\frac{\mathrm{d}u}{\mathrm{d}x} + p_0(x) = 0$$

and divide by p_0

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \frac{p_1(x)}{p_0(x)}\frac{\mathrm{d}u}{\mathrm{d}x} + \frac{p_2(x)}{p_0(x)}u = 0.$$

Multiply by an integrating factor

$$Q(x) = \exp\left(\int_a^x \frac{p_1(x)}{p_0(x)}\,\mathrm{d}x\right)$$

and combine the first two terms

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(Q(x)\frac{p_1(x)}{p_0(x)}\frac{\mathrm{d}u}{\mathrm{d}x}\right) + Q(x)\frac{p_2(x)}{p_0(x)}u = 0.$$

Example. Consider the Hermite equation

$$y'' - 2xy' + \lambda y = 0.$$

We can put it into self-adjoint form by multiplying by

$$\mathrm{e}^{\int_{-\infty}^{x} -2s\,\mathrm{d}s} = \mathrm{e}^{-x^2}.$$

In this case, we have that

$$\begin{aligned} \mathrm{e}^{-x^2}\left[y'' - 2xy' + \lambda y\right] &= \mathrm{e}^{-x^2} y'' - 2x\,\mathrm{e}^{-x^2} y' + \lambda\,\mathrm{e}^{-x^2} y \\ &= \left(\mathrm{e}^{-x^2} y'\right)' + \lambda\,\mathrm{e}^{-x^2} y. \end{aligned}$$

The Hermite equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{-x^2}\frac{\mathrm{d}u'}{\mathrm{d}x}\right)' = -\lambda\,\mathrm{e}^{-x^2} y.$$

is now in self-adjoint form. ◄

Mathematical detour. The Gram–Schmidt process allows us to create an orthogonal set of basis functions using an arbitrary set of basis functions by using the inner product to project out the non-orthogonal components. Suppose that we have the functions $\{u_1, u_2, u_3, \ldots\}$ and we want the closest set of mutually orthogonal basis functions $\{v_1, v_2, v_3, \ldots\}$. Start by taking

$$v_1 = u_1.$$

(We can't get any closer than this.) Now, define v_2 as the closest function to u_2 that is orthogonal to v_1. We can do this by projecting the v_1 component out of u_2.

$$v_2 = u_2 - \left(\frac{v_1}{\|v_1\|}, u_2\right)\frac{v_1}{\|v_1\|} = u_2 - v_1\frac{(v_1, u_2)}{\|v_1\|^2}.$$

Once we have v_2 we can get v_3 by starting with u_3 projecting out any components in the v_1 and v_2 directions:

$$v_3 = u_3 - v_1 \frac{(v_1, u_3)}{\|v_1\|^2} - v_2 \frac{(v_2, u_3)}{\|v_3\|^2}.$$

We continue in this manner to get the other basis functions.

The Legendre equation can be solved using the method of Frobenius to get the Legendre polynomials.Another approach to generating Legendre polynomials is to use the Gram–Schmidt process. Putting the Legendre equation into Sturm–Liouville form $(pu')' + qu = \lambda wu$ we have

$$((1 - x^2)y')' = -m(m + 1)y.$$

We note that that $p(x) = (1 - x^2)$, eigenvalues are given by $-m(m + 1)$, and the weight $w(x) = 1$. Since $p(1) = p(-1) = 0$, the Sturm–Liouville operator is self-adjoint with respect to the inner product

$$(u, v) = \int_{-1}^{1} uv \, \mathrm{d}x.$$

The eigenfunctions of the Lengendre equation are orthogonal in this basis. Let's start with the basis of monomials $\{1, x, x^2, x^3, \dots\}$ and extract the Legendre polynomials from them. Starting with $m = 0$ we have that $\mathrm{P}_0(x) = 1$ is a solution to the Legendre equation. Let's find the solution for $m = 1$. The solution will be the function that is closest to x and orthogonal to $\mathrm{P}_0 = 1$.

$$\mathrm{P}_1(x) = x - \mathrm{P}_0(x) \frac{(\mathrm{P}_0, x)}{\| \mathrm{P}_0 \|^2} = x - 1 \frac{(1, x)}{\|1\|^2} = x.$$

$\mathrm{P}_2(x)$ will be the closest quadratic polynomial to x^2 that is orthogonal to $\mathrm{P}_0(x)$ and $\mathrm{P}_1(x)$

$$\begin{aligned} \mathrm{P}_2(x) &= x^2 - \mathrm{P}_0(x) \frac{(\mathrm{P}_0, x^2)}{\| \mathrm{P}_0 \|^2} - \mathrm{P}_1 \frac{(\mathrm{P}_1, x^2)}{\| \mathrm{P}_1 \|^2} \\ &= x^2 - 1 \frac{(1, x^2)}{\|1\|^2} - x \frac{(x, x^2)}{\|x\|^2} \\ &= x^2 - 1 \frac{4/3}{2} - 0 = x^2 - \frac{2}{3}. \end{aligned}$$

Getting high Legendre polynomials $\mathrm{P}_3(x)$, $\mathrm{P}_4(x)$, and higher using the Gram–Schmidt process requires quite a bit of work. Recursion formulas, which we'll come to later, are much faster. ◀

CHAPTER 6

Bessel Functions

Bessel's equation

$$x^2\,\mathrm{J}_m'' + x\,\mathrm{J}_m' + (x^2 - m^2)\,\mathrm{J}_m = 0,$$

which we had earlier used to model the displacement of a circular drum head, arises in separation of variables for Laplace equation and Helmholtz equation in spherical or cylindrical coordinates. A such it is also important in solutions involving electromagnetic waves, heat conduction, vibration, and Schrödinger's equation. In this chapter, we examine the Bessel function $\mathrm{J}_m(x)$ and different expressions for the Bessel function in depth.

6.1 Generating function

We call $g(x,t)$ a *generating function* of the functions $P_m(x)$ if

$$g(x,t) = \sum_{m=-\infty}^{\infty} P_m(x)t^m.$$

That is, $g(x,t)$ is a generating function of $P_m(x)$, if the coefficients of the Laurent series of $g(x,t)$ are the functions $P_m(x)$ for integer values m. Many generating functions can be derived from physical principles. The generating function for the Bessel functions can be derived by expressing the plane wave solution to the Helmholtz equation as a Bessel function expansion. Because such a derivation (called the a Jacobi–Anger expression) would be a substantial detour for us, we'll simply state the generating function and confirm that it agrees with the solution (4.6) we obtained using the method of Frobenius.

The generating function for the Bessel functions is given by

$$g(x,t) = \mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^m. \tag{6.1}$$

To see this

$$\begin{aligned}
g(x,t) &= \mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \mathrm{e}^{xt/2}\,\mathrm{e}^{-x/2t} \\
&= \left(\sum_{j=0}^{\infty} \frac{1}{j!}\left(\frac{x}{2}\right)^{j} t^{j}\right)\left(\sum_{k=0}^{\infty} \frac{(-1)^k}{k!}\left(\frac{x}{2}\right)^{k} t^{-k}\right) \\
&= \sum_{m=-\infty}^{\infty}\left(\sum_{\substack{j-k=m\\ j,k\geq 0}} \frac{(-1)^k}{j!k!}\left(\frac{x}{2}\right)^{j+k}\right) t^m \\
&= \sum_{m=-\infty}^{\infty}\left(\sum_{k=0}^{\infty} \frac{(-1)^k}{(m+k)!k!}\left(\frac{x}{2}\right)^{2k+m}\right) t^m \\
&= \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^m .
\end{aligned}$$

Furthermore, note that

$$\mathrm{J}_{-m}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(-m+k)!}\left(\frac{x}{2}\right)^{-m+2k} .$$

Because the factorial of a negative number is infinite, we can start the sum at m:

$$\mathrm{J}_{-m}(x) = \sum_{k=m}^{\infty} \frac{(-1)^k}{k!(-m+k)!}\left(\frac{x}{2}\right)^{-m+2k} .$$

Shifting the indices $k \longrightarrow k+m$, we get

$$\begin{aligned}
\mathrm{J}_{-m}(x) &= \sum_{k=0}^{\infty} \frac{(-1)^{k+m}}{(k+m)!k!}\left(\frac{x}{2}\right)^{m+2k} \\
&= (-1)^m\,\mathrm{J}_m(x).
\end{aligned}$$

Also, note that m need not be integer valued. For general m we replace the factorial with the corresponding gamma function

$$\mathrm{J}_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(m+k+1)}\left(\frac{x}{2}\right)^{2k+m} .$$

Example. Generating functions allow us to quickly derive many useful expressions for special functions. In particular, if we take $t = \mathrm{e}^{-\mathrm{i}\theta}$, we have

$$\mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \mathrm{e}^{\frac{1}{2}x(\mathrm{e}^{\mathrm{i}\theta}-\mathrm{e}^{-\mathrm{i}\theta})} = \mathrm{e}^{\mathrm{i}x\sin\theta} .$$

This means that

$$\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)\, \mathrm{e}^{\mathrm{i}m\theta} = \mathrm{e}^{\mathrm{i}x\sin\theta}$$

is the discrete Fourier transform of the the Bessel function. ◄

6.2 Recursion formulae

We can use the generating function to find a recursion formula for the Bessel functions. By differentiating the generating function (6.1) with resepect to t we get

$$\begin{aligned}
\frac{\partial g}{\partial t} &= \frac{x}{2}(1+t^{-2})\,\mathrm{e}^{\frac{1}{2}x(t-t^{-1})}\\
&= \frac{x}{2}(1+t^{-2})g(x,t)\\
&= \frac{x}{2}(1+t^{-2})\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^m\\
&= \frac{x}{2}\left(\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^m + \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^{m-2}\right)\\
&= \frac{x}{2}\left(\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^m + \sum_{m=-\infty}^{\infty} \mathrm{J}_{m+2}(x)t^{m}\right)\\
&= \frac{x}{2}\sum_{m=-\infty}^{\infty} \big(\mathrm{J}_m(x) + \mathrm{J}_{m+2}(x)\big)t^m.
\end{aligned}$$

Similarly, differentiating the expression in (6.1) we get

$$\frac{\partial g}{\partial t} = \sum_{m=-\infty}^{\infty} m\,\mathrm{J}_m(x)t^{m-1} = \sum_{m=-\infty}^{\infty} (m+1)\,\mathrm{J}_{m+1}(x)t^m.$$

Both derivatives are the same, so

$$\frac{x}{2}\sum_{m=-\infty}^{\infty} (\mathrm{J}_m(x) + \mathrm{J}_{m+2}(x))\,t^m = \sum_{m=-\infty}^{\infty} (m+1)\,\mathrm{J}_{m+1}(x)t^m.$$

Because this equality holds for all values t, the coefficients must be equal

$$\frac{x}{2}\,(\mathrm{J}_m(x) + \mathrm{J}_{m+2}(x)) = (m+1)\,\mathrm{J}_{m+1}(x).$$

Equivalently,

$$\mathrm{J}_{m+1} + \mathrm{J}_{m-1} = \frac{2m}{x}\,\mathrm{J}_m$$

giving us a recursion formula for the Bessel functions.

We can get a second recursion formula by taking the partial derivative of the generating function with respect to x:

$$\begin{aligned}
\frac{\partial g}{\partial x} &= \sum_{m=-\infty}^{\infty} \mathrm{J}'_m(x) t^m \\
&= \tfrac{1}{2}\left(t - t^{-1}\right) \mathrm{e}^{\frac{1}{2}x(t-t^{-1})} \\
&= \tfrac{1}{2}\left(t - t^{-1}\right) g(x,t) \\
&= \tfrac{1}{2}\left(t - t^{-1}\right) \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^m \\
&= \tfrac{1}{2}\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^{m+1} - \tfrac{1}{2}\sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^{m-1} \\
&= \tfrac{1}{2}\sum_{m=-\infty}^{\infty} \mathrm{J}_{m-1}(x) t^{m} - \tfrac{1}{2}\sum_{m=-\infty}^{\infty} \mathrm{J}_{m+1}(x) t^{m}.
\end{aligned}$$

So,

$$\sum_{m=-\infty}^{\infty} \mathrm{J}'_m(x) t^m = \tfrac{1}{2}\sum_{m=-\infty}^{\infty} \left(\mathrm{J}_{m-1}(x) - \mathrm{J}_{m+1}(x)\right) t^m.$$

The sum holds for all t, so it follows that

$$\mathrm{J}'_m(x) = \tfrac{1}{2}\,\mathrm{J}_{m-1}(x) - \tfrac{1}{2}\,\mathrm{J}_{m+1}(x).$$

6.3 Integral representation

Starting with the generating function

$$\mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^m$$

and taking $t = e^{-\mathrm{i}\theta}$ gives us

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}x\sin\theta} &= \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)\,\mathrm{e}^{\mathrm{i}m\theta} \\
&= \mathrm{J}_0(x) + \sum_{m=-\infty}^{\infty} \left(\mathrm{J}_m(x)\,\mathrm{e}^{\mathrm{i}m\theta} + \mathrm{J}_{-m}(x)\,\mathrm{e}^{-\mathrm{i}m\theta}\right) \\
&= \mathrm{J}_0(x) + \sum_{m=-\infty}^{\infty} \left(\mathrm{J}_m(x)\,\mathrm{e}^{\mathrm{i}m\theta} + (-1)^m\,\mathrm{J}_m(x)\,\mathrm{e}^{-\mathrm{i}m\theta}\right) \\
&= \mathrm{J}_0(x) + \sum_{m=-\infty}^{\infty} \mathrm{J}_{2m}(x)\left(\mathrm{e}^{\mathrm{i}2m\theta} + \mathrm{e}^{-\mathrm{i}2m\theta}\right) \\
&\qquad + \sum_{m=-\infty}^{\infty} \mathrm{J}_{2m+1}(x)\left(\mathrm{e}^{\mathrm{i}(2m+1)\theta} - \mathrm{e}^{-\mathrm{i}(2m+1)\theta}\right) \\
&= \mathrm{J}_0(x) + 2\sum_{m=-\infty}^{\infty} \mathrm{J}_{2m}\cos(2m\theta) \\
&\qquad + 2\mathrm{i}\sum_{m=-\infty}^{\infty} \mathrm{J}_{2m+1}\sin((2m+1)\theta)
\end{aligned}$$

The left-hand side can be expanded

$$\mathrm{e}^{\mathrm{i}x\sin\theta} = \cos(x\sin\theta) + \mathrm{i}\sin(x\sin\theta).$$

Equating the real and imaginary parts we get

$$\begin{aligned}
\mathrm{J}_0(x) + 2\sum_{m=1}^{\infty} \mathrm{J}_{2m}(x)\cos(2m\theta) &= \cos(x\sin\theta) \\
2\sum_{m=1}^{\infty} \mathrm{J}_{2m-1}(x)\sin((2m-1)\theta) &= \sin(x\sin\theta)
\end{aligned}$$

By orthogonality of sine and cosine,

$$\begin{aligned}
\int_0^\pi \cos n\theta\cos m\theta\,\mathrm{d}\theta &= \frac{\pi}{2}\delta_{nm} \\
\int_0^\pi \sin n\theta\sin m\theta\,\mathrm{d}\theta &= \frac{\pi}{2}\delta_{nm},
\end{aligned}$$

we have that

$$\int_0^\pi \cos(x\sin\theta)\cos(m\theta)\,\mathrm{d}\theta = \begin{cases} \mathrm{J}_m(x), & n \text{ even} \\ 0, & n \text{ odd} \end{cases}$$

$$\int_0^\pi \sin(x\sin\theta)\sin(m\theta)\,\mathrm{d}\theta = \begin{cases} 0, & n \text{ even} \\ \mathrm{J}_m(x), & n \text{ odd.} \end{cases}$$

Adding these expressions together gives us

$$\begin{aligned} \mathrm{J}_m(x) &= \frac{1}{\pi}\int_0^\pi \cos(x\sin\theta)\cos(m\theta) + \sin(x\sin\theta)\sin(m\theta)\,\mathrm{d}\theta \\ &= \frac{1}{\pi}\int_0^\pi \cos(m\theta - x\sin\theta)\,\mathrm{d}\theta \end{aligned}$$

and

$$\mathrm{J}_0(x) = \frac{1}{2\pi}\int_0^\pi \cos(x\sin\theta)\,\mathrm{d}\theta.$$

6.4 Schläfli integral representation

The representation of a function using a contour integral is called the *Schläfli integral*. Divide the generating function for the Bessel function

$$g(x,t) = \mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^m$$

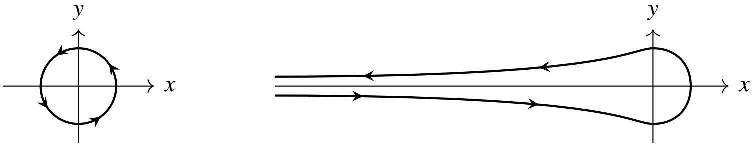
by t^{n+1} for some n and consider the contour integral which avoids the origin

$$\begin{aligned} \oint \mathrm{e}^{\frac{1}{2}x(t-t^{-1})}\, t^{-n-1}\,\mathrm{d}t &= \oint \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)t^{m-n-1}\,\mathrm{d}t \\ &= \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)\oint t^{m-n-1}\,\mathrm{d}t \\ &= \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x)2\pi\mathrm{i}\delta_{mn} \\ &= 2\pi\mathrm{i}\,\mathrm{J}_n(x) \end{aligned}$$

So,

$$\mathrm{J}_n(x) = \frac{1}{2\pi\mathrm{i}}\oint \mathrm{e}^{\frac{1}{2}x(t-t^{-1})}\, t^{-n-1}\,\mathrm{d}t$$

This integral representation is the Schläfli integral. We can continue this representation to non-integer n. In this case there is a branch cut, and we need to take the contour to avoid it.



When x is small ($x \ll 1$), we can use the series representation of the Bessel function

$$\mathrm{J}_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(m+k)!} \left(\frac{x}{2}\right)^{m+2k}$$

to determine an approximation

$$\mathrm{J}_m(x) \approx \frac{1}{m!} \left(\frac{x}{2}\right)^{m} = \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^{m}.$$

When x is large ($x \gg 1$), we can use the method of steepest descent on the Schläfli integral representation to approximate the Bessel function. Recall the method of steepest descent (for $s \gg 1$):

$$\int_C g(z)\,\mathrm{e}^{sf(z)}\,\mathrm{d}z \approx \frac{\sqrt{2\pi} g(z_0) e^{sf(z_0)} \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2}}{\sqrt{|sf''(z_0)|}}$$

where $\theta = \arg f''(z_0)$. Now,

$$f(t) = \tfrac{1}{2}(t - t^{-1}) \quad \text{and} \quad g(t) = t^{-(n+1)}.$$

We compute

$$f'(t) = \tfrac{1}{2}(1 + t^{-2})$$
$$f''(t) = -t^{-3}$$

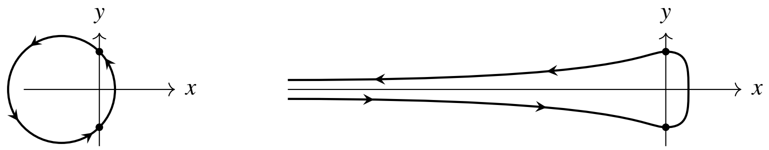
The function $f(t)$ has a saddle point when $f'(t) = 0$. From

$$\tfrac{1}{2}(1 + t^{-2}) = 0$$

we have $t = \mathrm{i}$ and $t = -\mathrm{i}$. In this case, $f(t)$ has two saddle points and we must compute the contribution from both. At $t = \mathrm{i}$ and $t = -\mathrm{i}$, we have

$$f(\mathrm{i}) = \tfrac{1}{2}(\mathrm{i} + \mathrm{i}) = \mathrm{i} \qquad f(-\mathrm{i}) = \tfrac{1}{2}(-\mathrm{i} - \mathrm{i}) = -\mathrm{i}$$
$$f''(\mathrm{i}) = -\mathrm{i} \qquad f''(-\mathrm{i}) = \mathrm{i}$$
$$g(\mathrm{i}) = \mathrm{e}^{-(n+1)\mathrm{i}\pi/2} \qquad g(-\mathrm{i}) = \mathrm{e}^{(n+1)\mathrm{i}\pi/2}$$
$$\theta = \arg f''(\mathrm{i}) = -\pi/2 \qquad \theta = \arg f''(-\mathrm{i}) = \pi/2$$

The direction of the of steepest descent at the saddle point is given by $\alpha = \pi/2 - \theta/2$ We will need to deform our contour so that it goes through the sadde point at $t = \mathrm{i}$ at angle $\alpha = 3\pi/4$ and the saddle point at $t = -\mathrm{i}$ at angle $\alpha = \pi/4$.



In this case, from the method of steepest descent

$$\int_C g(z)\,\mathrm{e}^{sf(z)}\,\mathrm{d}z \approx \frac{\sqrt{2\pi}g(z_0)e^{sf(z_0)}\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta/2}}{\sqrt{|sf''(z_0)|}} = I_{z_0}$$

we get the contribution

$$\begin{aligned} I_{\mathrm{i}} &= \frac{\sqrt{2\pi}\,\mathrm{e}^{-(n+1)\mathrm{i}\pi/2}\,e^{-\mathrm{i}x}\mathrm{i}\,\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{x}} = \frac{\sqrt{2\pi}\mathrm{i}\,\mathrm{e}^{-\mathrm{i}(n\pi/2+x-\pi/4)}}{\sqrt{x}} \\ I_{-\mathrm{i}} &= \frac{\sqrt{2\pi}\,\mathrm{e}^{(n+1)\mathrm{i}\pi/2}\,e^{\mathrm{i}x}(-\mathrm{i})\,\mathrm{e}^{-\mathrm{i}\pi/4}}{\sqrt{x}} = \frac{\sqrt{2\pi}\mathrm{i}\,\mathrm{e}^{+\mathrm{i}(n\pi/2+x-\pi/4)}}{\sqrt{x}}. \end{aligned}$$

Combining these values gives us

$$\begin{aligned} \mathrm{J}_n(x) &\approx \frac{1}{2\pi\mathrm{i}}(I_{\mathrm{i}} + I_{-\mathrm{i}}) \\ &= \left(\frac{1}{2\pi\mathrm{i}}\right)\frac{\sqrt{2\pi}}{\sqrt{x}}\mathrm{i}\left(\mathrm{e}^{-\mathrm{i}(n\pi/2+x-\pi/4)} + \mathrm{e}^{\mathrm{i}(n\pi/2+x-3\pi/4)}\right) \\ &= \sqrt{\frac{2}{\pi x}}\cos(x + n\pi/2 - \pi/4). \end{aligned}$$

6.5 Neumann functions

For integer values of m, the method of Frobenius produces only one linearly independent solution to Bessel's equation, called the Bessel function of the first kind. Using this solution we were able to compute a second solution

$$\begin{aligned} y(x) &= A\,\mathrm{J}_m(x) + B\,\mathrm{J}_m(x)\int_0^x \frac{1}{x\,\mathrm{J}_m^2(x)}\,\mathrm{d}x \\ &= A'\,\mathrm{J}_m(x) + B'\,\mathrm{Y}_m(x) \end{aligned}$$

where Y_m is called the Bessel function of the second kind or the Neumann function. For integer values of m, the Neumann function has a singularity at the origin and hence it is unphysical in the solution to the circular drum problem.

For non-integer values of m, the Neumann function can be defined as

$$\mathrm{Y}_m(x) = \frac{\mathrm{J}_m(x)\cos(m\pi) - \mathrm{J}_{-m}(x)}{\sin(m\pi)}.$$

Because this expression is simply a combination of Bessel functions, the Neumann function is a solution to Bessel's equation. When m is an integer,

$$\mathrm{Y}_m(x) = \frac{\mathrm{J}_m(x)\cos(m\pi) - \mathrm{J}_{-m}(x)}{\sin(m\pi)} = \frac{\mathrm{J}_m(x)(-1)^m - (-1)^m\,\mathrm{J}_m(x)}{\sin(m\pi)} = \frac{0}{0}$$

and the function is formally undefined. But we can use l'Hôpital's rule (differentiating the numerator and denominator with respect to m) and substitute the resulting expression into the derivative of Bessel's equation with respect to m. The whole process is more or less straight-forward but a little tedious, so we'll skip the derivation.

Whereas

$$\begin{aligned}
\mathrm{J}_m(x) &\approx \frac{1}{\Gamma(m+1)}\left(\frac{x}{2}\right)^m && x \ll 1\\
\mathrm{J}_m(x) &\approx \sqrt{\frac{2}{\pi x}}\cos(x - n\pi/2 - \pi/4) && x \gg 1,
\end{aligned}$$

for Neumann functions

$$\begin{aligned}
\mathrm{Y}_m(x) &\approx -\frac{\Gamma(m)}{\pi}\left(\frac{2}{x}\right)^m, \quad \text{for } m > 0 && x \ll 1\\
\mathrm{Y}_m(x) &\approx \sqrt{\frac{2}{\pi x}}\sin(x - n\pi/2 - \pi/4) && x \gg 1
\end{aligned}$$

Notice that far from the origin $\mathrm{J}_m(x)$ and $\mathrm{Y}_m(x)$ behave as complementary decaying trigonometric functions.

6.6 Hankel transform

Just as we can express the exponential function in terms of trigonometric functions

$$\mathrm{e}^{\pm\mathrm{i}\theta} = \cos\theta \pm \mathrm{i}\sin\theta$$

we can analogously define the *Hankel function* (sometimes called the Bessel function of the third kind) as

$$\mathrm{H}_m^{(1)}(x) = \mathrm{J}_m(x) + \mathrm{i}\,\mathrm{Y}_m(x) \tag{6.2}$$

$$\mathrm{H}_m^{(2)}(x) = \mathrm{J}_m(x) - \mathrm{i}\,\mathrm{Y}_m(x). \tag{6.3}$$

Because $Y_m(x)$ has a singularity at the origin, it is a bad idea to use the Hankel function approximation (in lieu of a Bessel function approximation) near the origin when solving a problem numerically.

So far we have seen that the Fourier functions $\sin nx$ and $\cos nx$ are the eigenfunctions for the harmonic oscillator equation, which we used to model wave propagation on a the one-dimensional string. When the ends of the guitar string were clamped, the solution were a made up of sine functions

$$u(t,x) = \sum_{n=0}^{\infty} a_n \cos n\pi t \sin n\pi x$$

where the coefficients a_n are determined by the sine transform

$$a_m = 2\,(\sin m\pi x, f(x)) = 2\int_0^1 f(x)\sin m\pi x\,\mathrm{d}x.$$

If the string had infinite length extending from $-\infty$ to ∞, the solution would be a combination of sine and cosine functions, and coefficients could be determined using a Fourier transform (a combination of a sine transform and a cosine transform)

$$a_m = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-\mathrm{i}mx}\,\mathrm{d}x.$$

We also saw that the Bessel functions $J_n(x)$ are the eigenfunctions of the Bessel equation, which gave us the radial component for the two-dimensional wave propagation solution to the drum. For a radially symmetric initial condition,

$$u(t,x) = \sum_{n=0}^{\infty} a_n \cos n\pi t\, J_n(x).$$

Because the circular drum is clamped down around its circumference, we must stretch the domain for each Bessel function so that their zeros coincide with the domain boundary (say at $x = 1$). As we saw earlier, by taking $x = \alpha s$ in Bessel's equation we have

$$s^2\frac{\mathrm{d}^2 y}{\mathrm{d}s^2} + s\frac{\mathrm{d}y}{\mathrm{d}s} + (\alpha^2 s^2 - m^2)y = 0,$$

which in Sturm–Liouville form is

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(s\frac{\mathrm{d}y}{\mathrm{d}s}\right) - \frac{m^2}{s}y = \alpha^2 s y.$$

The Bessel functions are orthogonal under the inner-product

$$(u,v) = \int_0^1 uvs\,\mathrm{d}s.$$

Specifically,

$$\int_0^1 \mathrm{J}_m(\alpha_j x)\,\mathrm{J}_m(\alpha_k x) x\,\mathrm{d}x = \tfrac{1}{2}\,\mathrm{J}_{m+1}(\alpha_j)\delta_{jk},$$

when α_j and α_k are zeros of $\mathrm{J}_m(x)$.

Now, we can expand a function in a Fourier–Bessel series in terms of the Bessel function of order m as

$$f(x) = \sum_{n=0}^{\infty} a_n\,\mathrm{J}_m(\alpha_n x)$$

where a_n are found using the *Hankel transform* (of order m)

$$a_n = \int_0^{\infty} f(r)\,\mathrm{J}_m(\alpha_n r) r\,\mathrm{d}r.$$

Example. The Fourier transform is related to the zero-order Hankel transform. To see this, note that the two-dimensional Fourier transform is given by

$$F(k_x, k_y) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x,y)\,\mathrm{e}^{-\mathrm{i}k_x x}\,\mathrm{e}^{-\mathrm{i}k_y y}\,\mathrm{d}x\,\mathrm{d}y.$$

which in polar coordinates equals

$$\frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} f(x,\theta)\,\mathrm{e}^{-\mathrm{i}k\sin\theta}\,r\,\mathrm{d}r\,\mathrm{d}\theta. \qquad (6.4)$$

Recall the Bessel function

$$\mathrm{J}_n(x) = \frac{1}{2\pi\mathrm{i}}\oint \mathrm{e}^{(x/2)(t-1/t)}\,t^{-n-1}\,\mathrm{d}t.$$

By taking $t = \mathrm{e}^{\mathrm{i}\theta}$ in the Schläfli integral, we have

$$\mathrm{J}_n(x) = \frac{1}{2\pi}\oint \mathrm{e}^{\mathrm{i}x\sin\theta}\,\mathrm{e}^{-\mathrm{i}n\theta}\,\mathrm{d}\theta.$$

It follows that for $n = 0$

$$\mathrm{J}_0(x) = \frac{1}{2\pi}\oint \mathrm{e}^{\mathrm{i}x\sin\theta}\,\mathrm{d}\theta.$$

If the function f is radially symmetric, so that $f(x,\theta) \equiv f(x)$, then (6.4) becomes

$$\begin{aligned}
F(k_x, k_y) &= \frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} f(x,\theta)\,\mathrm{e}^{-\mathrm{i}k\sin\theta}\,r\,\mathrm{d}r\,\mathrm{d}\theta \\
&= \frac{1}{2\pi}\int_0^{\infty} f(r) r \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}k\sin\theta}\,\mathrm{d}\theta\,\mathrm{d}r \\
&= \frac{1}{2\pi}\int_0^{\infty} f(r)\,\mathrm{J}_0(kr) r\,\mathrm{d}r.
\end{aligned}$$

This shows us that the Fourier transform is now really just the zero-order Hankel transform. ◀

Here are useful formulas for the Bessel function:

differential equation	$x^2\,\mathrm{J}_m'' + x\,\mathrm{J}_m' + (x^2 - m^2)\,\mathrm{J}_m = 0$
series solution	$\mathrm{J}_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(m+k)!} \left(\frac{x}{2}\right)^{m+2k}$
generating function	$\mathrm{e}^{\frac{1}{2}x(t-t^{-1})} = \sum_{m=-\infty}^{\infty} \mathrm{J}_m(x) t^m$
recursion formula	$2\,\mathrm{J}_m'(x) = \mathrm{J}_{m-1}(x) - \mathrm{J}_{m+1}(x)$
recursion formula	$\mathrm{J}_{m+1}(x) + \mathrm{J}_{m-1}(x) = \frac{2m}{x}\,\mathrm{J}_m(x)$
Schläfli integral	$\mathrm{J}_m(x) = \frac{1}{2\pi\mathrm{i}} \oint \mathrm{e}^{(x/2)(t-1/t)}\, t^{-(m+1)}\,\mathrm{d}t$
integral representation	$\mathrm{J}_m(x) = \frac{1}{\pi} \int_0^{\pi} \cos(m\theta - x\sin\theta)\,\mathrm{d}\theta$
	$\mathrm{J}_0(x) = \frac{1}{2\pi} \int_0^{\pi} \cos(x\sin\theta)\,\mathrm{d}\theta$

CHAPTER 7

Orthogonal Polynomials

In this final chapter, we examine the Legendre, Hermite, Laguerre, and Chebyshev orthogonal polynomials. These polynomials are important both in physics and in mathematics as basis functions for solutions to Laplace's equation $\nabla^2\psi = 0$, Poisson's equation $\nabla^2\psi = f(x)$, Helmholtz's equation $\nabla^2\psi = -k^2\psi$, and Schrödinger's equation $\nabla^2\psi = -f(x)\psi$, along with their time-dependent counterparts. Solutions to these equations are linear combinations of Fourier polynomials (sines and cosines) in Cartesian coordinates, Legendre polynomials in spherical system, Bessel functions in cylindrical coordinates, and Chebyshev polynomials in an elliptical coordinate system. Let's start by examining the spherical harmonics which arise in a spherical coordinate system.

7.1 Spherical harmonics

A function that satisfies Laplace's equation $\nabla^2\psi = 0$ is called a *harmonic function*. We've already encountered two-dimensional harmonic functions when studying analytic (complex) functions. Solutions to the two-dimensional Laplace's equation $\psi_{xx} + \psi_{yy} = 0$ are harmonic conjugates of analytic functions $u(x, y) = \psi + \mathrm{i}\phi$, which satisfy the Cauchy–Riemann equations. In this section, we examine three-dimensional spherical harmonic functions.

Example. As a review let's solve the two-dimensional Laplace's equation in polar coordinates

$$\nabla^2\psi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} = 0$$

using separation of variables. Taking $\psi(r,\theta) = u(r)v(\theta)$ gives us

$$v\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}u}{\mathrm{d}r}\right) + \frac{1}{r^2}u\frac{\mathrm{d}^2v}{\mathrm{d}\theta^2} = 0.$$

After separating out the variables $u(r)$ and $v(\theta)$ we get

$$-\frac{v''}{v} = \frac{r(ru')'}{u} = \lambda$$

for an arbitrary constant λ. Solving $v'' + \lambda v = 0$, we get $v(\theta) = \mathrm{e}^{\pm i\sqrt{\lambda}\theta}$. Take with $\lambda = n^2$ for integer values n to satisfy the periodic boundary conditions in the angular direction. For $u(r)$

$$r(ru')' - n^2 u = 0,$$

which has the solution $u(r) = r^n$. So,

$$\psi(r,\theta) = \sum_{n=-\infty}^{\infty} a_n r^n \,\mathrm{e}^{in\theta} = a_n z^n$$

for $z = r\,\mathrm{e}^{\mathrm{i}\theta}$ where coefficients a_n are determined from boundary conditions. ◄

Let's now look at the three-dimensional Laplace's equation in spherical coordinates. With $\psi(r,\theta,\psi)$ we have

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} = 0.$$

Take

$$\psi(r,\theta,\phi) = u(r)y(\theta,\phi) = u(r)v(\theta)w(\phi).$$

Then

$$y\frac{1}{r^2}(r^2u_r)_r + \frac{u}{r^2}\left[\frac{1}{\sin\theta}(\sin\theta y_\theta)_\theta\right] + \frac{u}{r^2}\frac{1}{\sin^2\theta}y_{\phi\phi} = 0$$

So,

$$\frac{(r^2u_r)_r}{u} = -\frac{\frac{1}{\sin\theta}(\sin\theta y_\theta)_\theta + \frac{1}{\sin^2\theta}y_{\phi\phi}}{y} = \lambda$$

Let's first find the solution for u:

$$(r^2u')' - \lambda u = 0$$

Taking the ansatz that $u = r^n$, then $n(n+1)r^n = \lambda r^n$. So, $\lambda = n(n+1)$.

Now, let's find y:

$$\frac{1}{\sin\theta}(\sin\theta y_\theta)_\theta + \frac{y_{\phi\phi}}{\sin^2\theta} = -n(n+1)y.$$

Taking $y(\phi,\theta) = v(\theta)w(\phi)$ gives us

$$\sin\theta w(\sin\theta v')' + vw'' + n(n+1)\sin^2\theta vw = 0.$$

Dividing by $y = vw$:

$$\frac{\sin\theta(\sin\theta v')' + n(n+1)\sin^2\theta v}{v} = -\frac{w''}{w} = \gamma$$

for some γ. The solution to $w'' + \gamma w = 0$ is $w = \mathrm{e}^{\pm \mathrm{i}\sqrt{\gamma}\phi}$. The value $\sqrt{\gamma}$ must be an integer to satisfy periodic boundary conditions, and therefore $\gamma = m^2$.

Finally, we solve

$$\sin\theta(\sin\theta v')' + n(n+1)\sin^2\theta v = -m^2 v$$

for $v(\theta)$. We can simplify this by making the change of variables $x = \cos\theta$ for which

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}\theta} = -\sin\theta\frac{\mathrm{d}}{\mathrm{d}x}.$$

Starting with

$$\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}v}{\mathrm{d}\theta}\right) + n(n+1)\sin^2\theta v = -m^2 v$$

and making the change of variable we get

$$-\sin^2\theta\frac{\mathrm{d}}{\mathrm{d}x}\left(-\sin^2\theta\frac{\mathrm{d}v}{\mathrm{d}x}\right) + n(n+1)\sin^2\theta v = -m^2 v.$$

Because $\sin^2\theta = 1 - \cos^2\theta = 1 - x^2$, we have

$$(1-x)^2((1-x^2)v')' + n(n+1)(1-x^2)v + m^2 v = 0$$

$$((1-x)^2 v')' + \left[n(n+1) - \frac{m^2}{1-x^2}\right]v = 0. \tag{7.1}$$

We call this equation the associated Legendre equation. The solution

$$\mathrm{P}_n^m(x) = \mathrm{P}_n^m(\cos\theta)$$

is called the associated Legendre polynomial.

The solution to the three-dimensional Laplace's equation is

$$\begin{aligned}\psi(r,\theta,\phi) &= \sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty} a_{nm} r^n \,\mathrm{e}^{\mathrm{i}m\phi}\,\mathrm{P}_n^m(\cos\theta)\\ &= \sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty} a_{nm} r^n \,\mathrm{Y}_n^m(\theta,\phi).\end{aligned}$$

The functions $\mathrm{Y}_n^m(\theta,\phi) = \mathrm{e}^{\mathrm{i}m\phi}\,\mathrm{P}_n^m(\cos\theta)$ are called *spherical harmonics*.

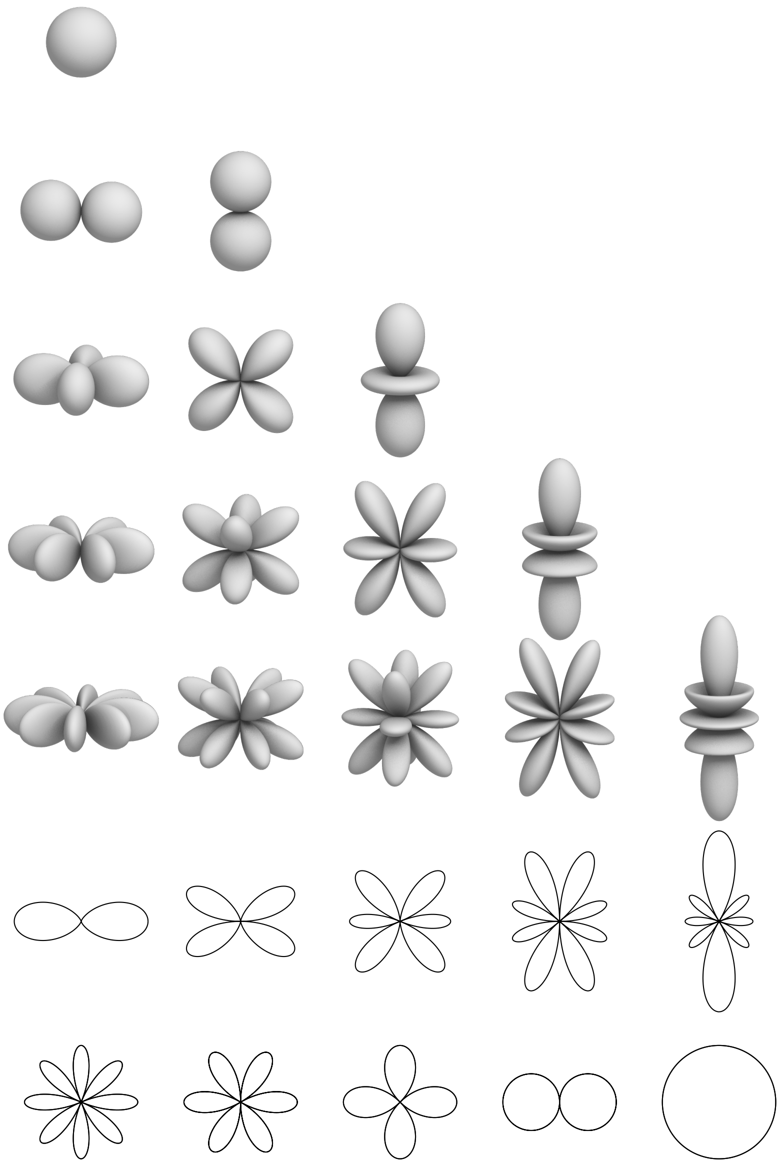


Figure 7.1: Real part of the spherical harmonic function $Y_n^m(\theta, \phi) = e^{im\phi} P_n^m(\cos\theta)$ for $n = 0, 1, 2, 3, 4$ top-to-bottom and $m = 0, 1, \ldots, n$ right-to-left.

If we happen to have radial symmetry in along the ϕ axis, then $m = 0$. In this case, the associated Legendre equation (7.1) is now simply the Legendre equation

$$((1 - x^2)v')' + n(n+1)v = 0.$$

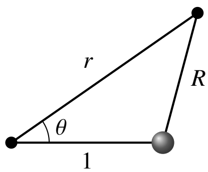
which has the Legendre polynomial solutions

$$\mathrm{P}_n(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{(2n-2k)!}{2^n k!(n-2k)!(n-k)!} x^{n-2k}.$$

7.2 Legendre polynomial

Generating function

Suppose that we have a point charge located one unit from the origin along the x-axis. The electrostatic Coulomb potential $\varphi(r,\theta)$ is proportional to $1/R$ where R is distance to the point charge. We can use the law of cosines to get that



$$\varphi(r,\theta) = \frac{C}{R} = \frac{C}{\sqrt{r^2 + 1 - 2r\cos\theta}}$$

where C is a constant determined by the magnitude of the point charges and Coulomb's constant. The electrostatic potential satisfies Poisson's equation, so we have that

$$\varphi(r,\theta) = \frac{C}{\sqrt{r^2 + 1 - 2r\cos\theta}} = \sum_{n=0}^{\infty} a_n \, \mathrm{P}_n(\cos\theta) r^n.$$

for some coefficients a_n. The constant C is merely a scaling factor, so we can leave it out of the discussion by rescaling $\{a_n\}$ appropriately

$$\varphi(r,\theta) = \frac{1}{\sqrt{r^2 + 1 - 2r\cos\theta}} = \sum_{n=0}^{\infty} a_n \, \mathrm{P}_n(\cos\theta) r^n.$$

If we take $\theta = 0$, then

$$\frac{1}{\sqrt{r^2 + 1 - 2r}} = \sum_{n=0}^{\infty} a_n \, \mathrm{P}_n(1) r^n.$$

We can (and do) normalize the Legendre polynomials so that $\mathrm{P}_n(1) = 1$. So, we have

$$\frac{1}{\sqrt{r^2 + 1 - 2r}} = \sum_{n=0}^{\infty} a_n r^n$$

The left hand side simplifies to $1/|1-r|$ which can be expanded as a power series

$$\frac{1}{1-r} = 1 + r + r^2 + r^3 + \cdots$$

It follows that $a_n = 1$ for all $n = 0, 1, \ldots$. Hence,

$$\frac{1}{\sqrt{r^2 + 1 - 2r\cos\theta}} = \sum_{n=0}^{\infty} \mathrm{P}_n(\cos\theta) r^n.$$

Take $t = 1/r$ and $x = \cos\theta$. Then

$$g(x,t) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} \mathrm{P}_n(x) t^n$$

giving us the generating function for the Legendre polynomials.

Three term recurrence

We can derive a three term recurrence for the Legendre polynomials by examining the partial derivative of $g(x,t)$ with respect to t. We have that

$$\frac{\partial g}{\partial t} = \frac{x - t}{(1 - 2tx + t^2)^{3/2}} = \sum_{n=1}^{\infty} n\,\mathrm{P}_n(x) t^{n-1}.$$

Equivalently, we have

$$\frac{x - t}{(1 - 2tx + t^2)^{1/2}} = (1 - 2tx + t^2) \sum_{n=1}^{\infty} n\,\mathrm{P}_n(x) t^{n-1}$$

which we can rewrite as

$$(x - t) g(x,t) = (1 - 2tx + t^2) \sum_{n=1}^{\infty} n\,\mathrm{P}_n(x) t^{n-1}$$

or

$$(x - t) \sum_{n=0}^{\infty} \mathrm{P}_n(x) t^n = (1 - 2tx + t^2) \sum_{n=1}^{\infty} n\,\mathrm{P}_n(x) t^{n-1}.$$

Distributing terms ino the sums (and defining $\mathrm{P}_n \equiv \mathrm{P}_n(x)$ to simplify notation) gives us

$$\sum_{n=0}^{\infty} x\,\mathrm{P}_n\,t^n - \sum_{n=0}^{\infty} \mathrm{P}_n\,t^{n+1} = \sum_{n=1}^{\infty} n\,\mathrm{P}_n\,t^{n-1} - 2\sum_{n=1}^{\infty} nx\,\mathrm{P}_n\,t^n + \sum_{n=1}^{\infty} \mathrm{P}_n\,t^{n+1}.$$

Let's shift the indices n so that we can combine the sums

$$\sum_{n=0}^{\infty} x\,P_n\,t^n - \sum_{n=0}^{\infty} P_{n-1}\,t^n$$
$$= \sum_{n=0}^{\infty}(n+1)\,P_{n+1}\,t^n - 2\sum_{n=0}^{\infty} nx\,P_n\,t^n + \sum_{n=0}^{\infty} P_{n-1}\,t^n.$$

It is understood that $P_{-1}(x) = 0$. Now, combining

$$\sum_{n=0}^{\infty} [x\,P_n - P_{n-1} - (n+1)\,P_{n+1} + 2nx\,P_n - P_{n-1}]\,t^n = 0.$$

We simplify the expression to get

$$\sum_{n=0}^{\infty} \Big[(x+1)\,P_n(x) - (n+1)\,P_{n+1}(x) + n\,P_{n-1}\Big] t^n = 0.$$

Because this expression is true for all t, it follows that

$$(x+1)\,P_n(x) - (n+1)\,P_{n+1}(x) + n\,P_{n-1}(x) = 0.$$

Hence,

$$(n+1)\,P_{n+1}(x) = (2n+1)x\,P_n(x) - n\,P_{n-1}(x)$$

and the first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \tfrac{1}{2}(3x^2-1), \quad P_2(x) = \tfrac{1}{2}(5x^3-3x).$$

Contour Integral

We can divide the generating function

$$g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n$$

by t^{m+1} and integrate around a contour about the origin in the complex plane

$$\oint_\gamma \frac{1}{t^{m+1}\sqrt{1-2xt+t^2}}\,\mathrm{d}t = \oint_\gamma \sum_{n=0}^{\infty} P_n(x) t^{n-(m+1)}\,\mathrm{d}t = 2\pi\mathrm{i}\,P_m(x)$$

giving us

$$P_n(x) = \frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{1}{t^{m+1}\sqrt{1-2xt+t^2}}\,\mathrm{d}t.$$

The function $\sqrt{1-2xt+t^2}$ has branch points at $t = x \pm \mathrm{i}\sqrt{1-x^2}$. By taking $x = \cos\theta$, we see that the branch points are at $t = \cos\theta \pm \mathrm{i}\sin\theta$. In other words, they lie on the unit circle. We can take one branch cut between the two branch points (instead of two branch cuts from each of the branch points to infinity). Now, we just need to choose the contour γ to avoid the branch cut. For example, we could take γ to be the unit circle.

Rodrigues' Formula

The binomial expansion of $(1-x^2)$ is given by

$$(1-x^2)^n = \sum_{k=0}^{n}(-1)^k\binom{n}{k}x^{2(n-k)} = \sum_{k=0}^{n}(-1)^k\frac{n!}{(n-k)!k!}x^{2(n-k)}.$$

If we differentiate n times we get

$$\begin{aligned}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x^2)^n &= \sum_{k=0}^{n}(-1)^k\frac{n!}{(n-k)!k!}\frac{(2n-2k)!}{(n-2k)!}x^{n-2k}\\ &= n!\sum_{k=0}^{[n/2]}(-1)^k\frac{(2n-2k)!}{k!(n-k)!(n-2k)!}x^{n-2k}.\end{aligned}$$

The series representation of the Legendre polynomial is

$$\mathrm{P}_n(x) = \sum_{k=0}^{[n/2]}(-1)^k\frac{(2n-2k)!}{2^n k!(n-2k)!(n-k)!}x^{n-2k}.$$

Therefore,

$$\mathrm{P}_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x^2)^n.$$

We call this formula the *Rodriques' formula*. We can use the Rodrigues' formula to derive the Schläfli integral. Recall Cauchy's integral formula

$$f^{[n]}(x) = \frac{n!}{2\pi\mathrm{i}}\oint\frac{f(t)}{(t-x)^{n+1}}\,\mathrm{d}t.$$

Hence,

$$\mathrm{P}_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x^2)^n = \frac{1}{2^{n+1}\pi\mathrm{i}}\oint\frac{(1-t^2)^n}{(t-x)^{n+1}}\,\mathrm{d}t.$$

We can extend the Legendre polynomials to noninteger values n using the Schläfli representation directly or the Rodriques' formula using fractional calculus.

Orthogonality

The Sturm–Liouville form of the Legendre equation is given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{P}_n(x)\right] + n(n+1)\,\mathrm{P}_n(x) = 0.$$

If we define the domain $x \in [-1, 1]$ and the weight $w = 1$, then

$$(\mathrm{P}_n, \mathrm{P}_m) = \int_{-1}^{1} \mathrm{P}_n(x)\,\mathrm{P}_m(x)\,\mathrm{d}x = 0$$

for $n \neq m$. What is the normalization constant? We can use the Rodrigue's formula to show that the Legendre polynomials are in fact orthogonal over the interval $(-1, 1)$ and to determine the normality constant.

Theorem. *If* $\mathrm{P}_m(x)$ *and* $\mathrm{P}_n(x)$ *are mth degree and nth degree Legendre polynomials, then*

$$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x = \frac{2}{2m+1}\delta_{nm}.$$

Proof. Without loss of generality suppose that $n \leq m$. Then

$$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x = \frac{1}{2^{m+n}m!n!}\int_{-1}^{1} \frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^2-1)^m \frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\,\mathrm{d}x.$$

Because $(x^2-1)^m$ has an mth order zeros at $x = -1$ and $x = +1$, it follows that the boundary terms resulting from integration by parts is zero. After integrating by parts once we have

$$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x = \frac{-1}{2^{m+n}m!n!}\int_{-1}^{1} \frac{\mathrm{d}^{m-1}}{\mathrm{d}x^{m-1}}(x^2-1)^m \frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}(x^2-1)^n\,\mathrm{d}x.$$

If we continue integrating by parts the boundary terms will again be zero because $(x^2-1)^{m-1}$ has an $m-1$th order zeros at $x = -1$ and $x = +1$. By continuing integration be parts a total of n times we have

$$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x = \frac{(-1)^n}{2^{m+n}m!n!}\int_{-1}^{1} \frac{\mathrm{d}^{m-n}}{\mathrm{d}x^{m-n}}(x^2-1)^m \frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}(x^2-1)^n\,\mathrm{d}x \tag{7.2}$$

If $m = n$ then

$$\frac{\mathrm{d}^{2m}}{\mathrm{d}x^{2m}}(x^2-1)^m = \frac{\mathrm{d}^{2m}}{\mathrm{d}x^{2m}}(x^{2m}+\cdots) = (2m)!$$

and (7.2) becomes

$$\begin{aligned}
\int_{-1}^{1} (\mathrm{P}_m)^2 \,\mathrm{d}x &= \frac{(-1)^m}{2^{2m}(m!)^2}(2m)! \int_{-1}^{1} (x^2-1)^m \,\mathrm{d}x \\
&= \frac{(-1)^m}{2^{2m}(m!)^2}(2m)! \int_{-1}^{1} (x+1)^m (x-1)^m \,\mathrm{d}x \\
&= \frac{(-1)^{2m}}{2^{2m}(m!)^2}(2m)! \frac{(m!)^2}{(2m)!} \int_{-1}^{1} (x-1)^2 m \,\mathrm{d}x \\
&= \frac{1}{2^{2m}} \frac{2^{2m+2}}{2m+1} \\
&= \frac{2}{2m+1}.
\end{aligned}$$

If $m \neq n$ it follows that $m < n$, in which case we can integrate (7.2) by parts at least once more. By integrating by parts again we have

$$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x =$$
$$\frac{(-1)^{n+1}}{2^{m+n} m! n!} \int_{-1}^{1} \frac{\mathrm{d}^{m-n+1}}{\mathrm{d}x^{m-n+1}}(x^2-1)^m \frac{\mathrm{d}^{2n+1}}{\mathrm{d}x^{2n+1}}(x^2-1)^n \,\mathrm{d}x.$$

The term $\frac{\mathrm{d}^{2n+1}}{\mathrm{d}x^{2n+1}}(x^2-1)^n = 0$ because a polynomial of degree $2n$ is annihilated by a derivative of order greater than $2n$. So, it follows that the whole integral is zero. Therefore, $(\mathrm{P}_n, \mathrm{P}_m) = \dfrac{2}{2m+1}\delta_{nm}$. □

Fourier–Legendre series

Recall the harmonic oscillator equation

$$u'' + n^2 u = 0,$$

which has the solutions $u_n = \mathrm{e}^{\mathrm{i}nx}$ that are orthogonal using the inner product

$$(u, v) = \frac{1}{2\pi} \int_{-\pi}^{\pi} uv \,\mathrm{d}x.$$

The Fourier series of a function $f(x)$ is given by

$$f(x) = \sum_{n=-\infty}^{\infty} \left(f, \mathrm{e}^{-\mathrm{i}nx}\right) \mathrm{e}^{\mathrm{i}nx}.$$

We can similarly define a Fourier-Legendre series. We have just seen that the set of Legendre polynomials $\{\mathrm{P}_n\}$ is orthogonal: $(\mathrm{P}_n, \mathrm{P}_m) = \frac{2}{2m+1}\delta_{nm}$. The Legendre polynomials are also complete. This means that any function can be expressed as a linear combination of the basis elements $\{\mathrm{P}_n\}$:

$$f(x) = \sum_{n=0}^{\infty} a_n \, \mathrm{P}_n(x)$$

for some a_n. Let's determine the $\{a_n\}$. Consider the inner product of $f(x)$ with an arbitrary Legendre polynomial $\mathrm{P}_m(x)$:

$$\begin{aligned}(f, \mathrm{P}_m) &= \left(\sum_{n=0}^{\infty} a_n \, \mathrm{P}_n, \mathrm{P}_m\right) = \sum_{n=0}^{\infty} a_n \, (\mathrm{P}_n, \mathrm{P}_m) \\ &= \sum_{n=0}^{\infty} a_n \frac{2}{2m+1}\delta_{nm} = a_m \frac{2}{2m+1}\end{aligned}$$

The coefficient

$$a_m = \frac{2m+1}{2}\,(f, \mathrm{P}_m)$$

is the projection of f onto P_m. From this we have that

$$f(x) = \sum_{n=0}^{\infty} \frac{2n+1}{2}\,(f, \mathrm{P}_n)\,.$$

Here are useful formulas for the Legendre polynomial:

differential equation	$(1-x^2)\,\mathrm{P}_m'' - 2x\,\mathrm{P}_m' + m^2\,\mathrm{P}_m = 0$
series solution	$\mathrm{P}_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k(2n-2k)!}{2^n k!(n-2k)!(n-k)!} x^{n-2k}$
generating function	$\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{m=0}^{\infty} \mathrm{P}_m(x) t^m$
recursion formula	$(n+1)\,\mathrm{P}_{n+1} = (2n+1)x\,\mathrm{P}_n - n\,\mathrm{P}_{n-1}$
orthogonality	$\int_{-1}^{1} \mathrm{P}_m(x)\,\mathrm{P}_n(x)\,\mathrm{d}x = \frac{2}{2m+1}\delta_{mn}$
Rodriques formula	$\mathrm{P}_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n$
Schläfli integral	$\mathrm{P}_n(x) = \frac{1}{2^{n+1}\pi\mathrm{i}} \oint \frac{(1-t^2)^n}{(t-x)^{n+1}}\,\mathrm{d}t$

7.3 Hermite polynomial

In this section we look at the solutions to the Hermite differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}y - 2x\frac{\mathrm{d}}{\mathrm{d}x}y + 2ny = 0.$$

The solutions to the Hermite differential equation can be found using the method of Frobenius to get

$$\mathrm{H}_n(x) = \sum_{k=0}^{\infty}(-1)^k(2x)^{n-2k}\frac{n!}{k!(n-2k)!}.$$

If n is an integer, the series terminates after $n/2$ terms. Otherwise, the series is divergent (and non-physical). Therefore, we can define the Hermite polynomials as

$$\mathrm{H}_n(x) = \sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k(2x)^{n-2k}\frac{n!}{k!(n-2k)!}$$

for integer n where $\lfloor n/2\rfloor$ is the floor function: $\lfloor n/2\rfloor = n/2$ if n is even and $\lfloor n/2\rfloor = (n-1)/2$ if n is odd.

By multiplying the Hermite equation by the integrating factor e^{-x^2} we can put it in Sturm–Liouville form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(e^{-x^2}\frac{\mathrm{d}}{\mathrm{d}x}y\right) + 2ne^{-x^2}y = 0.$$

By inspection of this equation—wth weight $w(x) = e^{-x^2}$ and domain $x \in (-\infty,\infty)$—we note that the eigenfunction solutions are orthogonal in the inner product

$$(u,v)_w = \int_{-\infty}^{\infty} uv\,\mathrm{e}^{-x^2}\,\mathrm{d}x.$$

Hence, we have the orthogonality condition

$$\int_{-\infty}^{\infty}\mathrm{H}_m(x)\,\mathrm{H}_n(x)\,\mathrm{e}^{-x^2}\,\mathrm{d}x = 0 \qquad \text{if } n \neq m.$$

Often, the usual Euclidean inner product is more meaningful in application than a weighted inner product. Note that by defining $\psi_n(x) = \mathrm{e}^{-x^2/2}\,\mathrm{H}_n$, we have class of functions that are orthogonal over the whole real line under the Euclidean inner product

$$\int_{-\infty}^{\infty}\psi_m(x)\psi_n(x)\,\mathrm{d}x = \int_{-\infty}^{\infty}\mathrm{H}_m(x)\,\mathrm{H}_n(x)\,\mathrm{e}^{-x^2}\,\mathrm{d}x = 0.$$

What differential equation does this new function $\psi_n(x)$ solve? If we take $\psi(x) = \mathrm{e}^{-x^2/2}\,\mathrm{H} = \mathrm{e}^{-x^2/2}\,y$, then

$$y' = \left(\mathrm{e}^{x^2/2}\,\psi\right)' = \mathrm{e}^{x^2/2}\,\psi' + x\,\mathrm{e}^{x^2/2}\,\psi$$
$$y'' = \mathrm{e}^{x^2/2}\,\psi'' + 2x\,\mathrm{e}^{x^2/2}\,\psi' + (x^2+1)\,\mathrm{e}^{x^2/2}\,\psi.$$

With these substitutions, the Hermite equation $y'' - 2xy' + 2ny = 0$ becomes

$$\mathrm{e}^{x^2/2}\,\psi'' + 2x\,\mathrm{e}^{x^2/2}\,\psi' + (x^2+1)\,\mathrm{e}^{x^2/2}\,\psi$$
$$- 2x\,\mathrm{e}^{x^2/2}\,\psi' - 2x^2\,\mathrm{e}^{x^2/2}\,\psi + 2n\,\mathrm{e}^{x^2/2}\,\psi = 0$$

which simplifies to

$$\mathrm{e}^{x^2/2}\,\psi'' + (-x^2+1+2n)\,\mathrm{e}^{x^2/2}\,\psi = 0.$$

Dividing by $\mathrm{e}^{x^2/2}$ gives us the equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n + \left(2n+1-x^2\right)\psi_n = 0. \tag{7.3}$$

Of course, the solutions to this equation are simply $\psi_n(x) = \mathrm{e}^{-x^2/2}\,\mathrm{H}_n(x)$.

Example. **Quantum Oscillator.** The one-dimensional Schrödinger equation for a particle subject to a potential is given by

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) \tag{7.4}$$

where $V(x)$ is the potential, m is the particle mass, and and $\hbar$ is the reduced Planck constant. We can solve (7.4) by using separation of variables setting $\Psi(x,t) = u(t)\psi(x)$ to get

$$\frac{\mathrm{i}\hbar u'}{u} = \frac{-\frac{\hbar}{2m}\psi'' + V(x)\psi}{\psi} = E$$

where the constant E gives the energy of a state. From $i\hbar u' = Eu$ we have

$$u(t) = a\,\mathrm{e}^{\mathrm{i}\hbar Et}\,.$$

Let's consider the time-independent Schrödinger equation

$$-\frac{\hbar}{2m}\psi'' + V(x)\psi = E\psi$$

The operator $H = -\frac{\hbar}{2m}\frac{\mathrm{d}}{\mathrm{d}x} + V(x)$ is the Hamiltonian operator. The potential of a harmonic oscillator is given by Hooke's law $V(x) = \frac{1}{2}kx^2$ where k is the spring constant. We can express the constant k in terms of the angular frequency $\omega = \sqrt{k/m}$. In this case, the potential is given by $V(x) = \frac{1}{2}m\omega^2 x^2$, and the Schrödinger equation is

$$-\frac{\hbar}{2m}\psi'' + \tfrac{1}{2}m\omega^2 x^2 \psi = E\psi$$

which we can rewrite as

$$\psi'' + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\psi = 0.$$

Making the change of variable $\tilde{x} = \sqrt{m\omega/\hbar}x$ to simplify the expression, we have

$$\psi'' + \left(\frac{2E}{\hbar\omega} - \tilde{x}^2\right)\psi = 0.$$

Comparing this expression with (7.3), we have that

$$\psi_n(\tilde{x}) = \mathrm{e}^{-\tilde{x}^2/2}\,\mathrm{H}_n(\tilde{x})$$

where

$$\frac{2E}{\hbar\omega} = 2n + 1.$$

Physically meaningful (non-divergent) solutions to the Hermite equation have the restriction that n be an integer. In this case, we have that

$$E_n = (n + \tfrac{1}{2})\hbar\omega$$

resulting in discrete energy states. The solution can finally be written as

$$\Psi(x,t) = \sum_{n=0}^{\infty} a_n\,\mathrm{e}^{\mathrm{i}\hbar^2\omega(n+\frac{1}{2})t}\,\mathrm{e}^{-\frac{1}{2}m\omega\hbar^{-1}x^2}\,\mathrm{H}_n\left(\sqrt{m\omega\hbar^{-1}}x\right).$$ ◄

Generating function

The generating function for the Hermite polynomials is given by

$$g(x,t) = \mathrm{e}^{-(t-x)^2}\,\mathrm{e}^{x^2} = \mathrm{e}^{-t^2+2tx} = \sum_{n=0}^{\infty}\mathrm{H}_n(x)\frac{t^n}{n!}.$$

We can differentiate the generating function m times with respect to t

$$e^{x^2}\frac{d^n}{dt^n}e^{-(t-x)^2} = H_m(x) + H_{m+1}(x)t + \frac{1}{2}H_{m+2}(x)t^2 + \cdots$$

Setting $t = 0$ gives us

$$e^{x^2}\frac{d^n}{dt^n}e^{-(t-x)^2}\Big|_{t=0} = H_m(x)$$

Making the change of variable $s = x - t$ with $d^n/\,dt^n = (-1)^n\, d^n/\,ds^n$

$$(-1)^n e^{x^2}\frac{d^n}{ds^n}e^{-s^2}\Big|_{s=x} = H_m(x).$$

Equivalently,

$$(-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} = H_m(x).$$

So, we have the Rodrigues' formula

$$H_m(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}.$$

We can also derive the Schläfli integral from the generating function. Divide by t^{m+1} and integrate along a contour γ about the origin.

$$\begin{aligned}\oint_\gamma \frac{e^{-t^2+2tx}}{t^{m+1}}\,dt &= \oint_\gamma \sum_{n=0}^{\infty} H_n(x)\frac{t^{(n-m)-1}}{n!}\,dt \\ &= \sum_{n=0}^{\infty}\frac{H_n(x)}{n!}\oint_\gamma t^{(n-m)-1}\,dt \\ &= \sum_{n=0}^{\infty}\frac{H_n(x)}{n!}2\pi i\delta_{nm}.\end{aligned}$$

Hencce,

$$H_m(x) = \frac{n!}{2\pi i}\oint_\gamma \frac{e^{-t^2+2tx}}{t^{m+1}}\,dt.$$

Example. Find $H_n(0)$. From the generating function we have that

$$g(0,t) = e^{-t^2} = \sum_{n=0}^{\infty} H_n\frac{t^n}{n!}.$$

The Taylor series representation also gives us

$$e^{-t^2} = \sum_{m=0}^{\infty} (-1)^n \frac{t^{2m}}{m!}.$$

So,

$$H_{2n+1}(0) = 0 \quad \text{and} \quad H_{2n}(0) = (-1)^n (2n)! \qquad \blacktriangleleft$$

Recurrence relation

Taking the derivative of the generating function with respect to x gives us

$$\frac{\partial g}{\partial x} = 2t\, e^{-t^2+2tx} = 2\sum_{n=0}^{\infty} H_n' \frac{t^n}{n!}$$

$$2t\sum_{n=0}^{\infty} H_n \frac{t^n}{n!} = 2\sum_{n=0}^{\infty} H_n' \frac{t^{n+1}}{n!}$$

$$2\sum_{n=0}^{\infty} H_n \frac{t^{n+1}}{n!} = 2\sum_{n=0}^{\infty} H_n' \frac{t^{n+1}}{n!}.$$

Shift the indices on the left

$$2\sum_{n=0}^{\infty} H_{n-1} \frac{nt^n}{n!} = 2\sum_{n=0}^{\infty} H_n' \frac{t^{n+1}}{n!}.$$

Therefore,

$$H_n' = 2n\, H_{n-1}\,.$$

Taking the derivative of the generating function with respect to t gives

$$\frac{\partial g}{\partial t} = (-2t + 2x)\, e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n \frac{t^{n-1}}{(n-1)!}$$

$$(-2t + 2x)\sum_{n=0}^{\infty} H_n \frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n \frac{t^{n-1}}{(n-1)!}$$

$$-2\sum_{n=0}^{\infty} H_n \frac{t^{n+1}}{n!} + 2\sum_{n=0}^{\infty} x\, H_n \frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n \frac{t^{n-1}}{(n-1)!}.$$

Shift the indices n so that the powers of t are the same:

$$-2\sum_{n=1}^{\infty} H_{n-1} \frac{nt^n}{n!} + 2\sum_{n=0}^{\infty} x\, H_n \frac{t^n}{n!} = \sum_{n=-1}^{\infty} H_{n+1} \frac{t^n}{n!}.$$

It follows that

$$\mathrm{H}_{n+1}(x) = 2x\,\mathrm{H}_n(x) - 2n\,\mathrm{H}_{n-1}(x).$$

Here are useful formulas for the Hermite polynomial:

differential equation	$\mathrm{H}_n'' - 2x\,\mathrm{H}_n\, y + 2n\,\mathrm{H}_n = 0$
series solution	$\mathrm{H}_n(x) = \sum_{k=0}^{[n/2]} (-1)^k (2x)^{n-2k} \dfrac{n!}{k!(n-2k)!}$
generating function	$\mathrm{e}^{-t^2+2tx} = \sum_{n=0}^{\infty} \mathrm{H}_n(x) \dfrac{t^n}{n!}$
recursion formulae	$\mathrm{H}_n' = 2n\,\mathrm{H}_{n-1}$
	$\mathrm{H}_{n+1}(x) = 2x\,\mathrm{H}_n(x) - 2n\,\mathrm{H}_{n-1}(x)$
orthogonality	$\int_{-\infty}^{\infty} \mathrm{H}_m(x)\,\mathrm{H}_n(x)\,\mathrm{e}^{-x^2}\,\mathrm{d}x = n!2^n\sqrt{\pi}\delta_{mn}$
Rodrigues formula	$\mathrm{H}_m(x) = (-1)^n\,\mathrm{e}^{x^2} \dfrac{\mathrm{d}^n}{\mathrm{d}x^n}\,\mathrm{e}^{-x^2}$
Schläfli integral	$\mathrm{H}_m(x) = \dfrac{n!}{2\pi \mathrm{i}} \oint \dfrac{\mathrm{e}^{-t^2+2tx}}{t^{m+1}}\,\mathrm{d}t$

7.4 Laguerre polynomial

Solutions to the Laguerre equation

$$xy'' + (1-x)y' + ny = 0$$

can be found using the method of Frobenius. The series terminates as polynomials for integer values n:

$$\mathrm{L}_n(x) = \sum_{k=0}^{n} \frac{(-1)^k n! x^k}{(n-k)!(k!)^2}.$$

Otherwise, the series diverges. The generalized (or associated) Laguerre polynomials $L_n^{(\alpha)}(x)$ are solutions to a similar equation

$$xy'' + (\alpha + 1 - x)y' + ny = 0$$

for an arbitrary real number α.

By multiplying the Laguerre equation by the integrating factor e^{-x} and simplifying we get

$$[(1-x)e^{-x}y']' + ne^{-x}y = 0.$$

By inspection we note that the Laguerre polynomials are orthogonal over the domain $x \in [0, \infty)$ with weight $w(x) = e^{-x}$

$$\int_0^\infty \mathrm{L}_m(x)\,\mathrm{L}_n(x)\,\mathrm{e}^{-x}\;\mathrm{d}x = 0$$

if $m \neq n$.

The generating function for the Laguerre polynomials is given by

$$g(x,t) = \frac{\mathrm{e}^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} \mathrm{L}_n(x) t^n.$$

Note

$$g(0,z) = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n$$

so $\mathrm{L}_n(0) = 1$.

We can use the generating function to derive the Schläfli and Rodriques' representations. Divide the generating function by t^{m+1} and integrate about a contour about the origin that avoid the (essential) singularity at $t = 1$:

$$\begin{aligned}
\oint \frac{g(x,z)}{z^{m+1}}\,\mathrm{d}z &= \oint \sum_{n=0}^{\infty} \mathrm{L}_n(x) z^{n-m-1}\,\mathrm{d}z \\
&= \sum_{n=0}^{\infty} \mathrm{L}_n(x) \oint z^{n-m-1}\,\mathrm{d}z \\
&= 2\pi \mathrm{i}\, \mathrm{L}_m(x)
\end{aligned}$$

Hence, the Schläfli integral is

$$\mathrm{L}_m(x) = \frac{1}{2\pi i} \oint_{|z|=1/2} \frac{\mathrm{e}^{-xz/(1-z)}}{(1-z)z^{n_1}}\,\mathrm{d}z.$$

Take $z = (s-x)/s$ and use the Cauchy integral formula

$$\mathrm{L}_m(x) = \frac{\mathrm{e}^s}{2\pi \mathrm{i}} \oint \frac{s^n\,\mathrm{e}^{-s}}{(s-x)^{m+1}}\,\mathrm{d}s = \frac{\mathrm{e}^x}{m!} \frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^m\,\mathrm{e}^{-x}),$$

which is Rodrigue's formula.

We can also get the recursion formulas from the generating function. Differentiating the generating function with respect to x gives us

$$\left(\frac{t}{1-t}\right) \frac{\mathrm{e}^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} \mathrm{L}'_n(x) t^n.$$

Equivalently,

$$t\sum_{n=0}^{\infty} \mathrm{L}_n(x)t^n = (1-t)\sum_{n=0}^{\infty} \mathrm{L}'_n(x)t^n.$$

or

$$\sum_{n=0}^{\infty} \mathrm{L}_n(x)t^{n+1} = \sum_{n=0}^{\infty} \mathrm{L}'_n(x)t^n - \sum_{n=0}^{\infty} \mathrm{L}'_n(x)t^{n+1}.$$

By shifting the indices n for that the powers of t are the same, we can easily combine the sums

$$\sum_{n=0}^{\infty} \left(\mathrm{L}_{n-1} - \mathrm{L}'_n + \mathrm{L}'_{n-1}\right) t^{n+1} = 0.$$

Hence,

$$x\,\mathrm{L}'_n = n\,\mathrm{L}_n - n\,\mathrm{L}_{n-1}\,.$$

Here are useful formulas for the Laguerre polynomial:

differential equation	$x\,\mathrm{L}''_n + (1-x)\,\mathrm{L}'_n + n\,\mathrm{L}_n = 0$
series solution	$\mathrm{L}_n(x) = \sum_{k=0}^{n} \frac{(-1)^k n! x^k}{(n-k)!(k!)^2}$
generating function	$\left(\frac{t}{1-t}\right) \frac{\mathrm{e}^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} \mathrm{L}_n(x)t^n$
orthogonality	$\int_0^{\infty} \mathrm{L}_m(x)\,\mathrm{L}_n(x)\,\mathrm{e}^{-x}\,\mathrm{d}x = \delta_{mn}$
Rodriques formula	$\mathrm{L}_m(x) = \frac{\mathrm{e}^x}{m!}\frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^m\,\mathrm{e}^{-x})$
Schläfli integral	$\mathrm{L}_m(x) = \frac{1}{2\pi i}\oint_{\lvert z\rvert=1/2} \frac{\mathrm{e}^{-xz/(1-z)}}{(1-z)z^{n_1}}\,\mathrm{d}z$

7.5 Chebyshev polynomial

Consider the polynomials formed by taking

$$\mathrm{T}_n(\cos\theta) = \cos n\theta$$

That is, take $x = \cos\theta$ and consider

$$\mathrm{T}_0(x) = \cos 0 = 1$$
$$\mathrm{T}_1(x) = \cos\theta = x$$

Now consider $\cos 2\theta$:

$$\cos 2\theta = \cos^2\theta - \sin^2\theta = 2\cos^2\theta - 1 = 2x^2 - 1.$$

Then

$$\mathrm{T}_2(x) = 2x^2 - 1$$

What is $\cos 3\theta$?

$$\cos 3\theta + \mathrm{i}\sin 3\theta = \mathrm{e}^{\mathrm{i}3\theta} = (\cos\theta + \mathrm{i}\sin\theta)^3$$

So,

$$\begin{aligned}
\mathrm{T}_3(\cos\theta) &= \operatorname{Re}(\cos + \mathrm{i}\sin\theta)^3 \\
&= \operatorname{Re}(\cos^3\theta + 3\mathrm{i}\sin\theta\cos^2\theta - 3\sin^2\theta\cos\theta - \mathrm{i}\sin^3) \\
&= \cos^3\theta - 3(1 - \cos^2\theta)\cos\theta \\
&= 4\cos^3\theta - 3\cos\theta.
\end{aligned}$$

Therefore,

$$\mathrm{T}_3(x) = 4x^3 - 3.$$

What is $\cos n\theta$? It will be easier to compute a general $\mathrm{T}_n(x)$ by using a recursion formula. By adding the two identities

$$\begin{aligned}
\cos(n+1)\theta &= \cos n\theta\cos\theta - \sin n\theta\sin\theta \\
\cos(n-1)\theta &= \cos n\theta\cos\theta + \sin n\theta\sin\theta
\end{aligned}$$

we get

$$\cos(n+1)\theta + \cos(n-1)\theta = 2\cos n\theta\cos\theta$$

and therefore

$$\mathrm{T}_{n+1}(x) + \mathrm{T}_{n-1}(x) = 2x\,\mathrm{T}_n(x)$$

So,

$$\mathrm{T}_{n+1}(x) = 2x\,\mathrm{T}_n(x) - \mathrm{T}_{n-1}(x).$$

For example,

$$\begin{aligned}
\mathrm{T}_4(x) &= 2x\,\mathrm{T}_3(x) - \mathrm{T}_2(x) = 2x(4x^3 - 3) - (2x^2 - 1) \\
&= 8x^4 - 2x^2 - 6x + 1.
\end{aligned}$$

Using this recursion, we can also note that $\mathrm{T}_n(x)$ has a leading coefficient 2^{n-1} and $\mathrm{T}_n(\pm 1) = 0$.

> There are 40 different ways to spell "Chebyshev" but there is only one way to spell "Pafnuty."

The Chebyshev polynomials $\mathrm{T}_n(\cos\theta) = \cos n\theta$ clearly satisfy the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}\,\mathrm{T}_n + n^2\,\mathrm{T}_n = 0.$$

From

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}\theta} = -\sin\theta\frac{\mathrm{d}}{\mathrm{d}x}$$

it follows that

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}\theta^2} &= \frac{\mathrm{d}}{\mathrm{d}x}\left(-\sin\theta\frac{\mathrm{d}}{\mathrm{d}x}\right)\\ &= -\cos\theta\frac{\mathrm{d}}{\mathrm{d}x} - \sin\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\mathrm{d}}{\mathrm{d}x}\\ &= -x\frac{\mathrm{d}}{\mathrm{d}x} + (1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}.\end{aligned}$$

So, the Chebyshev polynomials $\mathrm{T}_n(x)$ solve the equation

$$(1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\mathrm{T}_n - x\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{T}_n + n^2\,\mathrm{T}_n = 0.$$

We can put this equation in Sturm–Liouville form by multiplying by the integrating factor $(1-x^2)^{1/2}$:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\sqrt{1-x^2}\frac{\mathrm{d}}{\mathrm{d}x}u\right) + \frac{n^2}{\sqrt{1-x^2}} = 0.$$

So, we have that the Chebyshev polynomials are orthogonal with respect to the inner product

$$(u,v) = \int_{-1}^{1} uv\frac{\mathrm{d}x}{\sqrt{1-x^2}}.$$

Note that because $x = \cos\theta$:

$$\int_0^\pi \mathrm{T}_n(\cos\theta)\,\mathrm{T}_m(\cos\theta)\,\mathrm{d}\theta = \int_0^\pi \cos n\theta)\cos m\theta\,\mathrm{d}\theta = \begin{cases}0, & n \neq m\\ \pi, & n = m\\ \pi/2, & n = m \neq 0\end{cases}$$

Here are useful formulas for the Chebyshev polynomial:

differential equation	$x\,\mathrm{T}_n'' + (1-x)\,\mathrm{T}_n' + n\,\mathrm{T}_n = 0$
series solution	$\mathrm{T}_n(x) = \sum_{k=0}^{n} \frac{(-1)^k n! x^k}{(n-k)!(k!)^2}$
generating function	$\frac{1-t}{1-2xt+t^2} = \mathrm{T}_0(x) + 2\sum_{n=1}^{\infty} \mathrm{T}_n(x) t^n$
recursion formula	$\mathrm{T}_{n+1}(x) = 2x\,\mathrm{T}_n(x) - \mathrm{T}_{n-1}(x)$
orthogonality	$\int_{-1}^{1} \mathrm{T}_n\,\mathrm{T}_m (1-x^2)^{-1/2}\,\mathrm{d}x = \pi\delta_{nm}$

CHAPTER 8

Self Test

8.1 Problems

1. a) **true** or **false** A function is analytic at $z = z_0$ only if it has a Taylor series representation at z_0.

   b) **true** or **false** If a function is analytic at $z = z_0$, then the derivative of the function must be analytic at $z = z_0$.

   c) **true** or **false** All analytic functions satisfy the Cauchy-Riemann conditions.

   d) **true** or **false** The function $\cos z$ has an essential singularity at infinity.

   e) Each of the following functions has a singularity at the origin. Classify the singularity as either a removable singularity, a regular singularity (simple pole, double pole, etc.) or an essential singularity.

      - $\sin(1/z)$
      - $z/\sin z$
      - $1/\sin z$

   f) Compute the residue of $\dfrac{e^z}{z^5}$ at $z = 0$.

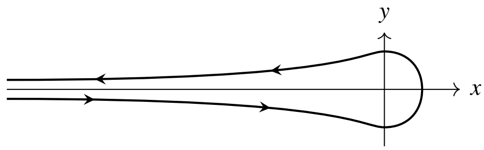
2. a) Locate all the poles of $\dfrac{1}{\sin z}$.

   b) Compute $\displaystyle\oint_{|z|=10} \frac{1}{\sin z}\, dz$ where the contour is taken in the counter-clockwise direction.

3. a) Locate all the poles of the gamma function $\Gamma(z)$.

   b) Compute the residues for each of the poles.

c) Compute the contour integral $\oint_\gamma \Gamma(z)\,\mathrm{d}z$ for the contour shown below that encircles the negative real axis.



4. Compute $\int_0^\infty \mathrm{e}^{-x^{2/3}}\,\mathrm{d}x$.

5. Compute $\int_0^\infty \frac{\sqrt{x}}{x^2+1}\,\mathrm{d}x$.

6. Short answer questions. Be precise and concise.

   a) Give an example of a function with a branch cut in the complex plane

   b) Define removable singularity, a regular singularity, and an essential singularity. Give examples (functions) for each.

   c) Explain the concept of analytic continuation.

   d) Under what conditions does Fuch's theorem assure us that the differential equation
   $$p_0(x)u'' + p_1(x)u' + p_2(x)u = 0$$
   has a series solution $u(x) = \sum_{k=0}^\infty a_k x^{k+r}$.

   e) Under what conditions is the Sturm-Liouville operator
   $$\mathrm{L}\,u = \frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u$$
   self-adjoint (Hermitian)

   f) Describe the behavior of the Bessel function $\mathrm{J}_m(x)$ as for $x \ll 1$ (x small).

7. Consider the function
   $$f(z) = \frac{\mathrm{e}^{-1/z^2}}{1+z^2}.$$

   a) Determine and classify (removable, regular, essential) all the singularities of $f(z)$.

   b) Determine the residue of $f(z)$ at $z = 0$.

   c) Determine $\int_0^\infty f(x)\,\mathrm{d}x$.

8. Find the solution to the Hermite equation:

$$\mathrm{H}''(x) - 2x\,\mathrm{H}'(x) + 2n\,\mathrm{H}(x) = 0$$

using the Method of Frobenius.

9. Find the solution to the Chebyshev equation:

$$(1 - x^2)\,\mathrm{T}_n'' - x\,\mathrm{T}_n' + n^2\,\mathrm{T}_n = 0$$

using the Method of Frobenius.

10. Let $\mathrm{H}_n(x)$ be a Hermite polynomial and take n, m as **arbitrary** integers.

    a) Compute $\displaystyle\int_{-\infty}^{\infty} xe^{-x^2}\,\mathrm{H}_n(x)\,\mathrm{d}x$.

    b) Compute $\displaystyle\int_{-\infty}^{\infty} xe^{-x^2}\,\mathrm{H}_n(x)\,\mathrm{H}_m(x)\,\mathrm{d}x$.

8.2 Solutions

1. a) True. The proof of this statement is on page 24.

   b) True. An analytic function is infinitely differentiable.

   c) True. See page 16.

   d) True. A function $f(z)$ has a singularity at $z = \infty$ if and only if $f(1/z)$ has an essential singularity at $z = 0$. The function $\cos(1/z)$ has an essential singularity at 0. See page 33.

   e)
   - $\sin(1/z)$ has an essential singularity at the origin because its Laurent series does not terminate as $n \to -\infty$.
   - $z/\sin z$ has a removable singularity at the origin. The function is analytic at the origin if we define its value there to equal its limit of 1.
   - $1/\sin z$ has a simple pole at the origin.

   f) The function $f(z) = \mathrm{e}^z/z^5$ has a fifth order pole at the origin. So, its residue is (see page 36)

$$\operatorname{Res}[f(z), 0] = \lim_{z\to z_0} \frac{1}{4!}\frac{\mathrm{d}^4}{\mathrm{d}z^4}[\mathrm{e}^z] = \frac{1}{24}.$$

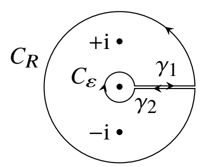
2. a) Poles of $1/\sin z$ coincide with zeros of $\sin z$: $n\pi$ for all integers n.

   b) The integral equals $2\pi\mathrm{i}$ times the sum of the residues of the seven poles contained within the circle of radius 10 (a little larger than 3π). The residue of each pole is 1, so the value of the integral is 14π. See page 35.

3. a) $\Gamma(z)$ has simple poles at $z = 0, -1, -2, -3, \ldots$. See page 68.
   b) If functions f and g are both analytic at $z = z_0$ and g has a simple zero at z_0, then $\operatorname{Res}[f(z)/g(z), z_0] = f(z_0)/g'(z_0)$. See page 36. Using Euler's reflection formula
   $$\Gamma(z) = \frac{\pi}{\Gamma(-z+1)\sin(\pi z)}.$$
   and the definition $n! = \Gamma(n+1)$, we get
   $$\operatorname{Res}[\Gamma(z), -n] = \frac{\pi}{n!\cos(\pi n)} = \pi\frac{(-1)^n}{n!}$$
   c) The contour contains all the non-positive integers (the poles of the gamma function):
   $$\oint_\gamma \Gamma(z)\,\mathrm{d}z = 2\pi\mathrm{i}\sum_{n=0}^{\infty}\pi\frac{(-1)^n}{n!} = 2\pi^2\mathrm{i}\,\mathrm{e}^{-1}\,.$$
   Note the Taylor series representation for $\exp(-1)$.

4. $\Gamma(\frac{5}{3})$. See page 70.

5. Note that $\sqrt{z} = \mathrm{e}^{\frac{1}{2}\log z}$, so there is a branch point at $z = 0$. Because we are integrating along the positive real axis, we will take the branch cut along the positive real axis. In this case, we have the keyhole contour which avoids the branch cut. The integrand has simple poles at $z = \pm\mathrm{i}$.



$$\begin{aligned}\oint_C f(z)\,\mathrm{d}z &= \left(\int_{C_\varepsilon} + \int_{C_R} + \int_{\gamma_1} + \int_{\gamma_2}\right) f(z)\,\mathrm{d}z\\ &= 2\pi\mathrm{i}\left(\operatorname{Res}\left[\frac{z^{1/2}}{z^2+1}, \mathrm{i}\right] + \operatorname{Res}\left[\frac{z^{1/2}}{z^2+1}, -\mathrm{i}\right]\right)\\ &= 2\pi\mathrm{i}\left(\frac{\left(\mathrm{e}^{\pi\mathrm{i}/2}\right)^{1/2}}{2\mathrm{i}} + \frac{\left(\mathrm{e}^{3\pi\mathrm{i}/2}\right)^{1/2}}{-2\mathrm{i}}\right)\\ &= 2\pi\mathrm{i}\frac{\mathrm{e}^{\mathrm{i}\pi/4} - \mathrm{e}^{3\mathrm{i}\pi/4}}{2\mathrm{i}} = 2\pi\mathrm{i}\,\mathrm{e}^{\mathrm{i}\pi/2}\,\frac{\mathrm{e}^{-\mathrm{i}\pi/4} - \mathrm{e}^{\mathrm{i}\pi/4}}{2\mathrm{i}}\\ &= 2\pi\sin(\pi/4) = \pi\sqrt{2}\end{aligned}$$

The ML-estimate gives us

$$\begin{aligned}\int_{C_R}\frac{z^{1/2}}{z^2+1}\,\mathrm{d}z &\le \left(\frac{R^{1/2}}{R^2-1}\right)\pi R\\ &= \frac{\pi R^{3/2}}{R^2-1} \approx \pi R^{-1/2} \to 0 \quad \text{as} \quad R\to\infty\end{aligned}$$

and

$$\int_{C_\varepsilon} \frac{z^{1/2}}{z^2+1}\,\mathrm{d}z \leq \left(\frac{\varepsilon^{1/2}}{1-\varepsilon^2}\right)\pi\varepsilon$$
$$= \frac{\pi\varepsilon^{3/2}}{1-\varepsilon^2} \approx \pi\varepsilon^{3/2} \longrightarrow 0 \quad \text{as} \quad \varepsilon \longrightarrow 0.$$

Along γ_1 we have $z = r$:

$$\int_{\gamma_1} \frac{z^{1/2}}{z^2+1}\,\mathrm{d}z = \int_0^R \frac{r^{1/2}}{r^2+1}\,\mathrm{d}r.$$

Along γ_2 (remembering not to cross the branch cut) we have $z = r\,\mathrm{e}^{\mathrm{i}2\pi}$:

$$\int_{\gamma_1} \frac{z^{1/2}}{z^2+1}\,\mathrm{d}z = \int_R^0 \frac{r^{1/2}\,\mathrm{e}^{\mathrm{i}\pi}}{r^2+1}\,\mathrm{d}r$$
$$= -\int_R^0 \frac{r^{1/2}}{r^2+1}\,\mathrm{d}r = \int_0^R \frac{r^{1/2}}{r^2+1}\,\mathrm{d}r.$$

Therefore,

$$2\int_0^R \frac{r^{1/2}}{r^2+1}\,\mathrm{d}r + \left(\int_{C_R} + \int_{C_\varepsilon}\right) f(z)\,\mathrm{d}z = \oint_C f(z)\,\mathrm{d}z = \pi\sqrt{2}.$$

In the limit as $R \longrightarrow \infty$, it follows that

$$\int_0^\infty \frac{r^{1/2}}{r^2+1}\,\mathrm{d}r = \pi/\sqrt{2}.$$

6. a) The logarithm function $\log z$ and root functions $z^{1/p} = \exp(\frac{1}{p}\log z)$ have branch cut from the origin to infinity.

   b) A singularity is any point z_0 at which a function $f(z)$ is undefined. Let $\sum_{n=-\infty}^{\infty} a_n(z-z_0)^n$ be the Laurent series representation of $f(z)$. If z_0 is a removable singularity, then $a_n = 0$ for all $n < 0$. If z_0 is a regular singularity, then there is a negative integer N such that $a_N \neq 0$ and $a_n = 0$ for all $n < N$. If z_0 is an essential singularity, then for all negative integers N there is some $n < N$ such that $a_n \neq 0$.

   c) If an two analytic functions are identical in some open subset of the complex plane, then they are identical over a larger domain over which they are defined. For example, we can use analytic continuation to extend the define the gamma function and Riemann zeta function.

   d) If $p_1(x)/p_0(x)$ has at most a simple pole $x = 0$ and $p_2(x)/p_0(x)$ has at most a double pole at $x = 0$, then Fuch's theorem says that a series solutions exists. See page 95.

e) Let the domain be $[a, b]$. The Sturm–Liouville operator is self-adjoint under any of the following conditions: $p(x)$ vanishes on the boundaries $p(a) = p(b) = 0$, the solution $u(x)$ has Dirichlet boundary conditions $u(a) = u(b) = 0$, the solution $u(x)$ has Neumann boundary condition $u'(a) = u'(b) = 0$, or the solution has periodic boundary conditions $u(a) = u(b)$ and $u'(a) = u'(b)$. See page **??**.

f) $\mathrm{J}_m(x) \approx \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m$. See page 115.

7. a) $f(z)$ has two regular singularities (simple poles at $z = +\mathrm{i}$ and $z = -\mathrm{i}$) and a removable singularity at $z = 0$. We can remove the singularity at $z = 0$ by noting that $\lim_{z\to 0} f(z) = 0$ and defining $f(0) = 0$.

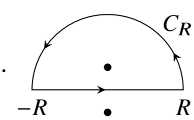
b) The singularity at $z = 0$ is removable, so the residue is zero.

c) $f(z)$ is an even function, so let's compute

$$\frac{1}{2}\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z.$$

Take a contour that is the semicircle in the upper half-plane:

$$\oint \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z = \int_{-R}^{+R} \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z + \int_{C_R} \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z.$$



Because $|\,\mathrm{e}^{-1/z^2}\,| \le 1$ in the upper half plane, we have the ML-estimate

$$\left|\int_{C_R} \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z\right| \le \frac{1}{R^2-1}\pi R \to 0 \quad \text{as } R \to \infty.$$

Now we just need to evaluate the contour integral

$$\oint \frac{\mathrm{e}^{-1/z^2}}{1+z^2}\,\mathrm{d}z = 2\pi\mathrm{i}\,\mathrm{Res}\left[\frac{\mathrm{e}^{-1/z^2}}{1+z^2}, \mathrm{i}\right]$$

$$= 2\pi\mathrm{i}\left(\left.\frac{f(z)}{g'(z)}\right|_{z=i}\right) = 2\pi\mathrm{i}\left.\frac{\mathrm{e}^{-1/z^2}}{2z}\right|_{z=\mathrm{i}} = \pi\,\mathrm{e}$$

It follows that

$$\int_0^{\infty} \frac{\mathrm{e}^{-1/x^2}}{1+x^2}\,\mathrm{d}x = \tfrac{1}{2}\pi\,\mathrm{e}\,.$$

8. Take the solution of the form

$$\mathrm{H}(x) = \sum_{k=0}^{\infty} a_k x^{k+r}$$

where $\{a_k\}$ and r are unknown and $a_0 \neq 0$. Substituting the solution into the Hermite equation gives us

$$\sum_{k=2}^{\infty} a_k(k+r)(k+r-1)x^{k+r-2} - 2x\sum_{k=1}^{\infty} a_k(k+r)x^{k+r-1} + 2n\sum_{k=0}^{\infty} a_k x^{k+r} = 0$$

Equivalently,

$$\sum_{k=0}^{\infty} a_{k+2}(k+r+2)(k+r+1)x^{k+r} - 2\sum_{k=1}^{\infty} a_k(k+r)x^{k+r} + 2n\sum_{k=0}^{\infty} a_k x^{k+r} = 0$$

or

$$\sum_{k=1}^{\infty}\big((k+r+2)(k+r+1)a_{k+2} + 2(n-k-r)a_k\big)x^{k+r} = 0$$

Because the solution is valid for all x in the domain, we must have that the coefficients

$$(k+r+2)(k+r+1)a_{k+2} + 2(n-k-r)a_k = 0.$$

Because $a_0 \neq 0$, $a_{-1} = 0$, and $a_{-2} = 0$, it follows from setting $k = -2$ in the above expression that $r(r-1) = 0$ from which we have that $r = 0$ or $r = 1$. Take $r = 0$, then

$$(k+2)(k+1)a_{k+2} + 2(n-k)a_k = 0$$

from which

$$a_{k+2} = -\frac{2(n-k)}{(k+2)(k+1)}a_k.$$

Starting with a_0, we have

$$\begin{aligned} a_2 &= -na_0 \\ a_4 &= -\frac{2(n-2)}{4\cdot 3}a_2 = +\frac{2^2 n(n-2)}{4!}a_0 \\ a_6 &= -\frac{2(n-4)}{6\cdot 5}a_4 = -\frac{2^3 n(n-2)(n-4)}{6!}a_0 \end{aligned}$$

and in general

$$a_{2k} = (-1)^k \frac{2^k n!!}{(2k)!(n-2k)!!} a_0.$$

The series will diverge unless n is a positive even integer. When n is a positive even integer, the solution will be a polynomial with $n/2 + 1$ terms:

$$\mathrm{H}_n(x) = \sum_{k=0}^{n/2} (-1)^k \frac{2^k n!!}{(2k)!(n-2k)!!} x^{2k}$$

We can simplify this expression by using the identity $(2m)!! = 2^m m!$:

$$\mathrm{H}_n(x) = \sum_{k=0}^{n/2} (-1)^k \frac{(n/2)!}{(2k)!(n/2-k)!} (2x)^{2k}.$$

By reversing the order of the sum $k \mapsto n/2 - k$, we have:

$$\mathrm{H}_n(x) = \sum_{k=0}^{n/2} (-1)^k \frac{(n/2)!}{(n-2k)!k!} (2x)^{n-2k}.$$

We can derive a similar solution for odd integers n by starting with a_1.

9. Take the solution of the form

$$\mathrm{T}_n(x) = \sum_{m=0}^{\infty} a_m x^{m+k}$$

where $\{a_m\}$ and k are unknown. Let's furthermore set $m' = m + k$ to help keep our derivations as clean as possible. Substituting the solution into the Chebyshev equation gives us

$$(1-x^2) \sum_{m=0}^{\infty} m'(m'-1) a_m x^{m'-2} - x \sum_{m=0}^{\infty} m' a_m x^{m'-1} + n^2 \sum_{m=0}^{\infty} a_m x^{m'} = 0.$$

Equivalently,

$$\sum_{m=0}^{\infty} m'(m'-1) a_m x^{m'-2} - \sum_{m=0}^{\infty} m'(m'-1) a_m x^{m'} - \sum_{m=0}^{\infty} m' a_m x^{m'} + \sum_{m=0}^{\infty} n^2 a_m x^{m'} = 0$$

or

$$\sum_{m=0}^{\infty} m'(m'-1)a_m x^{m'-2} + \sum_{m=0}^{\infty} \left[-m'(m'-1) - m' + n^2\right] a_m x^{m'} = 0.$$

In order to more easily combine the two sums, we will shift the m in the second sum to be $m-2$ (and taking $a_{-1} = 0$ and $a_{-2} = 0$), we have

$$\sum_{m=0}^{\infty} m'(m'-1)a_m x^{m'-2} + \sum_{m=0}^{\infty} \left[-(m'-2)(m'-3) - (m'-2) + n^2\right] a_{m-2} x^{m'-2} = 0.$$

Now, we can combine the sums

$$\sum_{m=0}^{\infty} \Bigg(m'(m'-1)a_m - \left[(m'-2)(m'-3) + (m'-2) - n^2\right] a_{m-2} \Bigg) x^{m'-2} = 0.$$

Because expression must be true for all x in the domain, we must have

$$m'(m'-1)a_m + \left[-(m'-2)(m'-3) - (m'-2) + n^2\right] a_{m-2} = 0.$$

Take $m = 0$. Then (remembering that $m' = m + k$ and $a_{-2} = 0$)

$$k(k-1)a_0 = 0.$$

This indicial equation says that either $k = 0$ or $k = 1$, because by assumption $a_0 \neq 0$. Let's look at the solutions for $k = 0$:

$$m(m-1)a_m + \left[-(m-2)(m-3) - (m-2) + n^2\right] a_{m-2} = 0$$

which simplifies to

$$m(m-1)a_m + \left[n^2 - (m-2)^2\right] a_{m-2} = 0$$

or

$$a_m = -\frac{n^2 - (m-2)^2}{m(m-1)} a_{m-2}.$$

We can shift m back to $m+2$ to make it a little easier to compute each of the coefficients a_m

$$a_{m+2} = -\frac{n^2 - m^2}{(m+2)(m+1)} a_m.$$

We can also factor the numerator (not an obviously simplification—except in retrospect after finding the solution)

$$a_{m+2} = -\frac{(n-m)(n+m)}{(m+2)(m+1)} a_m.$$

We have that

$$\begin{aligned}
a_2 &= -\frac{n^2}{2} a_0 \\
a_4 &= -\frac{(n-2)(n+2)}{4 \cdot 3} a_2 = +n\frac{(n-2)n(n+2)}{4 \cdot 3 \cdots 2} a_0 \\
a_6 &= -\frac{(n-4)(n+4)}{6 \cdot 4} a_4 = -n\frac{(n-4)(n-2)n(n+2)(n+4)}{6!} a_0
\end{aligned}$$

If $n > 0$ is even, then the sequence truncates with $a_{n+2} = 0$. Otherwise, the sequences does not terminate and the coefficients $|a_n| \to 1$ as $n \to \infty$. Subsequently, the series does not converge. In general (for even n)

$$\begin{aligned}
a_{2m} &= (-1)^m 2^m n \frac{(n-m+1)\dots(n+m-1)}{(2m)!} a_0 \\
&= (-1)^m 2^m n \frac{(n+m+1)!}{(n-m)!(2m)!} a_0
\end{aligned}$$

So, for even n

$$\mathrm{T}_n(x) = a_0 n \sum_{m=0}^{n/2} (-1)^m 2^m \frac{(n+m+1)!}{(n-m)!(2m)!} x^m$$

In a similar fashion we can get the odd-order Chebyshev polynomials by considering $k = 1$.

10. Let $\mathrm{H}_n(x)$ be a Hermite polynomial and take n, m as arbitrary integers.

    a) Compute $\int_{-\infty}^{\infty} x e^{-x^2} \mathrm{H}_n(x)\,\mathrm{d}x$.

    b) Compute $\int_{-\infty}^{\infty} x e^{-x^2} \mathrm{H}_n(x)\,\mathrm{H}_m(x)\,\mathrm{d}x$.

$$\mathrm{H}_{n+1}(x) = 2x\,\mathrm{H}_n(x) - 2n\,\mathrm{H}_{n-1}(x)$$

$$\int_{-\infty}^{\infty} e^{-x^2}(\tfrac{1}{2}\,\mathrm{H}_{n+1}(x) - n\,\mathrm{H}_{n-1}(x))\,\mathrm{H}_m(x)$$

$$\int_{-\infty}^{\infty} \mathrm{H}_m(x)\,\mathrm{H}_n(x)\,\mathrm{e}^{-x^2}\,\mathrm{d}x = n!2^n\sqrt{\pi}\delta_{mn}$$

$$\int_{-\infty}^{\infty} \mathrm{H}_m(x)\,\mathrm{H}_n(x)x\,\mathrm{e}^{-x^2}\,\mathrm{d}x = \begin{cases}(n+1)!2^{n+1}\sqrt{\pi}, & m = n+1\\ (n-1)!2^{n-1}\sqrt{\pi}, & m = n-1\\ 0, & \text{otherwise}\end{cases}$$

References

The following resources may be useful for further study.

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Index

Special Functions of Mathematical Physics

A Tourist's Guidebook

Strum a guitar. Bang a drum. The sound of one is a combination of sine functions and the other a combination of Bessel functions. While every scientist and engineer knows the sine function, not as many are familiar with Bessel functions or the broader class of special functions that frequently arise in mathematical physics. This book provides a guided tour through the important special functions and develops the mathematical tools and intuition for working with them.

Kyle Novak has over twenty years of experience applying mathematics, decision analysis, modeling, and scientific computing on a wide range topics from autonomous navigation systems and cryptanalysis to superconducting materials and multiscale networks.

Cover illustration: The spherical harmonic function $F_3^0(\theta, \phi)$ and the equipotentials of the gamma function in the complex plane.