



Function Analysis in DROP

v4.57 30 November 2019



Gamma Function

Introduction and Background

- 1. Extension to the Factorial Function: The *gamma function* represented by Γ is one of a number of extensions to the factorial function with its argument shifted down by 1, to real and complex numbers (Wikipedia (2019)).
- 2. <u>First Expression for Gamma Function</u>: Derived by Daniel Bernoulli, if *n* is positive,

$$\Gamma(n) = (n-1)!$$

Although other extensions do exist, this particular function is the most popular and useful.

- 3. <u>Defined over the Full Complex Plane</u>: The gamma function is defined for all complex numbers except for non-positive numbers.
- 4. <u>Second Expression for Gamma Function</u>: For complex numbers with a real positive part, it is defined in the convergent improper integral

$$\Gamma(z) = \int_{0}^{\infty} x^{z-1} e^{-x} dx$$

5. <u>Analytic Continuation onto Complex Plane</u>: This integral function is extended by analytic continuation to all complex numbers except for non-positive integers – where this function has simple poles – yielding the meromorphic function that is now known as the gamma function.



6. Third Expression for Gamma Function: It has no zeros, so the reciprocal function $\frac{1}{\Gamma(z)}$ is a holomorphic function. In fact, the gamma function corresponds to the Mellin transform of the negative exponential function

$$\Gamma(z) = \{\mathcal{M}e^{-x}\}(z)$$

7. <u>Applicable Domain of Gamma Function</u>: The gamma function is a component in various probability distribution functions, and as such, it is applicable in the fields of probability and statistics, as well as combinatorics.

Motivation

1. Gamma Function as Interpolation Problem: The gamma function can be seen as a solution to the following interpolation problem: Find a smooth curve that connects the points (x, y) given by

$$y = (x - 1)!$$

at the positive integer values for x.

- 2. Expression Representing the Factorial Function: A plot of the first few factorials makes it clear that such a curve can be drawn, but it would be preferable to have an expression that describes the curve, in which the number of operations do not depend on the size of *x*.
- 3. <u>Inadequacy of Integer Factorial Expression</u>: The simple formula

$$x! = 1 \times 2 \times \cdots \times x$$

cannot be used for then factorial values of x since it works only when x is a natural number, i.e., a positive integer.



- 4. Factorial Representation for Real Numbers: There are, relatively speaking, no such simple solutions for factorials. No finite combinations, of sums, products, powers, exponential functions, or logarithms will suffice to express x!, but it is possible to find a general formula for factorials using tools from calculus such as integrals and limits. A good solution to this is the gamma function (Davis (1959)).
- 5. <u>Infinite Solutions to the Problem</u>: There are infinitely many continuous extensions to the factorials of non-integers; infinitely many curves can be drawn through any of isolated points.
- 6. Ways to Characterize Gamma Function: The gamma function is the most useful solution in practice, being analytic except at non-positive integers and can be characterized in several ways.
- 7. Origin of the Non-Uniqueness: However, it is not the only analytic function that extends the factorial, as adding it to any analytics function that is zero at the non-positive integers, such as $k \sin m\pi x$, with give another function with that property (Davis (1959)).
- 8. <u>First Criterion for the Function</u>: A more restrictive property than satisfying the above interpolation is to satisfy the recurrence relation defining a translated version of the factorial function;

$$f(1) = 1$$

$$f(x+1) = xf(x)$$

for x equal to any positive integer.

- 9. Insufficiency of the First Criterion: But this would allow for multiplication by any periodic analytic function which evaluates to one on the non-positive integers, such as $e^{k \sin m\pi x}$.
- 10. Conditions of Bohr-Mollerup Theorem: There is a final way to address all this ambiguity; Bohr-Mollerup theorem states that when the condition that f be



logarithmically convex – or super-convex (Kingman (1961)) - is added, it uniquely determines f for positive, real inputs.

- 11. Extension to Real/Complex Numbers: From there, the gamma function can be extended to all real and complex values except the negative integers and zero by using the unique analytic continuation of f.
- 12. <u>Asymptotic Requirement of the Euler Product</u>: Also see Euler's infinite product definition below where the properties

$$f(1) = 1$$

and

$$f(x+1) = xf(x)$$

together with the asymptotic requirement that

$$\lim_{n \to \infty} \frac{(n-1)! \, n^x}{f(n+x)} = 1$$

uniquely define the same function.

Main Definition

1. Euler Integral of Second Kind: The notation $\Gamma(z)$ is due to Legendre (Davis (1959)). If the real part of the complex number z is positive –

- then the integral



$$\Gamma(z) = \int_{0}^{\infty} x^{z-1} e^{-x} dx$$

converges absolutely, and is known as the *Euler Integral of the Second Kind* – the Euler Integral of the First Kind defines the beta function (Davis (1959)).

2. <u>Integrating Gamma Function by Parts</u>: Using integration by parts, one sees that

$$\Gamma(z+1) = \int_{0}^{\infty} x^{z} e^{-x} dx = [-x^{z} e^{-x}]_{0}^{\infty} + \int_{0}^{\infty} z x^{z-1} e^{-x} dx$$
$$= \lim_{x \to \infty} [-x^{z} e^{-x}] - [0e^{-0}] + z \int_{0}^{\infty} x^{z-1} e^{-x} dx$$

3. Recovery of the Recurrence Relation: Recognizing that

$$\lim_{x \to \infty} \left[-x^z e^{-x} \right] \to 0$$

$$\Gamma(z+1) = z \int_{0}^{\infty} x^{z-1} e^{-x} dx = z \Gamma(z)$$

4. $\underline{n} = 1$ Limit of the Gamma Function: One can calculate $\Gamma(1)$ as

$$\Gamma(1) = \int_{0}^{\infty} x^{1-1} e^{-x} dx = [-e^{-x}]_{0}^{\infty} = \lim_{x \to \infty} [-e^{-x}] - [e^{-0}] = 0 - (-1) = 1$$

5. Proof by Induction for n > 1: Given that

$$\Gamma(1) = 1$$



and

$$\Gamma(n+1) = n\Gamma(n)$$

$$\Gamma(n) = 1 \cdot 2 \cdot 3 \cdots (n-1) = (n-1)!$$

for all positive integers n. This can be seen as an example of proof by induction.

6. Meromorphic Extension to Complex Plane: The identity

$$\Gamma(z) = \frac{\Gamma(z+1)}{z}$$

can be used – or yielding the same result, the analytic continuity can be used – to uniquely extend the integral formulation of $\Gamma(z)$ to a meromorphic function defined for all complex numbers z, except integers less than or equal to zero (Davis (1959)). It is this extended version that is commonly referred to as the gamma function (Davis (1959)).

Alternate Definitions: Euler's Definition as an Infinite Product

1. Approximating z! form Complex Numbers: When seeking to approximate z! For a complex number z, it turns out that it is effective to compute first n! For some large integer n, and then use that value to approximate a value for (n + z)!, and then use the recursion relation

$$m! = m(m-1)!$$



backwards n times, to unwind it to an approximation for z!. Furthermore, this approximation is exact in the limit as n goes to infinity.

2. <u>Integer Limits Extension to Complex Numbers</u>: Specifically, for a fixed integer *m*, it is the case that

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

and one can ask if the same expression is obeyed when the arbitrary integer m is replaced by the arbitrary complex number z

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

3. <u>Infinite Product Expression for z!</u>: Multiplying both sides by z! gives

$$z! = \frac{Limit}{n \to \infty} n! \frac{z!}{(z+m)!} (n+1)^z = \frac{Limit}{n \to \infty} \frac{1 \cdots n}{(1+z) \cdots (n+z)} (n+1)^z$$
$$= \frac{Limit}{n \to \infty} \frac{1 \cdots n}{(1+z) \cdots (n+z)} \left[\left(1 + \frac{1}{1} \right) \left(1 + \frac{1}{2} \right) \cdots \left(1 + \frac{1}{n} \right) \right]^z$$
$$= \prod_{n=1}^{\infty} \left[\frac{1}{\left(1 + \frac{z}{n} \right)} \left(1 + \frac{1}{n} \right)^z \right]$$

4. <u>Convergence of the Infinite Product</u>: This infinite product converges for all complex *z* except negative integers, which fails because using the recurrence relation

$$m! = m(m-1)!$$

backwards through the value



$$m = 0$$

involves a division by zero.

5. <u>Gamma Function as Infinite Product</u>: Similarly, for the gamma function, the definition as an infinite product due to Euler is valid for all complex numbers *z* except for non-positive integers

$$\Gamma(z) = \frac{1}{z} \prod_{n=1}^{\infty} \left[\frac{\left(1 + \frac{1}{n}\right)^{z}}{\left(1 + \frac{z}{n}\right)} \right]$$

6. <u>Uniqueness of Euler's Infinite Product</u>: By this construction, the gamma function is the unique function that simultaneously satisfies

$$\Gamma(1) = 1$$

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

for all complex numbers z except the non-positive integers, and

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

for all complex numbers z (Davis (1959)).

Weierstrass Definition

The definition for the gamma function due to Weierstrass is also valid for all complex numbers *z* except the non-positive integers:

$$\Gamma(z) = \frac{e^{-\gamma z}}{z} \prod_{n=1}^{\infty} \left[\frac{e^{-\frac{z}{n}}}{\left(1 + \frac{z}{n}\right)} \right]$$

where

$$\gamma \cong 0.577216$$

is the Euler-Mascheroni constant.

In Terms of Generalized Laguerre Polynomials

1. <u>Laguerre Polynomials – Incomplete Gamma Function</u>: A parametrization of the incomplete gamma function in terms of the generalized Laguerre polynomials is

$$\Gamma(z,x) = x^z e^{-x} \sum_{n=0}^{\infty} \frac{\mathcal{L}_n^z(x)}{n+z}$$

which converges for

$$Re(z) > -1$$

and

(National Institute of Standards and technology (2019)).



Laguerre Polynomials - Complete Gamma Function: A somewhat unusual
parametrization of the gamma function in terms of the Laguerre polynomials is given
by

$$\Gamma(z) = t^{z} \sum_{n=0}^{\infty} \frac{\mathcal{L}_{n}^{z}(t)}{n+z}$$

which converges for

$$Re(z) < \frac{1}{2}$$

General Properties

1. <u>Euler's Reflection and Duplication Formula</u>: Other important functional equations for the gamma function are the Euler's reflection formula

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

$$z \notin \mathbb{Z}$$

which implies

$$\Gamma(\epsilon - n) = (-1)^{n-1} \frac{\Gamma(-\epsilon)\Gamma(1+\epsilon)}{\Gamma(n+1-\epsilon)}$$

and the duplication formula

$$\Gamma(z)\Gamma\left(z+\frac{1}{2}\right) = 2^{1-2z}\sqrt{\pi}\Gamma(2z)$$

2. <u>Duplication Formula and Multiplication Theorem</u>: The duplication formula is a special case of the multiplication theorem (National Institute of Standards and technology (2019))

$$\prod_{k=0}^{m-1} \Gamma\left(z + \frac{k}{m}\right) = m^{\frac{1}{2} - mz} (2\pi)^{\frac{m-1}{2}} \Gamma(2z)$$

3. <u>Complex Conjugate of the Gamma Function</u>: A simple but useful property, which can be seen from the limit definition, is

$$\overline{\Gamma(z)} = \Gamma(\bar{z}) \Rightarrow \Gamma(z)\Gamma(\bar{z}) \in \mathbb{R}$$

4. Modulus of the Gamma Function: In particular, with

$$z = a + bi$$

this product is

$$|\Gamma(a+bi)|^2 = |\Gamma(a)|^2 \prod_{k=0}^{\infty} \frac{1}{1 + \frac{b^2}{(a+k)^2}}$$

$$|\Gamma(bi)|^2 = \frac{\pi}{b \sinh(\pi b)}$$

$$\left|\Gamma\left(\frac{1}{2} + bi\right)\right|^2 = \frac{\pi}{\cosh(\pi b)}$$



5. Special Gamma Function Value $x = \frac{1}{2}$: Perhaps the best-known value of the gamma function at a non-integer is

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

which can be found by setting

$$z=\frac{1}{2}$$

in the reflection or the duplication formulas, or by using the relation to the beta function given below with

$$x = y = \frac{1}{2}$$

or by simply making the substitution

$$u = \sqrt{x}$$

in the integral definition of the gamma function.

6. Special Gamma Function Value $x = \frac{1}{2} \pm n$: In general, for non-negative integer values of n one has

$$\Gamma\left(\frac{1}{2} + n\right) = \frac{(2n)!}{4^n n!} \sqrt{\pi} = \frac{(2n-1)!!}{2^n} \sqrt{\pi} = \binom{n-\frac{1}{2}}{n} n! \sqrt{\pi}$$

$$\Gamma\left(\frac{1}{2} - n\right) = \frac{(-4)^n n!}{(2n)!} \sqrt{\pi} = \frac{(-2)^n}{(2n-1)!!} \sqrt{\pi} = \frac{\sqrt{n\pi}}{n!}$$



where n!! denotes the double factorial of n and, when

$$n = 0$$

$$n!! = 1$$

7. <u>Special Gamma Function Value Rational *x*</u>: It might be tempting to generalize the result that

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

by looking for a formula for other individual values $\Gamma(r)$, where r is rational.

8. Transcendental Nature of the Gamma Function: It has been proved that $\Gamma(n+r)$ is a transcendental number and algebraically independent of π for any integer n and each of the fractions

$$r = \frac{1}{6}, \frac{1}{4}, \frac{1}{3}, \frac{2}{3}, \frac{3}{4}, \frac{5}{6}$$

(Waldschmidt (2008)). In general, when computing the values of the gamma function, one must settle for numerical approximations.

9. <u>Asymptotic Approximation for the Gamma Function</u>: Another useful limit for the asymptotic approximation is

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

$$\alpha\in\mathbb{C}$$



10. <u>Polygamma Functions: Derivatives of Gamma</u>: The derivatives of the gamma function are described in terms of the polygamma function. For example,

$$\Gamma'(z) = \Gamma(z)\psi_0(z)$$

11. <u>Gamma Derivative for Positive Integers</u>: For a positive integer *m* the derivatives of the gamma function can be calculated as follows:

$$\Gamma'(m+1) = m! \left(-\gamma + \sum_{k=1}^{m} \frac{1}{k}\right)$$

12. Gamma Function Derivatives when Re(z) > 0: When

the nth derivative of the gamma function is

$$\frac{\partial^n}{\partial z^n}\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}(\ln t)^n dt$$

This can be derived by differentiating the integral form of gamma with respect to z, the technique of differentiation under the integral sign.

13. Polynomial Series for Gamma Functions: Using the identity

$$\left. \frac{\partial^n}{\partial z^n} \Gamma(z) \right|_{z=1} = (-1)^n n! \sum_{\pi \vdash n} \prod_{i=1}^r \frac{\zeta^*(a_i)}{k_i! \cdot a_i}$$

$$\zeta^*(z) \coloneqq \begin{cases} \zeta(z) \ z \neq 1 \\ \gamma \quad z = 1 \end{cases}$$



where $\zeta(z)$ is the Riemann zeta function with partitions

$$\pi = \left(\underbrace{a_1, \cdots, a_1}_{k_1}, \cdots, \underbrace{a_r, \cdots, a_r}_{k_1}\right)$$

one has in particular

$$\zeta(z) = \frac{1}{z} - \gamma + \frac{1}{2} \left(\gamma^2 + \frac{\pi^2}{6} \right) z - \frac{1}{6} \left[\gamma^3 + \frac{\pi^2 \gamma}{2} + 2\zeta(3) \right] z^2 + \mathcal{O}(z^3)$$

Inequalities

- Characterizing Strictly Logarithmically Convex Functionality: When restricted to
 positive real numbers, the gamma function is a strictly logarithmically convex
 function. This property may be stated in any of the following three equivalent ways.
- 2. Characterization via Exponentially Convex Inequality: For any two positive real numbers x_1 and x_2 , and for any

$$t \in [0, 1]$$

$$\Gamma(tx_1+[1-t]x_2)\leq \Gamma^t(x_1)\Gamma^{1-t}(x_2)$$

Moreover, the inequality is strict for

$$t \in (0,1]$$

3. Characterization via Spaced Point Pair: For any two positive numbers x and y with

$$\left[\frac{\Gamma(y)}{\Gamma(x)}\right]^{\frac{1}{y-x}} > e^{\frac{\Gamma'(x)}{\Gamma(x)}}$$

4. Characterization via First/Second Derivatives: For any positive real number x,

$$\Gamma''(x)\Gamma(x) > \Gamma'(x)$$

- 5. Strict Positivity of the First Derivative: The last of the statements is, essentially by definition, the same as the statement that $\psi_1(x)$ where ψ_1 is the polygamma function of order 1. To prove the logarithmic convexity of the gamma function, it therefore suffices to observe that ψ_1 has a series representation which, fort positive real x, consists of only positive terms.
- 6. Convexity Extension to Multi-point Interpolant: Logarithmic convexity and Jensen's inequality together imply, for any positive real numbers x_1, \dots, x_n and a_1, \dots, a_n

$$\Gamma\left(\frac{a_1x_1 + \dots + a_nx_n}{a_1 + \dots + a_n}\right) \le \left[\Gamma(x_1) \cdots \Gamma(x_n)\right]^{\frac{1}{a_1 + \dots + a_n}}$$

7. <u>Bounds on Gamma - Gautschi Inequality</u>: There are also bounds on the ratios of gamma functions. The best-known is the Gautschi's inequality, which says that for any positive real number *x* and

$$s \in (0,1)$$

$$x^{1-s} < \frac{\Gamma(x+1)}{\Gamma(x+s)} < (x+1)^{1-s}$$

Stirling's Formula



- 1. Asymptotic Growth of the Gamma Function: The behavior of $\Gamma(z)$ for an increasing positive variable is simple; it grows quickly, faster than an exponential function.
- 2. Asymptotic Approximation using Stirling's Formula: Asymptotically, as

$$z \to \infty$$

the magnitude of the gamma function is given by the formula

$$\Gamma(z+1) \sim \sqrt{2\pi e} \left(\frac{z}{e}\right)^z$$

where the symbol \sim means that the ratio of the two sides converges to 1 (Davis (1959)) or asymptotically converges.

Residues

1. <u>Analytic Continuity into Negative Planes</u>: The behavior of non-positive *z* is more intricate. Euler's integral does not converge for

but the function it defines in the positive convex half-plane has a unique analytic continuation to the negative half-plane.

2. Repeated Application of the Recurrence: One way to find that analytic continuation is to use Euler's integral for positive arguments and extend the domain to negative numbers by repeated application of the recurrence formula (Davis (1959))

$$\Gamma(z) = \frac{\Gamma(z+n+1)}{z(z+1)\cdots(z+n)}$$



choosing n such that z + n is positive.

- 3. Meromorphic in the Negative Half Plane: The product in the denominator is zero if z equals any of the integers $0, -1, \cdots$ Thus, the gamma function must be undefined at these points to avoid division by zero; it is a meromorphic function with simple poles at the non-positive integers (Davis (1959)).
- 4. Residue Conducive Expansion for Gamma: The definition can be re-written as

$$(z+n)\Gamma(z) = \frac{\Gamma(z+n+1)}{z(z+1)\cdots(z+n-1)}$$

5. <u>Formal Definition of the Residue</u>: For a function f of a complex variable z, at a simple pole c, the residue of f is given by:

$$Residue(f,c) = \underset{z \to c}{limit} [(z-c)f(z)]$$

6. Residue Numerator and Denominator Values: When

$$z = -n$$

$$\Gamma(z + n + 1) = \Gamma(1) = 1$$

and

$$z(z+1)\cdots(z+n-1) = (-1)^n n!$$

7. <u>Gamma Function Residue at Poles</u>: So, the residues of the gamma function at those points are:



$$Residue(\Gamma, -n) = \frac{(-1)^n}{n}$$

8. <u>Holomorphic Nature of Reciprocal Gamma</u>: The gamma function is non-zero everywhere along the real line, although it comes arbitrarily close to zero as

$$z \to -\infty$$

There is in fact, no complex number z for which

$$\Gamma(z) = 0$$

and hence the reciprocal gamma function $\frac{1}{\Gamma(z)}$ is an entire function, with zeros at

$$z = 0, -1, \cdots$$

(Davis (1959)).

Minima

1. <u>Gamma Function Minimum Inside [0, 1]</u>: The gamma function has a local minimum at

$$z_{MIN} \approx 1.46163$$

where it attains the value

$$\Gamma(z_{MIN}) \approx 0.885603$$



2. Gamma Function Minimum between Poles: The gamma function must alternate the signs between the poles because the product in the forward recurrence contains an odd number of negative factors if the number of poles between z and z + n is odd, and even number of poles if their number is even.

Integral Representations

- 1. <u>Alternate Integral Representations of Gamma</u>: There are many formulations, besides the Euler's Integrals of the second kind, that express gamma function as an integral.
- 2. <u>Log Reciprocal Representation in [0, 1]</u>: For instance, when the real part of z is positive (Whittaker and Watson (1996)):

$$\Gamma(z) = \int_{0}^{1} \left(\log \frac{1}{t}\right)^{z-1} dt$$

3. <u>Binet's First Integral Representation</u>: Binet's first integral formula for the gamma function states that, when the real part of z is positive, then (Whittaker and Watson (1996)):

$$\log \Gamma(z) = \left(z - \frac{1}{2}\right) \log z - z + \frac{1}{2} \log 2\pi + \int_{0}^{\infty} \left(\frac{1}{2} - \frac{1}{t} + \frac{1}{e^{t} - 1}\right) \frac{e^{-tz}}{t} dt$$

4. <u>Laplacian of the Error Term</u>: The integral on the right-hand side may be interpreted as a Laplace transform. That is,

$$\log\left[\Gamma(z)\left(\frac{e}{z}\right)^{z}\sqrt{2\pi e}\right] = \mathfrak{L}\left(\frac{1}{2t} - \frac{1}{t^{2}} + \frac{1}{t[e^{t} - 1]}\right)(z)$$



5. <u>Binet's Second Integral Representation Form</u>: Binet's second integral formula states that, again when the real part of *z* is positive,

$$\log \Gamma(z) = \left(z - \frac{1}{2}\right) \log z - z + \frac{1}{2} \log 2\pi + 2 \int_{0}^{\infty} \frac{\arctan\left(\frac{t}{z}\right)}{e^{2\pi t} - 1} dt$$

- 6. Reimann Sphere Hankel Contour Transform: Let \mathcal{C} be a Hankel contour, meaning a path the begins and ends at the point ∞ in the Riemann sphere, whose unit tangent vector converges to -1 at the start of the path and at +1 at the end, which has a winding number of 1 around 0, and which does not cross $[0, \infty)$.
- 7. Specification of the Contour Branch: Fix a branch of log(-t) to be real when -t is on the negative real axis. Assume z is not an integer.
- 8. <u>Hankel's Formula for Gamma Function</u>: Then the Hankel's formula for the gamma function is (Whittaker and Watson (1996)):

$$\Gamma(z) = -\frac{1}{2i\sin(\pi z)} \oint_{\mathcal{C}}^{\mathcal{C}} (-t)^{z-1} e^{-t} dt$$

where $(-t)^{z-1}$ is interpreted as $e^{(z-1)\log(-t)}$

9. <u>Application of the Reflection Formula</u>: The reflection formula leads to the closely related expression

$$\Gamma(z) = \frac{i}{2\pi} \oint_{c}^{c} (-t)^{-z} e^{-t} dt$$

again, valid wherever z is not an integer.

Fourier Series Expansion



The logarithm of the gamma function has the following Fourier series expansion for

$$\log \Gamma(z) = \left(z - \frac{1}{2}\right) (\gamma + \log z) + (1 - z) \log \pi - \frac{1}{2} \log(\sin(\pi z))$$
$$+ \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{\log n}{n} \sin(2\pi nz)$$

which was, for a long time, attributed to Ernst Kummer, who derived it in 1847 (Bateman and Erdelyi (1955), Shrivastava and Choi (2001)). However, Blagouchine (2014) discovered that Carl Johann Malmsten first derived this series in 1842.

Raabe's Formula

In 1840, Joseph Ludwig Raabe proved that

$$\int_{a}^{a+1} \ln \Gamma(z) dz = \frac{1}{2} \log(2\pi) + a \log a - a$$

In particular, if

$$a = 0$$

then

$$\int_{0}^{1} \ln \Gamma(z) dz = \frac{1}{2} \log(2\pi)$$

Pi Function

1. <u>Definition of the Pi Function</u>: A alternative notation, which was originally introduced by Gauss and which was sometimes used is the *Pi function*, which in terms of the gamma function is

$$\Pi(z) = \Gamma(z+1) = z\Gamma(z) = \int_{0}^{\infty} e^{-t}t^{z}dz$$

so that

$$\Pi(n) = n!$$

For every non-negative integer n.

2. <u>Applying Reflection Formula/Multiplication Theorem</u>: Using the Pi function, the reflection formula takes on the form

$$\Pi(z)\Pi(-z) = \frac{\pi z}{\sin(\pi z)} = \frac{1}{\sin z}$$

where $sinc\ z$ is the normalized sine function, while the multiplication theorem takes on the form

$$\Pi\left(\frac{z}{m}\right)\Pi\left(\frac{z-1}{m}\right)\cdots\Pi\left(\frac{z-m+1}{m}\right) = (2\pi)^{\frac{m-1}{2}}m^{-z-\frac{1}{2}}\Pi(z)$$



3. Reciprocal of the Pi Function: One also sometimes finds

$$\pi(z) = \frac{1}{\Pi(z)}$$

which is entire function, defined for every complex number, just like the reciprocal gamma function. That $\pi(z)$ is entire entails that it has no poles, so $\Pi(z)$, like $\Gamma(z)$, has no zeros.

4. <u>Volume of the n-Ellipsoid</u>: The volume of the n-ellipsoid with radii r_1, \dots, r_n can be expressed as

$$V(r_1, \dots, r_n) = \frac{\pi^{\frac{n}{2}}}{\prod \left(\frac{n}{2}\right)} \prod_{k=1}^{n} r_k$$

Relation to Other Functions

- 1. <u>Upper/Lower Incomplete Gamma Functions</u>: In the first integral above, which defines the gamma function, the limits of integration are fixed. The upper and the lower incomplete gamma functions are the functions obtained by allowing the lower or upper (respectively) limits of integration to vary.
- 2. Relation of Beta to Gamma: The gamma function is related to the Beta function by

$$\mathcal{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

 Gamma Function Derivatives - Digamma Polygamma: The logarithmic derivative of the gamma function is called the digamma function; higher derivatives are the polygamma functions.



- 4. <u>Gamma Function vs. Exponential Sum</u>: The analog of the gamma function over a finite field or a finite ring is the Gaussian sum, a type of exponential sum.
- 5. <u>Reciprocal of the Gamma Function</u>: The reciprocal gamma function is an entire function and has been studied as a specific, separate topic.
- 6. Gamma vs. Reimann Zeta Function: The gamma function also shows up in an important relation with the Reimann zeta function $\zeta(z)$.

$$\pi^{-\frac{z}{2}}\Gamma\left(\frac{z}{2}\right)\zeta(z) = \pi^{-\frac{1-z}{2}}\Gamma\left(\frac{1-z}{2}\right)\zeta(1-z)$$

7. Product of Gamma and Reimann Zeta: It also appears in the following formula:

$$\Gamma(z)\zeta(z) = \int_{0}^{\infty} \frac{u^{z}}{e^{u} - 1} \frac{du}{u}$$

which is only valid for

8. <u>Log of the Gamma Function</u>: The logarithm of the gamma function satisfies the following relation:

$$\log \Gamma(z) = \zeta_H{}'(0,z) - \zeta'(0)$$

where ζ_H is the Hurwitz zeta function, ζ is the Reimann zeta function, and the prime denotes differentiation in the first variable.

9. <u>Moments of Stretched Exponential Function</u>: The gamma function is related to the stretched exponential function. For instance, moments of that function are

$$\langle \tau^n \rangle = \int\limits_0^\infty dt \ t^{n-1} e^{-\left(\frac{t}{\tau}\right)^{\beta}} = \frac{\tau^n}{\beta} \Gamma\left(\frac{n}{\beta}\right)$$

Particular Values

1. <u>Some Specific Gamma Function Values</u>: Some particular values of the gamma function are:

$$\Gamma\left(-\frac{3}{2}\right) = \frac{4}{3}\sqrt{\pi} \approx 2.633\ 271\ 801\ 207$$

$$\Gamma\left(-\frac{1}{2}\right) = -2\sqrt{\pi} \approx -3.544\,907\,701\,811$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \approx 1.772 \ 453 \ 850 \ 906$$

$$\Gamma(1) = 0! \approx 1$$

$$\Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\sqrt{\pi} \approx 0.886\ 226\ 925\ 453$$

$$\Gamma(2)=1!\approx 1$$

$$\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi} \approx 1.329\ 340\ 388\ 179$$

$$\Gamma(3) = 2! \approx 2$$

$$\Gamma\left(\frac{7}{2}\right) = \frac{15}{8}\sqrt{\pi} \approx 3.323\ 350\ 970\ 448$$

$$\Gamma(4) = 3! \approx 6$$

- Undefined for Non-Positive Numbers: The complex gamma function is undefined for non-positive integers, but in these cases, the values can be defined in the Reimann sphere as ∞.
- 3. <u>Holomorphic Nature of Reciprocal Gamma</u>: The reciprocal gamma is well-defined, and analytic at these values and in the entire complex plane:

$$\frac{1}{\Gamma(-3)} = \frac{1}{\Gamma(-2)} = \frac{1}{\Gamma(-2)} = \frac{1}{\Gamma(0)} = 0$$

The Log-Gamma Function

- Rationale behind the Log-Gamma Function: Because the gamma and the factorial
 functions grow so rapidly for moderately large arguments, many computing
 environments include a function that return the natural logarithm of the gamma
 function often given as *lgamma* or *lngamma* in programming environments, or
 gammaln in spreadsheets this grows much more slowly, and for combinatorial
 calculations allows adding and subtracting logs instead of multiplying and dividing
 by very large values.
- 2. <u>Definition of Log-Gamma Function</u>: It is often defined as

$$\log \Gamma(z) = -\gamma z - \log z + \sum_{k=1}^{\infty} \left[\frac{z}{k} - \log \left(1 + \frac{z}{k} \right) \right]$$



- 3. <u>Digamma Function Derivative of Log Gamma</u>: The digamma function, which is a derivative of this function, is also commonly seen.
- 4. <u>Single Strip Function Value</u>: In the context of technical and physical applications, e.g., wave propagation, the functional equation

$$\log \Gamma(z) = \log \Gamma(z+1) - \log z$$

is often used since it allows one to determine the functional values in one strip of width 1 in z from the neighboring strip.

- 5. <u>Large z as Starting Point</u>: In particular, starting with a good approximation for a z with large real part, one may go step-by-step down to the derived z.
- 6. Rocktaeschel Proposal for $\log \Gamma(z)$ Approximation: Following an indication of Carl Friedrich Gauss, Rocktaeschel (1922) proposed for $\log \Gamma(z)$ an approximation for large Re(z):

$$\log \Gamma(z) \approx \left(z - \frac{1}{2}\right) \log z - z + \frac{1}{2} \log(2\pi)$$

7. Approximation for Smaller z: This can be used to accurately approximate $\log \Gamma(z)$ for z with smaller Re(z) via Bohmer (1939):

$$\log \Gamma(z - m) = \log \Gamma(z) - \sum_{k=1}^{m} \log(z - k)$$

8. Approximation using Higher Order Terms: A more accurate approximation can be obtained from the asymptotic expansions of $\log \Gamma(z)$ and $\Gamma(z)$, which are based on Stirling's approximation:

$$\Gamma(z) \sim z^{z-\frac{1}{2}} e^{-z} 2\pi \left(1 + \frac{1}{12z} + \frac{1}{288z^2} - \frac{139}{51840z^3} - \frac{571}{2488320z^4}\right)$$



as

$$|z| \to \infty$$

at constant

$$|\arg z| < \pi$$

9. <u>Approximation using Log Gamma Series</u>: In a more *natural* presentation:

$$\log \Gamma(z) \approx z \log z - z + \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5}$$

as

$$|z| \to \infty$$

at constant

$$|\arg z| < \pi$$

10. Coefficients in the Polynomial Expansion: The coefficients of the terms with

of z^{1-k} in the last expansion are simply $\frac{B_k}{k(k-1)}$ where B_k are the Bernoulli numbers.

The Log-Gamma Function Properties



- Log-Gamma Bohr-Mollerup Theorem: The Bohr-Mollerup theorem states that, among all functions extending factorial functions to positive real numbers, only the gamma function is log-convex, that is, its natural logarithm is convex on the positive real axis.
- 2. <u>Log-Gamma using Riemann Zeta</u>: In a certain sense, the log gamma function is the more natural form; it makes some intrinsic attributes of the function clearer. A striking example of the Taylor series of log Γ around 1:

$$\log \Gamma(z) = -\gamma z + \sum_{k=2}^{\infty} \frac{\zeta(k)}{k} (-z)^k \ \forall \ |z| < 1$$

with $\zeta(k)$ denoting the Riemann zeta function at k.

3. <u>Integral Representation for Log-Gamma</u>: So, using the following property

$$\zeta(z)\Gamma(z) = \int_{0}^{\infty} \frac{u^{z}}{e^{u} - 1} \frac{du}{u}$$

one can find the integral representation for the $\log \Gamma(z)$ function:

$$\log \Gamma(1+z) = -\gamma z + \int_{0}^{\infty} \frac{e^{-zt} - 1 + zt}{t(e^t - 1)} dt$$

or, setting

$$z = 1$$

and calculating γ ,

$$\log \Gamma(1+z) = \int_{0}^{\infty} \frac{e^{-zt} - ze^{-t} - 1 + z}{t(e^t - 1)} dt$$

4. <u>Log-Gamma for Rational z</u>: There also exist special formulas for the logarithm of gamma function for rational z. For instance, if k and n are integers with

and

$$k \neq \frac{n}{2}$$

then

$$\begin{split} \log \Gamma\left(\frac{k}{n}\right) &= \frac{(n-2k)\log(2\pi)}{2n} + \frac{1}{2} \left\{ \log \pi - \log \left(\sin \frac{\pi k}{n}\right) \right\} \\ &+ \frac{1}{\pi} \sum_{r=1}^{n-1} \frac{\gamma + \log r}{r} \cdot \sin \frac{2\pi kr}{n} - \frac{1}{2\pi} \cdot \sin \frac{2\pi kr}{n} \int\limits_{0}^{\infty} \frac{e^{-nx} \log x}{\cosh x - \cdot \cos \frac{2\pi k}{n}} dx \end{split}$$

(Blagouchine (2015)). This formula is sometimes used for numerical computation, since the integrand decreases very quickly.

Integration Over Log-Gamma

1. <u>Log-Gamma Integral from Barnes G</u>: The integral $\int_0^z \Gamma(x) dx$ can be expressed in terms of the Barnes G-function (Alexejweski (1894), Barnes (1899))



$$\int_{0}^{z} \Gamma(x)dx = \frac{z}{2}\log 2\pi + \frac{z(1-z)}{2} + z\Gamma(z) - \ln G(z+1)$$

where

$$Re(z) > -1$$

2. <u>Log-Gamma Integral from Hurwitz Zeta</u>: It can also be written in terms of the Hurwitz zeta function (Gosper (1997), Adamchik (1998)):

$$\int_{0}^{z} \Gamma(x)dx = \frac{z}{2}\log 2\pi + \frac{z(1-z)}{2} - \zeta'(-1) + \zeta'(-1,z)$$

Approximations

- 1. <u>Arbitrary Precision using Stirling/Lanczos</u>: Complex values of the gamma function can be computed numerically to arbitrary precision using Stirling's approximation or Lanczos approximation.
- 2. Fixed Precision Estimate for $Re(z) \in [1,2]$: The gamma function can be computed to fixed precision for

$$Re(z) \in [1,2]$$

by applying integration by parts to the Euler's integral.

3. <u>Breaking Down the Integral Form</u>: For any positive number *x* the gamma function can be written as

$$\Gamma(z) = \int_{0}^{x} e^{-t} t^{z} \frac{dt}{t} + \int_{x}^{\infty} e^{-t} t^{z} \frac{dt}{t} = e^{-x} x^{z} \sum_{n=0}^{\infty} \frac{x^{n}}{z(z+1)\cdots(z+n)} + \int_{x}^{\infty} e^{-t} t^{z} \frac{dt}{t}$$

4. Custom N-bit Precision Estimate: When

$$Re(z) \in [1,2]$$

and

$$x \ge 1$$

the absolute value of the last integral is smaller than $(x + 1)e^{-x}$. By choosing a large enough x, the last expression can be smaller than 2^{-N} for any desired value N. Thus, the gamma function can be evaluated to N bits of precision with the above series.

- 5. <u>Karatsuba Algorithm for Euler Gamma</u>: A fast algorithm for the calculation of the Euler gamma function for any algebraic argument including rational was constructed by Karatsuba (1991a, 1991b).
- 6. Estimates using Arithmetic-Geometric Iterations: For arguments that are integer multiples of ¹/₂₄, the gamma function can also be evaluated quickly using arithmetic-geometric mean iterations see the Section on Particular Values of the Gamma Function, as well as Borwein and Zucker (1992).

Applications – Integration Problems

1. <u>Special Nature of the Gamma Function</u>: The gamma functions have been described as arguably the most common special function, or at least the *least* special of them. The other transcendental functions are special because one could conceivably avoid them



- by staying away from many specialized mathematical topics. On the other hand, the gamma function is the most difficult to avoid.
- 2. Range of Gamma Function Application: The gamma function finds applications in such diverse areas such as quantum physics, astrophysics, and fluid dynamics (Chaudhry and Zubair (2001)).
- 3. <u>Gamma Distribution Usage in Statistics</u>: The gamma distribution, which is formulated in terms of the gamma function, is used in statistics to model a wide range of processes; for example, the time between the occurrences of the earthquakes (Rice (2010)).
- 4. Rationale Behind Gama Functions' Usefulness: The primary reason for the Gamma function's usefulness in such contexts is the prevalence of expressions of the type $f(t)e^{-g(t)}$ which describe processes that decay exponentially in space or time.
- 5. <u>Reduction into Gamma-Type Integrals</u>: Integrals of such expressions can be occasionally solved in terms of gamma function when no elementary solution exists.
- 6. Example Power Source Function Decay: For example, if *f* is a power function and *g* is a linear function, a simple change of variables gives the evaluation

$$\int_{0}^{\infty} t^{b} e^{-at} dt = \frac{\Gamma(b+1)}{a^{b+1}}$$

- 7. <u>Significance of Real Positive Integration</u>: The fact that the integration is performed along the entire real positive line might signify that the gamma function represents the combination of a time-dependent process that continuous indefinitely, or the value might be the total of a distribution in an infinite space.
- 8. Complete vs. Incomplete Gamma Function: It is of course frequently useful to take limits of integration other 0 ad ∞ to describe the cumulation of a finite process, in which case the ordinary gamma function is no longer a solution; the solution is then called an incomplete gamma function.



- 9. Gaussian Category of Exponentially Decaying Functions: An important category of exponentially decaying functions is that of the Gaussian functions $ae^{-\frac{(x-b)^2}{2}}$ and integrals thereof, such as the error function. There are many inter-relations between these functions and the gamma function, notably, $\sqrt{\pi}$ obtained by evaluating $\Gamma\left(\frac{1}{2}\right)$ is the *same* as that found in the normalizing factor of the error distribution and the normal distribution.
- 10. <u>Gamma Function from Algebraic Integrals</u>: The integrals discuss so far involve transcendental functions, but the gamma function also arises from integrals of purely algebraic functions.
- 11. Arc Lengths, Surfaces, and Volumes: In particular, the arc lengths of the ellipses and the lemniscates, which are curves defined by algebraic equations, are given by elliptic integrals that in special cases can be evaluated in terms of the gamma functions. The gamma function also be used to calculate *volume* and *area* of *n*-dimensional hyperspheres.
- 12. <u>Definition of the Beta Function</u>: Another important special case is that of the beta function:

$$\mathcal{B}(x,y) = \int_{0}^{1} t^{x-1} (1-t)^{y-1} dt = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

Calculating Products

 Gamma Function as Generalized Factorial: The gamma function's ability to generalize factorial products immediately leads to applications in many areas of mathematics, in combinatorics, and by extension in areas such as probability theory and the calculation of power series.



 Gamma Function for Binomial Coefficient: Many expressions involving products of successive integers can be written as some combination of factorials, the most important example being that of the binomial coefficient

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

3. Interpretation Suitability for Binomial Coefficient: The example of binomial coefficient motivates why the properties of gamma functions are natural when extended to negative numbers. A binomial coefficient gives the number of ways to choose k elements from n elements; if

there are of course no ways. If

(n-k)! is the factorial of a negative integer, and hence infinite if the gamma function's definition of the integral is used – dividing by infinity gives the expected value of 0.

- 4. Extension to Rational Function Products: One can replace the factorial by a gamma function to extend any such formula to complex numbers. Generally, this works for any product where each factor is a rational function of the index variable, by factoring the rational functions into linear expressions.
- 5. <u>Polynomial Quotient Using Gamma Functions</u>: If P and Q are monic polynomials with degree m and n and respective roots p_1, \dots, p_m and q_1, \dots, q_n , one has

$$\prod_{i=a}^{b} \frac{P(i)}{Q(i)} = \left[\prod_{j=1}^{m} \frac{\Gamma(b-p_j+1)}{\Gamma(a-p_j)} \right] \left[\prod_{k=1}^{n} \frac{\Gamma(a-q_k)}{\Gamma(b-q_k+1)} \right]$$



- 6. Advantage of the Gamma Function Representation: If there is a way to calculate the gamma function numerically, it is a breeze to calculate numerical values of such products. The number of gamma functions on the right depend upon only the degree of polynomials, so it does not matter whether b a equals 5 or 10^5
- 7. <u>Handling Product Poles and Zeros</u>: By taking appropriate limits, the equation can also be made to hold even when the left-hand product contains zeros and poles.
- 8. Extension to Infinite Rational Products: By taking limits, certain rational products of infinitely many factors can be evaluated in terms of gamma function as well. Due to the Weierstrass factorization theorem, analytic functions can be written as infinite products, and these can sometimes be represented as finite products or quotients of the gamma function.
- 9. <u>Example Sine Function Using Gamma</u>: Already one striking example has been seen; the reflection formula essentially represents the sine function as a product of two gamma functions.
- 10. Exponential, Trigonometric, and Hyperbolic Functions: Starting from this expression, the exponential function as well as all the trigonometric and the hyperbolic functions can be expressed using gamma functions.
- 11. <u>Mellin-Barnes Complex Contour Integrals</u>: More functions yet, including the hypergeometric functions and special cases thereof, can be represented by means of complex contour integrals of the products and the quotients of the gamma functions, called the Mellin-Barnes integrals.

Analytic Number Theory

- 1. <u>Study of Riemann Zeta Function</u>: An elegant and deep application of the gamma function is in the study of the Riemann zeta function.
- 2. <u>Reimann Zeta Function Functional Equation</u>: A fundamental property of the Riemann zeta function is its functional form:

$$\Gamma\left(\frac{s}{2}\right)\zeta(s)\pi^{-\frac{s}{2}} = \Gamma\left(\frac{1-s}{2}\right)\zeta(1-s)\pi^{-\frac{1-s}{2}}$$

- 3. <u>Reimann Zeta Function Analytic Continuation</u>: Among other things, this provides an explicit form for analytic continuation of the zeta function to a meromorphic function in the complex plane and leads to an immediate proof that the zeta function has infinitely many so-called *trivial* zeros on the real line.
- 4. <u>Reimann Zeta Function Property #2</u>: Another property of the Riemann zeta function is

$$\Gamma(s)\zeta(s) = \int_{0}^{\infty} \frac{t^{s}}{e^{t} - 1} \frac{dt}{t}$$

- 5. <u>Analytic Number Theory Developmental Milestone</u>: Both formulas were derived by Bernhard Riemann in his seminal 1859 paper (Riemann (1859)), one of the milestones in the development of analytic number theory the branch of mathematics that studies prime numbers using the tools of mathematical analysis.
- 6. <u>Riemann Extension to Factorial Numbers</u>: Factorial numbers, considered as discrete objects, are an important concept in classical number theory, because they contain many prime factors, but Riemann found a use for their continuous extension that arguably turned out to be even more important.

References

Adamchik, V. S. (1998): Polygamma Functions of Negative Order *Journal of Computational and Applied Mathematics* 100 (2) 191-199



- Alexejewski, W. P. (1894): Uber eine Klasse von Funktionen, die der Gammafunktion Analog Sid Leipzig Weidmannsche Buchhandluns 46 268-275
- Barnes, E. W. (1899): The Theory of the G-Function *Quarterly Journal of Pure and Applied Mathematics* **31** 264-314
- Bateman, H., A. Erdelyi (1955): Higher Transcendental Functions McGraw Hill
- Blagouchine, I. V. (2014): Re-discovery of Malmsten's Integrals, their Evaluation by Contour Integration Methods, and some Related Results *Ramanujan Journal* **35** (1) 21-110
- Blagouchine, I. V. (2015): <u>A Theorem for the Closed-form Evaluation of the First</u>
 Generalized Stieljes Constant at Rational Arguments and Related Summations arXiv
- Bohmer, P. E. (1939): Differenzengleichungen und Bestimmte Integrale Kohler-Verlag Leipzig
- Borwein, J. M., And I. J. Zucker (1992): Fast Evaluation of the Gamma Function for Small Rational Fractions using Complete Elliptical Integrals of the First Kind *IMA Journal of Mathematical Analysis* 12 519-526
- Chaudhry, S. M., and M. A. Zubair (2003): On a Class of Incomplete Gamma Functions with Applications Chapman & Hall/CRC
- Davis, P. J. (1959): Leonhard Euler's Integral A Historical Profile of the Gamma
 Function American Mathematical Monthly 66 (10) 849-869
- Gosper, R. W. (1997): $\int_{\frac{m}{4}}^{\frac{n}{6}} \log \Gamma(z) dz$ in: Special Functions, Q-Series, and Related Topics, Ismail, M., D. Masson, and M. Rahman, editors Fields Institute of Communication, American Mathematical Society
- Karatsuba, E. A. (1991a): Fast Evaluation of Transcendental Functions *Problems of Information Transmission* **27 (4)** 339-360
- Karatsuba, E. A. (1991b): On a New Method for Fast Evaluation of Transcendental Functions *Russian Mathematical Surveys* **46** (2) 246-247
- Kingman, J. F. C. (1961): A Convexity Property of Positive Matrices Quarterly Journal of Mathematics 12 (1) 283-284



- National Institute for Standards and Technology (2019): <u>Incomplete Gamma and</u>
 Related Functions
- Rice, J. A. (2010): *Mathematical Statistics and Data Analysis 3rd Edition* **Duxbury Advanced Series**
- Riemann, B. (1859)): <u>Ueber die Anzahl der Primzahlen Unter Einer Gegebenen</u> Grosse
- Rocktaeschel, O. R. (1922): Methoden zur Berechnung der Gammafunktion fur Komplexes Argument **Technical University** Dresden
- Shrivastava, H. M., and J. Choi (2001): Series Associated with Zeta and Related Functions Kluwer Academic Netherlands
- Waldschmidt, M. (2006): Transcendence of Periods: The State of the Art *Pure and Applied Mathematics Quarterly* **2** (2) 435-463
- Whittaker, E. T., and G. N. Watson (1996): A Course on Modern Analysis 4th Edition
 Cambridge University Press
- Wikipedia (2019): Gamma Function



Stirling's Approximation

Introduction and Overview

- 1. <u>Approximation for Factorials and Gamma</u>: *Stirling's approximation* (or *Stirling's formula*) is an approximation for factorials.
- 2. Accuracy for Small *n* Values: It is a good approximation, leading to accurate results even for small values of *n*. It is named after James Stirling, although it was first stated by Abraham de Moivre (Pearson (1924), Le Cam (1986), Dutka (1991), Wikipedia (2019)).
- 3. <u>Typical Version of Stirling's Approximation</u>: The version of the formula typically used in applications is

$$\ln n! = n \ln n - n + \mathcal{O}(\ln n)$$

in the big- \mathcal{O} notation, as

$$n \rightarrow \infty$$

By changing the base of the logarithm, for instance, in the worst case lower bound for comparison sorting, it becomes

$$log_2n! = n log_2n - (log_2e) n + \mathcal{O}(log_2n)$$



4. Constant Term in the Approximation: Specifying the constant in the $O(\ln n)$ error term gives $\frac{1}{2}\ln(2\pi n)$ yielding the more precise formula

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$$

where the sign \sim means that the two quantities are asymptotic, i.e., their ratio tends to 1 as n tends to infinity.

5. <u>Upper/Lower Bounds on the Approximation</u>: One may also give simple bounds valid for all positive integers *n*, rather than for only large *n*:

$$\sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} \le n! \le e n^{n+\frac{1}{2}} e^{-n}$$

for

$$n = 1, 2, 3, \cdots$$

These follow from the more precise error bounds discussed below in this chapter.

Derivation

1. <u>Summation of the Logs as an Integral</u>: Roughly speaking, the simplest version of Stirling's formula can be obtained by approximating the sum

$$\ln n! = \sum_{j=1}^{n} \ln j$$



by an integral

$$\sum_{j=1}^{n} \ln j \approx \int_{0}^{1} \ln x \, dx = n \ln n - n + 1$$

2. <u>Sum of the Log Terms</u>: The full formula, together with an estimate of its error, can be derived as follows. Instead of approximating n!, one considers its natural log as this slowly varying function:

$$\ln n! = \ln 1 + \dots + \ln n$$

3. <u>Trapezoidal Approximation of the Integral</u>: The right-hand side of the equation minus

$$\frac{1}{2}(\ln 1 + \ln n) = \frac{1}{2}\ln n$$

is the approximation by the trapezoidal rule of the integral

$$\ln n! - \frac{1}{2} \ln n \approx \int_{0}^{1} \ln x \, dx = n \ln n - n + 1$$

and the error in this approximation is given by the Euler-MacLaurin formula

$$\ln n! - \frac{1}{2} \ln n = \frac{1}{2} \ln 1 + \ln 2 + \dots + \ln(n-1) + \frac{1}{2} \ln n$$
$$= n \ln n - n + 1 + \sum_{k=2}^{m} \frac{(-1)^k B_k}{k(k-1)} + R_{m,n}$$



where B_k is the Bernoulli number and $R_{m,n}$ is the remainder term in the Euler-MacLaurin formula.

4. Integration Error Terms as $n \to \infty$: Take limits to find that

$$\lim_{n \to \infty} \left(\ln n! - n \ln n + n - \frac{1}{2} \ln n \right) = 1 - \sum_{k=2}^{m} \frac{(-1)^k B_k}{k(k-1)} + \lim_{n \to \infty} R_{m,n}$$

5. <u>Euler-MacLaurin Error Term Asymptote</u>: This limit is denoted as y. Because the remainder $R_{m,n}$ in the Euler-MacLaurin formula satisfies

$$R_{m,n} = \lim_{n \to \infty} R_{m,n} + \mathcal{O}\left(\frac{1}{n^m}\right)$$

where the big \mathcal{O} notation is used again, combining the equations above yields the approximation formula in its logarithmic form:

$$\ln n! = n \ln \left(\frac{n}{e}\right) + \frac{1}{2} \ln n + y + \sum_{k=2}^{m} \frac{(-1)^k B_k}{k(k-1)} + \mathcal{O}\left(\frac{1}{n^m}\right)$$

6. Exponentiation for the n! Expression: Taking exponential of both sides, and choosing a positive integer m, one gets an expression involving the unknown quantity e^y . For

$$m = 1$$

the expression becomes

$$n! = e^{y} \sqrt{n} \left(\frac{n}{e} \right)^{n} \left[1 + \mathcal{O} \left(\frac{1}{n} \right) \right]$$



7. Explicit Value of the Limit: The quantity e^y can be found by taking the limit on both sides as n tends to infinity and using Wallis' product, which shows that

$$e^y = \sqrt{2\pi}$$

Therefore, the Stirling's formula is obtained as

$$n! = \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \left[1 + \mathcal{O}\left(\frac{1}{n}\right)\right]$$

An Alternative Definition

1. <u>Starting Point – The Gamma Function</u>: An alternative formula for n! using the gamma function is

$$n! = \int_{0}^{\infty} x^{n} e^{-x} dx$$

This can be verified by repeated integration by parts.

2. Change of *x* to *ny*: Rewriting and arranging the variables as

$$x = ny$$

one gets

$$n! = \int_{0}^{\infty} e^{n \ln x - x} dx = n e^{n \ln n} \int_{0}^{\infty} e^{n(\ln y - y)} dy$$

3. Laplace's Method Recovers Stirling's Formula: Applying Laplace's method, one has

$$\int_{0}^{\infty} e^{n(\ln y - y)} dy \sim \sqrt{\frac{2\pi}{n}} e^{-n}$$

which recovers the Stirling formula

$$n! \sim ne^{n \ln n} \sqrt{\frac{2\pi}{n}} e^{-n} = \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$$

 Two Orders of Laplace Correction: Further corrections can be obtained by using the Laplace's method. For example, computing two-order expansion using Laplace's method yields

$$\int_{0}^{\infty} e^{n(\ln y - y)} dy \sim \sqrt{\frac{2\pi}{n}} e^{-n} \left(1 + \frac{1}{12n} \right)$$

and gives Stirling's formula to two-orders as

$$n! \sim ne^{n\ln n} \sqrt{\frac{2\pi}{n}} e^{-n} \left(1 + \frac{1}{12n}\right) = \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \left(1 + \frac{1}{12n}\right)$$

5. Complex Analysis Using Cauchy's Integral: A complex analysis version of this method (Flajolet and Sedgewick (2009)) is to consider $\frac{1}{n!}$ as a Taylor coefficient of the exponential function



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

computed by Cauchy's integral formula as

$$\frac{1}{n!} = \frac{1}{2\pi i} \oint_{|z|=r}^{|z|=r} \frac{e^z}{z^{n+1}} dz$$

6. <u>Approximation Using the Saddle Point Method</u>: The line integral can then be approximated using the addle point method with an appropriate choice of the contour radius

$$r = r_n$$

The dominant portion of the integral near the saddle point is then approximated by a real integral and Laplace's method, while the remaining portion of the integral can be bounded above to give an error term.

Speed of Convergence and Error Estimates

1. <u>Stirling Series for Factorial Approximation</u>: Stirling's formula is in fact the first approximation to the following series called the *Stirling Series* (National Institute of Standards and Technology (2018)):

$$n! = \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \left(1 + \frac{1}{12n} + \frac{1}{288n^2} - \frac{139}{51840n^3} - \frac{571}{2488320n^4} + \cdots\right)$$



- 2. <u>Structure of the Stirling Errors</u>: An explicit formula for the coefficients of this series was given by Nemes (2010). As illustrated in Wikipedia (2019), the relative error vs. *n* for 1 through 5 terms listed above have very characteristic error structure features.
- 3. Asymptotic Expansion of Stirling Series: As

$$n \rightarrow \infty$$

the error in the truncated series is asymptotically equal to the first term. This is an example of an asymptotic expansion.

- 4. <u>Stirling Series is not Convergent</u>: It is not a convergent series; for any *particular* value of *n* there are only so many terms of the series that improve the accuracy, after which point the accuracy actually gets worse.
- 5. Errors due to Alternating Signs: Rewriting Stirling's series in the form

$$\ln n! \sim n \ln n - n + \frac{1}{2} \ln(2\pi n) + \frac{1}{12n} - \frac{1}{360n^3} + \frac{1}{1260n^5} - \frac{1}{1680n^7} + \cdots$$

it is known that the error in truncating the series is always of the opposite sign and at most the same magnitude of the first omitted term.

6. <u>Precise Estimates of Lower/Upper Bounds</u>: More precise bounds, due to Robbins (1955), that are valid for all positive integers *n* are:

$$\sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} e^{\frac{1}{12n+1}} < n! < \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} e^{\frac{1}{12n}}$$

Stirling's Formula for the Gamma Function



1. Review – Gamma Function Definition: For all positive integers

$$n! = \Gamma(n+1)$$

where Γ denotes the gamma function.

- 2. <u>Differences between Gamma and Factorial</u>: However, the gamma function, unlike the factorial, is more broadly defined for all complex numbers other than non-positive integers; nevertheless, Stirling's formula may still be applied.
- 3. Starting Expression for $\ln \Gamma(z)$ Term: If

then

$$\ln \Gamma(z) = z \ln z - z + \frac{1}{2} \ln \frac{2\pi}{z} + \int_{0}^{\infty} \frac{2 \arctan \frac{t}{z}}{e^{2\pi t} - 1} dt$$

4. Repeated Integration by Parts: Repeated integration by parts results in

$$\ln \Gamma(z) \sim z \ln z - z + \frac{1}{2} \ln \frac{2\pi}{z} + \sum_{n=1}^{N-1} \frac{B_{2n}}{2n(2n-1)z^{2n-1}}$$

where B_n is the n^{th} Bernoulli number. Note that the limit of the sum as

$$N \to +\infty$$

is not convergent, so this expression is just an asymptotic expansion.

5. <u>z Validity Range for Asymptotic Expansion</u>: The formula is valid for z large enough in absolute value when

$$|\arg(z)| < \pi - \varepsilon$$

where ε is positive with an error term of $\mathcal{O}(z^{-2N+1})$. The corresponding approximation may now be written as

$$\Gamma(z) = \sqrt{\frac{2\pi}{z}} \left(\frac{z}{e}\right)^z \left[1 + \mathcal{O}\left(\frac{1}{z}\right)\right]$$

6. Riemann-Siegel Theta Function over Varying Im(z): A further application of this asymptotic expansion is for complex argument z with constant Re(z). See, for example, the Stirling formula applied in

$$Im(z) = t$$

of the Riemann-Siegel theta function on the straight line $\frac{1}{4} + it$.

Error Bounds

1. <u>Explicit Expression for the Residuals</u>: For any positive integer *N*, the following notation is introduced:

$$\ln \Gamma(z) \sim z \ln z - z + \frac{1}{2} \ln \frac{2\pi}{z} + \sum_{n=1}^{N-1} \frac{B_{2n}}{2n(2n-1)z^{2n-1}} + R_N(z)$$

and

$$\Gamma(z) = \sqrt{\frac{2\pi}{z}} \left(\frac{z}{e}\right)^z \left[\sum_{n=0}^{N-1} \frac{a_n}{z^n} + \tilde{R}_N(z)\right]$$

2. Residuals of $\Gamma(z)$ and $\ln \Gamma(z)$: Then, from Schafke and Sattler (1990) and Memes (2015):

$$|R_N(z)| \le \frac{B_{2N}}{2N(2N-1)|z|^{2N-1}} \begin{cases} 1 & |\arg(z)| \le \frac{\pi}{4} \\ |\csc(\arg z)| & \frac{\pi}{4} < |\arg(z)| < \frac{\pi}{2} \\ \sec^{2N}\left(\frac{\arg(z)}{2}\right) & |\arg(z)| < \pi \end{cases}$$

$$\left| \tilde{R}_N(z) \right| \leq \left(\frac{|a_N|}{|z|^N} + \frac{|a_{N+1}|}{|z|^{N+1}} \right) \begin{cases} 1 & |\operatorname{arg}(z)| \leq \frac{\pi}{4} \\ |\operatorname{csc}(\operatorname{arg} z)| & \frac{\pi}{4} < |\operatorname{arg}(z)| < \frac{\pi}{2} \end{cases}$$

A Convergent Version of the Sterling's Formula

1. <u>Convergent Version Using Raabe's Integral</u>: Obtaining a convergent version of the Sterling's formula entails evaluating Raabe's integral:

$$\int_{0}^{\infty} \frac{2 \arctan \frac{t}{x}}{e^{2\pi t} - 1} dt = \ln \Gamma(x) - x \ln x + x - \frac{1}{2} \ln \frac{2\pi}{x}$$

2. <u>Use of Inverted Rising Exponentials</u>: One way to do this is by means of a convergent series of inverted rising exponentials. If

$$z^{\bar{n}} = z(z+1)\cdots(z+n-1)$$

then

$$\int_{0}^{\infty} \frac{2 \arctan \frac{t}{x}}{e^{2\pi t} - 1} dt = \sum_{n=1}^{\infty} \frac{C_n}{(x+1)^{\overline{n}}}$$

where

$$C_n = \frac{1}{n} \int_{0}^{1} x^{\bar{n}} \left(x - \frac{1}{2} \right) dx = \frac{1}{2} \sum_{k=1}^{n} \frac{k |S(n,k)|}{(k+1)(k+2)}$$

where S(n, k) denotes the Stirling's numbers of the first kind.

3. <u>Convergent Version of the Stirling Series</u>: From this, one obtains a version of the Stirling's series

$$\ln \Gamma(x) = x \ln x - x + \frac{1}{2} \ln \left(\frac{2\pi}{x}\right) + \frac{1}{12(x+1)} + \frac{1}{12(x+1)(x+2)} + \frac{59}{360(x+1)(x+2)(x+3)} + \frac{29}{60(x+1)(x+2)(x+3)} + \cdots$$

which converges when



Versions Suitable for Calculators

1. <u>Hyperbolic Sine Function Based Version</u>: The approximation

$$\Gamma(z) \approx \sqrt{\frac{2\pi}{z}} \left(\frac{z}{e} \sqrt{z \sinh \frac{1}{z} + \frac{1}{810z^6}} \right)^z$$

and its equivalent form

$$2 \ln \Gamma(z) \approx \ln(2\pi) - \ln z \left[2 \ln z + \ln \left(z \sinh \frac{1}{z} + \frac{1}{810z^6} \right) - 2 \right]$$

can be obtained by re-arranging Stirling's extended formula and observing the coincidence between the resultant power series and the Taylor series expansion of the hyperbolic sine function.

- 2. Memory Efficient Computation of Gamma: This approximation is good to more than 8 decimal digits for z with a real part greater than 8. Toth (2016) indicates that this was suggested by Robert Windschitl in 2002 for computing gamma functions with fair accuracy on calculators with limited program or register memory.
- 3. <u>Nemes Simplified Gamma Function Version</u>: Nemes (2010) proposed an approximation which gives the same number of exact digits as the Windschitl approximation, but is much simpler.

$$\Gamma(z) \approx \sqrt{\frac{2\pi}{z}} \left[\frac{1}{e} \left(z + \frac{1}{12z - \frac{1}{10z}} \right) \right]^z$$

or equivalently

$$\ln \Gamma(z) \approx \frac{1}{2} (\ln 2\pi - \ln z) + z \left[\ln \left(z + \frac{1}{12z - \frac{1}{10z}} \right) - 1 \right]$$

4. Ramanujan's Simplified Expression for $\Gamma(1+x)$: An alternative approximation for the gamma function stated by Ramanujan is

$$\Gamma(1+x) \approx \sqrt{\pi} \left(\frac{x}{e}\right)^x \left(8x^3 + 4x^2 + x + \frac{1}{30}\right)^{\frac{1}{6}}$$

for

$$x \ge 0$$

5. Ramanujan's Simplified Expression for $\ln n!$: The equivalent approximation for $\ln n!$ Has an approximate error of $\frac{1}{1400n^3}$ and is given by

$$\ln n! \approx n \ln n - n + \frac{1}{6} \ln \left(8x^3 + 4x^2 + x + \frac{1}{30} \right) + \frac{1}{2} \ln \pi$$

6. <u>Ramanujan's Approximation - Lower/Upper Bounds</u>: The approximation may be made more precise by giving paired upper and lower bounds; one such inequality is (Karatsuba (2001), Mortici (2011a, 2011b, 2011c))

$$\sqrt{\pi} \left(\frac{x}{e}\right)^x \left(8x^3 + 4x^2 + x + \frac{1}{100}\right)^{\frac{1}{6}} < \Gamma(1+x) < \sqrt{\pi} \left(\frac{x}{e}\right)^x \left(8x^3 + 4x^2 + x + \frac{1}{30}\right)^{\frac{1}{6}}$$

References



- Dutka, J. (1991): The Early History of the Factorial Function Archive for History of Exact Sciences 43 (3) 225-249
- Flajolet, P., and R. Sedgewick (2009): Analytic Combinatorics Cambridge
 University Press New York
- Karatsuba, E. (2001): On the Asymptotic Representation of the Euler Gamma
 Function by Ramanujan *Journal of Computational and Applied Mathematics* 135 (2) 225-240
- Le Cam, L. (1986): The Central Limit Theorem around 1935 *Statistical Science* **1** (**1**) 78-96
- Mortici, C. (2011a): Ramanujan's Estimate for the Gamma Function via Monotonicity Arguments *Ramanujan Journal* **25** (2) 149-154
- Mortici, C. (2011b): Improved Asymptotic Formulas for the Gamma Function
 Computers and Mathematics with Applications 61 (11) 3364-3369
- Mortici, C. (2011c): On Ramanujan's Large Argument Formula for the Gamma Function Ramanujan Journal 26 (3) 185-192
- National Institute of Standards and Technology (2018): <u>NIST Digital Library of</u>
 <u>Mathematical Functions</u>
- Nemes, G. (2010): On the Coefficients of the Asymptotic Expansion of n! arXiv
- Pearson, K. (1924): Historical Note on the Origin of the Normal Curve of Errors
 Biometrika 16 (3) 402-404
- Robbins, H. (1955): A Remark on Stirling's Formula American Mathematical Monthly 62 (1) 26-29
- Schafke, F. W., and A. Sattler (1990): Restgliedabschatzungen für die Sterlingsche Reine *Note di Matematica* **10 (2)** 453-470
- Toth V. T. (2016): <u>Programmable Calculators The Gamma Function</u>
- Wikipedia (2019): <u>Stirling's Approximation</u>



Lanczos Approximation

Introduction

- 1. <u>Numerical Approximation to Gamma Function</u>: The Lanczos is a method for computing the gamma function numerically. It is a practical alternative to the more popular Stirling's approximation for calculating the gamma function with a fixed precision (Wikipedia (2019)).
- 2. <u>Principal Expression for the Lanczos Approximation</u>: The Lanczos approximation consists of the formula

$$\Gamma(z+1) = \sqrt{2\pi} \left(z+g+\frac{1}{2}\right)^{z+\frac{1}{2}} e^{-\left(z+g+\frac{1}{2}\right)} A_g(z)$$

for the gamma function, with

$$A_g(z) = \frac{1}{2}p_0(g) + p_1(g)\frac{z}{z+1} + p_2(g)\frac{z(z-1)}{(z+1)(z+2)} + \cdots$$

3. <u>Usage of the Control Constant g</u>: Here, g is a constant that may be chosen arbitrarily subject to the restriction that'

$$Re(z) > \frac{1}{2}$$



- (Pugh (2004)). The coefficients p_i are slightly more difficult to calculate, as shown in the next section.
- 4. Extension to the Full Complex Plane: Although the expression as states here is only valid for the components in the right complex half-plane, it can be extended to the entire half plane by the reflection formula

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

- 5. Truncation to obtain Suitable Precision: The series A is convergent and may be truncated to obtain an approximation to the desired precision. By choosing an appropriate g − typically a small integer − only 5 − 10 terms of the series are required to compute the gamma function with typical single or double floating-point precision.
- 6. <u>Pre-calculation of the Series Coefficients</u>: If a fixed *g* is chosen, the coefficients can be calculated in advance, and the sum is re-cast into the following form:

$$A_g = c_0 + \sum_{k=1}^{N} \frac{c_k}{z + k}$$

7. Popularization by Numerical Recipes: Thus, computing the gamma function becomes a matter of evaluating only a small number of elementary functions and multiplying by stored constants. The Lanczos approximation was popularized by Press, Teukolsky, Vetterling, and Flannery (2007), according to whom computing the gamma function becomes "not much more difficult than other built-in functions taken for granted, such as $\sin x$ or e^x ". This method is also implemented in the GNU Scientific Library.



Coefficients

1. Expression for the Lanczos Coefficients: The coefficients are given by

$$p_k(g) = \sum_{a=0}^k C(2k+1, 2a+1) \frac{\sqrt{2}}{\pi} \left(a - \frac{1}{2}\right)! \left(a + g + \frac{1}{2}\right)^{-\left(a + \frac{1}{2}\right)} e^{a + g + \frac{1}{2}}$$

with C(i,j) denoting the $(i,j)^{th}$ element of the Chebyshev polynomial coefficient matrix which can be calculated recursively from the identities

$$C(1,1) = 1$$

$$C(2,2) = 1$$

$$C(i,1) = -C(i-2,1) \quad i = 3,4,\cdots$$

$$C(i,j) = -2C(i-1,j-1) \quad i = j = 3,4,\cdots$$

$$C(i,j) = -2C(i-1,j-1) - C(i-2,j) \quad i > j = 2,3,\cdots$$

2. <u>Paul Godfrey's Coefficient Computation Scheme</u>: Godfrey (2001) describes how to obtain the coefficients as well as the value of the truncated series *A* as a matrix product.

Derivation



1. Lanczos derived the formula from the Euler's integral

$$\Gamma(z+1) = \int_{0}^{\infty} t^{z} e^{-t} dt$$

performing a basic sequence of manipulations to obtain

$$\Gamma(z+1) = (z+g+1)^{z+1}e^{-(z+g+1)} \int_{0}^{e} [v(1-\log v)]^{z} v^{g} dv$$

and then deriving a series for the integral.

References

- Godfrey, P. (2001): <u>Lanczos Implementation of the Gamma Function</u>
- Press, W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery (2007):
 Numerical Recipes: The Art of Scientific Computing 3rd Edition Cambridge
 University Press New York
- Pugh, G. R. (2004): An Analysis of the Lanczos Gamma Approximation Ph. D.
 University of British Columbia
- Wikipedia (2019): <u>Lanczos Approximation</u>



Incomplete Gamma Function

Introduction and Overview

- 1. <u>Lower/Upper Incomplete Gamma Functions</u>: In mathematics, the *upper* and the *lower incomplete gamma functions* are types of special functions which arise as solutions to various mathematical problems, such as certain integrals (Wikipedia (2019b)).
- 2. <u>Origin of the Term *Incomplete*</u>: Their respective names stem from their integral definitions, which are defined similarly to the gamma functions, but with different or *incomplete* integrals.
- 3. <u>Lower Gamma Function Integration Limits</u>: The gamma function is defined as an integral from zero to infinity. This contrasts with the lower incomplete gamma function, which is defined as an integral from zero to a variable upper limit.
- 4. <u>Upper Gamma Function Integration Limits</u>: Similarly, the upper incomplete gamma function is defined as an integral from a variable lower limit to infinity.

Definition

The upper incomplete gamma function is defined as

$$\Gamma(s,x) = \int_{x}^{\infty} t^{s-1} e^{-t} dt$$

whereas the lower incomplete gamma function is defined as

$$\gamma(s,x) = \int_{0}^{x} t^{s-1}e^{-t}dt$$

Properties

- 1. <u>Positive Real Part of s</u>: In both cases above, s is a positive complex number, such that the real part of s is positive.
- 2. <u>Recurrence for Lower/Upper Gamma</u>: On integrating by parts, one finds the recurrence relations

$$\Gamma(s+1,x) = s\Gamma(s,x) + x^s e^{-x}$$

and

$$\gamma(s+1,x) = s\gamma(s,x) - x^s e^{-x}$$

3. Equivalence across Upper/Lower/Parent: Since the ordinary gamma function is defined as



$$\Gamma(s) = \int_{0}^{\infty} t^{s-1} e^{-t} dt$$

one has

$$\Gamma(s) = \Gamma(s,0) = \lim_{x \to \infty} \Gamma(s,x)$$

and

$$\Gamma(s,x) + \gamma(s,x) = \Gamma(s)$$

Continuation to Complex Values

- 1. <u>Development of the Holomorphic Equivalents</u>: The lower and the upper incomplete gamma functions, as defined above for real, positive *s* and *x*, can be developed into holomorphic functions for both *x* and *s*, as well as defined for almost all combinations of complex *x* and *s* (National Institute of Standards and Technology (2019a)).
- 2. <u>Complex Analysis of Holomorphic Counterparts</u>: Complex analysis shows how the properties of real incomplete gamma functions extend to their holomorphic counterparts.

Lower Incomplete Gamma Function – Holomorphic Extensions



1. <u>Recurrence Applied to Lower Gamma</u>: Repeated application of the recurrence relation to the *lower incomplete gamma* function leads to the power series expansion (National Institute of Standards and Technology (2019a))

$$\gamma(s,x) = \sum_{k=0}^{\infty} \frac{x^{s} e^{-x} x^{k}}{s(s+1)\cdots(s+k)} = x^{s} \Gamma(s) e^{-x} \sum_{k=0}^{\infty} \frac{x^{k}}{\Gamma(s+k-1)}$$

2. Well-definedness of the Sum: Given the rapid growth of the absolute value of $\Gamma(z+k)$ when

$$k \to \infty$$

and the fact that the reciprocal of $\Gamma(z)$ is an entire function, the coefficients in the right-most sum are well-defined, and locally the sum converges uniformly for all complex s and x.

3. <u>Property of the Limiting Function</u>: By the theorem of Weierstrass (Marshall (2009)), the limiting function, sometimes denoted as γ^*

$$\gamma^*(s,z) = e^{-z} \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(s+k-1)}$$

(National Institute of Standards and Technology (2019a)) is entire with respect to both z for fixed s and s for fixed z (National Institute of Standards and Technology (2019a)), and, thus holomorphic on $\mathbb{C} \times \mathbb{C}$ by Hartog's theorem (Garrett (2005)).

4. Holomorphicity of the Lower Gamma Function: Hence, the following decomposition

$$\gamma(s,x) = x^s e^{-x} \gamma^*(s,x)$$



(National Institute of Standards and Technology (2019a)) extends the real lower incomplete gamma function as a holomorphic function, both jointly and separately in z and s.

5. <u>Singularities and Zeroes of γ </u>: It follows from the properties of z^s and the Γ-function, that the first two terms capture the singularities of γ – at

$$z = 0$$

or at s a non-positive integer – whereas the last term γ^* contributes to its zeroes.

Multi-Valuedness

1. <u>Multi-Valuedness Inherent in Complex Logarithms</u>: The complex logarithm

$$\log z = \log |z| + i \arg z$$

is determined only upto a multiple of $2\pi i$, which renders it multi-valued. Functions involving complex logarithms typically inherit this property. Among these are the complex power, and since z^s appears in its decomposition, the γ function will too.

- Indeterminacy of Multi-Valued Functions: The indeterminacy of multi-valued functions introduces complications, since it must be stated how to select the value. Two strategies are presented below to handle this.
- 3. Replacement using $\mathbb{C} \times \mathbb{C}$ Riemann Manifold: The most general way is to replace the domain \mathbb{C} of the multi-valued function by a suitable manifold in $\mathbb{C} \times \mathbb{C}$ called the Reimann surface. While this removes multi-valuedness, aspects of the theory behind it have to be closely followed (Teleman (2003)).



- 4. <u>Decomposition into Single-Valued Branches</u>: Restrict the domain such that the multi-valued function decomposes into separate single-valued branches, which can be handled individually.
- 5. <u>Terminology Used in this Section</u>: The following set of rules are used to interpret the formulations of this Section, unless explicitly stated otherwise.

Sectors

1. <u>Domains Suitable for Complex Expressions</u>: Sectors in C having their vertex at

$$z = 0$$

often prove to be appropriate domains for complex expressions.

2. Sub-sector within the Main Sector \mathbb{C} : A sector D consists of all complex z fulfilling

$$z \neq 0$$

and

$$\alpha - \delta < \arg z < \alpha + \delta$$

with some α , and

$$0 < \delta \le \pi$$

Often α can be arbitrarily chosen, and is not specified.



3. <u>Default Value for δ </u>: If δ is not given, it is often assumed to be π , and the sector is in fact the whole plane \mathbb{C} , with the exception of a half-line originating at

$$z = 0$$

and pointing into the direction of $-\alpha$, usually serving as a branch-cut.

4. Sector Centered around Positive Real: Note: In many applications and texts, α is silently taken to be 0, which centers the sector around the positive real axis.

Branches

- 1. Single-Valued and Holomorphic Logarithm: In particular, a single-valued and holomorphic logarithm exists on any such sector D having its imaginary part bounded to the range $(\alpha \delta, \alpha + \delta)$.
- 2. Single Valued and Holomorphic Incomplete Gamma: Based on such a restricted logarithm, z^s and the incomplete gamma functions collapse to single-valued, holomorphic functions on D ($\mathbb{C} \times D$), called branches of their multi-valued counterparts on D.
- 3. Fixing the Branch by Setting α : Adding a multiple of 2π to α yields a different set of correlated branches on the same set D. However, in any given context here, α is assumed fixed, and all branches involved are associated with it.
- 4. <u>Defining the Principal Branch</u>: If

 $|\alpha| < \delta$



the branches are called principal, because they equal their real analogons on the positive real axis. Note: In many applications and texts, the formulations hold only for principal branches.

Relation between Branches

The values of different branches of both the complex power function and the lower incomplete gamma function can be easily derived from each other by multiplication of $e^{2\pi iks}$ (National Institute of Standards and Technology (2019a)).

Behavior near the Branch Point

1. Asymptotic Gamma Behavior near z = 0: The decomposition above further shows that γ behaves near

$$z = 0$$

asymptotically as

$$\gamma(z,x) \to z^s e^{-z} \gamma^*(z,0) = z^s \frac{\Gamma(s)}{\Gamma(s+1)} = \frac{z^s}{s}$$

2. Real/Complex Realm Behavioral Differences: For positive and real x, y, and s,



$$\frac{z^y}{y} \to 0$$

when

$$(x,y) \rightarrow (0,s)$$

This seems to justify setting

$$\gamma(s,0)=0$$

for real

However, matters are somewhat different in the complex realm.

3. Conditions to be Satisfied for Convergence: Only if a) the real part of s is positive, and b) the values u^v are taken from just a finite set of branches, are they guaranteed to converge to zero, as

$$(u,v) \rightarrow (0,s)$$

in which case, so does $\gamma(u, v)$.

4. Results for a Single Branch: On a single branch of γ , the criterion b) is naturally fulfilled, so

$$\gamma(s,0)=0$$



for *s* with positive real part, and it is a continuous limit. Also note that such a continuation is by no means an analytic one.

Algebraic Relations

- 1. Algebraic Relations and Differential Equations: All algebraic relations and differential equations observed by the real $\gamma(s,z)$ hold for its holomorphic counterpart as well.
- 2. <u>Holomorphic Extension using Identity Theorem</u>: This is a consequence of the identity theorem that states that equations between holomorphic functions valid on a real interval hold everywhere.
- 3. <u>Branch Preservation of Recurrences/Derivatives</u>: In particular, the recurrence relation and

$$\frac{\partial \gamma(s,z)}{\partial z} = z^{s-1}e^{-z}$$

(National Institute of Standards and Technology (2019a)) are preserved on their corresponding branches.

Integral Representation



- 1. γ as a Holomorphic Anti-derivative: The last relation clearly indicates that, for a fixed s, γ is a primitive or an anti-derivative of the holomorphic function $z^{s-1}e^{-z}$.
- 2. <u>Integration inside a Single Branch</u>: Consequently, for any complex

$$u, v \neq 0$$

$$\int_{u}^{v} t^{s-1}e^{-t}dt = \gamma(s,v) - \gamma(s,u)$$

holds as long as the path of the integration is contained entirely inside the domain of a branch of the integrand.

3. Complex Integral Definition of γ : If, additionally, the real part of s is positive, then the limit

$$\gamma(s,u)\to 0$$

for

$$u \rightarrow 0$$

applies, finally aiming at the complex integral definition of γ

$$\gamma(s,z) = \int_{0}^{z} t^{s-1}e^{-t}dt$$

(National Institute of Standards and Technology (2019a)).



4. Inclusion of z = 0 at Start: Any path of the integration containing only 0 at the beginning, otherwise restricted to the domain of a branch of the integrand, is valid here, for example, the line connecting 0 and z.

Limit for $z \to \pm \infty$ - Real Values

Given the integral representation of the principal branch of γ , the equation holds for all positive real s and x.

$$\Gamma(s,z) = \int_{0}^{\infty} t^{s-1}e^{-t}dt = \lim_{x \to \infty} \gamma(s,z)$$

(National Institute of Standards and Technology (2019b)).

Limit for $z \to \pm \infty$ - Complex Values

1. Extending $z \to \pm \infty$ Limit to Complex s: This result extends to complex s. Assume first

$$1 \le Re(s) \le 2$$

and



Then

$$|\gamma(s,b) - \gamma(s,a)| \le \int_{a}^{b} |t^{s-1}| e^{-t} dt = \int_{a}^{b} t^{\Re s - 1} e^{-t} dt \le \int_{a}^{b} t e^{-t} dt$$

where

$$|z^{s}| = |z^{\Re s}| \cdot e^{-\Im s \arg z}$$

(National Institute of Standards and Technology (2019c)) has been used in the middle.

2. Skip Convergence as $x \to +\infty$: Since the final integral becomes arbitrarily small if only a is small enough, $\gamma(s, x)$ converges uniformly for

$$x \to +\infty$$

on the strip

towards a holomorphic function (Marshall (2009)), which must be $\Gamma(s)$ because of the identity theorem.

3. Convergence Outside the Strip as $x \to +\infty$: Taking the limit in the recurrence relation

$$\gamma(s, x) = (s - 1)\gamma(s - 1, x) - x^{s - 1}e^{-x}$$

and noting that



$$\lim_{x\to\infty} x^{s-1}e^{-x}\to 0$$

for all n shows that $\gamma(s,x)$ converges outside the strip too, towards a function obeying the recurrence relation of the Γ -function.

4. $\Gamma(s)$ Limit Using the Identity Theorem: It follows that

$$\Gamma(s) = \frac{Limit}{x \to \infty} \gamma(s, x)$$

for all complex s not a non-positive integer, x real, and y principal.

Sector-wise Convergence

1. $\gamma(s, u)$ Convergence inside Principal Sector: Let u be from the sector

$$\arg z < \delta < \frac{\pi}{2}$$

with some fixed δ keeping

$$\alpha = 0$$

 γ is the principal branch on this sector, and this section looks at

$$\Gamma(s) - \gamma(s, u) = \Gamma(s) - \gamma(s, |u|) + \gamma(s, |u|) - \gamma(s, u)$$



2. Gamma Difference across Imaginary u: As shown above, the first difference can be made arbitrarily small if |u| is sufficiently large. The second difference allows for the following estimation:

$$\gamma(s,|u|) - \gamma(s,u) \le \int_{u}^{|u|} |x^{z-1}e^{-z}| dz = \int_{u}^{|u|} |z|^{\Re s} \cdot e^{-\Im s \arg z} \cdot e^{-\Re s} dz$$

where the integral representation of γ and the expression regarding $|z|^s$ have been used.

3. <u>Integrating across the Arc</u>: On integrating along the arc with radius

$$R = |u|$$

around 0 connecting u and |u|, the last integral becomes

$$\int_{u}^{|u|} |z|^{\Re s} \cdot e^{-\Im s \arg z} \cdot e^{-\Re s} dz \le R \cdot |\arg u| \cdot R^{\Re s - 1} \cdot e^{\Im s |\arg u|} \cdot e^{-R \cos(\arg u)}$$

$$\le \delta \cdot R^{\Re s} \cdot e^{\Im s \delta} \cdot e^{-R \cos \delta} = M \cdot (R \cos \delta)^{\Re s} \cdot e^{-R \cos \delta}$$

where

$$M = \delta(\cos \delta)^{-Re(s)} e^{-Im(s\delta)}$$

is a constant independent of u or R. Again, using

$$\lim_{x \to \infty} x^{s-1} e^{-x} \to 0$$



for all n, it can be seen that the last expression approaches 0 as R increases towards $+\infty$.

4. Convergence on the Principal Domain: In total, one now has

$$\Gamma(s) = \underset{|z| \to \infty}{limit} \gamma(s, z)$$

$$|\arg z| < \frac{\pi}{2} - \epsilon$$

if s is not a non-negative integer,

$$0 < \epsilon < \frac{\pi}{2}$$

is arbitrarily small but fixed, and γ denotes the principal branch on this domain.

Lower Incomplete Gamma Function – Overview

 $\gamma(s,z)$ is:

- i. Entire in z, for a fixed positive integer s
- ii. Multi-valued holomorphic in z for fixed s not an integer
- iii. On each branch, it is meromorphic in s for fixed

$$z \neq 0$$

with simple poles at non-positive integers s.



Upper Incomplete Gamma Function

1. <u>Upper Incomplete Gamma – Holomorphic Extension</u>: As for the *upper incomplete gamma function*, a holomorphic extension, with respect to z or s, is given by

$$\Gamma(s,z) = \Gamma(s) - \gamma(s,z)$$

(National Institute of Standards and Technology (2019a)) at points (s, z) where the right-hand side exists.

- 2. Single-Valued, and Restricted to Principal Branch: Since γ is multi-valued, the same holds for Γ , but a restriction to principal values only yields the single-valued principal branch of Γ .
- 3. <u>Behavior under Non-Positive s</u>: When s is a non-positive integer in the above equation, neither part of the difference is defined, and a limiting process, developed here for

$$s \rightarrow 0$$

fills in the missing values.

4. Upper Gamma Bound as $s \to 0$: Complex analysis guarantees holomorphicity, since $\Gamma(s,z)$ proves to be bounded in the neighborhood of

$$s \to 0$$

for fixed z.

5. Power Series Expansion for γ : To determine that limit, the power series of γ^* at

$$z = 0$$

turns out useful. When replacing e^{-x} by its power series in the integral definition of γ , one obtains – assuming x and s to be positive reals for now –

$$\gamma(s,z) = \int_{0}^{x} t^{s-1}e^{-t}dt = \int_{0}^{x} \sum_{k=0}^{\infty} (-1)^{k} \frac{t^{s+k-1}}{k!}dt = \sum_{k=0}^{\infty} (-1)^{k} \frac{x^{s+k}}{k!(s+k)}$$
$$= x^{s} \sum_{k=0}^{\infty} \frac{(-x)^{k}}{k!(s+k)}$$

or

$$\gamma^* = \sum_{k=0}^{\infty} \frac{(-x)^k}{k! (s+k)}$$

(National Institute of Standards and Technology (2019a)) which, as a series representation of the entire γ^* function, converges for all complex x (and all complex s not a non-positive integer).

6. Extending from *s* to *z*: With its restriction to real values lifted, the series allows the expansion:

$$\gamma(s,z) - \frac{1}{s} = -\frac{1}{s} + z^s \sum_{k=0}^{\infty} \frac{(-z)^k}{k! (s+k)} = \frac{z^s - 1}{s} + z^s \sum_{k=1}^{\infty} \frac{(-z)^k}{k! (s+k)}$$

$$\Re(s) > -1$$

$$s \neq 0$$



7. $\underline{s} \rightarrow 0$ Limit for Upper Gamma: When

$$s \rightarrow 0$$

$$\frac{z^s - 1}{s} \to \ln z$$

$$\Gamma(s) - \frac{1}{s} = \frac{1}{s} - \gamma + \mathcal{O}(s) - \frac{1}{s} \rightarrow -\gamma$$

(Wikipedia (2019a)) where γ is the Euler-Mascheroni constant, hence

$$\Gamma(0,z) = \lim_{s \to 0} \left[\Gamma(s) - \frac{1}{s} - \left\{ \gamma(s,z) - \frac{1}{s} \right\} \right] = -\gamma - \ln z - \sum_{k=1}^{\infty} \frac{(-z)^k}{k! \, k}$$

is the limiting function to the upper incomplete gamma function as

$$s \to 0$$

also known as the exponential integral $E_1(z)$ (National Institute of Standards and Technology (2019a)).

8. Recurrence Relation Based Values for $\Gamma(-n,z)$: By the way of recurrence relation, the values of $\Gamma(-n,z)$ for positive integers can be obtained from this result (National Institute of Standards and Technology (2019a))

$$\Gamma(-n,z) = \frac{1}{n!} \left[\frac{e^{-z}}{z^n} \sum_{k=0}^{n-1} (-1)^k (n-k-1)! \, z^k + (-1)^n \Gamma(0,z) \right]$$

Thus, the upper incomplete gamma function proves to exist and be holomorphic, with respect to both *z* and *s*, for all *s* and



$$z \neq 0$$

- 9. Characteristics of Upper Gamma Function: $\Gamma(s, z)$ is:
 - a. Entire in z for fixed positive integer s.
 - b. Multi-valued holomorphic in z for fixed s not zero and not a positive integer, with a branch point at-

$$z = 0$$

c.

$$\Gamma(s,z) = \Gamma(s)$$

for s with positive real part and

$$z = 0$$

– the limit when

$$(s_i, z_i) \rightarrow (s, 0)$$

but this is a continuous extension, not an analytic one, i.e., it does not hold for

Special Values



1. Compendium of Special $\Gamma(s, x)$ Values:

a.

$$\Gamma(s) = (s-1)!$$

if s is a positive integer

b.

$$\Gamma(s,x) = (s-1)! e^{-x} \sum_{k=0}^{s-1} \frac{x^k}{k!}$$

if s is a positive integer

c.

$$\Gamma(s,0) = \Gamma(s)$$

$$\Re(s) > 0$$

d.

$$\Gamma(1,x)=e^{-x}$$

e.

$$\gamma(1,x) = 1 - e^{-x}$$

f.

$$\Gamma(0,x) = -Ei(-x)$$

for

g.

$$\Gamma(s,x) = x^2 E_{1-s}(x)$$



h.

$$\Gamma\left(\frac{1}{2},x\right) = \sqrt{\pi} \ erfc(\sqrt{x})$$

i.

$$\gamma\left(\frac{1}{2},x\right) = \sqrt{\pi} \ erf\left(\sqrt{x}\right)$$

2. <u>Terminologies Associated with Special Functions</u>: Here, Ei is the exponential integral, E_n is the generalized exponential integral, erf is the error function, and erfc is the complementary error function

$$erfc(x) = 1 - erf(x)$$

Asymptotic Behavior

a.

$$\frac{\gamma(s,x)}{x^s} \to \frac{1}{s}$$

as

$$x \to 0$$

b.

$$\frac{\Gamma(s,x)}{x^s} = -\frac{1}{s}$$



as

 $x \to 0$

and

$$\Re(s) > 0$$

For real *s*, the error of

$$\Gamma(s,x)=-\frac{x^s}{s}$$

is of the order of $\mathcal{O}(x^{\min(s+1,0)})$ if

 $s \neq -1$

and $O(\ln x)$ if

s = -1

c.

 $\gamma(s,x) \to \Gamma(s)$

as

 $\chi \to \infty$

d.



$$\frac{\Gamma(s,x)}{x^{s-1}e^{-x}} \to 1$$

as

$$\chi \to \infty$$

e.

$$\Gamma(s,z) \to z^{s-1} e^{-z} \sum_{k=0}^{\infty} \frac{\Gamma(s)}{\Gamma(s-k)} z^{-k}$$

as an asymptotic series where

$$|z| \to \infty$$

and

$$|\arg z| < \frac{3\pi}{2}$$

(National Institute of Standards and Technology (2019a)).

Evaluation Formulas

 Lower Gamma Power Series Expansion: The lower incomplete gamma function can be evaluated using the power series expansion (National Institute of Standards and Technology (2019a))



$$\gamma(s,z) = \sum_{k=0}^{\infty} \frac{z^s e^{-z} z^k}{s(s+1)\cdots(s+k)} = z^s e^{-z} \sum_{k=0}^{\infty} \frac{z^k}{s^{k+1}}$$

where $s^{\overline{k+1}}$ is the Pochhammer symbol.

2. <u>Using Kummer's Confluent Hyper-geometric Function</u>: An alternative expansion is

$$\gamma(s,z) = \sum_{k=0}^{\infty} \frac{(-1)^k z^{s+k}}{k(s+k)} = \frac{z^s}{s} M(s,s+1,z)$$

where *M* is Kummer's Confluent Hyper-geometric function.

Connection with Kummer's Confluent Hyper-geometric Function

1. Positive Real Part of z: When the real part of z is positive,

$$\gamma(s,z) = s^{-1}z^s e^{-z} M(1,s+1,z)$$

where

$$M(1,s+1,z) = 1 + \frac{z}{s+1} + \frac{z^2}{(s+1)(s+2)} + \frac{z^3}{(s+1)(s+2)(s+3)} + \cdots$$

has an infinite radius of convergence.

2. <u>Upper Gamma from Kummer's Identity</u>: Again, using confluent hyper-geometric functions and employing Kummer's identity

$$\Gamma(s,z) = e^{-z}U(1-s,1-s,z) = \frac{z^s e^{-z}}{\Gamma(1-s)} \int_0^\infty \frac{e^{-u}}{u^s(z+u)} du = e^{-z} z^s U(1,1+s,z)$$
$$= e^{-z} \int_0^\infty e^{-u} (z+u)^{s-1} du = e^{-z} z^s \int_0^\infty e^{-zu} (1+u)^{s-1} du$$

γ from Continued Gauss Fraction: For actual computation of numerical values,
 Gauss' continued fraction provides a useful expansion:

$$\gamma(s,z) = \frac{z^{s}e^{-z}}{s - \frac{sz}{s+1 + \frac{z}{s+2 - \frac{(s+1)z}{s+3 + \frac{2z}{s+4 - \frac{(s+2)z}{s+6 - \ddots}}}}}$$

- 4. <u>Convergence for all Complex z</u>: The above continuous fraction converges for all complex z, provided that s is not a negative integer.
- 5. $\Gamma(s,z)$ from Continued Fraction Expressions: The upper gamma function has the continued fraction expression (Abramowitz and Stegun (2007))

$$\Gamma(s,z) = \frac{z^s e^{-z}}{z + \frac{1-s}{1 + \frac{1}{z + \frac{2-s}{1 + \frac{2}{z + \frac{3-s}{1 + \frac{1}{z}}}}}}}$$

$$\Gamma(s,z) = \frac{z^s e^{-z}}{1 + z - s + \frac{s - 1}{3 + z - s + \frac{2(s - 2)}{5 + z - 3 + \frac{3(s - 3)}{7 + z - s + \frac{4(s - 4)}{9 + z - s + \ddots}}}$$

Multiplication Theorem

The following multiplication theorem holds true:

$$\Gamma(s,z) = \frac{1}{t^s} \sum_{i=0}^{\infty} \frac{\left(1 - \frac{1}{t}\right)^i}{i!} \Gamma(s+i,tz) = \Gamma(s,tz) - (tz)^s e^{-tz} \sum_{i=0}^{\infty} \frac{\left(\frac{1}{t} - 1\right)^i}{i} L_{i-1}^{s-1}(tz)$$

Software Implementation

- 1. <u>Availability in Computer Algebra Systems</u>: The incomplete gamma functions are available in a variety of computer algebra systems.
- γ from Other Special Functions: Even if unavailable directly, however, incomplete
 function values can be calculated using functions commonly included in spreadsheets
 and computer algebra packages. In Excel, for example, these can be calculated using
 the Gamma function combined with the Gamma distribution function.
- 3. γ from Cumulative Distribution Function: The lower incomplete function is given by



$$\gamma(s,x) = \exp(GammaLn(s)) \times Gamma.Dist(x,s,1,TRUE)$$

The upper incomplete function is given by

$$\Gamma(s,x) = \exp(GammaLn(s)) \times [1 - Gamma.Dist(x,s,1,TRUE)]$$

Regularized Gamma Functions and Poisson Random Variables

1. <u>Regularized Gamma Functions *P* and *Q*</u>: Two related functions are the regularized Gamma functions:

$$P(s,x) = \frac{\gamma(s,x)}{\Gamma(s)}$$

$$Q(s,x) = \frac{\Gamma(s,x)}{\Gamma(s)} = 1 - P(s,x)$$

- 2. CDF for Random Gamma Variables: P(s, x) is the cumulative distribution function for Gamma random variables with shape parameter s and scale parameter 1.
- 3. <u>CDF for Poisson Random Variables</u>: When s is an integer, $Q(s, \lambda)$ is the cumulative distribution function for Poisson random variables. If x is a $Poisson(\lambda)$ random variable, then

$$\mathbb{P}[X,s] = \sum_{j < s} e^{-\lambda} \frac{\lambda^j}{j!} = \frac{\Gamma(s,\lambda)}{\Gamma(s)} = Q(s,\lambda)$$



This formula can be derived by repeated integration by parts.

Derivatives

1. <u>Upper Gamma Function wrt x</u>: Using the integral representation above, the derivative of the upper gamma incomplete function $\Gamma(s,x)$ with respect to x is

$$\frac{\partial \Gamma(s,x)}{\partial x} = -x^{s-1}e^{-x}$$

2. <u>Upper Gamma Function wrt s</u>: The derivative with respect to its first argument x is given by (Geddes, Glasser, Moore, and Scott (1990))

$$\frac{\partial \Gamma(s, x)}{\partial s} = \ln x \Gamma(s, x) + x T(3, s, x)$$

and the second derivative by

$$\frac{\partial^2 \Gamma(s,x)}{\partial s^2} = \ln^2 x \Gamma(s,x) + 2x [\ln x T(3,s,x) + T(4,s,x)]$$

where the function T(m, s, x) is a special case of the Meijer G-function

$$T(m, s, x) = G_{m-1,m}^{m,0} \begin{pmatrix} 0, 0, \dots, 0 \\ s - 1, -1, \dots, -1 \end{pmatrix} x$$

3. <u>Special Case of Meijer G-Function</u>: This particular function has internal *closure* properties of its own because it can be used to express all successive derivatives.



4. Derivative of $\Gamma(s, x)$ wrt s: In general,

$$\frac{\partial^{m} \Gamma(s,x)}{\partial s^{m}} = \ln^{m} x \Gamma(s,x) + mx \ln x T(3+n,s,x) \sum_{n=0}^{m-1} P_{n}^{m-1} \ln^{m-n-1} x T(3+n,s,x)$$

where P_i^n is the permutation defined by the Pochhammer symbol

$$P_j^n = \binom{n}{j} n! = \frac{n!}{(n-j)!}$$

5. $\underline{\Gamma(s,x)}$ Derivatives in Succession Form: All such derivatives can be generated in the succession form

$$\frac{\partial T(m,s,x)}{\partial s} = \ln x T(m,s,x) + (m-1)T(m+1,s,x)$$

and

$$\frac{\partial T(m,s,x)}{\partial x} = -\frac{1}{x} [T(m-1,s,x) + T(m,s,x)]$$

6. Computing the Special Function T(m, s, z): This function T(m, s, z) can be computed from its series representation valid for

$$T(m,s,z) = -\frac{(-1)^{m-1}}{(m-2)!} \left\{ \frac{d^{m-2}}{dt^{m-2}} \left[\Gamma(s-t)z^{t-1} \right] \right\} \bigg|_{t=0} + \sum_{n=0}^{\infty} \frac{(-1)^n z^{s-1+n}}{n! (-s-n)^{m-1}}$$

with the understanding that s is not a negative number or zero.



7. Handling Negative or Zero s: In such a case, one my use a limit. Results for

$$|z| \ge 1$$

can be obtained by analytic continuation.

8. <u>Simplification under Certain Special Cases</u>: Some special cases of this function can be simplified. For example,

$$T(2, s, x) = \frac{T(s, x)}{x}$$

and

$$xT(3,1,x) = E_1(x)$$

where $E_1(x)$ is the Exponential Integral.

9. Functions Dependent on $\Gamma(s,x)$ Derivatives: These derivatives and the function T(m,s,x) provide exact solutions to a number of integrals by repeated differentiation of the integral definition of the upper incomplete gamma function (Milgram and Milgram (1985), Mathar (2010)). For example,

$$\int_{x}^{\infty} e^{-t}t^{s-1} \ln^{m} t \, dt = \frac{d^{m}}{ds^{m}} \int_{x}^{\infty} e^{-t}t^{s-1} dt = \frac{d^{m}}{ds^{m}} \Gamma(s, x)$$

- 10. <u>Class of Laplace/Mellin Transforms</u>: This formula can be further *inflated* or generalized to a huge class of Laplace transforms and Mellin transforms.
- 11. <u>Definite Integrals in Computer Algebra</u>: When combined with a computer algebra system, the exploitation of special functions provides a powerful method for solving definite integrals, in particular those encountered by practical engineering applications.



Indefinite and Definite Integrals

1. <u>Incomplete Gamma Function Power Integrand</u>: The following indefinite integrals are readily obtained using integration by parts – with the constant of integration omitted in both cases.

$$\int x^{b-1}\gamma(s,x)dx = \frac{1}{b}\left[x^b\gamma(s,x) + \Gamma(s+b,x)\right]$$

$$\int x^{b-1}\Gamma(s,x)dx = \frac{1}{b}\left[x^b\Gamma(s,x) - \Gamma(s+b,x)\right]$$

2. <u>Lower/Upper Gamma Fourier Connection</u>: The lower and the upper incomplete Gamma function are connected via the Fourier transform

$$\int_{-\infty}^{+\infty} \frac{\gamma\left(\frac{s}{2}, \pi z^2\right)}{(\pi z^2)^{\frac{s}{2}}} e^{-2\pi i k z} dz = \frac{\gamma\left(\frac{1-s}{2}, \pi k^2\right)}{(\pi k^2)^{\frac{1-s}{2}}}$$

This follows, for example, using a suitable specialization of the technique illustrated in Gradshteyn, Ryzhik, Geronimus, Tseytlin, and Jeffrey (2015).

References



- Abramowitz, M., and I. A. Stegun (2007): Handbook of Mathematics Functions
 Dover Book on Mathematics
- Garrett, P. (2005): <u>Hartog's Theorem: Separate Analyticity Implies Joint</u>
- Geddes, K. O., M. L. Glasser, R. A. Moore, and T. C. Scott (1990): Evaluation of Classes of Definite Integrals involving Elementary Functions via Differentiation of Special Functions *Applicable Algebra in Engineering, Communications, and* Computing 1 (2) 149-165
- Gradshteyn, I. S., I. M. Ryzhik, Y. V. Geronimus, M. Y. Tseytlin, and A. Jeffrey (2015): *Tables of Integrals, Series, and Products* **Academic Press**
- Marshall, D. E. (2009): Complex Analysis
- Mathar, R. J. (2010): Numerical Evaluation of the Oscillatory Integral over $e^{i\pi x} x^{\frac{1}{x}}$ between 1 and ∞ arXiV
- Milgram, and M. S. Milgram (1985): The Generalized Integro-exponential Function
 Mathematics of Computation 44 (170) 443-458
- National Institute of Standards and Technology (2019a): <u>Incomplete Gamma and</u> <u>Related Functions</u>
- National Institute of Standards and Technology (2019b): Gamma Functions
- National Institute of Standards and Technology (2019c): <u>Elementary Functions</u>
- Teleman, C. (2003): Riemann Surfaces
- Wikipedia (2019a): Gamma Function
- Wikipedia (2019b): <u>Incomplete Gamma Functions</u>



Digamma Function

Introduction and Overview

1. <u>Definition of the Digamma Function</u>: The *digamma function* is defined as the logarithmic derivative of the gamma function (Abramowitz and Stegun (2007), Wikipedia (2019)).

$$\psi(x) = \frac{d}{dx} \log \Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}$$

This is the first of the polygamma function.

2. Representation of the Digamma Function: The digamma function is often denoted as $\psi_0(x)$, $\psi^{(0)}(x)$, or F - the upper-case form of the archaic Greek consonant digamma meaning double gamma.

Relation to the Harmonic Series

1. Equation of the Gamma Function: The gamma function obeys the equation

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



2. <u>Derivative of the Gamma Function</u>: Taking derivative with respect to z gives

$$\Gamma'(z+1) = z\Gamma'(z) + \Gamma(z)$$

3. Recurrence Relation for the Digamma Function: Dividing by $\Gamma(z+1)$ or the equivalent $z\Gamma(z)$ results in:

$$\frac{\Gamma'(z+1)}{\Gamma(z+1)} = \frac{\Gamma'(z)}{\Gamma(z)} + \frac{1}{z}$$

or

$$\psi(z+1) = \psi(z) + \frac{1}{z}$$

4. <u>Digamma Function using Harmonic Series</u>: Since the harmonic series are defined for positive integers *n* as

$$H_n = \sum_{k=1}^n \frac{1}{k}$$

the digamma function is related to them by

$$\psi(n)=H_{n-1}-\gamma$$

where

$$H_0 = 0$$



and γ is the Euler-Mascheroni constant.

 Digamma Function for Half-Integers: For half-integer arguments, the digamma function takes the values

$$\psi\left(n + \frac{1}{2}\right) = -\gamma - 2\log 2 + \sum_{k=1}^{n} \frac{2}{2k-1}$$

Integral Representations

1. <u>Gauss Integral for Digamma Function</u>: if the real part of *z* is positive, then the digamma function has the following integral representation due to Gauss (Whittaker and Watson (1996)):

$$\psi(z) = \int_{0}^{\infty} \left(\frac{e^{-t}}{t} - \frac{e^{-zt}}{1 - e^{-t}} \right) dt$$

2. Incorporating Euler Mascheroni Integral Identity: Combining the above expression with an integral identity for the Euler-Mascheroni constant γ gives:

$$\psi(z+1) = -\gamma + \int_{0}^{\infty} \frac{1-t^{z}}{1-t} dt$$

3. <u>Difference between the Harmonic Terms</u>: The integral is Euler's harmonic number H_z , so the previous formula may also be written as

$$\psi(z+1) = -\gamma + H_z$$

A consequence is the following generalization of the recurrence relation:

$$\psi(w+1) - \psi(z+1) = H_w - H_z$$

4. <u>Digamma Function Dirichlet Integral Representation</u>: An integral representation due to Dirichlet is (Whittaker and Watson (1996)):

$$\psi(z) = \int_{0}^{\infty} \left(e^{-t} - \frac{1}{[1-t]^z}\right) \frac{dt}{t}$$

5. <u>Asymptotic Integral for Digamma Function</u>: Gauss' integral representation can be manipulated to give the start of the asymptotic expansion of $\psi(z)$ (Whittaker and Watson (1996)):

$$\psi(z) = \log z - \frac{1}{z} - \int_{0}^{\infty} \left(\frac{1}{2} - \frac{1}{t} + \frac{1}{e^{t} - 1}\right) e^{-zt} dt$$

- Gamma Function using Binet's First Integral: The above expression is a consequence
 of the Binet's first integral for the gamma function. The integral may be recognized
 as Laplace transform.
- 7. Gamma Function Binet's Second Integral: Binet's second integral for the gamma function gives a different formula for $\psi(z)$, which also gives the first few terms of the asymptotic expansion (Whittaker and Watson (1996)):

$$\psi(z) = \log z - \frac{1}{2z} - 2\int_{0}^{\infty} \frac{t}{(z^2 + t^2)(e^{2\pi t} - 1)} dt$$



Infinite Product Representation

The function $\frac{\psi(z)}{\Gamma(z)}$ is an entire function (Mezo and Hoffman (2017)), and it can be represented by the infinite product

$$\frac{\psi(z)}{\Gamma(z)} = -e^{2\gamma z} \prod_{k=0}^{\infty} \left(1 - \frac{z}{x_k}\right) e^{\frac{z}{x_k}}$$

Here x_k is the k^{th} zero of $\psi(z)$ (see below).

Series Formula

 Euler Product Formula Based Digamma Function: Euler's product formula for digamma function, combined with the functional equation and an identity for the Euler Mascheroni constant, yields the following expression for the digamma function, valid in the complex plane outside the negative integers (Abramowitz and Stegun (2007)):

$$\psi(z+1) = -\gamma + \sum_{n=1}^{\infty} \left(\frac{1}{n} - \frac{1}{n+z} \right) = -\gamma + \sum_{n=1}^{\infty} \frac{z}{n(n+z)}$$

$$z \neq -1, -2, \cdots$$

2. Alternate Euler Product Digamma Formula: Equivalently,

$$\psi(z) = -\gamma + \sum_{n=0}^{\infty} \left(\frac{1}{n+1} - \frac{1}{n+z} \right) = -\gamma + \sum_{n=1}^{\infty} \frac{z-1}{(n+1)(n+z)}$$

$$z \neq 0, -1, -2, \cdots$$

Evaluation of Sums of Rational Functions

1. <u>Sum of Rational Functions – Setup</u>: The above identity can be used to evaluate sums of the form

$$\sum_{n=0}^{\infty} u_n = \sum_{n=0}^{\infty} \frac{p(n)}{q(n)}$$

where p(n) and q(n) are polynomials of n.

2. <u>Criterion for Rational Series Convergence</u>: For the series to converge,

$$\lim_{n \to \infty} nu_n \to 0$$

otherwise the series will be greater than the harmonic series, and thus diverge.

3. <u>Digamma Based Rational Series Sum</u>: Hence,



$$\sum_{k=1}^{m} a_k = 0$$

and

$$\sum_{n=0}^{\infty} u_n = \sum_{n=0}^{\infty} \sum_{k=1}^{m} \frac{a_k}{n+b_k} = \sum_{n=0}^{\infty} \sum_{k=1}^{m} a_k \left(\frac{1}{n+b_k} - \frac{1}{n+1} \right)$$

$$= \sum_{k=1}^{m} \left[a_k \sum_{n=0}^{\infty} \left(\frac{1}{n+b_k} - \frac{1}{n+1} \right) \right] = -\sum_{k=1}^{m} a_k [\psi(b_k) + \gamma]$$

$$= -\sum_{k=1}^{m} a_k \psi(b_k)$$

4. <u>Polygamma Based Rational Series Sum</u>: With the series expansion of higher rank polygamma function, a generalized formula may be given as

$$\sum_{n=0}^{\infty} u_n = \sum_{n=0}^{\infty} \sum_{k=1}^{m} \frac{a_k}{(n+b_k)^{r_k}} = \sum_{k=1}^{m} \frac{(-1)^{r_k}}{(r_k-1)!} a_k \psi^{r_k-1}(b_k)$$

provided the series on the left converges.

Taylor Series

 Digamma using Rational Zeta Series: The digamma has a rational zeta series, given by the Taylor series at



$$z = 1$$

This is

$$\psi(z+1) = -\gamma + \sum_{k=1}^{\infty} \zeta(k+1)(-z)^k$$

which converges for

2. <u>Derivation of the Taylor Series Above</u>: Here, $\zeta(n)$ is the Riemann Zeta function. This series is easily derived from the corresponding Taylor's series and the Hurwitz zeta function.

Newton Series

1. <u>Newton/Stern Series for Digamma</u>: The Newton series for digamma, sometimes referred to as the *Stern series* (Norlund (1924), Blagouchine (2018)), reads as

$$\psi(z+1) = -\gamma + \sum_{k=1}^{\infty} \frac{(-1)^k}{k} {s \choose k}$$

where $\binom{s}{k}$ is the binomial coefficient.

2. Generalization of the above Series: It may also be generalized to



$$\psi(z+1) = -\gamma - \frac{1}{m} \sum_{k=1}^{\infty} \frac{m-k}{s+k} - \frac{1}{m} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left\{ {s+m \choose k+1} - {s \choose k+1} \right\}$$

Series with Gregory's Coefficients, Cauchy Numbers, and Bernoulli Polynomials of the Second Kind

- 1. <u>Using Rational Coefficients for Rational Series</u>: There exist various series for the digamma containing only rational coefficients for rational arguments.
- 2. <u>Digamma Function using Gregory's Coefficients</u>: In particular, the series version of the Gregory's coefficient G_n is

$$\psi(v) = \log v - \sum_{n=1}^{\infty} \frac{|G_n|(n-1)!}{(v)_n}$$

$$\Re(v)>0$$

$$\psi(v) = 2\log\Gamma(v) - 2v\log v + 2v + 2\log v - \log 2\pi - \sum_{n=1}^{\infty} \frac{|G_n(2)|(n-1)!}{(v)_n}$$

$$\Re(v) > 0$$

$$\psi(v) = 3\log\Gamma(v) - 6\zeta'(-1, v) + 3v^2\log v - \frac{3}{2}v^2 + 6v\log v + 3v + 3\log v$$
$$+ \frac{3}{2}\log 2\pi + \frac{1}{2} - 3\sum_{n=1}^{\infty} \frac{|G_n(3)|(n-1)!}{(v)_n}$$



$$\Re(v) > 0$$

where $(v)_n$ is the rising factorial

$$(v)_n = v(v+1)\cdots(v+n-k)$$

 $G_n(k)$ are the Gregory coefficients of higher order with

$$G_n(1) = G_n$$

 Γ is the gamma function, and ζ is the Hurwitz zeta function (Blagouchine (2016, 2018)).

3. <u>Using Cauchy's Numbers of the Second Kind</u>: Similar series with the Cauchy numbers of the second kind C_n reads (Blagouchine (2016, 2018))

$$\psi(v) = \log(v - 1) - \sum_{n=1}^{\infty} \frac{C_n(n-1)!}{(v)_n}$$

$$\Re(v) > 1$$

4. <u>Digamma Function using Bernoulli Polynomials</u>: A series with the Bernoulli polynomials of the second kind has the following form (Blagouchine (2018)):

$$\psi(v) = \log(v+a) - \sum_{n=1}^{\infty} \frac{(-1)^n \varphi_n(a)(n-1)!}{(v)_n}$$

$$\Re(v) > -a$$

where $\varphi_n(a)$ are the *Bernoulli polynomials of the Second Kind* defined by the generating equation



$$\frac{z(1+z)^a}{\log(1+z)} = \sum_{n=0}^{\infty} z^n \varphi_n(a)$$

5. Generalization of the above Series: It may be generalized to

$$\psi(v) = \frac{1}{r} \sum_{l=0}^{r-1} \log(v + a + l) + \frac{1}{r} \sum_{n=1}^{\infty} \frac{(-1)^n N_{n,r}(a)(n-1)!}{(v)_n}$$

$$\Re(v) > -a$$

$$r = 1, 2, 3, \cdots$$

where the polynomials $N_{n,r}(a)$ are given by the following generating equation

$$\frac{(1+z)^{a+m}-(1+z)^a}{\log(1+z)} = \sum_{n=0}^{\infty} z^n N_{n,m}(a)$$

so that

$$N_{n,l}(a) = \varphi_n(a)$$

(Blagouchine (2018)).

6. <u>Series for Log Gamma Function</u>: Similar expressions for the logarithm of the gamma function produce the following (Blagouchine (2018)):



$$\psi(v) = \frac{1}{v+a-\frac{1}{2}} \left\{ \log \Gamma(v+a) + v - \frac{1}{2} \log 2\pi - \frac{1}{2} - \sum_{n=1}^{\infty} \frac{(-1)^n \varphi_{n+1}(a)(n-1)!}{(v)_n} \right\}$$

$$\Re(v) > -a$$

and

$$\psi(v) = \frac{1}{v+a-1+\frac{1}{2}r} \left\{ \log \Gamma(v+a) + v - \frac{1}{2} \log 2\pi - \frac{1}{2} + \frac{1}{r} \sum_{n=0}^{r-2} (r-n-1) \log(v+a+n) + \frac{1}{r} \sum_{n=1}^{\infty} \frac{(-1)^n N_{n+1,r}(a)(n-1)!}{(v)_n} \right\}$$

$$\Re(v) > -a$$

Reflection Formula

The digamma function satisfies a reflection formula similar to that of the gamma function

$$\psi(1-z) - \psi(z) = \pi \cot \pi z$$

Recurrence Formula and Characterization



1. <u>Recurrence Relation for Digamma Function</u>: The digamma function satisfies the recurrence relation

$$\psi(x+1) = \psi(x) + \frac{1}{x}$$

2. <u>Digamma Function Telescoping for $\frac{1}{x}$ </u>: Thus, it can be said to *telescope* $\frac{1}{x}$, for one has

$$\Delta[\psi](x) = \frac{1}{x}$$

where Δ is the forward difference operator.

3. <u>Partial Harmonic Sum Recurrence Relation</u>: This satisfies the recurrence relation of a partial sum of the harmonic series, thus implying the formula

$$\psi_n = H_{n-1} - \gamma$$

4. Generalization of the Harmonic Sum: More generally, one has

$$\psi(1+z) = -\gamma + \sum_{k=1}^{\infty} \left(\frac{1}{k} - \frac{1}{z-k}\right)$$

for

$$\Re(z) > 0$$

5. <u>Bernoulli Number Digamma Series Expansion</u>: Another series expansion is

$$\psi(1+z) = \log(z) + \frac{1}{2z} - \sum_{j=1}^{\infty} \frac{B_{2j}}{2j z^{2j}}$$

where B_{2j} are the Bernoulli numbers. This series diverges for all z and is known as the *Stirling series*.

6. <u>Uniqueness of the Telescoped Solution</u>: Actually, ψ is the only solution of the functional equation

$$F(x+1) = F(x) + \frac{1}{x}$$

that is monotonic on \mathbb{R}^+ and satisfies

$$F(1) = -\gamma$$

This follows immediately from the uniqueness of the gamma function, given its recurrence relation and the convexity restriction.

7. Digamma Function Difference Equation: This implies the useful difference equation

$$\psi(x+N) - \psi(x) = \sum_{k=0}^{N-1} \frac{1}{x+k}$$

Some Finite Sums involving the Digamma Function

1. Digamma Function Gaussian Summation Formulas:



$$\sum_{r=0}^{m} \psi\left(\frac{r}{m}\right) = -m(\gamma + \log m)$$

$$\sum_{r=0}^{m} \psi\left(\frac{r}{m}\right) \cdot e^{\frac{2\pi i k r}{m}} = -m \log\left(1 - e^{\frac{2\pi i k}{m}}\right)$$

 $k \in \mathbb{Z}$

 $m \in \mathbb{N}$

 $k \neq m$

$$\sum_{r=0}^{m} \psi\left(\frac{r}{m}\right) \cdot \cos\frac{2\pi kr}{m} = -m\log\left(2\sin\frac{2\pi k}{m}\right) + \gamma$$

$$k = 1, 2, \dots, m - 1$$

$$\sum_{r=0}^{m} \psi\left(\frac{r}{m}\right) \cdot \sin\frac{2\pi kr}{m} = \frac{\pi}{2}(2k - m)$$

$$k = 1, 2, \dots, m - 1$$

are due to Gauss (Campbell (1966), Shrivastava and Choi (2001)).

2. <u>Digamma Function Blagouchine Summation Formula</u>: More complicated formulas, such as

$$\sum_{r=0}^{m-1} \psi\left(\frac{2r+1}{m}\right) \cdot \cos\frac{(2r+1)\pi k}{m} = m \log\left(\tan\frac{\pi k}{2m}\right)$$



$$k = 1, 2, \dots, m - 1$$

$$\sum_{r=0}^{m-1} \psi\left(\frac{2r+1}{m}\right) \cdot \sin\frac{(2r+1)\pi k}{m} = -\frac{\pi m}{2}$$

$$k = 1, 2, \dots, m - 1$$

$$\sum_{r=0}^{m-1} \psi\left(\frac{r}{m}\right) \cdot \cot\frac{\pi r}{m} = -\frac{\pi(m-1)(m-2)}{6}$$

$$\sum_{r=0}^{m-1} \psi\left(\frac{r}{m}\right) \cdot \frac{r}{m} = -\frac{\gamma}{2}(m-1) - \frac{m}{2}\log m - \frac{\pi}{2}\sum_{r=1}^{m-1} \frac{r}{m} \cdot \cot \frac{\pi r}{m}$$

$$\sum_{r=1}^{m-1} \psi\left(\frac{r}{m}\right) \cdot \cos\frac{(2l+1)\pi r}{m} = -\frac{\pi}{m} \sum_{r=1}^{m-1} \frac{r \cdot \sin\frac{2\pi r}{m}}{\cos\frac{2\pi r}{m} - \cos\frac{(2l+1)\pi}{m}}$$

$$l \in \mathbb{Z}$$

$$\sum_{r=1}^{m-1} \psi\left(\frac{r}{m}\right) \cdot \sin\frac{(2l+1)\pi r}{m}$$

$$= -(\gamma + \log 2m) \cot\frac{(2l+1)\pi}{2m}$$

$$+ \sin\frac{(2l+1)\pi}{m} \sum_{r=1}^{m-1} \frac{\log \sin\frac{\pi r}{m}}{\cos\frac{2\pi r}{m} - \cos\frac{(2l+1)\pi}{m}}$$

 $l \in \mathbb{Z}$

$$\sum_{r=1}^{m-1} \psi^2 \left(\frac{r}{m}\right) = (m-1)\gamma^2 + m(2\gamma + \log 4m)\log m - m(m-1)\log^2 2$$
$$-\frac{\pi^2(m^2 - 3m + 2)}{12} + m\sum_{l=1}^{m-1} \log^2 \sin \frac{\pi l}{m}$$

are due to the works of certain modern authors (e.g., Blagouchine (2015)).

Gauss Digamma Theorem

For positive integers r and m

the digamma function may be expressed in terms of Euler's constant and a finite number of elementary functions.

$$\psi\left(\frac{r}{m}\right) = -\gamma - \log 2m - \frac{\pi}{2}\cot\frac{\pi r}{m} + 2\sum_{n=1}^{\left[\frac{m-1}{2}\right]} \frac{r}{m} \cdot \cos\frac{2\pi nr}{m}\log\sin\frac{\pi n}{m}$$

Asymptotic Expansion



1. <u>Asymptotic Expansion using Bernoulli/Reimann Zeta</u>: The digamma function has the asymptotic expansion

$$\psi(z) \to \log(z) - \frac{1}{2z} + \sum_{j=1}^{\infty} \frac{\zeta(1-2n)}{z^{2j}} = \log(z) - \frac{1}{2z} - \sum_{j=1}^{\infty} \frac{B_{2j}}{2j z^{2j}}$$

where B_k is the k^{th} Bernoulli number, and ζ is the Riemann zeta function.

2. Asymptotic Expansion of Series Terms: The first few terms of this expansion are:

$$\psi(z) \to \log(z) - \frac{1}{2z} - \frac{1}{12z^2} + \frac{1}{120z^4} - \frac{1}{252z^6} + \frac{1}{240z^8} - \frac{5}{660z^{10}} + \frac{691}{32760z^{12}} - \frac{1}{12z^{14}} + \cdots$$

- 3. <u>Convergence of the above Series</u>: Although the infinite sum does not converge for any *z*, any finite partial sum becomes increasingly accurate as *z* increases.
- 4. <u>Infinite Series using Euler MacLaurin Formula</u>: The above series can be found by applying the Euler-MacLaurin formula to the sum (Bernardo (1976)) $\sum_{n=1}^{\infty} \left(\frac{1}{n} \frac{1}{z+n}\right)$
- 5. <u>Binet's Second Integral Series Expansion</u>: The expansion can also be derived from the integral representation coming from Binet's second integral formula for the gamma function.
- 6. Application of Bernoulli's Numbers to Geometric Series: Expanding $\frac{t}{(z^2+t^2)}$ as a geometric series, and substituting the integral representation of the Bernoulli numbers leads to the same asymptotic series as above. Furthermore, expanding only finitely many terms of the series gives a formula with an explicit error term:

$$\psi(z) = \log(z) - \frac{1}{2z} - \sum_{j=1}^{\infty} \frac{B_{2j}}{2j z^{2j}} + (-1)^{N+1} \frac{2}{z^{2N}} \int_{0}^{\infty} \frac{t^{2N+1}}{(z^2 + t^2)(e^{2\pi t} - 1)} dt$$



Inequalities

1. LTE Inequality for Digamma Function: When

the function $\log(z) - \frac{1}{2z} - \psi(z)$ is completely monotonic, and in particular, positive.

- Consequence of Bernstein's Theorem: This is a consequence of Bernstein's theorem
 on monotone functions applied to the integral representation coming from Binet's
 first integral for the gamma function.
- 3. Upper Bound on the Integral: Additionally, by the convexity inequality

$$1 + t \le e^t$$

the integrand in this representation is bounded above by $\frac{e^{-tz}}{2}$.

- 4. GTE Inequality for Digamma Function: Consequently, $\frac{1}{z} \log(z) + \psi(z)$ is also completely monotone.
- 5. <u>Alzer Inequality for Digamma Differences</u>: This recovers the theorem of Alzer (1997), who also showed that, for

$$s \in (0,1)$$

$$\frac{1-s}{1+s} < \psi(z+1) - \psi(z+s)$$



6. <u>Elezovic-Giordano-Pecaric Digamma Bounds</u>: Related bounds were obtained by Elezovic, Giordano, and Pecaric (2000), who proved that, for

$$\log\left(z+\frac{1}{2}\right)-\frac{1}{z}<\psi(z)<\log(z+e^{-\gamma})-\frac{1}{z}$$

where γ is the Euler-Mascheroni constant. The constants appearing in these bounds are the best possible (Qi and Guo (2009)).

7. <u>Gautschi Inequality for Digamma Ratio</u>: The mean-value theorem implies the following analog of Gautschi's inequality. If

where

$$c \approx 1.461$$

is the unique positive real root of the digamma function, and if

then

$$e^{(1-s)\frac{\psi'(z+1)}{\psi(z+1)}} \le \frac{\psi(z+1)}{\psi(z+s)} \le e^{(1-s)\frac{\psi'(z+s)}{\psi(z+s)}}$$

Moreover, the equality holds if and only if

$$s = 1$$



(Laforgia and Natalini (2013)).

8. <u>Digamma Harmonic Mean Value Inequality</u>: Inspired by the harmonic mean value inequality for the classical gamma function, Alzer and Jameson (2017) showed, among other things, a harmonic mean value inequality for the digamma function:

$$-\gamma \le \frac{2\psi(z)\psi\left(\frac{1}{z}\right)}{\psi(z) + \psi\left(\frac{1}{z}\right)}$$

for

$$z \ge 0$$

The inequality holds if and only if

$$z = 1$$

Computation and Approximation

1. Asymptotic Expansion using Recurrence Relation: The asymptotic expansion gives an easy way to compute $\psi(z)$ when the real part of z is large. To compute $\psi(z)$ for small z, the recurrence relation

$$\psi(z) + 1 = \psi(z) + \frac{1}{z}$$



can be used to shift the value of z higher.

- 2. <u>Usage for Higher z Values</u>: Beal (2003) suggests using the above recurrence to shift to a value greater than 6 and then applying the above expansion with terms over the z^{14} cutoff, which yields *more than enough precision* at least 12 digits except near the zeros.
- 3. Bounds on $\psi(z)$ as $z \to \infty$: As z goes to infinity, $\psi(z)$ gets arbitrarily close to both $\log\left(z-\frac{1}{2}\right)$ and $\log z$. Going down from z+1 to z, $\psi(z)$ decreases by $\frac{1}{z}$, $\log\left(z-\frac{1}{2}\right)$ decreases by $\frac{\log(z+\frac{1}{2})}{z-\frac{1}{2}}$, which is more than $\frac{1}{z}$, and $\log z$ decreases by $\log\left(1+\frac{1}{z}\right)$, which is less than $\frac{1}{z}$.
- 4. $\psi(z)$ Bounds for $z > \frac{1}{2}$: From this, it can be seen that for any positive z greater than $\frac{1}{2}$,

$$\psi(z) \in \left(\log\left(z - \frac{1}{2}\right), \log z\right)$$

or, for any positive z,

$$e^{\psi(z)} \in \left(z - \frac{1}{2}, z\right)$$

5. $e^{\psi(z)}$ as $z \to \infty$ and $z \to 0$: The exponential $e^{\psi(z)}$ is approximately $z - \frac{1}{2}$ for large z, but gets closer to z at small z, approaching 0 at

$$z = 0$$

6. $\psi(z)$ Bounds for $z \in (0,1)$: For z < 1 the limits can be calculated based on the fact that, between 1 and 2, as

$$\psi(z)\in (-\gamma,1-\gamma)$$



SO

$$\psi(z) \in \left(-\frac{1}{z} - \gamma, 1 - \frac{1}{z} - \gamma\right)$$

$$z \in (0,1)$$

or

$$e^{\psi(z)} \in \left(e^{-\frac{1}{z}-\gamma}, e \cdot e^{-\frac{1}{z}-\gamma}\right)$$

7. Asymptotic Series Expansion for $e^{\psi(z)}$: From the above asymptotic series for $\psi(z)$, one can derive an asymptotic series for $e^{-\psi(z)}$. The series matches the overall behavior well, that is, it behaves asymptotically as it should for large arguments, and has poles of unbounded multiplicity at the origin.

$$\frac{1}{e^{\psi(z)}} \sim \frac{1}{x} + \frac{1}{2 \cdot x^2} + \frac{5}{4 \cdot 3! \cdot x^3} + \frac{3}{2 \cdot 4! \cdot x^4} + \frac{47}{48 \cdot 5! \cdot x^5} - \frac{5}{16 \cdot 6! \cdot x^6} + \cdots$$

8. Convergence Behavior of the Above Series: This is similar to the Taylor expansion of $e^{-\psi(\frac{1}{y})}$ at

$$y = 0$$

but it does not converge. However, if it converged to a function f(y), then $\log \frac{f(y)}{y}$ would have the same MacLaurin series as $\log \frac{1}{y} - \psi \left(\frac{1}{y}\right)$ But this does not converge because the series given above does not converge – the function is not analytic at infinity. A similar series exists for $e^{\psi(z)}$, which starts at

$$e^{\psi(z)} \sim z - \frac{1}{2}$$

9. Asymptotic Series for $\psi\left(z+\frac{1}{2}\right)$ and $e^{\psi\left(z+\frac{1}{2}\right)}$: If one calculates the asymptotic series for $\psi\left(z+\frac{1}{2}\right)$ it turns out there are no odd powers of z, i.e., there is no z^{-1} term. This leads to the following asymptotic expansion, which saves computing terms of even order:

$$e^{\psi\left(z+\frac{1}{2}\right)} \sim x + \frac{1}{4! \cdot x} - \frac{37}{8 \cdot 6! \cdot x^3} + \frac{10313}{72 \cdot 8! \cdot x^5} - \frac{5509121}{384 \cdot 10! \cdot x^7} + \cdots$$

Special Values

1. <u>Special Values from Gauss Theorem</u>: The digamma function has values in closed form for rational numbers, as a result of Gauss' theorem. Some are listed below:

$$\psi(1) = -\gamma$$

$$\psi\left(\frac{1}{2}\right) = -2\ln 2 - \gamma$$

$$\psi\left(\frac{1}{3}\right) = -\frac{\pi}{2\sqrt{3}} - \frac{3\ln 3}{2} - \gamma$$

$$\psi\left(\frac{1}{4}\right) = -\frac{\pi}{2} - 3\ln 2 - \gamma$$

$$\psi\left(\frac{1}{6}\right) = -\frac{\pi\sqrt{3}}{2} - 2\ln 2 - \frac{3\ln 3}{2} - \gamma$$

$$\psi\left(\frac{1}{8}\right) = -\frac{\pi}{2} - 4\ln 2 - \frac{\pi + \log(2 + \sqrt{2}) - \log(2 - \sqrt{2})}{\sqrt{2}} - \gamma$$

2. <u>Values at Imaginary Unit</u>: Moreover, by the series representation, it can be easily deduced that at the imaginary unit,

$$\Re(\psi(i)) = -\gamma - \sum_{n=0}^{\infty} \frac{n-1}{n^3 + n^2 + n + 1}$$

$$\Im(\psi(i)) = \sum_{n=0}^{\infty} \frac{1}{n^2 + 1} = \frac{1}{2} + \frac{\pi}{2} \coth \pi$$

Regularization

The digamma function appears in the regularization of divergent integrals $\int_0^\infty \frac{dx}{x+a}$, this integral can be approximated by a divergent general Harmonic series, but the following value can be attached to the series

$$-\psi(a) = \sum_{n=0}^{\infty} \frac{1}{n+a}$$



Roots of the Digamma Function

- Complex Gamma Function Saddle Point: The roots of the digamma function are the saddle points of the complex-valued gamma function. Thus, they all lie on the real axis.
- 2. <u>Positive and Negative Digamma Roots</u>: The only one on the positive real axis is the unique minimum of the real-valued gamma function at \mathbb{R}^+ at

$$x_0 = 1.461632144968 \cdots$$

All others occur between the single poles on the negative axis.

$$x_1 = -0.504083008 \cdots$$

$$x_2 = -1.573498473 \cdots$$

$$x_3 = -2.610720868 \cdots$$

$$x_4 = -3.635293366 \cdots$$

3. Hermite Approximation of Digamma Roots: Charles Hermite (1881) observed that

$$x_n = -n + \frac{1}{\ln n} + \mathcal{O}\left(\frac{1}{\ln^2 n}\right)$$

holds asymptotically.

4. <u>Analytic Improvement over Hermite Roots</u>: A better approximation of the location of the roots is given by



$$x_n \approx -n + \frac{1}{\ln n} + \frac{1}{\pi} \arctan\left(\frac{\pi}{\ln n}\right)$$

$$n \ge 2$$

and using a further term it becomes still better

$$x_n \approx -n + \frac{1}{\ln n} + \frac{1}{\pi} \arctan\left(\frac{\pi}{\ln n + \frac{1}{8n}}\right)$$

$$n \ge 1$$

which both spring off of the reflection formula via

$$0 = \psi(1 - x_n) = \psi(x_n) + \frac{\pi}{\tan \pi x_n}$$

and substituting $\psi(x_n)$ by its most convergent asymptotic expansion.

- 5. Adjusted Digamma Expansion for Roots: The correct second term of this expansion is $\frac{1}{2n}$, where the given one works good to approximate roots with small n.
- 6. Enhancement to the Hermite Roots: Another improvement of the Hermite's formula was given by Mezo and Hoffman (2017):

$$x_n = -n + \frac{1}{\ln n} - \frac{1}{2n \ln^2 n} + \mathcal{O}\left(\frac{1}{n^2 \ln^2 n}\right)$$



7. <u>Digamma Roots - Infinite Sum Identities</u>: Regarding the zeros, the following infinite sum identities were recently proved by Mezo and Hoffman (2017):

$$\sum_{n=0}^{\infty} \frac{1}{x_n^2} = \gamma^2 + \frac{\pi^2}{2}$$

$$\sum_{n=0}^{\infty} \frac{1}{x_n^3} = -4\zeta(3) - \gamma^3 - \frac{\pi^2 \gamma}{2}$$

$$\sum_{n=0}^{\infty} \frac{1}{x_n^4} = \gamma^4 + \frac{\pi^4}{9} + \frac{2\pi^2 \gamma^2}{3} + 4\gamma \zeta(3)$$

8. <u>Digamma Roots - Higher Order Terms</u>: In general, the function

$$\varpi(k) = \sum_{n=0}^{\infty} \frac{1}{x_n^k}$$

can be determined, and it has been studied in detail by Mezo and Hoffman (2017).

9. <u>Reciprocal Quadrature Root Polynomial Sums</u>: Further, Mezo and Hoffman (2017) show that



$$\sum_{n=0}^{\infty} \frac{1}{x_n^2 + x_n} = -2$$

and

$$\sum_{n=0}^{\infty} \frac{1}{{x_n}^2 + x_n} = \gamma + \frac{\pi^2}{6\gamma}$$

also holds true.

References

- Abramowitz, M., and I. A. Stegun (2007): Handbook of Mathematics Functions
 Dover Book on Mathematics
- Alzer, H. (1997): On some Inequalities for the Γ and the ψ Functions *Mathematics of Computation* **66 (217)** 373-389
- Alzer, H., and G. Jameson (2017): A Harmonic Mean Inequality for the Digamma
 Function and Related Results *Rendiconti del Seminaro Matematico della Universita di Padova* 70 (201) 203-209
- Bernardo, J. M. (1976): Algorithm AS03 ψ (Digamma Function) Computation Applied Statistics **25** 315-317



- Blagouchine, I. V. (2015): <u>A Theorem for the Closed-Form Evaluation of the First</u>
 Generalized Stieltjes Constant at Rational Arguments and some Related Summations

 arXiv
- Blagouchine, I. V. (2016): <u>Two Series Expansions for the Logarithm of the Gamma Function involving Stirling Numbers and containing only Rational Coefficients for certain argument related π^{-1} arXiv</u>
- Blagouchine, I. V. (2018): <u>Three Notes on Ser's and Hasse's Representations for the</u>
 <u>Zeta-Functions</u> arXiv
- Campbell, R. (1966): Les Integrales Euleriennes et Leurs Applications **Dunod** Paris
- Elezovic, N., C. Giordano, J. Pecaric (2000): The Best Bounds in Gautschi's Inequality Mathematical Inequalities and Applications 3 (2) 239-252
- Hermite, C. (1881): Sur l'integrale Eulerienne de Seconde Espace Journal fur die Reine und Angewandte Mathematik 90 332-338
- Laforgia, A., and P. Natalini (2013): Exponential, Gamma, and Polygamma
 Functions: Simple Proofs of Classical and New Inequalities *Journal of Mathematical Analysis and Applications* 407 (2) 495-504
- Mezo, I., and M. E. Hoffman (2017): Zeros of the Digamma Function and its Barnes
 G-function Analogue *Integral Transforms and Special Functions* 28 (28) 846-858
- Norlund, N. E. (1924): Vorlesungen über Differenzenrechnung Springer Berlin
- Qi, F., and B. N. Guo (2009): <u>Sharp inequalities for the psi function and harmonic numbers arXiv</u>
- Shrivastava, H. M., and J. Choi (2001): Series Associated with the Zeta and the Related Functions Kluwer Academic Publishers Netherlands
- Whittaker, E. T., and G. N. Watson (1996): A Course on Modern Analysis 4th Edition
 Cambridge University Press
- Wikipedia (2019): <u>Digamma Function</u>



Beta Function

Introduction and Overview

1. <u>Definition of the Beta Function</u>: The *beta function*, also called the Euler integral of the first kind, is a special function defined by

$$\mathcal{B}(x,y) = \int_{0}^{1} t^{x-1} (1-t)^{y-1} dt$$

For

$$\Re(x) > 0$$

$$\Re(y)>0$$

(Wikipedia (2019)).

2. Origin of the Symbol: The beta function was studied by Euler and Legendre and was given its name by Jacques Binet; the symbol \mathcal{B} is a Greek Capital beta rather than the Latin Capital B or the Greek lower-case β .



Properties

1. Symmetric Nature of the Beta Function: The beta function is symmetric, meaning that

$$\mathcal{B}(x,y) = \mathcal{B}(y,x)$$

(Abramowitz and Stegun (2007)).

2. Relation to the Gamma Function: A key property of the beta function is its relationship to the gamma function; proof is given below in the section on the relationship between the beta and the gamma functions (Abramowitz and Stegun (2007)):

$$\mathcal{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

3. <u>Beta Function - Key Property Lemmas</u>: When x and y are positive integers, it follows from the definition of the gamma function that (Abramowitz and Stegun (2007)):

$$\mathcal{B}(x,y) = \frac{(x-1)!(y-1)!}{(x+y-1)!}$$



$$\mathcal{B}(x,y) = 2\int_{0}^{\frac{\pi}{2}} (\sin\theta)^{2x-1} (\cos\theta)^{2y-1} d\theta$$

$$\Re(x) > 0$$

$$\Re(y) > 0$$

$$\mathcal{B}(x,y) = 2 \int_{0}^{\frac{\pi}{2}} \frac{t^{x-1}}{(1+t)^{x+y}} d\theta$$

$$\Re(x) > 0$$

$$\Re(y)>0$$

$$\mathcal{B}(x,y) = n \int_{0}^{1} t^{nx-1} (1 - t^{n})^{y-1} d\theta$$

$$\Re(x) > 0$$

$$\Re(y)>0$$



$$\mathcal{B}(x,y) = \sum_{n=0}^{\infty} \frac{\binom{n-y}{n}}{x+n}$$

$$\mathcal{B}(x,y) = \frac{x+y}{xy} \prod_{n=1}^{\infty} \left[1 + \frac{xy}{n(x+y+n)} \right]^{-1}$$

4. <u>Beta Function - Key Identity Lemmas</u>: The beta function satisfies several interesting identities, including:

$$\mathcal{B}(x,y) = \mathcal{B}(x,y+1) + \mathcal{B}(x+1,y)$$

$$\mathcal{B}(x+1,y) = \mathcal{B}(x,y) \cdot \frac{x}{x+y}$$

$$\mathcal{B}(x, y + 1) = \mathcal{B}(x, y) \cdot \frac{y}{x + y}$$

$$\mathcal{B}(x,y)\cdot \left(t\mapsto t_+^{x+y-1}\right)=\left(t\mapsto t_+^{x-1}\right)\times \left(t\mapsto t_+^{y-1}\right)$$



$$x \ge 1$$

$$y \ge 1$$

$$\mathcal{B}(x,y) \cdot \mathcal{B}(x+y,1-y) = \frac{\pi}{x \sin(\pi y)}$$

$$\mathcal{B}(x,1-x) = \frac{\pi}{\sin(\pi x)}$$

$$\mathcal{B}(1,x) = \frac{1}{x}$$

where

$$t\mapsto t_+^x$$

is a truncated power function, and \times denotes convolution.

5. <u>Applications for Deriving *n*-ball Volumes</u>: The lower-most identity above shows, in particular, that

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$



Some of these identities, e.g., the trigonometric formula, can be applied for deriving the volume of a *n*-ball in Cartesian coordinates.

6. Beta Function Pochhammer Contour Integral: Euler's integral for the beta function can be converted to an integral over the Pochhammer contour C as

$$(1 - e^{2\pi i\alpha})(1 - e^{2\pi i\beta})\mathcal{B}(\alpha,\beta) = \oint_{\mathcal{C}}^{\mathcal{C}} t^{\alpha}(1 - t)^{\beta} dt$$

This Pochhammer integral contour converges for all values of α and β , and so gives the analytic continuation of the beta function.

7. Gamma Factorial vs Beta Binomial Coefficient: Just as the gamma function for integers describes factorials, the beta function can define the binomial coefficient after adjusting the indices:

$$\binom{n}{k} = \frac{1}{(n+1)\mathcal{B}(n-k+1,k+1)}$$

8. <u>Binomial Coefficient Continuous Interpolant Function</u>: Moreover, for integer n, \mathcal{B} can be factored to give a closed form, an interpolation function for continuous values of k:

$$\binom{n}{k} = (-1)^n n! \frac{\sin(\pi k)}{\pi \prod_{i=0}^n (k-i)}$$



9. <u>Applications of the Beta Function</u>: The beta function was the first known scattering amplitude in string theory, first conjectured by Gabriele Veneziano. It also occurs in the theory of the preferential attachment process, a type of stochastic urn process.

Relationship between Gamma Function and Beta Function

1. <u>Product of Two Gamma Functions</u>: To derive the integral representation of the beta function, the product of the two factorials are written as

$$\Gamma(x)\Gamma(y) = \int_{u=0}^{\infty} e^{-u}u^{x-1}du \cdot \int_{v=0}^{\infty} e^{-v}v^{y-1}dv = \int_{u=0}^{\infty} \int_{v=0}^{\infty} e^{-u-v}u^{x-1}v^{y-1}dudv$$

2. Reduction into Beta and Gamma: Changing variables by using

$$u = f(z, t) = zt$$

and

$$v = g(z, t) = z(1 - t)$$

shows that this is

$$\Gamma(x)\Gamma(y) = \int_{u=0}^{\infty} \int_{t=0}^{1} e^{-z}(zt)^{x-1} [z(1-t)]^{y-1} |J(z,t)| dt dz$$

$$= \int_{u=0}^{\infty} \int_{t=0}^{1} e^{-z}(zt)^{x-1} [z(1-t)]^{y-1} z dt dz$$

$$= \int_{u=0}^{\infty} e^{-z} z^{x+y-1} dz \int_{t=0}^{1} t^{x-1} (1-t)^{y-1} dt = \Gamma(x+y) \mathcal{B}(x,y)$$

where |J(z,t)| is the absolute value of the Jacobian determinant of

$$u = f(z, t)$$

and

$$v = g(z, t)$$

3. <u>Generalization Integral of a Convolution</u>: The stated identity may be seen as a particular case of the identity for the integral of a convolution. Taking

$$f(u) \coloneqq e^{-u}u^{x-1}\mathbb{R}_+$$

and

$$g(v) \coloneqq e^{-v}v^{y-1}\mathbb{R}_+$$

one has

$$\Gamma(x)\Gamma(y) = \int_{\mathbb{R}}^{\mathbb{R}} f(u)du \cdot \int_{\mathbb{R}}^{\mathbb{R}} g(u)du = \int_{\mathbb{R}}^{\mathbb{R}} (f \times g)(u)du = \Gamma(x+y)\mathcal{B}(x,y)$$

Derivatives

One has

$$\frac{\partial}{\partial x}\mathcal{B}(x,y) = \mathcal{B}(x,y)\left[\frac{\Gamma'(x)}{\Gamma(x)} - \frac{\Gamma'(x+y)}{\Gamma(x+y)}\right] = \mathcal{B}(x,y)[\psi(x) - \psi(x+y)]$$

where $\psi(x)$ is the digamma function.

Integrals

The Norlund-Rice integral is a contour integral involving the beta function.



Approximation

1. Stirling's Approximation Expression for Beta:

$$\mathcal{B}(x,y) \sim \frac{x^{x-\frac{1}{2}}y^{y-\frac{1}{2}}}{(x+y)^{x+y-\frac{1}{2}}}$$

for large x and large y.

2. Large x and Fixed y: If, on the other hand, x is large and y is fixed, then

$$\mathcal{B}(x,y) \sim \Gamma(y)e^{-y}$$

Incomplete Beta Function

1. <u>Definition of Incomplete Beta Function</u>: The *incomplete beta function*, a generalization of the beta function, is defined as



$$\mathcal{B}(x; a, b) = \int_{0}^{x} t^{a-1} (1-t)^{b-1} dt$$

For

$$x = 1$$

the incomplete beta function coincides with the complete beta function.

- Similarity to Incomplete Gamma Function: The relationship between the two
 functions is like the relationship between the gamma function and its generalization –
 the incomplete gamma function.
- 3. <u>Regularized Incomplete Beta Function Definition</u>: The *regularized incomplete beta function* or the *regularized beta function* is defined in terms of the incomplete beta function and the complete beta function:

$$I_{x}(a,b) = \frac{\mathcal{B}(x; a,b)}{\mathcal{B}(a,b)}$$

4. The Cumulative Binomial Distribution Function: The regularized incomplete beta function is the cumulative distribution function of the beta distribution, and is related to the cumulative distribution of a random variable *X* from a binomial distribution, where the *probability of success* is *p* and the sample size is *n*:

$$F(k;n,p) = \mathbb{P}[X \le k] = I_{1-p}(n-k,k+1) = 1 - I_p(k+1,n-k)$$



Properties

$$I_0(a,b) = 0$$

$$I_1(a,b)=1$$

$$I_{x}(a,1) = x^{a}$$

$$I_{x}(1,b) = 1 - (1-x)^{b}$$

$$I_x(a,b) = 1 - I_{1-x}(b,a)$$

$$I_x(a+1,b) = I_x(a,b) - \frac{x^a(1-x)^b}{a\mathcal{B}(a,b)}$$

$$I_x(a, b + 1) = I_x(a, b) + \frac{x^a(1 - x)^b}{b\mathcal{B}(a, b)}$$

$$\mathcal{B}(x;\ a,b) = (-1)^a \mathcal{B}\left(\frac{x}{x-1};\ a,1-a-b\right)$$



Multi-variate Beta Function

The beta function can be extended to a function with more than two arguments:

$$\mathcal{B}(\alpha_1, \dots, \alpha_n) = \frac{\Gamma(\alpha_1) \dots \Gamma(\alpha_n)}{\Gamma(\alpha_1 + \dots + \alpha_n)}$$

This multivariate beta function is used in the definition of the Dirichlet distribution.

Software Implementation

- 1. <u>Computing Beta from Other Functions</u>: Even if unavailable directly, the complete and the incomplete beta function values can be calculated using functions commonly included in spreadsheet or computer algebra systems.
- 2. <u>Complete Beta Functions in Excel</u>: In Excel, for example, the complete beta function value can be calculated from the *GammaLn* value:

$$Value = Exp[GammaLn(a) + GammaLn(b) - GammaLn(a + b)]$$



3. <u>Incomplete Beta Function in Excel</u>: The incomplete beta function value can be calculated as

$$Value = BetaDist(x, a, b)$$

$$\times Exp[GammaLn(a) + GammaLn(b) - GammaLn(a + b)]$$

These results follow from the properties listed above.

4. MATLAB, GNU, R, SciPy, Mathematica: Similarly, betainc – the incomplete beta function – in MATLAB and GNU Octave, pbeta – probability of beta distribution – in R, or special.betainc in Python's SciPy package compute the regularized incomplete beta function – which is, in fact, the cumulative beta distribution – and so, to get the actual incomplete beta function, one must multiply the result of betainc by the result returned by the corresponding beta function. In Mathematica, Beta(x, a, b) and BetaRegularized(x, a, b) give $\mathcal{B}(x; a, b)$ and $I_x(a, b)$, respectively.

References

- Abramowitz, M., and I. A. Stegun (2007): Handbook of Mathematics Functions
 Dover Book on Mathematics
- Wikipedia (2019): Beta Function



Hypergeometric Function

Introduction and Overview

- 1. <u>Hypergeometric Function and Series</u>: The Gaussian or ordinary *hyper-geometric* function ${}_{1}^{2}F(a,b;c;z)$ is a special function represented by the *hypergeometric series* that includes many other functions as limiting or special cases (Wikipedia (2019)).
- 2. <u>Solution to Linear, Second Order ODE</u>: It is a solution to a second-order linear ordinary differential equation (ODE). Every second-order linear ODE with 3 regular singular points can be transformed into this equation.
- 3. <u>Identities involving Hypergeometric Function</u>: For a systematic list of many thousands of published identities involving the hypergeometric function, one refers to the works of Erdelyi, Magnus, Oberhettinger, and Tricomi (1953), and National Institute of Standards and Technology (2019).
- 4. Algorithmic Generation of the Identities: There is no known system for organizing all of the identities; indeed, there is no known system that can generate all the identities, a number of different algorithms are known that generate different series of identities. The theory of algorithmic discovery of these identities remains an active research topic.

The Hypergeometric Series

1. <u>Definition of Hypergeometric Series</u>: The hypergeometric series is defined for

|z| < 1

by the power series



$${}_{1}^{2}F(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_{n}(b)_{n}}{(c)_{n}} \frac{z^{n}}{n!}$$

It is undefined – or infinite – if c equals a non-positive integer.

2. <u>Definition of the Rising Exponent/Pochhammer Symbol</u>: Here $(q)_n$ is a rising Pochhammer symbol, which is defined by

$$(q)_n = \begin{cases} 1 & n = 0 \\ q(q+1)\cdots(q+n-1) & n > 0 \end{cases}$$

3. Reduction to a Polynomial: The series terminates if α or b is a non-positive integer, in which case the function reduces to a polynomial

$${}_{1}^{2}F(-m,b;c;z) = \sum_{n=0}^{m} (-1)^{n} {m \choose n} \frac{(b)_{n}}{(c)_{n}} z^{n}$$

4. Analytic Continuation for Complex Arguments: For complex arguments z with

$$|z| \ge 1$$

it can be analytically continued along any path in the complex plane that avoids the branch points at 1 and ∞ .

5. <u>Limits Under Non-negative *c*</u>: As

$$c \rightarrow -m$$

where m is a non-negative integer

$$_{1}^{2}F(a,b;-m;z)\rightarrow\infty$$



but on dividing by $\Gamma(c)$ the following limit arises:

$$\frac{{}_{1}^{2}F(a,b;c;z)}{\Gamma(c)} = \frac{(a)_{m+1}(b)_{m+1}}{(m+1)!} z^{m+1} {}_{1}^{2}F(a+m+1,b+m+1;m+2;z)$$

6. $\frac{q}{p}F(a,b;c;z)$ – Generalized Hypergeometric Series: ${}_{1}^{2}F(a,b;c;z)$ is the most Usual type of hypergeometric series ${}_{p}^{q}F(a,b;c;z)$, and is often denoted simply as F(a,b;c;z)

Differentiation Formulas

1. <u>Higher Order Hypergeometric Function Differentiation</u>: Using the identity

$$(a)_m = a \cdot (a)_{m+1}$$

it is easily shown that

$$\frac{\partial}{\partial z} {}_{1}^{2}F(a,b;c;z) = \frac{ab}{c} {}_{1}^{2}F(a+1,b+1;c+1;z)$$

and, more generally

$$\frac{\partial^n}{\partial z^n} {}_{1}^{2}F(a,b;c;z) = \frac{(a)_n(b)_n}{(c)_n} {}_{1}^{2}F(a+n,b+n;c+n;z)$$

2. First Order Differentiation - Special Case: In the special case that

$$c = a + 1$$



one has

$$\frac{\partial}{\partial z} {}_{1}^{2}F(a,b;a+1;z) = \frac{\partial}{\partial z} {}_{1}^{2}F(b,a;c;z) = a \frac{(1-z)^{-a} - {}_{1}^{2}F(a,b;1+a;z)}{z}$$

Special Cases

 Hypergeometric Function – Typical Case: Many of the common mathematical functions can be expressed in terms of hypergeometric functions, or as limiting cases of it. Some examples are

$$ln(1+z) = z_1^2 F(1,1;2;-z)$$

$$(1-z)^{-a} = {}_{1}^{2}F(a, 1; 1; z)$$

$$sin^{-1}(z) = z_1^2 F\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z^2\right)$$

2. <u>Hypergeometric Function: Limiting Cases</u>: The confluent hypergeometric function (or Kummer's function) can be given as a limit of the hypergeometric function

$$M(a,c,z) = \underset{b \to \infty}{\underset{1}{limit}} {_{2}} F(a,b;c;b^{-1}z)$$

Thus, all functions that are essentially special cases of it, such as Bessel function, can be expressed as limits of hypergeometric function. These include most of the commonly used functions of mathematical physics.

3. <u>Legendre Functions - Hypergeometric Representation</u>: Legendre functions are solutions of second-order differential equations with 3 regular singular points, so they can be expressed in terms of the hypergeometric function in many ways, for example:

$$_{1}^{2}F(a, 1-a; c; z) = \Gamma(c) z^{\frac{1-c}{2}} (1-z)^{\frac{c-1}{2}} P_{-a}^{1-c} (1-2z)$$

4. <u>Jacobi Polynomial and its Derivatives</u>: Several orthogonal polynomials, including the Jacobi polynomials $P_n^{(\alpha,\beta)}$ and their special cases Legendre polynomials, Chebyshev polynomials, and Gegenbauer polynomials can be written in terms of their hypergeometric functions using

$$_{1}^{2}F(-n,\alpha+1+\beta;\alpha+1;z) = P_{n}^{(\alpha,\beta)}(1-2z)$$

- Krawtchouk and Meixner Polynomial Families: Other polynomials that are special cases include Krawtchouk polynomials, Meixner polynomials, and Meixner-Pollaczek polynomials.
- 6. Representation of Elliptic Modular Functions: Elliptic modular functions can sometimes be expressed as the inverse functions of ratios of hypergeometric functions whose arguments a, b, and c are $1, \frac{1}{2}, \frac{1}{3}, \cdots$, or 0. For example, if

$$\tau = \frac{{}_{1}^{2}F\left(\frac{1}{2}, \frac{1}{2}; 1; 1 - z\right)}{{}_{1}^{2}F\left(\frac{1}{2}, \frac{1}{2}; 1; z\right)}$$

then

$$z = \kappa^2(\tau) = \frac{\theta_2(\tau)^4}{\theta_3(\tau)^4}$$

is an elliptic modular function of τ .

7. Representation of Incomplete Beta Function: Incomplete beta functions $\mathcal{B}_{x}(p,q)$ are related by

$$\mathcal{B}_{x}(p,q) = \frac{x^{p}}{q} {}_{1}^{2} F(p, 1-q; p+1; x)$$

8. Representation of Complete Elliptic Integrals: The complete elliptic integrals *K* and *E* are given by

$$K(k) = \frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}; 1; k^2\right)$$

and

$$E(k) = \frac{\pi}{2} F\left(-\frac{1}{2}, \frac{1}{2}; 1; k^2\right)$$

The Hypergeometric Differential Equation

1. <u>Euler's Hypergeometric Differential Equation</u>: The hypergeometric function is a solution to the Euler's hypergeometric differential equation

$$z(1-z)\frac{\partial^2 w}{\partial z^2} + [c - (a+b+1)z]\frac{\partial w}{\partial z} - ab w = 0$$

which has three regular singular points; $0, 1, and \infty$.

- 2. <u>Generalization using Riemann's Differential Equation</u>: The generalization of this equation to three arbitrary regular singular points is given by Riemann's differential equation.
- 3. <u>Second-Order ODE with Three Singularities</u>: Any second-order differential equation with three regular singular points can be converted to the hypergeometric differential equation by a change of variables.

Solutions at the Singular Points



- 1. <u>Solution using Hypergeometric Series</u>: Solutions to the hypergeometric differential equation are built out of the hypergeometric series ${}_{1}^{2}F(a,b;c;z)$. The equation has two linearly independent solutions.
- 2. Structure of the Special Solutions: At each of the three singular points $0, 1, and \infty$, there are usually two solutions of the form x^s times a holomorphic function of x, where s is one of the two roots of the indicial equation, and x is a local variable vanishing at the regular singular point. This gives

$$3 \times 2 = 6$$

special solutions, as follows.

3. <u>Independent Solutions at z = 0</u>: Around the point

$$z = 0$$

the two independent solutions are, if c is not a non-positive integer, ${}_{1}^{2}F(a,b;c;z)$ and, on the condition that c is not an integer, $z^{1-c}\,{}_{1}^{2}F(1+a-c,1+b-c;2-c;z)$.

- 4. Solution when c is a Non-Positive Integer: If c is a non-positive integer 1 m, then the first of these solutions does not exist, and must be replaced by $z^{m} {}_{1}^{2}F(a+m,b+m;1+m;z)$.
- 5. <u>Solution when *c* is an Integer Greater than 1</u>: The second solution does not exist when *c* is an integer greater than 1, and is equal to the first solution, or its replacement, when *c* is any other integer.
- 6. <u>Complication when *c* is an Integer</u>: Thus, when *c* is an integer, a more complicated expression must be used for the second solution, equal to the first solution multiplied



by $\ln z$, power another series in powers of z, involving the digamma function. See (National Institute of Standards and Technology (2019)) for details.

7. Independent Solutions at z = 1: Around

$$z = 1$$

if c - a - b is not an integer, one has two independent solutions;

$$_{1}^{2}F(a,b;1+a+b-c;1-z)$$

and

$$(1-z)^{c-a-b} {}_{1}^{2}F(c-a,c-b;1+c-a-b;1-z)$$

8. Independent Solutions at $z = \infty$: Around

$$z = \infty$$

if a - b is not an integer, one has two independent solutions;

$$z^{-a}$$
 ${}_{1}^{2}F(a, 1+a-c; 1+a-b; z^{-1})$ and z^{-b} ${}_{1}^{2}F(b, 1+b-c; 1+b-a; z^{-1})$

9. <u>Non-integer Conditions Not Met</u>: Again, when conditions of non-integrality are not met, there exist other solutions that are more complicated.



10. <u>Connection Formulas - Linear Relations between the Solutions</u>: Any 3 of the above 6 solutions satisfy a linear relation as the space of the solutions is two-dimensional, giving

$$\binom{6}{3} = 20$$

linear relations between them called *connection formulas*.

Kummer's 24 Solutions

- 1. Second-Order Function Equation Isomorphism: A second-order Fuchsian equation with n singular points has a group of symmetries acting projectively on its solutions, isomorphic to the Coxeter group D_n of order $n! \, 2^{n-1}$.
- 2. <u>Isomorphism for Hypergeometric Equation</u>: For the hypergeometric equation

$$n = 3$$

- so then group is of order 24 and is isomorphic to the symmetry group on 4 points, and was first described by Kummer.
- 3. Extension using Klein-4 Group: The isomorphism with the symmetry group is accidental and has no analogue for more than 3 singular points, and is sometimes better to think of the group as an extension of the symmetry group on 3 points –



acting as the permutation on the 3 singular points – by a Klein-4 group – whose elements change the signs of the differences of the exponents at an even number of singular points.

4. <u>Kummer's Group of 24 Transformations</u>: Kummer's group of 24 transformations is generated by the three transformations taking a solution of ${}_{1}^{2}F(a,b;c;z)$ to one of

$$(1-z)^{-a} {}_{1}^{2}F\left(a,c-b;c;\frac{z}{z-1}\right)$$

$$_{1}^{2}F(a,b;1+a+b-c;1-z)$$

and

$$(1-z)^{-b} {}_{1}^{2}F\left(c-a,b;c;\frac{z}{z-1}\right)$$

which correspond to the transpositions (12), (23), and (34) under an isomorphism with the symmetric group in 4 points 1, 2, 3, 4.

- 5. Characteristics of the Kummer Transformation: The first and the third of these are actually equal to ${}_{1}^{2}F(a,b;c;z)$ whereas the second is an independent solution to the differential equation.
- 6. Corresponding Euler and Pfaff Transformations: Applying Kummer's

$$24 = 6 \times 4$$



transformations to the hypergeometric function gives the

$$6 = 2 \times 3$$

solutions above to each of the 2 possible exponents at each of the 3 singular points, each of which appears 4 times because of the identities:

a. Euler Transformation:

$$_{1}^{2}F(a,b;c;z) = (1-z)^{c-a-b} _{1}^{2}F(c-a,c-b;c;z)$$

b. Pfaff Transformation:

$$_{1}^{2}F(a,b;c;z) = (1-z)^{-a} _{1}^{2}F\left(a,c-b;c;\frac{z}{z-1}\right)$$

c. Pfaff Transformation:

$$_{1}^{2}F(a,b;c;z) = (1-z)^{-b} _{1}^{2}F\left(c-a,b;c;\frac{z}{z-1}\right)$$

Q-Form



Transformation to the Q-form: The hypergeometric equation may be brought into the Q-form

$$\frac{\partial^2 u}{\partial z^2} + Q(z)u(z) = 0$$

by making the substitution

$$w = uv$$

and eliminating the first-derivative term.

2. Resulting Q(z) and v(z): One finds that

$$Q(z) = \frac{z^2[1 - (a-b)^2] + z[2c(a+b-1) - 4ab] + c(2-c)}{4z^2(1-z)^2}$$

and v(z) is given by the solution to

$$\frac{\partial}{\partial z} \log v(z) = -\frac{c - z(a+b+1)}{2z(1-z)} = -\frac{c}{2z} - \frac{a+b+1-c}{2(z-1)}$$

which is

$$v(z) = z^{-\frac{c}{2}} (1-z)^{\frac{c-a-b-1}{2}}$$

3. <u>Importance for the Schwarzian Derivative</u>: The Q-form is significant in its relation to the Schwarzian derivative (Hille (1976)).

Schwarz Triangle Maps

1. <u>Schwarz Triangle Maps as Solution Ratios</u>: The *Schwarz triangle maps* or *Schwarz s- functions* are ratios of the pairs of solutions

$$s_k = \frac{\phi_k^{(1)}(z)}{\phi_k^{(0)}(z)}$$

where k is one of the points $0, 1, \infty$.

2. Connection Coefficients as Mobius Transformations: The notation

$$D_k(\lambda, \mu, \nu; z) = s_k(z)$$

is also sometimes used. Note that the connection coefficients become Mobius transformations on the triangle maps.



3. Regularity of the Triangle Map: Note that each triangle map is regular at

$$z \in \{0, 1, \infty\}$$

respectively, with

$$s_0(z) = z^{\lambda}[1 + \mathcal{O}(z)]$$

$$s_1(z) = (1-z)^{\mu}[1+\mathcal{O}(z)]$$

$$s_{\infty}(z) = (1-z)^{\nu} [1 + \mathcal{O}(z)]$$

4. Conformal Maps of the Upper Half Plane: In the special case of λ , μ , and ν being real, with

$$0 \le \lambda, \mu, \nu < 1$$

the s-maps are conformal maps of the upper half plane \mathbf{H} to triangles in the Riemann sphere, bounded by circular arcs.

5. <u>Generalization of Schwarz-Christoffel Mapping</u>: The mapping is a generalization of the Schwarz-Christoffel mapping to triangles with circular arcs. The singular points



- $0, 1, \infty$ are set to the triangle vertexes. The angles of the triangle are $\pi\lambda, \pi\mu, \pi\nu$ respectively.
- 6. <u>Tiling the Spheres and Planes</u>: Furthermore, in the case of

$$\lambda = \frac{1}{p}$$

$$\mu = \frac{1}{q}$$

and

$$v = \frac{1}{r}$$

for integers p, q, and r, the triangle tiles the sphere, the complex plane, or the upper half plane according to whether $\lambda + \mu + \nu - 1$ is positive, zero, or negative; the smaps are inverse functions of automorphic functions for the triangle group

$$\langle p, q, r \rangle = \Delta(p, q, r)$$

Monodromy Group



- 1. Change on Loops around Singularity: The Monodromy of a hypergeometric equation describes how fundamental solutions change when continued analytically in the paths around the z-plane that return to the same point. That is when the paths wind around a singularity of ${}_{1}^{2}F(a,b;c;z)$, the value at the end-point will differ from the starting point.
- Relations between the Fundamental Solutions: Two fundamental solutions of the hypergeometric equation are related to each other by a linear transformation; thus, the Monodromy is a mapping – a group homomorphism –

$$\pi_1(\mathbb{C}\setminus\{0,1\},z_0)\to GL(2,\mathbb{C})$$

where π_1 is a fundamental group. In other words, the Monodromy is a twodimensional linear representation of the fundamental group.

- 3. Group Generated by the Monodromy Matrices: The Monodromy group of this equation is the image of this map, i.e., the group generated by the Monodromy matrices. The Monodromy representation of the fundamental group can be computed explicitly in terms of the exponents at the singular points (Ince (1944)).
- 4. Monodromy Matrices around 0/1 Loops: If (α, α') , (β, β') , and (γ, γ') are the exponents at 0, 1, and ∞ , then, taking z_0 around 0, the loops around 0 and 1 have monodromy matrices

$$g_0 = \begin{pmatrix} e^{2\pi i\alpha} & 0\\ 0 & e^{2\pi i\alpha'} \end{pmatrix}$$

and

$$g_{1} = \begin{pmatrix} \frac{\mu e^{2\pi i\beta} - e^{2\pi i\beta'}}{\mu - 1} & \frac{\mu \left[e^{2\pi i\beta} - e^{2\pi i\beta'}\right]}{[\mu - 1]^{2}} \\ e^{2\pi i\beta'} - e^{2\pi i\beta} & \frac{\mu e^{2\pi i\beta'} - e^{2\pi i\beta}}{\mu - 1} \end{pmatrix}$$

where

$$\mu = \frac{\sin \pi (\alpha + \beta' + \gamma') \sin \pi (\alpha' + \beta + \gamma')}{\sin \pi (\alpha' + \beta' + \gamma') \sin \pi (\alpha + \beta + \gamma')}$$

5. Finiteness of the Monodromy Group: If 1 - a, c - a - b, and a - b are non-integer rational numbers with denominators k, l, and m, the monodromy group is finite if and only if

$$\frac{1}{k} + \frac{1}{l} + \frac{1}{m} > 1$$

Integral Formulas – Euler Type

1. Euler Integral Hypergeometric Expression: If \mathcal{B} is the beta function, then

$$\mathcal{B}(b,c-b) \, {}_{1}^{2}F(a,b;c;z) = \int_{0}^{1} x^{b-1} \, (1-x)^{c-b-1} \, (1-zx)^{-a} dx$$

$$\Re(c) > \Re(b) > 0$$

provided that z is not a real number that is greater than or equal to 1. This can be proved by expanding $(1 - zx)^{-a}$ using the binomial theorem and integrating term by term for z with absolute value smaller than 1, and by analytic continuation elsewhere.

- 2. Analytic Continuation for Real z: When z is a real number greater than or equal to 1, analytic continuation must be used, because at some point (1 zx) is zero in the support of the integral, so the value of the integral may be ill-defined. This was given by Euler in 1748, and implies Euler's and Pfaff's hypergeometric transformations.
- 3. <u>Alternate Integrals using Monodromy Loops</u>: Other representations, corresponding to other branches, are given by taking the same integrand, but taking the path of the integral to be a closed Pochhammer cycle enclosing the singularities in various order. Such paths correspond to the monodromy action.

Barnes Integral

Barnes used the theory of residues to evaluate the Barnes integral

 $\frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} \frac{\Gamma(a+s)\Gamma(b+s)\Gamma(-s)}{\Gamma(c+s)} (-z)^s ds \text{ as } \frac{\Gamma(a)\Gamma(b)}{\Gamma(c)} \, {}_1^2F(a,b;c;z) \text{ where the contour is drawn to separate the poles } 0,1,2,\cdots \text{ from } -a,-a-1,\cdots,-b,-b-1,\cdots \text{ This is valid as long as } z \text{ is a non-negative real number.}$



John Transform

The Gauss hypergeometric function can be written as a John transform (Gelfand, Gindikin, and Graev (2003)).

Gauss' Contiguous Relation

- 1. <u>Gauss Contiguous Hypergeometric Functions</u>: The six functions ${}_{1}^{2}F(a \pm 1, b; c; z)$, ${}_{1}^{2}F(a, b \pm 1; c; z)$, and ${}_{1}^{2}F(a, b; c \pm 1; z)$ are called contiguous to ${}_{1}^{2}F(a, b; c; z)$.
- 2. <u>Linear Combination of the Contiguous Functions</u>: Gauss showed that ${}_{1}^{2}F(a,b;c;z)$ can be written as a linear combination of any of its two contiguous functions, with rational coefficients written in terms of a, b, c, and z.
- 3. <u>Derivatives Using the Contiguous Term</u>: This gives

$$\binom{6}{2} = 15$$

relations, given by any lines on the right-hand side of

$$\frac{\partial}{\partial z} {}_{1}^{2}F(a,b;c;z) = z\frac{ab}{c} {}_{1}^{2}F(a+1,b+1;c+1;z)$$

$$= a[{}_{1}^{2}F(a+1,b;c;z) - {}_{1}^{2}F(a,b;c;z)]$$

$$= b[{}_{1}^{2}F(a,b+1;c;z) - {}_{1}^{2}F(a,b;c;z)]$$

$$= (c-1)[{}_{1}^{2}F(a,b;c-1;z) - {}_{1}^{2}F(a,b;c;z)]$$

$$= \frac{(c-a){}_{1}^{2}F(a-1,b;c;z) + (a-c+bz){}_{1}^{2}F(a,b;c;z)}{1-z}$$

$$= \frac{(c-b){}_{1}^{2}F(a,b-1;c;z) + (b-c+az){}_{1}^{2}F(a,b;c;z)}{1-z}$$

$$= z\frac{(c-a)(c-b){}_{1}^{2}F(a,b;c+1;z) + c(a+b-c){}_{1}^{2}F(a,b;c;z)}{c(1-z)}$$

4. <u>Displaced Continuous Hypergeometric Form</u>: Repeatedly applying these relation gives a linear relation over $\mathbb{C}(z)$ between any three functions of the form ${}_{1}^{2}F(a+m,b+n;c+l;z)$ where m,n, and l are integers.

Gauss' Continued Fraction

Gauss used the contiguous relations to give several ways of writing a quotient of two hypergeometric functions as a continued fraction, for example:

$$\frac{{}_{1}^{2}F(a+1,b+1;c+1;z)}{{}_{1}^{2}F(a,b;c;z)} = \frac{1}{1+\frac{\dfrac{(a-c)b}{c(c+1)}z}{\dfrac{(b-c-1)(a+1)}{(c+1)(c+2)}z}} \\ 1 + \frac{1+\frac{\dfrac{(a-c)b}{c(c+1)}z}{\dfrac{(a-c-1)(b+1)}{(c+2)(c+3)}z}}{1+\frac{\dfrac{(a-c-1)(b+1)}{(c+2)(c+3)}z}{\dfrac{(c+3)(c+4)}{1+\ddots}z}}$$

Transformation Formula

Transformation formulas relate hypergeometric functions at two different values of z.

Fractional Linear Transformations

1. Euler Transformation of Hypergeometric Function: Euler's transformation is

$$_{1}^{2}F(a,b;c;z) = (1-z)^{c-a-b} _{1}^{2}F(c-a,c-b;c;z)$$

2. <u>Pfaff Linear Transformation</u>: It follows by combining the two Pfaff transformations

$$_{1}^{2}F(a,b;c;z) = (1-z)^{-b} _{1}^{2}F\left(b,c-a;c;\frac{z}{z-1}\right)$$

$$_{1}^{2}F(a,b;c;z) = (1-z)^{-a} _{1}^{2}F\left(a,c-b;c;\frac{z}{z-1}\right)$$

which in turn follow Euler's integral representation. For extension of Euler's first and second transformations, one refers to Rathie and Paris (2007) and Rakha and Rathie (2011).

Quadratic Transformation

- 1. Criteria for the Quadratic Transformation: If two of the numbers 1-c, c-1, a-b, b-a, a+b-c, and c-a-b are equal, or one of them is $\frac{1}{2}$, then there is a quadratic transformation of the hypergeometric function, connecting it to a different value of z related by a quadratic equation.
- 2. Example of a Quadratic Transformation: The first examples were given by Kummer (1836) and a more complete list was given by Goursat (1881). A typical example is

$$_{1}^{2}F(a,b;2b;z) = _{1}^{2}F\left(\frac{a}{2},b-\frac{a}{2};b+\frac{1}{2};\frac{z^{2}}{4z-4}\right)$$



Higher Order Transformations

- 1. <u>Criteria for Cubic Transformation</u>: If 1-c, a-b, or a+b-c differ by signs, or two of them are $\frac{1}{3}$ or $-\frac{1}{3}$, then there is a *cubic transformation* of the hypergeometric function, connecting it to a different value if z related by a cubic equation.
- 2. <u>Hypergeometric Cubic Transformation Example</u>: The first examples were given by Goursat (1881). One typical example is

$${}_{1}^{2}F\left(\frac{3}{2}a, \frac{1}{2}[3a-1]; a+\frac{1}{2}; -\frac{z^{2}}{3}\right) = {}_{1}^{2}F\left(a-\frac{1}{3}, a; 2a; \frac{2z[3+z^{2}]}{[1+z]^{-3}}\right)$$

3. <u>Rational and Higher Order Transformations</u>: There also exist transformations of degree 4 and 6 as well. Transformations of other degrees only exist if *a*, *b*, and *c* are certain rational numbers (Vidunas (2015)). For example,

$${}_{1}^{2}F\left(\frac{1}{4},\frac{3}{8};\frac{7}{8};z\right) \cdot \left[z^{4} - 60z^{3} + 134z^{2} - 60z + 1\right]^{\frac{1}{16}}$$

$$= {}_{1}^{2}F\left(\frac{1}{48},\frac{17}{48};\frac{7}{8};\frac{-432z(z-1)^{2}(z+1)^{8}}{\left[z^{4} - 60z^{3} + 134z^{2} - 60z + 1\right]^{3}}\right)$$

Values at Special Points



Slater (1966) contains a list of the summation formulas at special points, most of which appear in Bailey (1935). Gessel and Stanton (1982) give further evaluations at more points. Koepf (1995) shows how most of these identities can be verified by computer algorithms.

Special Values at z = 1

1. <u>Hypergeometric Estimate using Gauss Theorem</u>: Gauss' theorem is the identity

$${}_{1}^{2}F(a,b;c;z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}$$

$$\Re(c) > \Re(a+b)$$

which follows from the Euler's integral formula by setting

$$z = 1$$

It includes van der Monde identity as a special case.

2. Special case of a = -m: For the special case where

$$a = -m$$

$$_{1}^{2}F(-m,b;c;z) = \frac{(c-b)_{m}}{(c)_{m}}$$

Dougall's formula generalizes this to the bilateral hypergeometric series at

$$z = 1$$

Kummer's Theorem

1. Quadratic Transformation to z = +1: There are many cases where the hypergeometric functions can be evaluated at

$$z = -1$$

by using a quadratic transformation from change

$$z = -1$$



to

$$z = +1$$

and then using Gauss' theorem to evaluate the result.

2. <u>Kummer's Expression and its Generalization</u>: A typical example is Kummer's theorem, named for Ernst Kummer:

$${}_{1}^{2}F(a,b;1+a-b;-1) = \frac{\Gamma(1+a-b)\Gamma(1+\frac{a}{2})}{\Gamma(1+a)\Gamma(1+\frac{a}{2}-b)}$$

which follows from Kummer's quadratic transformations

$${}_{1}^{2}F(a,b;1+a-b;-1) = (1-z)^{-a} {}_{1}^{2}F\left(\frac{a}{2}, \frac{a+1}{2} - b; 1+a-b; -\frac{4z}{[1-z]^{2}}\right)$$
$$= (1+z)^{-a} {}_{1}^{2}F\left(\frac{a}{2}, \frac{a+1}{2} - b; 1+a-b; \frac{4z}{[1+z]^{2}}\right)$$

and Gauss' theorem by setting

$$z = -1$$



in the first identity. Lavoie, Grondin, and Rathie (1996) contain a generalization of Kummer's summation.

Special Values at $z = \frac{1}{2}$

1. <u>Gauss' Second Summation Theorem Expression</u>: Gauss' second summation theorem is

$${}_{1}^{2}F\left(a,b;\frac{1+a+b}{2};\frac{1}{2}\right) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1+a+b}{2}\right)}{\Gamma\left(\frac{1+a}{2}\right)\Gamma\left(\frac{1+b}{2}\right)}$$

2. Expression using Bailey's Theorem: Bailey's theorem is

$${}_{1}^{2}F\left(a,1-a;c;\frac{1}{2}\right) = \frac{\Gamma\left(\frac{c}{2}\right)\Gamma\left(\frac{1+c}{2}\right)}{\Gamma\left(\frac{c+a}{2}\right)\Gamma\left(\frac{1+c-a}{2}\right)}$$

3. <u>Other Generalizations</u>: For generalization of Gauss' second summation theorem, one refers to Lavoie, Grondin, and Rathie (1996).



Other Points

- 1. <u>Function Value at Special Points</u>: There are many other formulas giving the hypergeometric function as an algebraic number at special rational values of the parameters, some of which are listed in Gessel and Stanton (1982) and Koepf (1995).
- 2. Values at Special Points Example: Some typical examples are given by

$${}_{1}^{2}F\left(a,-a;\frac{1}{2};\frac{z^{2}}{4[z-1]}\right) = \frac{(1-z)^{-a} + (1-z)^{-b}}{2}$$

which can be re-stated as

$$T_a(\cos x) = {}_{1}^{2}F\left(a, -a; \frac{1}{2}; \frac{1}{2}[1 - \cos x]\right) = \cos(ax)$$

where

$$-\pi < x < \pi$$

and *T* is the generalized Chebyshev polynomial.



References

- Bailey, W. N. (1935): Generalized Hypergeometric Series Cambridge University
 Press
- Erdelyi, A., W. Magnus, F. Oberhettinger, and F. G. Tricomi (1953): Higher Transcendental Functions McGraw-Hill New York
- Gelfand, I. M., S. G. Gindikin, and M. I. Graev (2003): Selected Topics in Integral Geometry American Mathematical Society
- Gessel, I. and D. Stanton (1982): Strange Evaluations of Hypergeometric Series SIAM
 Journal on Mathematical Analysis 13 (2) 295-308
- Goursat, E. (1881): Sur l'Equation Différentielle Lineare, qui admit pour Integrale la Serie Hypergeometrique Annales Scientifiques de l'Ecole Normale Superieure 10 3-142
- Hille, E. (1976): Ordinary Differential Equations in the Complex Domain Dover
- Ince, E., L. (1944): Ordinary Differential Equations **Dover**
- Koepf, W (1995): Algorithms for m-fold Hypergeometric Summation Journal of Symbolic Computation 20 (4) 399-417
- Kummer, E. E. (1836): Uber die Hypergeometrische Reihe $1 + \frac{\alpha \cdot \beta}{1 \cdot \gamma} x + \frac{\alpha \cdot (\alpha+1) \cdot \beta \cdot (\beta+1)}{1 \cdot 2 \cdot \gamma \cdot (\gamma+1)} x^2 + \frac{\alpha \cdot (\alpha+1) \cdot (\alpha+2) \cdot \beta \cdot (\beta+1) \cdot (\beta+2)}{1 \cdot 2 \cdot 3 \cdot \gamma \cdot (\gamma+1) \cdot (\gamma+2)} x^3 + \cdots$ Journal fur die Reine und Angewandte Mathematik **15** 39-83, 127-172
- Lavoie, J. L., F. Grondin, and A. K. Rathie (1996): Generalization of Whipple's Theorem on the Sum of a ${}_{2}^{3}F(a,b;c;z)$ *Journal of Computational and Applied Mathematics* **72** 293-300
- National Institute of Standards and Technology (2019): Hypergeometric Function
- Rakha, M. A., and A. K. Rathie (2011): Extension of Euler's Type-II Transformation and Saalschutz's Theorem *Bulletin of the Korean Mathematical Society* 48 (1) 151-156



- Rathie, A. K., and R. B. Paris (2007): An Extension of the Euler's Type-II Transformation for the ${}_{2}^{3}F(a,b;c;z)$ Series Far East Journal of Mathematical Sciences 27 (1) 43-48
- Slater, L. J. (1966): Generalized Hypergeometric Functions Cambridge University
 Press
- Vidunas, R. (2005): <u>Transformations of some Gauss Hypergeometric Functions</u> arXiV
- Wikipedia (2019): <u>Hypergeometric Function</u>



Bessel Function

Introduction and Overview

1. Bessel Function Second-Order ODE: Bessel functions, first defined by the mathematician Daniel Bernoulli and generalized by Friedrich Bessel, are the canonical solutions y(x) of the Bessel's differential equations

$$x^{2}\frac{d^{2}y}{dx^{2}} + x\frac{dy}{dx} + (x^{2} - \alpha^{2})y = 0$$

for an arbitrary complex number α , the order of the Bessel equation (Wikipedia (2019)).

- 2. ODE Order Positive and Negative: Although α and $-\alpha$ produce the same differential equation, it is conventional to define Bessel functions for these two values in such a way that the Bessel functions are mostly smooth function of α .
- 3. <u>Important Cases of Order Value</u>: The most important cases are when α is an integer or a half-integer.
- 4. Integer Order Cylindrical Bessel Functions: Bessel functions for integer α are called the *cylindrical Bessel functions* or the *cylindrical harmonics* because they appear in the Laplace's solution in cylindrical coordinates.
- 5. <u>Half Integer Spherical Bessel Functions</u>: *Spherical Bessel functions* with half-integer α are obtained when the Helmholtz equation is solved in spherical coordinates.

Applications of Bessel Functions



- 1. <u>Separable Solutions in Cylindrical/Spherical Coordinates</u>: Bessel's equations arise when finding the separable solutions to the Laplace's equation and the Helmholtz equation on the cylindrical or spherical coordinates. Bessel functions are therefore especially important for many problems of wave propagation and static potentials.
- 2. <u>Orders under Cylindrical/Spherical Coordinates</u>: In solving problems in the cylindrical coordinate system, one obtains Bessel functions of integer order

$$\alpha = n$$

In spherical coordinates, one obtains half-integer orders

$$\alpha = n + \frac{1}{2}$$

- 3. Example Applications of Bessel Functions:
 - a. Electromagnetic waves in a cylindrical wave-guide
 - b. Pressure amplitudes of inviscid rotational flows
 - c. Heat conduction in a cylindrical object
 - d. Modes of vibration of a thin circular or annular acoustic membrane such as drum of other membranophane
 - e. Diffusion problems on a lattice
 - f. Solutions to the radian Schrodinger equation in spherical and cylindrical coordinates for a free particle
 - g. Solving for patterns of acoustical radiation
 - h. Frequency-dependent friction in circular pipelines
 - i. Dynamics of floating bodies
 - j. Angular resolution
 - k. Diffraction from helical objects, including DNA
- 4. <u>Bessel Functions is Signal Processing</u>: Bessel functions also appear in other problems such as signal processing, e.g., FM synthesis, Kaiser window, or Bessel filter.



Definitions

- 1. <u>Two Linearly Independent ODE Solutions</u>: Because this is a second-order differential equation, there must be two linearly independent solutions.
- Alternative Formulations of Bessel Solutions: Depending upon the circumstances, however, various formulations of these solutions are convenient. Different variations are summarized in the table below and described in the following sections.
- 3. Bessel Function Types and Solutions:

Туре	First Kind	Second Kind
Bessel Functions	J_{α}	Y_{α}
Modified Bessel Functions	I_{α}	K_{α}
Hankel Functions	$H_{\alpha}^{(1)} = J_{\alpha} + iK_{\alpha}$	$H_{\alpha}^{(2)} = J_{\alpha} - iK_{\alpha}$
Spherical Bessel Functions	j_n	y_n
Spherical Hankel Functions	$h_n^{(1)} = j_n + iy_n$	$h_n^{(2)} = j_n - iy_n$

4. Alternate Symbology for the Solutions: Bessel functions of the second kind and spherical Bessel functions of the second kind are sometimes denoted by N_n and n_n respectively, rather than by Y_n and y_n .

Bessel Functions of the First Kind J_{α}

1. <u>Definition as Solutions to ODE</u>: Bessel functions of the first kind, defined as $J_{\alpha}(x)$, are solutions to the Bessel's differential equation that are finite at the origin

$$x = 0$$



for integer or positive α and diverges as x approaches zero for negative non-integer α .

2. <u>Frobenius Series Expansion around x = 0</u>: It is possible to define the function by its series expansion around

$$x = 0$$

which can be found by applying the Frobenius method for the Bessel's equation (Abramowitz and Stegun (2007)):

$$J_{\alpha}(x) = \frac{(-1)^m}{m! \Gamma(m+\alpha+1)} \left(\frac{x}{2}\right)^{2m+\alpha}$$

where $\Gamma(z)$ is the gamma function, a shifted generalization of the factorial function to non-integer values.

- 3. Entire/Multi-valued Function Nature: The Bessel function of the first kind is an entire function if α is an integer, otherwise it is a multi-valued function with a singularity at zero.
- 4. <u>Similarities to Decaying Periodic Functions</u>: The graphs of Bessel functions look roughly like oscillating sine or cosine functions that decay proportionally to $\frac{1}{\sqrt{x}}$ their asymptotic forms are listed below although their roots are generally not periodic, except asymptotically for large x.
- 5. Successive Series Terms as Derivatives: The series above indicates that $-J_1(x)$ is the derivatives of $J_0(x)$, much like $-\sin x$ in the derivative of $\cos x$; more generally, the derivative of $J_n(x)$ can be expressed in terms of $J_{n\pm 1}(x)$ using the identities below.
- 6. <u>Linear Independence for Non-linear α </u>: For non-integer α , the functions $J_{\alpha}(x)$ and $J_{-\alpha}(x)$ are linearly independent, and are therefore the two solutions of the same differential equation.
- 7. Relationship for Integer α : On the other hand, the following relationship is valid (Abramowitz and Stegun (2007))

$$J_{-n}(x) = (-1)^n J_n(x)$$

Note that the gamma function has simple poles at each of the non-positive integers.

8. <u>Linearly Independent Solutions for Integer α </u>: This means that the two solutions above are no longer linearly independent. In this case, the second linearly independent solution is then found to be the Bessel function of the second kind, as discussed below.

Bessel's Integrals

1. <u>First Kind Integral Representation #1</u>: Another definition of the Bessel function, for integer values of *n*, is possible using an integral representation (Temme (1996)):

$$J_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos(n\tau - x \sin \tau) d\tau$$

2. <u>First Kind Integral Representation #2</u>: Another integral representation is (Temme (1996)):

$$J_n(x) = \frac{1}{2\pi} \int_{0}^{\pi} e^{i(x\sin\tau - n\tau)} d\tau$$

3. Representations for Non-Integer Integrals: The above was the approach that Bessel used, and from this definition, derived several properties of the function. The definition may be extended to non-integer orders by one of Schlafli's integrals (Watson (1995), Temme (1996), Lund (2000), Arfken and Weber (2005), Gerlach (2010)).

$$J_{\alpha}(x) = \frac{1}{\pi} \int_{0}^{\pi} \cos(\alpha \tau - x \sin \tau) d\tau - \frac{\sin \alpha \tau}{\tau} \int_{0}^{\pi} e^{-x \sinh \tau - \alpha \tau} d\tau$$

Relation to the Hypergeometric Series

The Bessel function can be expressed in terms of the generalized hypergeometric series as (Abramowitz and Stegun (2007))

$$J_{\alpha}(x) = \frac{\left(\frac{x}{2}\right)^{\alpha}}{\Gamma(\alpha+1)} \, {}_{0}^{1}F\left(\alpha+1; \, -\frac{x^{2}}{4}\right)$$

This function is related to the development of the Bessel function in terms of the Bessel-Clifford function.

Relation to the Laguerre Polynomials

In terms of the Laguerre polynomials L_k and an arbitrarily chosen parameter t, the Bessel function can be expressed as (Szego (1975))

$$\frac{J_{\alpha}(x)}{\left(\frac{x}{2}\right)^{\alpha}} = \frac{e^{-t}}{\Gamma(\alpha+1)} \sum_{k=0}^{\infty} \frac{L_{k}^{(\alpha)}\left(-\frac{x^{2}}{4}\right)}{\binom{k+\alpha}{k}} \frac{t^{k}}{k!}$$



Bessel Function of the Second Kind Y_{α}

1. <u>Bessel Function Second Kind Definition</u>: The Bessel functions of the second kind, denoted $Y_{\alpha}(x)$, and occasionally denoted instead by $N_{\alpha}(x)$, are solutions to the Bessel differential equation that have a singularity at the origin

$$x = 0$$

and are multi-valued. These are sometimes called *Weber functions*, as they were introduced by Weber (1873) and also as *Neumann functions* after Carl Neumann (Culham (2004)).

2. Relation between Y_{α} and J_{α} : For non-integer α , Y_{α} is related to J_{α} by

$$Y_{\alpha}(x) = \frac{J_{\alpha}(x)\cos\pi\alpha - J_{-\alpha}(x)}{\sin\pi\alpha}$$

3. $\underline{Y_n}$ for Integer α Values: In the case of integer order n, the function is defined by taking the limit as a non-integer α tends to n:

$$Y_n(x) = \frac{Limit}{\alpha \to n} Y_{\alpha}(x)$$

4. <u>Non-negative Integer Series Expansion</u>: If *n* is a non-negative integer, one has the following series (National Institute of Standards and Technology (2019)):



$$Y_n(z) = -\frac{\left(\frac{z}{2}\right)^{-n}}{\pi} \sum_{0 \le k \le n-1} \frac{(n-k-1)!}{k!} \left(\frac{z^2}{4}\right)^k + \frac{2}{\pi} J_n(z) \log \frac{z}{2}$$
$$-\frac{\pi}{2} \sum_{k \ge 0} [\psi(k+1) - \psi(n+k+1)] \frac{\left(-\frac{z^2}{4}\right)^k}{k! (n+k)!}$$

where $\psi(z)$ is the digamma function, the logarithmic derivative of the gamma function.

5. \underline{Y}_n Integral Form for Re(x) > 0: There is also a corresponding integral formula for

(Watson (1995)):

$$Y_n(x) = \frac{1}{\pi} \int_{0}^{\pi} \sin(x \sin \tau - n\tau) d\tau - \frac{1}{\pi} \int_{0}^{\infty} \left[e^{nt} + (-1)^n e^{-nt} \right] e^{-x \sinh t} dt$$

6. <u>Different Interpretations of $Y_{\alpha}(x)$ </u>: $Y_{\alpha}(x)$ is necessary as the second linearly independent solution of the Bessel's equation when α is an integer. But $Y_{\alpha}(x)$ has more meaning than that. It can be considered as a *natural* partner of $Y_{\alpha}(x)$. The section on Hankel functions contains more details.



7. Mirror Inverse Relationship for $Y_{\alpha}(x)$: When α is an integer, moreover, as was similarly the case for the functions of the first kind, the following relationship is valid:

$$Y_{-n}(x) = (-1)^n Y_n(x)$$

- 8. <u>Holomorphic Nature of the Functions</u>: Both $J_{\alpha}(x)$ and $Y_{\alpha}(x)$ are holomorphic functions of x on the complex plane cut along the negative axis. When α is an integer, the Bessel functions J are entire functions of x. If x is held fixed at a non-zero value, then the Bessel functions are entire functions of α .
- 9. Solution to the Fuch's Theorem: The Bessel functions of the second kind when α is an integer is an example of the second kind of solution in the Fuch's theorem.

Hankel Functions $H_{\alpha}^{(1)}$ and $H_{\alpha}^{(2)}$

1. <u>Definition of the Hankel Functions</u>: Another important formulation of the two independent solutions to the Bessel's equation are the *Hankel functions of the first* and the second kind $H_{\alpha}^{(1)}(x)$ and $H_{\alpha}^{(2)}(x)$, defined as (Abramowitz and Stegun (2007))

$$H_{\alpha}^{(1)}(x) = J_{\alpha}(x) + iK_{\alpha}(x)$$



and

$$H_{\alpha}^{(2)}(x) = J_{\alpha}(x) - iK_{\alpha}(x)$$

where i is the imaginary unit.

- 2. <u>Hankel Function Common Alternate Names</u>: These linear combinations are also known as the *Bessel functions of the third kind* they are linearly independent solutions to the Bessel's differential equation. They are named after Hermann Hankel.
- 3. Advantages of the Hankel Formulation: The importance of the Hankel functions of the first and the second kind lies more in theoretical development rather than in application. These forms of linear combinations satisfy numerous simple-looking properties, like asymptotic formulae or integral representations. Here *simple* means appearance of the factor of the form $e^{if(x)}$. The Bessel function of the second kind then can be thought to naturally appear as part of the Hankel functions.
- 4. <u>Outward and Inward Cylindrical Waves</u>: The Hankel functions are used to express outward- and inward- propagating cylindrical wave solutions to the cylindrical wave equation, respectively or vice versa depending on the sign convention for the frequency.
- 5. <u>Hankel's Function using Bessel's Combination</u>: Using the previous relationships, they can be expressed as

$$H_{\alpha}^{(1)}(x) = \frac{J_{-\alpha}(x) - e^{-i\pi\alpha}J_{\alpha}(x)}{i\sin\pi\alpha}$$

and

$$H_{\alpha}^{(2)}(x) = \frac{J_{-\alpha}(x) - e^{i\pi\alpha}J_{\alpha}(x)}{-i\sin\pi\alpha}$$

6. Positive/Negative α Hankel Expression: If α is an integer, a limit has to be used instead. The following relationships are valid whether α is an integer or not (Abramowitz and Stegun (2007)):

$$H_{-\alpha}^{(1)}(x) = e^{i\pi\alpha}H_{\alpha}^{(1)}(x)$$

$$H_{-\alpha}^{(2)}(x) = e^{-i\pi\alpha} H_{\alpha}^{(2)}(x)$$

7. <u>Half-Integer Hankel Function Expression</u>: In particular, if

$$\alpha = m + \frac{1}{2}$$

with α being a non-negative integer, the above relations imply directly that

$$J_{-\left(m+\frac{1}{2}\right)}(x)=(-1)^{m+1}Y_{m+\frac{1}{2}}(x)$$

$$Y_{-\left(m+\frac{1}{2}\right)}(x) = (-1)^{m+1} J_{m+\frac{1}{2}}(x)$$



These are useful in developing the spherical Bessel functions below.

8. <u>Imaginary Hankel Integral Contour Loops</u>: The Hankel functions admit the following integral representations for

(Abramowitz and Stegun (2007)):

$$H_{\alpha}^{(1)}(x) = \frac{1}{i\pi} \int_{-\infty}^{-\infty + i\pi} e^{x \sin \tau - \alpha \tau} d\tau$$

$$H_{\alpha}^{(2)}(x) = -\frac{1}{i\pi} \int_{-\infty}^{-\infty - i\pi} e^{x \sin \tau - \alpha \tau} d\tau$$

where the integral limits indicate integration along a contour that can be chosen as follows: from $-\infty$ to 0 along the negative real axis, and from $\pm i\pi$ to $\pm \infty \pm i\pi$ along a contour parallel to the real axis (Watson (1995)).

Modified Bessel Functions I_{α} , K_{α}



- 1. <u>Bessel Functions of Imaginary Argument</u>: The Bessel functions are valid even for complex arguments *x*, and an important special case of that is one using a purely imaginary argument.
- 2. <u>Modified First/Second Bessel Functions</u>: In this case, the solutions to the Bessel equations are called the *modified Bessel functions* or occasionally the *hyperbolic Bessel functions* of the first and the second kind and are defined as (Abramowitz and Stegun (2007))

$$I_{\alpha}(x) = i^{-\alpha} J_{\alpha}(x) = \sum_{m=0}^{\infty} \frac{1}{m! \Gamma(m+\alpha+1)} \left(\frac{x}{2}\right)^{2m+\alpha}$$

and

$$K_{\alpha}(x) = \frac{\pi}{2} \frac{I_{-\alpha}(x) - I_{\alpha}(x)}{\sin \pi \alpha}$$

when α is not an integer. When α is an integer, the limit is used.

- 3. Choice of the α Parameter: These are chosen to be real-valued for real and positive arguments x. The series expansion for $I_{\alpha}(x)$ is thus similar to that for $J_{\alpha}(x)$ but without the alternating $(-1)^m$ factor.
- 4. Expressions using First/Second Hankel: If

$$-\pi < \arg x \le \frac{\pi}{2}$$



 $K_{\alpha}(x)$ can be expressed as a Hankel function of the first kind

$$K_{\alpha}(x) = \frac{\pi}{2} i^{\alpha+1} H_{\alpha}^{(1)}(ix)$$

and if

$$-\frac{\pi}{2} < \arg x \le \pi$$

it can be expressed as a Hankel function of the second kind

$$K_{\alpha}(x) = \frac{\pi}{2} (-i)^{\alpha+1} H_{\alpha}^{(2)}(-ix)$$

5. <u>First/Second Bessel Function Re-cast</u>: The first and the second Bessel functions can also be expressed in terms of the modified Bessel functions. The following expressions are valid if

$$-\pi < \arg z \le \frac{\pi}{2}$$

(Abramowitz and Stegun (2007))



$$J_{\alpha}(iz) = e^{i\frac{\pi}{2}\alpha}I_{\alpha}(z)$$

$$Y_{\alpha}(iz) = e^{i\frac{\pi}{2}(\alpha+1)}I_{\alpha}(z) - \frac{2}{\pi}e^{-i\frac{\pi}{2}\alpha}K_{\alpha}(z)$$

6. Modified Bessel Function Second Order ODE: $I_{\alpha}(x)$ and $K_{\alpha}(x)$ are the two non-linearly independent solutions to the modified Bessel's equation (Abramowitz and Stegun (2007))

$$x^{2}\frac{d^{2}y}{dx^{2}} + x\frac{dy}{dx} - (x^{2} + \alpha^{2})y = 0$$

7. Asymptotic Properties of the Modified Bessel Functions: Unlike the ordinary Bessel functions which are oscillating functions of a real argument, I_{α} and K_{α} are exponentially growing and decaying functions, respectively. Like the ordinary Bessel function J_{α} , the function I_{α} goes to zero at

$$x = 0$$

for

 $\alpha > 0$



and is finite at

x = 0

for

 $\alpha = 0$

Analogously, K_{α} diverges at

x = 0

with the singularity being of the logarithmic type (Greiner and Reinhardt (2009)).

8. <u>Integral Expression for Modified Bessel</u>: Two integral formulas for the modified Bessel functions for

Re(z) > 0

are (Watson (1995)):

$$I_{\alpha}(x) = \frac{1}{\pi} \int_{0}^{\pi} e^{x \cos \theta} \cos \alpha \theta \, d\theta - \frac{\sin \pi \alpha}{\pi} \int_{0}^{\infty} e^{-x \cosh t - \alpha t} \, dt$$

$$K_{\alpha}(x) = \int_{0}^{\infty} e^{-x \cosh t} \cosh \alpha t \, dt$$

9. <u>Zeroth Order Modified Bessel Function</u>: In some calculations in physics, it can be useful to know that the following relation holds:

$$2K_0(\omega) = \int_{-\infty}^{+\infty} \frac{e^{i\omega t}}{\sqrt{t^2 + 1}} dt$$

It can be proven by showing equality to the above integral definition for K_0 . This is done by integrating along a closed curve in the first quadrant of the complex plane.

10. Expressions for $K_{\frac{1}{3}}$ and $K_{\frac{2}{3}}$: Modified Bessel functions for $K_{\frac{1}{3}}$ and $K_{\frac{2}{3}}$ can be represented in terms of rapidly convergently integrals (Khokonov (2004))

$$K_{\frac{1}{3}}(\xi) = \sqrt{3} \int_{0}^{\infty} e^{-\xi \left(1 + \frac{4x^2}{3}\right)\sqrt{1 + \frac{x^2}{3}}} dx$$

$$K_{\frac{2}{3}}(\xi) = \sqrt{3} \int_{0}^{\infty} \frac{2x^2 + 3}{\sqrt{1 + \frac{x^2}{3}}} e^{-\xi \left(1 + \frac{4x^2}{3}\right)\sqrt{1 + \frac{x^2}{3}}} dx$$



- 11. <u>Modified Bessel Function Alternate Names</u>: The *modified Bessel functions of the second kind* has been called by the following names although rare now.
 - a. <u>Basset Function</u> after Alfred Barnard Basset
 - b. Modified Bessel function of the Third Kind
 - c. Modified Hankel function (Teichroew (1957))
 - d. MacDonald function after Hector Munro MacDonald

Spherical Bessel Functions j_n and y_n

1. <u>Helmholtz Equation – Separation of Variables</u>: When solving the Helmholtz equation is spherical coordinates using separation of variables, the radial equation has the form

$$x^{2}\frac{d^{2}y}{dx^{2}} + 2x\frac{dy}{dx} - [x^{2} - n(n+1)]y = 0$$

2. <u>Linearly Independent Spherical Bessel Solutions</u>: The two linearly independent solutions to this equation are called the spherical Bessel functions j_n and y_n , and are related to the ordinary Bessel function J_n and Y_n by (Abramowitz and Stegun (2007))

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x)$$



and

$$y_n(x) = \sqrt{\frac{\pi}{2x}} Y_{n+\frac{1}{2}}(x) = (-1)^{n+1} \sqrt{\frac{\pi}{2x}} J_{-(n+\frac{1}{2})}(x)$$

- 3. <u>Alternate Terminology Spherical Neumann Functions</u>: y_n is also denoted n_n or η_n ; these are also referred to *Spherical Neumann Functions* sometimes.
- 4. <u>Spherical Bessel using Rayleigh Formulas</u>: The spherical Bessel functions can also be written using *Rayleigh formulas* as (Abramowitz and Stegun (2007))

$$j_n(x) = (-x)^n \left(\frac{1}{x} \frac{d}{dx}\right)^n \frac{\sin x}{x}$$

$$y_n(x) = -(-x)^n \left(\frac{1}{x} \frac{d}{dx}\right)^n \frac{\cos x}{x}$$

- 5. $j_0(x)$ becomes Unnormalized *sinc* Function: The first spherical Bessel function $j_0(x)$ is also known as the unnormalized *sinc* function.
- 6. <u>Leading Order Spherical Bessel Functions</u>: The first few spherical Bessel functions are (Abramowitz and Stegun (2007)):

$$j_0(x) = \frac{\sin x}{x}$$



$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$j_2(x) = \left(\frac{3}{x^2} - 1\right) \frac{\sin x}{x} - \frac{\cos x}{x^2}$$

$$j_2(x) = \left(\frac{15}{x^3} - \frac{6}{x}\right) \frac{\sin x}{x} - \left(\frac{15}{x^2} - 1\right) \frac{\sin x}{x}$$

and

$$y_0(x) = -j_{-1}(x) = -\frac{\cos x}{x}$$

$$y_1(x) = j_{-2}(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$y_2(x) = -j_{-3}(x) = \left(-\frac{3}{x^2} + 1\right) \frac{\cos x}{x} - 3\frac{\sin x}{x^2}$$

$$y_3(x) = j_{-4}(x) = \left(\frac{6}{x} - \frac{15}{x^3}\right) \frac{\cos x}{x} - \left(\frac{15}{x^2} - 1\right) \frac{\sin x}{x}$$



Generating Function

The spherical Bessel functions have the generating function (Abramowitz and Stegun (2007))

$$\frac{1}{z}\cos\sqrt{z^2 - 2zt} = \sum_{n=0}^{\infty} \frac{t^n}{n!} j_{n-1}(z)$$

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

Differential Relations

In the following, f_n is any of j_n , y_n , $h_n^{(1)}$, $h_n^{(2)}$ for

$$n = 0, \pm 1, \pm 2, \cdots$$

(Abramowitz and Stegun (2007)):

$$\left(\frac{1}{z}\frac{d}{dz}\right)^{n} z^{n+1} f_n(z) = z^{n-m+1} f_{n-m}(z)$$

$$\left(\frac{1}{z}\frac{d}{dz}\right)^n z^{-n} f_n(z) = (-1)^m z^{-n-m} f_{n+m}(z)$$

Spherical Hankel Functions

1. <u>Spherical Analogues of Hankel Function</u>: There are also spherical analogues of the Hankel functions:

$$h_n^{(1)}(z) = j_n(z) + iy_n(z)$$

$$h_n^{(2)}(z) = j_n(z) - iy_n(z)$$

- 2. <u>Spherical Hankel Closed Trigonometric Forms</u>: In fact, there are simple closed form expressions for Bessel functions of half-integer order in terms of the standard trigonometric functions, and therefore for the original Bessel functions.
- 3. Expression for Non-negative Integers: In particular, for non-negative integers n,

$$h_n^{(1)}(z) = (-i)^{n+1} \frac{e^{iz}}{z} \sum_{m=0}^n \frac{i^m}{m! (2z)^m} \frac{(n+m)!}{(n-m)!}$$



and $h_n^{(2)}(z)$ is the complex conjugate of this – for real z. It follows that, for example, that

$$j_0(x) = \frac{\sin x}{x}$$

and

$$y_0(x) = -\frac{\cos x}{x}$$

and so on.

4. <u>Usage of Spherical Hankel Functions</u>: The spherical Hankel functions appear in problems involving spherical wave propagation, for example, in the multi-pole expansion of the electromagnetic field.

Riccati-Bessel Functions - S_n, C_n, ξ_n, ζ_n

1. <u>Riccati-Bessel Functions – Standard Expressions</u>: Riccati-Bessel functions only differ slightly from spherical Bessel functions:

$$S_n(x) = x j_n(x) = \sqrt{\frac{\pi x}{2}} J_{n+\frac{1}{2}}(x)$$

$$C_n(x) = -xy_n(x) = -\sqrt{\frac{\pi x}{2}}Y_{n+\frac{1}{2}}(x)$$

$$\xi_n(x) = x h_n^{(1)}(x) = \sqrt{\frac{\pi x}{2}} H_{n+\frac{1}{2}}^{(1)}(x) = S_n(x) - iC_n(x)$$

$$\zeta_n(x) = x h_n^{(2)}(x) = \sqrt{\frac{\pi x}{2}} H_{n+\frac{1}{2}}^{(2)}(x) = S_n(x) + iC_n(x)$$

2. Riccati-Bessel Second-Order ODE: They satisfy the differential equation

$$x^{2}\frac{d^{2}y}{dx^{2}} + 2x\frac{dy}{dx} - [x^{2} - n(n+1)]y = 0$$

- 3. <u>Sample Usage #1 Schrodinger Equation</u>: This kind of equation appears in quantum mechanics while solving the radial component of the Schrodinger's equation with hypothetical cylindrical infinite potential barrier (Griffiths and Schroeter (2018)).
- 4. <u>Sample Usage #2 Spherical Setting</u>: The differential equation, as well as the Riccati-Bessel solutions, also arise in the problem of scattering of electromagnetic waves by a sphere, known as Mie scattering after the first publishes solution by Mie (1908). Du (2004) contains recent developments and references.



5. <u>Riccati-Bessel Function Alternate Symbology</u>: Following Debye, the notation ψ_n/χ_n are sometimes instead of S_n/C_n .

Asymptotic Forms

1. Small z Positive αJ_{α} : The Bessel functions have the following asymptotic forms. For small arguments

$$0 < z \ll \sqrt{\alpha + 1}$$

one obtains, where α is not a negative integer (Abramowitz and Stegun (2007)):

$$J_{\alpha}(z) \sim \frac{1}{\Gamma(\alpha+1)} \left(\frac{z}{2}\right)^{\alpha}$$

2. Negative Integer αJ_{α} Asymptote: When α is a negative integer, one gets

$$J_{\alpha}(z) \sim \frac{(-1)^{\alpha}}{(-\alpha)!} \left(\frac{2}{z}\right)^{\alpha}$$



3. Asymptotic Values for Y_{α} across α : For the Bessel function of the second kind, there are three cases:

$$Y_{\alpha}(z) \sim \begin{cases} \frac{2}{\pi} \left[\log \frac{z}{2} + \gamma \right] & \alpha = 0 \\ -\frac{\Gamma(\alpha)}{\pi} \left(\frac{2}{z} \right)^{\alpha} + \frac{1}{\Gamma(\alpha+1)} \left(\frac{2}{z} \right)^{\alpha} \cot \pi \alpha & \text{is a non-positive integer - one term dominates up a is a negative integer} \\ -\frac{(-1)^{\alpha} \Gamma(-\alpha)}{\pi} \left(\frac{z}{2} \right)^{\alpha} \end{cases}$$

where γ is the Euler-Mascheroni constant.

4. <u>Challenge Asymptoting for Large z</u>: For large real arguments

$$z \gg \left| \alpha^2 - \frac{1}{4} \right|$$

one cannot write a true asymptotic form for Bessel functions of the first and the second kind – unless α is a half-integer – because they have zeros all the way out to infinity, which would have to be matched by any asymptotic expansion.

5. Asymptote for a Fixed arg z: However, for a given value of arg z, one can write an equation in terms of $|z|^{-1}$ (Abramowitz and Stegun (2007)):

$$J_{\alpha}(z) \sim \sqrt{\frac{2}{\pi z}} \left[\cos \left(z - \frac{\pi \alpha}{2} - \frac{\pi}{4} \right) + e^{|Im(z)|} \mathcal{O}(|z|^{-1}) \right]$$

$$|\arg z| < \pi$$

$$Y_{\alpha}(z) \sim \sqrt{\frac{2}{\pi z}} \left[\sin \left(z - \frac{\pi \alpha}{2} - \frac{\pi}{4} \right) + e^{|Im(z)|} \mathcal{O}(|z|^{-1}) \right]$$

$$|\arg z| < \pi$$

6. <u>Verification of the Vanishing Asymptote</u>: For

$$\alpha = \frac{1}{2}$$

the last terms in these formulas drop out completely – see the spherical Bessel functions above.

7. Improved Approximation around Specific z: Even though the above expressions are true, better approximations may be available for specific complex z. For example, $J_0(z)$ when z is near the negative real-line is approximated better by

$$J_0(z) \approx \sqrt{\frac{-2}{\pi z}} \cos\left(z + \frac{\pi}{4}\right)$$

than by

$$J_0(z) \approx \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{\pi}{4}\right)$$

8. <u>Asymptotic Forms for Hankel Functions</u>: The asymptotic forms for Hankel functions are:

$$H_{\alpha}^{(1)}(z) \approx \sqrt{\frac{2}{\pi z}} e^{i\left(z - \frac{\pi \alpha}{2} - \frac{\pi}{4}\right)}$$

$$-\pi < \arg z < 2\pi$$

$$H_{\alpha}^{(2)}(z) \approx \sqrt{\frac{2}{\pi z}} e^{-i\left(z - \frac{\pi \alpha}{2} - \frac{\pi}{4}\right)}$$

$$-2\pi < \arg z < \pi$$

- 9. Extensions to other arg z Values: These can be extended to other values of arg z using equations relating $H_{\alpha}^{(1)}(ze^{i\pi m})$ and $H_{\alpha}^{(2)}(ze^{i\pi m})$ to $H_{\alpha}^{(1)}(z)$ and $H_{\alpha}^{(2)}(z)$ (National Institute of Standards and Technology (2019)).
- 10. Caveat Bessel Asymptote from Hankel: It is interesting that although the Bessel function of the first kind is the average of the two Hankel functions, $J_{\alpha}(z)$ is not asymptotic of the two asymptotic forms when z is negative, because one or the other will not be correct here, depending on arg z.



11. Asymptotic J_{α}/Y_{α} for Complex z: But the asymptotic forms of the Hankel functions permit the casting of the asymptotic forms of the Bessel functions of the first and the second kind for complex non-real z so long as |z| goes to infinity at a constant phase angle arg z - using the square root having the positive real part:

$$J_{\alpha}(z) \approx \sqrt{\frac{1}{2\pi z}} e^{i\left(z - \frac{\pi\alpha}{2} - \frac{\pi}{4}\right)}$$

$$-\pi < \arg z < 0$$

$$J_{\alpha}(z) \approx \sqrt{\frac{1}{2\pi z}} e^{-i\left(z - \frac{\pi\alpha}{2} - \frac{\pi}{4}\right)}$$

$$0 < \arg z < \pi$$

$$Y_{\alpha}(z) \approx -i \sqrt{\frac{1}{2\pi z}} e^{i\left(z - \frac{\pi\alpha}{2} - \frac{\pi}{4}\right)}$$

$$-\pi < \arg z < 0$$

$$Y_{\alpha}(z) \approx -i \sqrt{\frac{1}{2\pi z}} e^{-i\left(z - \frac{\pi\alpha}{2} - \frac{\pi}{4}\right)}$$

$$0 < \arg z < \pi$$

12. <u>Modified Bessel Functions' - Asymptotic Forms</u>: For modified Bessel functions, Hankel developed asymptotic large argument expressions as well (Abramowitz and Stegun (2007)):

$$I_{\alpha}(z) \sim \frac{e^{z}}{\sqrt{2\pi z}} \left[1 - \frac{4\alpha^{2} - 1}{8z} + \frac{(4\alpha^{2} - 1)(4\alpha^{2} - 9)}{2!(8z)^{2}} - \frac{(4\alpha^{2} - 1)(4\alpha^{2} - 9)(4\alpha^{2} - 25)}{3!(8z)^{3}} + \cdots \right]$$

for

$$|\arg z| < \frac{\pi}{2}$$

13. $\alpha = \frac{1}{2}$ Special Case for I/K: When

$$\alpha = \frac{1}{2}$$

all terms except the first vanish, and one has



$$I_{\alpha}(z) \sim \sqrt{\frac{2}{\pi z}} \sinh z \sim \frac{e^z}{\sqrt{2\pi z}}$$

for

$$|\arg z| < \frac{\pi}{2}$$

and

$$I_{\alpha}(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}$$

14. <u>Small z Expression for *I/K*</u>: For small arguments

$$0 < z \ll \sqrt{\alpha + 1}$$

one has

$$I_{\alpha}(z) \sim \frac{1}{\Gamma(\alpha+1)} \left(\frac{z}{2}\right)^{\alpha}$$

$$K_{\alpha}(z) \sim \begin{cases} -\ln \frac{z}{2} - \gamma & \alpha = 0\\ \frac{\Gamma(\alpha)}{2} \left(\frac{2}{z}\right)^{\alpha} & \alpha > 0 \end{cases}$$

Full Domain Approximations with Elementary Functions

Very good approximations – error below 0.3% of the maximum value 1 – of the Bessel function J_0 for an arbitrary value of the argument x maybe obtained using the elementary functions by joining the trigonometric approximations for small values of x with the expression containing attenuated cosine functions valid for large arguments with the usage of the smooth transition function $\frac{1}{1+\left(\frac{x}{7}\right)^{20}}$, i.e.,

$$\begin{split} J_0(x) &\approx \left(\frac{1}{6} + \frac{1}{3}\cos\frac{x}{2} + \frac{1}{3}\cos\frac{\sqrt{3}x}{2} + \frac{1}{6}\cos x\right) \frac{1}{1 + \left(\frac{x}{7}\right)^{20}} \\ &+ \sqrt{\frac{2}{\pi|x|}}\cos\left(x - sgn(x)\frac{\pi}{4}\right) \left[1 - \frac{1}{1 + \left(\frac{x}{7}\right)^{20}}\right] \end{split}$$

Properties



1. <u>Laurent-Series Based Generating Function</u>: For integer order

$$\alpha = n$$

 J_n is often defined via a Laurent series for a generating function

$$e^{\frac{x}{2}\left(t-\frac{1}{t}\right)} = \sum_{n=-\infty}^{+\infty} J_n(x)t^n$$

an approach used by P. A. Hansen in 1843. This can be generalized to non-integer order by contour integration or other methods.

2. <u>Integer Order Jacobi Anger Expansion</u>: Another important relation for the integer orders is the *Jacobi-Anger expansion*:

$$e^{iz\cos\phi} = \sum_{n=-\infty}^{+\infty} i^n J_n(z) e^{in\phi}$$

and

$$e^{\pm iz\sin\phi} = J_0(z) + 2\sum_{n=1}^{+\infty} J_{2n}(z)\cos 2n\phi \pm 2\sum_{n=0}^{+\infty} J_{2n+1}(z)\sin([2n+1]\phi)$$



which can be used to expand a plane wave as a sum of cylindrical waves, or to fund the Fourier series of a tone-modulated FM signal.

3. Neumann Expansion for a Function: More generally, the series

$$f(z) = a_{0,\nu}J_{\nu}(z) + 2\sum_{k=1}^{\infty} a_{k,\nu}J_{\nu+k}(z)$$

is called the Neumann expansion of f.

4. Series Coefficients using Neumann Polynomial: The coefficients for

$$\nu = 0$$

have the explicit form

$$a_{k,0} = \frac{1}{2\pi i} \oint_{|z|=c}^{|z|=c} f(z)O_k(z)dz$$

where O_k is the Neumann polynomial (Abramowitz and Stegun (2007)).

5. <u>Representation using the Neumann's Polynomial</u>: Selected functions admit the special representation

$$f(z) = \sum_{k=0}^{\infty} a_{k,\nu} J_{\nu+2k}(z)$$

with

$$a_{k,\nu} = 2(\nu + 2k) \int_{0}^{\infty} f(z) \frac{J_{\nu+2k}(z)}{z} dz$$

as a consequence of the orthogonality relation

$$\int_{0}^{\infty} \frac{J_{\alpha}(z)J_{\beta}(z)}{z} dz = \frac{2}{\pi} \frac{\sin\left(\frac{\pi}{2} [\alpha - \beta]\right)}{\alpha^{2} - \beta^{2}}$$

6. <u>Function Branch Points near Origin</u>: More generally, if *f* has a branch point near origin of such a nature that

$$f(z) = \sum_{k=0} a_k J_{\nu+k}(z)$$

then

$$\mathcal{L}\left[\sum_{k=0}^{\infty} a_k J_{\nu+k}\right](s) = \frac{1}{\sqrt{1+s^2}} \sum_{k=0}^{\infty} \frac{a_k}{\left(s+\sqrt{1+s^2}\right)^{\nu+k}}$$

or

$$\sum_{k=0} a_k \xi^{\nu+k} = \frac{1+\xi^2}{2\xi} \mathcal{L}[f] \left(\frac{1-\xi^2}{2\xi} \right)$$

where $\mathcal{L}[f]$ is the Laplace transform of f (Watson (1995)).

7. <u>Bessel Poison-Mehler-Sonine Form</u>: Another way to define the Bessel function is the Poisson representation formula and the Mehler-Sonine formula:

$$J_{\nu}(z) = \frac{\left(\frac{z}{2}\right)^{\nu}}{\Gamma\left(\nu + \frac{1}{2}\right)\sqrt{\pi}} \int_{-1}^{+1} e^{izs} (1 - s^2)^{\nu - \frac{1}{2}} ds = \frac{2}{\left(\frac{z}{2}\right)^{\nu} \sqrt{\pi} \Gamma\left(\frac{1}{2} - \nu\right)} \int_{1}^{\infty} \frac{\sin zu}{(u^2 - 1)^{\nu + \frac{1}{2}}} du$$

where

$$v > -\frac{1}{2}$$

and





- (Gradshteyn, Ryzhik, Geronimus, Tseytlin, and Jeffrey (2015)). This expression is particularly useful when working with Fourier transforms.
- 8. Orthogonality Consequence of Self-Adjointedness: Because Bessel's equation becomes Hermitian self-adjoint if divided by *z*, the solutions must satisfy an orthogonality relationship for appropriate boundary conditions.
- 9. Explicit Form for Orthogonality Constraint: In particular, it follows that

$$\int_{0}^{1} z J_{\alpha}(z u_{\alpha m}) J_{\alpha}(z u_{\alpha m}) dz = \frac{\delta_{mn}}{2} [J_{\alpha+1}(u_{\alpha m})]^{2} = \frac{\delta_{mn}}{2} [J_{\alpha}'(u_{\alpha m})]^{2}$$

where

$$\alpha > -1$$

 δ_{mn} is the Kronecker delta, and $u_{\alpha m}$ is the m^{th} zero of $J_{\alpha}(z)$.

- 10. Representations using Fourier-Bessel Series: This orthogonality relation can thus be used to extract coefficients in the Fourier-Bessel series, where a function is expanded in the basis of the functions $J_{\alpha}(zu_{\alpha m})$ for fixed α and varying m.
- 11. <u>Representation using Spherical Bessel Basis</u>: An analogous relationship for the spherical Bessel function follows immediately:

$$\int_{0}^{1} z^{2} j_{\alpha}(z u_{\alpha m}) j_{\alpha}(z u_{\alpha n}) dz = \frac{\delta_{mn}}{2} [j_{\alpha+1}(u_{\alpha m})]^{2}$$

12. <u>Hankel Transform of Boxcar Function</u>: Defining the boxcar function of z that depends on a small parameter ϵ as

$$f_{\epsilon}(z) = \epsilon \ rect \left(\frac{z-1}{\epsilon}\right)$$

where rect is the rectangle function, the Hankel transform of $f_{\epsilon}(z)$ of any given order

$$\alpha > -\frac{1}{2}$$

 $g_{\epsilon}(k)$ approaches $J_{\alpha}(k)$ as ϵ approaches zero, for any given k.

13. <u>Hankel Transform of the Result</u>: Conversely, the Hankel transform of the same order of $g_{\epsilon}(k)$ is $f_{\epsilon}(z)$:

$$\int_{0}^{\infty} k J_{\alpha}(kz) g_{\epsilon}(k) dk = f_{\epsilon}(z)$$

which is zero everywhere except near 1.



14. RHS of the Rectangle Function: As ϵ approaches zero, the right-hand side approaches $\delta(z-1)$, where δ is the Dirac delta function. This admits the limit in the distribution sense:

$$\int_{0}^{\infty} k J_{\alpha}(kz) J_{\alpha}(k) dk = \delta(z-1)$$

15. <u>Change of Variables Closure Equation</u>: A change of variables yields the *closure* equation (Arfken and Weber (2005)):

$$\int_{0}^{\infty} x J_{\alpha}(uz) J_{\alpha}(vz) dk = \frac{\delta(u-v)}{u}$$

for

$$\alpha > \frac{1}{2}$$

- 16. <u>Usage of the Hankel Function</u>: The Hankel transform can express a fairly arbitrary function as an integral of Bessel function of different scales.
- 17. <u>Spherical Bessel Function Closure Equation</u>: For spherical Bessel functions, the orthogonality relation is



$$\int_{0}^{\infty} x^{2} j_{\alpha}(uz) j_{\alpha}(vz) dk = \frac{\pi \delta(u-v)}{2u^{2}}$$

for

$$\alpha > -1$$

18. <u>Wronskian of the Bessel Solutions</u>: Another important property of Bessel's equations, which follows from Abel's identity, involves the Wronskian of the solutions:

$$A_{\alpha}(x)\frac{dB_{\alpha}(x)}{dx} - B_{\alpha}(x)\frac{dA_{\alpha}(x)}{dx} = \frac{C_{\alpha}}{x}$$

where A_{α} and B_{α} are any two solutions of the Bessel's equations, and C_{α} is a constant independent of x, but depends on α and the particular Bessel function considered.

19. Explicit Wronskian for Bessel Functions: In particular,

$$J_{\alpha}(x)\frac{dY_{\alpha}(x)}{dx} - Y_{\alpha}(x)\frac{dJ_{\alpha}(x)}{dx} = \frac{2}{\pi x}$$

and



$$I_{\alpha}(x)\frac{dK_{\alpha}(x)}{dx} - K_{\alpha}(x)\frac{dI_{\alpha}(x)}{dx} = -\frac{1}{x}$$

for

$$\alpha > -1$$

20. Zeros of the $x^{-\alpha}J_{\alpha}(x)$ Family: For

$$\alpha > -1$$

the even entire function of genus 1, $x^{-\alpha}J_{\alpha}(x)$ has only real zeros. Let

$$0 < j_{\alpha,1} < j_{\alpha,2} < \dots < j_{\alpha,n}$$

be all its positive zeros, then

$$J_{\alpha}(x) = \frac{\left(\frac{Z}{2}\right)^{\alpha}}{\Gamma(\alpha+1)} \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{j_{\alpha,n}^2}\right)$$



Similar to this, there are a large number of known integrals and identities that can be found in Wikipedia (2019).

Recurrence Relations

1. Adjacency Recurrence Relations for $J_{\alpha}/Y_{\alpha}/H_{\alpha}$: The functions J_{α} , Y_{α} , $H_{\alpha}^{(1)}$, and $H_{\alpha}^{(2)}$ all satisfy the recurrence relations (Abramowitz and Stegun (2007))

$$\frac{2\alpha}{z}Z_{\alpha}(z) = Z_{\alpha+1}(z) + Z_{\alpha-1}(z)$$

and

$$2\frac{dZ_{\alpha}(z)}{dz} = Z_{\alpha+1}(z) - Z_{\alpha-1}(z)$$

where Z_{α} denotes J_{α} , Y_{α} , $H_{\alpha}^{(1)}$, and $H_{\alpha}^{(2)}$.

2. <u>Higher Order Bessel Terms Expansion</u>: The above two expressions are often combined, i.e., added/subtracted, to yield various other relations. This way, Bessel functions of higher order – or higher derivatives – can be computed given the values at the lower orders or derivatives. It follows that (Abramowitz and Stegun (2007))

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m \left[z^{\alpha}Z_{\alpha}(z)\right] = z^{\alpha - m}Z_{\alpha - m}(z)$$

and

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m \left[z^{-\alpha}Z_{\alpha}(z)\right] = (-1)^m z^{-\alpha-m} Z_{\alpha+m}(z)$$

3. <u>Equivalent Modified Bessel Series Generators</u>: *Modified* Bessel functions follow similar relations:

$$e^{\frac{z}{2}\left(t-\frac{1}{t}\right)} = \sum_{n=-\infty}^{+\infty} I_n(z)t^n$$

and

$$e^{z\cos\theta} = I_0(z) + 2\sum_{n=1}^{+\infty} I_n(z)\cos n\theta$$

4. Adjacency Recurrence Relations for I_{α}/K_{α} : The recurrence relation reads

$$C_{\alpha-1}(z) - C_{\alpha+1}(z) = \frac{2\alpha}{z}C_{\alpha}(z)$$



and

$$C_{\alpha+1}(z) + C_{\alpha-1}(z) = 2\frac{dC_{\alpha}(z)}{dz}$$

where $C_{\alpha}(z)$ denotes $I_{\alpha}(z)$ or $e^{i\pi\alpha}C_{\alpha}(z)$. These recurrence relations are useful, among other situations, for discrete diffusion applications.

Multiplication Theorem

1. Multiplication Theorem for J_{ν} : The Bessel function obeys a multiplication theorem

$$\lambda^{-\nu} J_{\nu}(\lambda z) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{(1-\lambda^2)z}{2} \right]^n J_{\nu+n}(z)$$

where λ and ν maybe taken as arbitrary complex numbers (Truesdell (1950), Abramowitz and Stegun (2007)).

2. Multiplication Theorem for Y_{ν} : For

$$|\lambda^2 - 1| < 1$$



(Abramowitz and Stegun (2007)) the above expression also holds if J_{ν} is replaced by Y_{ν} .

3. <u>Multiplication Theorem I_{ν} for K_{ν} </u>: The analogous identities for modified Bessel functions where

$$|\lambda^2 - 1| < 1$$

are

$$\lambda^{-\nu} I_{\nu}(\lambda z) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{(\lambda^2 - 1)z}{2} \right]^n I_{\nu+n}(z)$$

and

$$\lambda^{-\nu} K_{\nu}(\lambda z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left[\frac{(\lambda^2 - 1)z}{2} \right]^n K_{\nu+n}(z)$$

Zeros of the Bessel Function – Bourget's Hypothesis



1. <u>Infinite Zeros of Bessel Functions</u>: Bessel himself originally established that for non-negative integers *n*, the equation

$$J_n(z) = 0$$

has an infinite number of solutions in z (Bessel (1824)). When the functions $J_n(z)$ are plotted on the same graph, though, none of the zeros coincide for different values of n except for the zero at

$$z = 0$$

This phenomenon is known as *Bourget's hypothesis* after the 19th century French mathematician who studied Bessel function.

2. <u>Statement of the Bourget Hypothesis</u>: Specifically, Bourget's hypothesis states that for any integers

$$n \ge 0$$

and

 $m \ge 1$



the functions $J_n(z)$ and $J_{n+m}(z)$ have no common zeros other than the one at

$$z = 0$$

This hypothesis was proved by Carl Ludwig Siegel in 1929 (Watson (1995)).

Numerical Approaches

For numerical studies of the zeros of the Bessel function, see Gil, Segura, and Temme (2007).

References

- Abramowitz, M., and I. A. Stegun (2007): Handbook of Mathematics Functions
 Dover Book on Mathematics
- Arfken, G. B., and H. J. Weber (2005): *Mathematical Methods for Physicists 6th Edition* **Harcourt** San Diego
- Bessel, F. W. (1824): <u>Untersuchung des Theils der planetarischen Störungen</u>
- Culham, J. R. (2004): Bessel Functions of the First and the Second Kind
- Du, H. (2004): Mie-scattering Calculation Applied Optics 43 (9) 1951-1956
- Gerlach, U. (2010): Properties of Hankel and Bessel Functions



- Gil, A., J. Segura, and N. M. Temme (2007): *Numerical Methods for Special Functions* Society for Industrial and Applied Mathematics
- Gradshteyn, I. S., I. M. Ryzhik, Y. V. Geronimus, M. Y. Tseytlin, and A. Jeffrey
 (2015): Tables of Integrals, Series, and Products Academic Press
- Greiner, W., and J. Reinhardt (2009): Quantum Electrodynamics Springer
- Griffiths, D. J., and D. F. Schroeter (2018): *Introduction to Quantum Mechanics 3rd Edition* **Cambridge University Press**
- Khokonov, M. K. (2004): Cascade Processes for Energy Loss by Emission of Hard Photons *Journal of Experimental and Theoretical Physics* **99** (4) 690-707
- Lund, M. (2000): <u>Integral Representations of the Bessel Functions</u>
- Mie, G. (1908): Bietrage zur Optik Truber Medien, Speziall Kolloidaler
 Metalosungen Annalen der Physik 330 (3) 377-445
- National Institute of Standards and Technology (2019): <u>Bessel Functions</u>
- Szego, G. (1975): Orthogonal Polynomials 4th Edition American Mathematical
 Society Providence, RI
- Teichroew, D. (1957): The Mixture of Normal Distribution with Different Variances

 Annals of Mathematical Statistics 28 (2) 510-512
- Temme N. M. (1996): Special Functions: An Introduction to the Classical Functions of Mathematical Physics 2nd Edition Wiley New York
- Truesdell, C. (1950): On Addition and Multiplication Theorems for the Special Functions
- Watson, G. N. (1995): A Treatise on the Theory of Bessel Functions Cambridge
 University Press
- Weber, H. (1873): Ueber eine Darstellung Willkurlicher Functionen durch Bessel'sche Functionen Mathematische Annalen 6 (2) 146-161
- Wikipedia (2019): Bessel Function



Stretched Exponential Function

Introduction and Overview

1. <u>Stretched Exponential Function – Power Law</u>: The stretched exponential function

$$f_{\beta}(t) = e^{-t^{\beta}}$$

is obtained by inserting a fractional power law into the exponential function (Wikipedia (2019)).

2. <u>Stretched Exponential Function - Support Range</u>: In most applications, it is meaningful only for arguments t between 0 and $+\infty$. With

$$\beta = 1$$

the usual exponential function is recovered.

- 3. Ordinate Range for Stretched Response: With the stretching exponent β between 0 and 1, the graph of $\log f$ versus t is characteristically stretched, hence the name of the function.
- 4. <u>Ordinate Range for Compressed Response</u>: The compressed exponential function with

$$\beta > 1$$

has less practical importance, with the notable exception of

$$\beta = 2$$



- which gives the normal distribution.
- 5. <u>Alternate Names and Characteristic Function</u>: The stretched exponential function is also known as the complementary cumulative Weibull distribution in mathematics. The stretched exponential function is also the characteristic function basically the Fourier transform of the Levy symmetric alpha-stable distribution.
- 6. <u>Formulating Relaxation in Disordered Systems</u>: In physics, the stretched exponential function is often used as a phenomenological description of disordered systems.
- 7. <u>Kohlrausch Function Capacitor Discharge Dynamics</u>: It was first introduced by Kohlrausch (1854) to describe the discharge of a capacitor; therefore it is also known as the Kohlrausch function.
- 8. <u>Kohlrausch-Williams-Watts (KWW) Function</u>: Williams and Watts (1970) used the Fourier transform of the stretched exponential to describe dielectric spectra of polymers; in this context, the stretched exponential or its Fourier transform is also called the Kohlrausch-Williams-Watts (KWW) function.
- 9. Practical Usage of Stretched Exponential: In phenomenological applications, it is often not clear whether the stretched exponential function should apply to the differential or the integral distribution function or to neither. In each case one gets the same asymptotic decay, but a different power-law pre-factor, which makes the fits more ambiguous than for simple exponentials. In a few cases (Donsker and Varadhan (1975), Shore and Zwanzig (1975), Takano, Nakanishi, and Miyashita (1988), Brey and Prados (1993)), it can be shown that the asymptotic decay is a stretched exponential, but the pre-factor is usually an unrelated power.

Mathematical Properties

- 1. Relaxation Time Distribution and Mean: Following the usual physical interpretation, the argument t is interpreted as a time, and $f_{\beta}(t)$ is the differential distribution.
- 2. Explicit Expression for the First Moment: One finds



$$\langle \tau \rangle = \int_{0}^{\infty} e^{-\left(\frac{t}{\tau_{K}}\right)^{\beta}} dt = \frac{\tau_{K}}{\beta} \Gamma\left(\frac{1}{\beta}\right)$$

where Γ is the gamma function. For the exponential decay,

$$\langle \tau \rangle = \tau_K$$

is observed.

3. Explicit Expression for Higher Moments: The higher moments of the stretched exponential function are (Gradshteyn, Ryzhik, Geronimus, Tseytlin, and Jeffrey (2015)):

$$\langle \tau^n \rangle = \int_{0}^{\infty} t^{n-1} e^{-\left(\frac{t}{\tau_K}\right)^{\beta}} dt = \frac{\tau_K^n}{\beta} \Gamma\left(\frac{n}{\beta}\right)$$

Mathematical Properties – Distribution Function

- <u>Linear Super-position of Decays</u>: In physics, attempts have been made to explain the stretched exponential behavior as a linear super-position of simple exponential decays.
- 2. <u>Distribution Function for Relaxation Times</u>: this requires a non-trivial distribution of relaxation times, $\rho(u)$, which is defined by

$$e^{-t^{\beta}} = \int_{0}^{\infty} \rho(u)e^{-\frac{t}{u}}dt$$

3. Alternate Relaxation Time Distribution Expression: Alternatively, the distribution

$$G(u) = u\rho(u)$$

is also used.

4. <u>Summation Series Expansion for $\rho(u)$ </u>: $\rho(u)$ can be computed from the series expansion (Lindsey and Patterson (1980), Berberan-Santos, Bodunov, and Valeur (2005))

$$\rho(u) = -\frac{1}{\pi u} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \sin(\pi \beta k) \Gamma(1 + \beta k) u^{\beta k}$$

5. Estimating $\rho(u)$ using Elementary Functions: For rational values of β , $\rho(u)$ can be calculated in terms of elementary functions. But the expression is in general too complex to be useful except for the case

$$\beta = \frac{1}{2}$$

where

$$G(u) = u\rho(u) = \frac{1}{2\sqrt{\pi}}\sqrt{u}e^{-\frac{u}{4}}$$

6. Dirac Delta Nature of G(u): Plotting the results for G(u) in both a linear and a logarithmic representation reveals that the corresponding curves converge to a Dirac delta function that peaks at

$$u = 1$$

as β approaches 1, corresponding to the simple exponential function.



7. Moments $\langle \tau^n \rangle$ using $\rho(\tau)$ Distribution: The moments $\langle \tau^n \rangle$ can also be expressed as

$$\langle \tau^n \rangle = \Gamma(n) \int_0^\infty t^n \rho(\tau) d\tau$$

8. Expansion for First Logarithm Moment: The first moment of the distribution of the simple exponential relaxation times is

$$\langle \log \tau \rangle = \left(1 - \frac{1}{\beta}\right) \gamma + \log \tau_K$$

where γ is the Euler-Mascheroni constant (Zorn (2002)).

Fourier Transform

- Series Expansion of Stretched Exponentials: To describe the results from
 spectroscopy or inelastic scattering, the sine or the cosine of the Fourier transform of
 the stretched exponential function is needed. It must be calculated either by numerical
 integration, or from a series expansion. The series here as well as the one used for
 the distribution function are special cases of the Fox-Wright function (Hilfer
 (2002)).
- 2. <u>Numerical Computation of the Fourier Transform</u>: For practical purposes, the Fourier transform may be approximated by the Havriliak-Negami function (Alvarez, Alegria, and Colmenero (1991)), though nowadays the numerical computation can be done efficiently (Wuttke (2002)) that there is no longer a reason not to use the Kohlrausch-Williams-Watts function in the frequency domain.

Further Applications



- Earlier Use of Stretched Exponentials: As seen earlier, the stretched exponential
 function was introduced to describe the discharge of a capacitor Leyden jar that
 used glass as dielectric medium. The next documented usage is by Friedrich
 Kohlrausch, son of Rudolf Kohlrausch, to describe torsional relaxation. A. Werner
 used it in 1907 to describe complex luminescence decays; Theodor Forster used ii in
 1949 as the fluorescence decay law of electronic energy donors.
- 2. <u>Usage Outside Condensed Matter Systems</u>: Outside condensed matter physics, the stretched exponential has been used to describe the removal rates of small, stray bodies in the solar system (Dobrovolskis, Alvarellos, and Lissauer (2007)), the diffusion-weighted MRI signals in the brain (Bennett, Schmainda, Tong, Rowe, Lu, and Hyde (2003)), and production from unconventional gas wells (Valko and Lee (2010)).

Use in Probability

If the integrated distribution is a stretched exponential, the normalized probability density function is given by

$$p(\tau|\lambda,\beta) = \frac{\lambda}{\Gamma\left(1 + \frac{1}{\beta}\right)} e^{-(\tau\lambda)^{\beta}}$$

It may be noted that some authors confusingly use the term *stretched exponential* to refer to the Weibull distribution (Sornette (2004)).

Modified Stretched Exponential

The modified stretched exponential function



$$f_{\beta}(t) = e^{-t^{\beta(t)}}$$

with a slowly t-dependent exponent $\beta(t)$ has been used for biological survival curves (Weon and Je (2009), Weon (2016)).

References

- Alvarez, F., A. Alegria, and J. Colmenero (1991): Relationship between the Time Domain Kohlrausch-Williams-Watts and the Frequency-Domain Havriliak-Negami Relaxation Functions *Physical Review B* 44 (14) 7306-7312
- Bennett, K. M., K. M. Schmainda, R. B. Tong, D. B. Rowe, H. Lu, and J. S. Hyde
 (2003): Characterization of Continuously Distributed Cortical Water Diffusion Rates
 with a Stretched-Exponential Model *Magnetic Resonance in Medicine* 50 (4) 727-734
- Berberan-Santos, M. N., E. N. Bodunov, and B. Valeur (2005): Mathematical
 Functions for the Analysis of Luminescence Decays with Underlying Distributions –
 Kohlrausch Decay Function (Stretched Exponential) *Chemical Physics* 315 (1) 171182
- Brey, J. J., and A. Prados (1993): Stretched Exponential Decay at Intermediate Times in the One-dimensional Ising Model at Low Temperatures *Physica A* 197 (4) 569-582
- Dobrovolskis, A. R., J. L. Alvarellos, and J. J. Lissauer (2007): Lifetimes of Small Bodies in Planeto-centric or Helio-centric Orbits *Icarus* 188 (2) 481-505
- Donsker, M. D., and S. R. S. Varadhan (1975): Asymptotic Evaluation of certain Markov Process Expectations for Large Time Communications on Pure and Applied Mathematics 28 (1) 1-47
- Gradshteyn, I. S., I. M. Ryzhik, Y. V. Geronimus, M. Y. Tseytlin, and A. Jeffrey (2015): *Tables of Integrals, Series, and Products* **Academic Press**



- Hilfer, J. (2002): H-function Representations for Stretched Exponential Relaxation and non-Debye Susceptibilities in Glassy Systems *Physical Review E* **65** (6) 061510
- Kohlrausch, R. (1854): Theorie des Elektrischen Ruckstandes in der Leidner Flasche
 Annalen der Physik und Chemie 91 56-82, 179-213
- Lindsey, C. P., and G. D. Patterson (1980): Detailed Comparison of the Williams-Watts and the Cole-Davidson Functions *Journal of Chemical Physics* 73 (7) 3348-3357
- Shore, J. E., and R. Zwanzig (1975): Dielectric Relaxation and Dynamic Susceptibility of a One-dimensional Model for Perpendicular Dipole Polymers Journal of Chemical Physics 63 (12) 5445-5458
- Sornette, D. (2004): Critical Phenomena in Natural Sciences Springer
- Takano, H., H. Nakanishi, and S. Miyashita (1988): Stretched Exponential Decay of the Spin-Correlation Function in the Kinetic Ising Model below the Critical Temperature *Physical Review B* 37 (7) 3716-3719
- Valko, P. P., and W. J. Lee (2010): <u>A Better Way To Forecast Production From</u> Unconventional Gas Wells
- Weon, B. M., and J. H. Je (2009): Theoretical Estimation of Maximum Human Lifespan *Biogerontology* **10** (1) 65-71
- Weon, B. M. (2016): Tyrannosaurs as long-lived species
- Wikipedia (2019): <u>Stretched Exponential Function</u>
- Williams, G., and D. C. Watts (1970): Non-symmetrical Dielectric Relaxation Behavior arising from a simple Empirical Decay Function *Transaction of the* Faraday Society 66 80-85
- Wuttke, J. (2012): Laplace-Fourier Transform of the Stretched Exponential Function: Analytic Error-Bounds, Double Exponential Transform, and Open Source Implementation libkww *Algorithm* 5 (4) 604-628
- Zorn, R. (2002): Logarithmic Moments of Relaxation Time Distributions *Journal of Chemical Physics* 116 (8) 3204-3209



Error Function

Introduction and Overview

- 1. What is an Error Function? The **error function** also called the **Gaussian Error Function** is a special non-elementary function of sigmoidal shape that occurs in probability, statistics, and partial differential equations describing diffusion (Wikipedia (2019)).
- 2. <u>Definition of the Error Function</u>: It is defined as (Greene (1993), Andrews (1998))

$$\operatorname{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^{x} e^{-t^2} dt = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt$$

- 3. Interpretation of the Error Function: In statistics, for non-negative values of x, the error function has the following interpretation: for a random variable Y that is normally distributed with a mean 0 and variance 0.5, describes the probability of Y falling in the range [-x, x].
- 4. <u>Function Related to erf</u>: There are several closely related functions, such as the complementary error function, the imaginary error function, and others.

Name



- 1. Origin of erf and erfc: The name *error function* and its abbreviation erf were proposed by J. W. L. Glaisher in 1871 on account of its connection with "the Theory of Probability, and notably the Theory of Errors" (Glaisher (1871a)). The error function complement was also discussed by Glaisher in a separate publication in the same year (Glaisher (1871b)).
- 2. <u>Error Density Law of Facility</u>: For the Law of Facility of errors whose density is given by a normal distribution

$$f(x) = \sqrt{\frac{c}{\pi}} e^{-cx^2}$$

Glaisher calculates the chance of an error lying between p and q as

$$\sqrt{\frac{c}{\pi}} p \int_{p}^{q} e^{-cx^{2}} dx = \frac{1}{2} \left[\operatorname{erf}(q\sqrt{c}) - \operatorname{erf}(p\sqrt{c}) \right]$$

Applications

1. Error Statistics Distribution from Measurements: When the results of a series of experiments is described by a normal distribution with standard deviation σ and expected value 0, then $\operatorname{erf}\left(\frac{a}{\sigma\sqrt{2}}\right)$ is the probability that the error of a single measurement lies between -a and +a for a positive a. This is useful, for example, in determining the bit error-rate if a digital communication system.



- 2. <u>Heaviside Step Function Boundary Conditions</u>: The error and the complementary error functions occur, for example, in solutions to the heat transfer equation when the boundary conditions are given by the Heaviside step function.
- 3. <u>Cumulative Probability such that X < L</u>: The error function and its approximations can be used to estimate results that hold with high probability. Given a variable

$$X \sim \mathcal{N}(\mu, \sigma)$$

and constant

$$L < \mu$$

$$\mathbb{P}[X \le L] = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{L - \mu}{\sqrt{2}\sigma}\right) \approx Ae^{-B\left(\frac{L - \mu}{\sigma}\right)^{2}}$$

where A and B are certain numeric constants.

4. <u>Asymptote of the Cumulative Probability</u>: If *L* is sufficiently far from the mean, i.e., if

$$\mu - L \ge \sigma \sqrt{\ln k}$$

then

$$\mathbb{P}[X \le L] \le Ae^{-B\ln k} = \frac{A}{k^B}$$

so the probability goes to 0 as

$$k \to \infty$$



Properties

1. erf is an Odd Function: The property

$$\operatorname{erf}(-z) = -\operatorname{erf}(z)$$

means that the error function is an odd function. This directly comes about from the fact that the integrand e^{-t^2} is an even function.

2. <u>erf is Self-Complex Conjugate</u>: For any complex number z

$$\operatorname{erf}(\bar{z}) = \overline{\operatorname{erf}(z)}$$

where \bar{z} is the complex conjugate of z.

3. <u>erf Asymptotic Behavior at $\pm \infty$ </u>: The error function at $+\infty$ is exactly 1. At the real axis, erf(z) approaches unity at

$$z \to +\infty$$

and -1 at

$$z \to -\infty$$

At the imaginary axis, it tends to $\pm i \infty$

Taylor Series



- erf Holomorphic Everywhere Except at ±∞: The error function is an entire function; it has no singularities except those at infinity, and its Taylor expansion always converges.
- 2. <u>MacLaurin Polynomial Series for erf</u>: The defining integral cannot be evaluated in closed form in terms of elementary functions, but by expanding the integrand e^{-x^2} into its MacLaurin series and integrating it term by term, one obtains the error function's MacLaurin series as:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{n+1}}{n! (2n+1)} = \frac{2}{\sqrt{\pi}} \left(z - \frac{z^3}{3} + \frac{z^5}{10} - \frac{z^7}{42} + \frac{z^9}{216} - \cdots \right)$$

which holds for every complex number z.

3. <u>Alternative Formulation of the MacLaurin Series</u>: For iterative calculation of the above series, the following alternative formulation may be useful.

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \left[z \prod_{k=1}^{n} \frac{-(2k-1)z^2}{k(2k+1)} \right] = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \left[\frac{z}{2n+1} \prod_{k=1}^{n} \frac{-z^2}{k} \right]$$

because $\frac{-(2k-1)z^2}{k(2k+1)}$ expresses the multiplier to turn the k^{th} term into the $(k+1)^{th}$ term, considering z as the first term.

4. <u>Imaginary Error Function MacLaurin Series</u>: The imaginary error function has a very similar MacLaurin series, which is

$$\operatorname{erfi}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{n+1}}{n! (2n+1)} = \frac{2}{\sqrt{\pi}} \left(z + \frac{z^3}{3} + \frac{z^5}{10} + \frac{z^7}{42} + \frac{z^9}{216} + \cdots \right)$$

which holds for every complex number z.



Derivative and Integral

1. <u>Derivative of the Error Function</u>: The derivative of the error function follows immediately from its definition:

$$\frac{d}{dz}\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}}e^{-z^2}$$

2. <u>Derivative of the Imaginary Error Function</u>: The derivative of the imaginary error function follows immediately from its definition:

$$\frac{d}{dz}\operatorname{erfi}(z) = \frac{2}{\sqrt{\pi}}e^{z^2}$$

- 3. <u>Anti-derivative of the Error Function</u>: An anti-derivative of the error function, obtainable by integration by parts, is $z \operatorname{erf}(z) + \frac{e^{-z^2}}{\sqrt{\pi}}$
- 4. <u>Anti-derivative of the Imaginary Error Function</u>: An anti-derivative of the error function, obtainable by integration by parts, is $z \operatorname{erfi}(z) \frac{e^{z^2}}{\sqrt{\pi}}$
- 5. <u>Higher Order Error Function Derivatives</u>: Higher order derivatives are given by

$$\operatorname{erf}_{k}(z) = \frac{2}{\sqrt{\pi}} \frac{d^{k-1}}{dz^{k-1}} e^{-z^{2}} = \frac{2(-1)^{k-1}}{\sqrt{\pi}} H_{k-1}(z) e^{-z^{2}}$$

where

$$k = 1, 2, \cdots$$



and *H* are the physicists' Hermite polynomials.

Burmann Series

1. <u>The Hans Heinrich Burmann Theorem</u>: An expansion, which converges more rapidly for all real values of *x* than the Taylor expansion, is obtained by using the Hans Heinrich Burmann's theorem (Schopf and Supancic (2014)):

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} sgn(x) \sqrt{1 - e^{-x^2}} \left[1 - \frac{1}{12} (1 - e^{-x^2}) - \frac{7}{480} (1 - e^{-x^2})^2 - \frac{5}{896} (1 - e^{-x^2})^3 - \frac{787}{276480} (1 - e^{-x^2})^4 - \dots \right]$$
$$= \frac{2}{\sqrt{\pi}} sgn(x) \sqrt{1 - e^{-x^2}} \left(\frac{\sqrt{\pi}}{2} + \sum_{k=1}^{\infty} c_k e^{-kx^2} \right)$$

2. <u>Approximation using the Two Leading Terms</u>: By keeping only the first two coefficients and choosing

$$c_1 = \frac{31}{200}$$

and

$$c_2 = -\frac{341}{8000}$$

the resulting approximation shows its largest relative error at

$$x = \pm 1.3796$$

where it is less than 3.6127×10^{-3} :

$$\operatorname{erf}(x) \approx \frac{2}{\sqrt{\pi}} sgn(x) \sqrt{1 - e^{-x^2}} \left(\frac{\sqrt{\pi}}{2} + \frac{31}{200} e^{-x^2} - \frac{341}{8000} e^{-2x^2} \right)$$

Inverse Functions

1. <u>Non-Unique Imaginary-Valued Solutions</u>: Given a complex number *z*, there is not a *unique* complex number *w* satisfying

$$\operatorname{erf}(w) = z$$

so a true inverse function would be multi-valued.

2. <u>Unique Real-Valued Inverse Solutions</u>: However, for

$$-1 < x < 1$$

there is a unique real number denoted $erf^{-1}(x)$ satisfying

$$\operatorname{erf}(\operatorname{erf}^{-1}(x)) = x$$

3. <u>Domain of the Inverse Error Function</u>: The **inverse error function** is usually defined in the domain (-1, 1), and it is restricted to this domain in many computer algebra systems.



4. Complex Domain of Error Functions: However, it can be extended to the disk

of the complex plane, using the MacLaurin series

$$\operatorname{erf}^{-1}(z) = \sum_{k=0}^{\infty} \frac{c_k}{2k+1} \left(\frac{\sqrt{\pi}}{2}z\right)^{2k+1}$$

where

$$c_0 = 1$$

and

$$c_k = \sum_{m=0}^{k-1} \frac{c_m c_{k-1-m}}{(m+1)2(m+1)} = \left\{1, 1, \frac{7}{6}, \frac{127}{90}, \frac{4369}{2520}, \frac{34807}{16200}, \dots\right\}$$

5. Polynomial Series Expansion of $erf^{-1}(z)$: Thus, one has the following series expansion. Note that the common factors have been canceled from the numerator and the denominator:

$$\operatorname{erf}^{-1}(z) = \frac{\sqrt{\pi}}{2} \left(z + \frac{\pi}{12} z^3 + \frac{7\pi^2}{480} z^5 + \frac{127\pi^3}{40320} z^7 + \frac{4369\pi^4}{5806080} z^9 + \frac{34807\pi^5}{182476800} z^{11} + \cdots \right)$$

Note that the error function's value at $\pm \infty$ is equal to ± 1 .

6. Caveat on Recovering the z: For



|z| < 1

one has

$$\operatorname{erf}(\operatorname{erf}^{-1}(z)) = z$$

7. The Inverse Complementary Error Function: The inverse complementary error function is defined as

$$\operatorname{erfc}^{-1}(1-z) = \operatorname{erf}^{-1}(z)$$

8. The Inverse Imaginary Error Function: For real x, there is a unique real number $erfi^{-1}(x)$ satisfying

$$erfi(erfi^{-1}(x)) = x$$

The inverse imaginary error function is defined as $erfi^{-1}(x)$ (Bergsma (2006)).

9. <u>MacLaurin Series Expansion for x</u>: For any real x, Newton's method can be used to compute $erfi^{-1}(x)$, and for

$$-1 \le x \le 1$$

the following MacLaurin series converges:

$$erfi^{-1}(x) = \sum_{k=0}^{\infty} \frac{(-1)^k c_k}{2k+1} \left(\frac{\sqrt{\pi}}{2}x\right)^{2k+1}$$

where c_k is defined as above.



Asymptotic Expansion

 Asymptotic Expansion for erfc(x): A useful asymptotic expansion of the complementary error function – and therefore also of the error function – for large real x is

$$\operatorname{erfc}(x) = \frac{e^{-x^2}}{x\sqrt{\pi}} \left[1 + \sum_{n=1}^{\infty} (-1)^n \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2x^2)^n} \right] = \frac{e^{-x^2}}{x\sqrt{\pi}} \left[\sum_{n=1}^{\infty} (-1)^n \frac{(2n-1)!!}{(2x^2)^n} \right]$$

where (2n-1)!! is the double factorial of (2n-1), which is the product of all odd numbers up to (2n-1).

2. Finite erfc Remainder Error in the Landau Notation: This series diverges for every finite x, and its meaning as asymptotic expansion is that, for any

$$N \in \mathbb{N}$$

on has

$$\operatorname{erfc}(x) = \frac{e^{-x^2}}{x\sqrt{\pi}} \left[\sum_{n=1}^{\infty} (-1)^n \frac{(2n-1)!!}{(2x^2)^n} \right] + R_N(x)$$

where the remainder, in Landau notation, is

$$R_N(x) = \mathcal{O}(x^{1-2N}e^{-x^2})$$

as



$$\chi \to \infty$$

3. Exact Value of the Error Remainder: Indeed, the exact value of the remainder is

$$R_N(x)
displane
eq \frac{(-1)^N}{\sqrt{\pi}} 2^{1-2N} \frac{(2N)!}{N!} \int_{x}^{\infty} t^{-2N} e^{-t^2} dt$$

which follows easily by induction, writing

$$e^{-t^2} = -(2t)^{-1} (e^{-t^2})'$$

and integrating by parts.

4. Approximation for Small/Large x: For large enough values of x, only the first few terms of this asymptotic expansion are needed to obtain a good approximate of erfc(x) while for not too large values for x, it can be noted that the above Taylor expansion at 0 provides a very fast convergence.

Continued Fraction Expansion

A continued fraction expansion of the complementary error function is (Cuyt, Petersen, Vigdis, Verdonk, Waadeland, and Jones (2008)):

$$\operatorname{erfc}(x) = \frac{z}{\sqrt{\pi}} e^{-x^2} \frac{1}{z^2 + \frac{a_1}{1 + \frac{a_2}{z^2 + \frac{a_3}{1 + \dots}}}}$$

$$a_m = \frac{m}{2}$$

Integral of Error Function with Gaussian Density Function

$$\int_{-\infty}^{\infty} \operatorname{erf}(ax+b) \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = \operatorname{erf}\left(\frac{a\mu+b}{\sqrt{1+2a^2\sigma^2}}\right)$$

$$a, b, \mu, \sigma \in \mathbb{R}$$

Factorial Series

1. The erfc Inverse Factorial Series: The inverse factorial series

$$\operatorname{erfc}(z) = \frac{e^{-z^2}}{z\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n Q_n}{(z^2+1)^{\bar{n}}} = \frac{e^{-z^2}}{z\sqrt{\pi}} \left[1 - \frac{1}{2} \frac{1}{(z^2+1)} + \frac{1}{2} \frac{1}{(z^2+1)(z^2+2)} + \cdots \right]$$

converges for

$$Re(z^2) > 0$$



2. <u>Definition of Rising Factorial Components</u>:

$$Q_n \triangleq \frac{1}{\Gamma\left(\frac{1}{2}\right)} \int_0^\infty \tau(\tau - 1) \cdots (\tau - n + 1) \frac{e^{-\tau}}{\sqrt{\tau}} d\tau = \sum_{k=0}^n \left(\frac{1}{2}\right)^{\bar{k}} s(n, k)$$

 $z^{\bar{n}}$ denotes the rising factorial, and s(n, k) denotes a signed Stirling number of the first kind (Schlomilch (1859), Nielson (1906)).

Numerical Approximations – Approximation with Elementary Functions

Abramowitz and Stegun Family of Functions: Abramowitz and Stegun (2007)
provide several approximations of varying accuracy. This allows one to choose the
fastest approximation suitable for a given application. In order of increasing accuracy,
they are:

a.

$$\operatorname{erf}(x) \approx 1 - \frac{1}{(1 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4)^4}$$

$$x \ge 0$$

with maximum error of 5×10^{-4} where

$$a_1 = 0.278393$$



$$a_2 = 0.230389$$

$$a_3 = 0.000972$$

$$a_4 = 0.078108$$

b.

$$\operatorname{erf}(x) \approx 1 - (1 + a_1 t + a_2 t^2 + a_3 t^3) e^{-x^2}$$

$$t = \frac{1}{1 + px}$$

$$x \ge 0$$

with maximum error of 2.5×10^{-5} where

$$a_1 = 0.3480242$$

$$a_2 = -0.0958798$$

$$a_3 = 0.7478556$$

$$p = 0.47047$$

c.

$$\operatorname{erf}(x) \approx 1 - \frac{1}{(1 + a_1 x + a_2 x^2 + \dots + a_6 x^6)^{16}}$$

$$x \ge 0$$



with maximum error of 3×10^{-7} where

$$a_1 = 0.0705230784$$

$$a_2 = 0.0422820123$$

$$a_3 = 0.0092705272$$

$$a_4 = 0.0001520143$$

$$a_5 = 0.0002765672$$

$$a_6 = 0.0000430638$$

d.

$$\operatorname{erf}(x) \approx 1 - (1 + a_1 t + a_2 t^2 + \dots + a_5 t^5) e^{-x^2}$$

$$t = \frac{1}{1 + px}$$

$$x \ge 0$$

with maximum error of 1.5×10^{-7} where

$$a_1 = 0.254829592$$

$$a_2 = -0.284496736$$

$$a_3 = 1.421413741$$

$$a_4 = -1.453152027$$

$$a_5 = 1.061405429$$

$$p = 0.3275911$$

2. <u>Usage for Positive Negative x</u>: All of the approximations are valid for

To use these approximations for negative x, use the fact that erf(x) is an odd function, so

$$\operatorname{erf}(x) = -\operatorname{erf}(-x)$$

3. <u>Pure Exponential Approximation and Bounds</u>: Exponential bounds and a pure exponential approximation for the complementary error function are given by Chiani, Dardari, and Simon (2003):

$$\operatorname{erfc}(x) \le \frac{1}{2}e^{-2x^2} + \frac{1}{2}e^{-x^2} \le e^{-x^2}$$

$$\operatorname{erfc}(x) \approx \frac{1}{2}e^{-x^2} + \frac{1}{2}e^{-\frac{4}{3}x^2}$$

4. <u>Karagiannidis and Lioumpas erfc Approximation</u>: A tight approximation of the complementary error function for



$$x \in [0, \infty)$$

is given by Karagiannidis and Lioumpas (2007) who showed that, for the appropriate choice of parameters $\{A, B\}$

$$\operatorname{erfc}(x) \approx e^{-x^2} \frac{1 - e^{-Ax}}{B\sqrt{\pi}x}$$

They determined that

$${A,B} = {1.98, 1.135}$$

which gave a good approximation for all

$$x \ge 0$$

5. <u>Single Term Lower erfc Bound</u>: A single-term lower bound is from Chang, Cosman, and Milstein (2011):

$$\operatorname{erfc}(x) \ge \sqrt{\frac{2e}{\pi}} \frac{\sqrt{\beta - 1}}{\beta} e^{-\beta x^2}$$

$$x \ge 0$$

$$\beta > 1$$

where the parameter β can be picked to minimize error on the desired interval of approximation.

6. Winitzki Approximation for erf: Another approximation is given by

$$\operatorname{erf}(x) \approx sgn(x) \sqrt{1 - e^{-x^2 \frac{\frac{4}{\pi} + ax^2}{1 + ax^2}}}$$

where

$$a = \frac{8(\pi - 3)}{3\pi(4 - \pi)} \cong 0.140012$$

7. Performance of the Winitzki Approximation: This is designed to be very accurate in the neighborhood of 0 and in the neighborhood of infinity, and the error is less than 0.00035 for all *x*. Using the alternate value

$$a \approx 0.147$$

reduces the maximum error to about 0.00012 (Winitzki (2008)).

8. <u>Winitzki Approximation for erf⁻¹</u>: This approximation can also be inverted to calculate the inverse error function:

$$\operatorname{erf}^{-1}(x) \approx sgn(x) \sqrt{\left[\frac{2}{\pi a} + \frac{\ln(1-x^2)}{2}\right]^2 - \frac{\ln(1-x^2)}{a}} - \left[\frac{2}{\pi a} + \frac{\ln(1-x^2)}{2}\right]$$

Polynomial



An approximation with a maximal error of 1.2×10^{-7} for any real argument (Press, Teukolsky, Vetterling, and Flannery (2007))

$$\operatorname{erf}(x) = \begin{cases} 1 - \tau & x \ge 0 \\ \tau - 1 & x < 0 \end{cases}$$

with

$$\tau = t \cdot \exp\{-x^2 - 1.26551223 + 1.00002368t + 0.37409196t^2 + 0.09678418t^3 - 0.18628806t^4 + 0.27886807t^5 - 1.13520398t^6 + 1.48851587t^7 - 0.82215223t^8 + 0.17087277t^9\}$$

and

$$t = \frac{1}{1 + 0.5|x|}$$

Table of Values

x	erf(x)	$1 - \operatorname{erf}(x)$
0.00	0	1



0.02	0.022 564 575	0.977 435 425
0.04	0.045 111 106	0.954 888 894
0.06	0.067 621 594	0.932 378 406
0.08	0.090 078 126	0.909 921 874
0.10	0.112 462 916	0.887 537 084
0.20	0.222 702 589	0.777 297 411
0.30	0.328 626 759	0.671 343 241
0.40	0.428 392 355	0.571 607 645
0.50	0.520 499 878	0.479 500 122
0.60	0.603 856 091	0.396 143 909
0.70	0.677 801 194	0.322 198 806
0.80	0.742 100 965	0.257 899 035
0.90	0.796 908 212	0.203 091 788
1.00	0.842 700 793	0.157 299 207
1.10	0.880 205 070	0.119 794 930
1.20	0.910 313 978	0.089 686 022
1.30	0.934 007 945	0.065 992 055
1.40	0.952 285 120	0.047 714 880
1.50	0.966 105 146	0.033 894 854
1.60	0.976 348 383	0.023 651 617



1.70	0.983 790 459	0.016 209 541
1.80	0.989 090 502	0.010 909 498
1.90	0.992 790 429	0.007 209 571
2.00	0.995 322 265	0.004 677 735
2.10	0.997 020 533	0.002 979 467
2.20	0.998 137 154	0.001 862 846
2.30	0.998 856 823	0.001 143 177
2.40	0.999 311 486	0.000 688 514
2.50	0.999 593 048	0.000 406 952
3.00	0.999 977 910	0.000 022 090
3.50	0.999 999 257	0.000 000 743

Related Functions – Complementary Error Function

 Scaled/Unscaled Complementary Error Function: The complementary error function, denoted erfc, is defined as

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^{2}} dt = e^{-x^{2}} \operatorname{erfcx}(x)$$



which also defines erfcx, the **scaled complementary error function** (Cody (1993)), which can be used instead of erfc to avoid arithmetic underflow (Cody (1993), Zaghloul (2007)).

2. Craig's Formula Version of erfc: Another form of erfc(x) for non-negative x is known as Craig's formula, after its discoverer (Craig (1991)):

$$\operatorname{erfc}(x|x \ge 0) = \frac{2}{\pi} \int_{0}^{\frac{\pi}{2}} e^{-\frac{x^2}{\sin^2 \theta}} d\theta$$

3. Benefits of using Craig's Formula: This expression is valid only for positive values of *x*, but it can be used in conjunction with

$$\operatorname{erfc}(x) = 2 - \operatorname{erfc}(-x)$$

to obtain $\operatorname{erfc}(x)$ for negative values. This form is advantageous in that the imaginary range of integration is fixed and finite.

Imaginary Error Function

1. <u>Definition of the Imaginary Error Function</u>: The **imaginary error function**, denoted erfi, is defined as

$$\operatorname{erfi}(x) = -i \cdot \operatorname{erf}(ix) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{t^{2}} dt = \frac{2}{\sqrt{\pi}} e^{x^{2}} D(x)$$



- where D(x) is the Dawson function, which can be used instead of erfi to avoid arithmetic overflow (Cody (1993)).
- 2. <u>erfi when x is Real</u>: Despite the name *imaginary error function*, erfi(x) is real when x is real.
- 3. <u>Faddeeva Complex Error Function Definition</u>: When the error function is evaluated for arbitrary complex arguments *z*, the resulting complex error function is usually discussed in a scaled form as the Faddeeva function:

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz) = \operatorname{erfcx}(-iz)$$

Cumulative Distribution Function

- 1. Standard Normal Cumulative Distribution Function: The error function is essentially identical to the standard normal cumulative distribution function, denoted Φ , also named norm (x) by software languages, as they differ only by scaling and translation.
- 2. Relation between CDF and erf: Indeed

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt = \frac{1}{2} \left[1 + \text{erf}\left(\frac{x}{\sqrt{2}}\right) \right] = \frac{1}{2} \text{erf}\left(-\frac{x}{\sqrt{2}}\right)$$

or, re-arranging for erf and erfc:

$$\operatorname{erf}(x) = 2 \cdot \Phi(x\sqrt{2}) - 1$$

$$\operatorname{erfc}(x) = 2 \cdot \Phi(-x\sqrt{2}) = 2[1 - \Phi(x\sqrt{2})]$$



3. <u>Relation between erf and Q-function</u>: Consequently, the error function is also closely related to the Q-function, which is the tail probability of the standard normal distribution. The Q-function can be expressed in terms of the error function as

$$Q(x) = \frac{1}{2} \left[1 - \operatorname{erf}\left(\frac{x}{\sqrt{2}}\right) \right] = \frac{1}{2} \operatorname{erfc}\left(\frac{x}{\sqrt{2}}\right)$$

4. Relation between erf⁻¹ and Probit: The inverse of Φ is known as the normal quantile function, or the probit function, and may be expressed in terms of the inverse error function as

$$Probit(p) = \Phi^{-1}(p) = \sqrt{2} \operatorname{erf}^{-1}(2p - 1) = -\sqrt{2} \operatorname{erfc}^{-1}(2p)$$

- 5. <u>Usage of CDF and erf</u>: The standard normal CDF is used more often in probability and statistics, and the error function is used more often in other branches of mathematics.
- 6. Special Case of Mittag-Lefler Function: The error function is a special case of the Mittag-Lefler function, and can also be expressed as a confluent hypergeometric function (Kummer's function):

$$\operatorname{erf}(x) = \frac{2x}{\sqrt{\pi}} \mathcal{M}\left(\frac{1}{2}, \frac{3}{2}, -x^2\right)$$

This has a simple expression in terms of the Fresnel integral.

 Relation between erf and Gamma Function: In terms of the regularized gamma function P and the regularized gamma function γ

$$\operatorname{erf}(x) = \operatorname{sgn}(x)\mathcal{P}\left(\frac{1}{2}, x^2\right) = \frac{\operatorname{sgn}(x)}{\sqrt{\pi}}\gamma\left(\frac{1}{2}, x^2\right)$$



where sgn(x) is the sign function.

Generalized Error Functions

1. <u>Expression for Generalized Error Function</u>: Some authors discuss the more general functions:

$$E_n(x) = \frac{n!}{\sqrt{\pi}} \int_0^x e^{-t^n} dt = \frac{n!}{\sqrt{\pi}} \sum_{p=0}^{\infty} (-1)^p \frac{x^{np+1}}{(np+1)p!}$$

- 2. Special Cases of Generalized Error Functions:
 - a. $E_0(x)$ is a straight line through the origin:

$$E_0(x) = \frac{x}{\sqrt{\pi}}$$

- b. $E_2(x)$ is the error function erf(x)
- 3. Similarity Among Odd/Even Error Exponents: After division by n!, all E_n for odd n look similar but not identical to each other. Similarly, all E_n for even n look similar but not identical to each other after a division by n!. All other generalized error functions look similar to each other on the positive x side of the graph.
- 4. <u>From Standard/Incomplete Gamma Function</u>: These generalized functions can be equivalently expressed for



using the gamma function and the incomplete gamma function:

$$E_n(x) = \frac{1}{\sqrt{\pi}} \Gamma(n) \left[\Gamma\left(\frac{1}{n}\right) - \Gamma\left(\frac{1}{n}, x^n\right) \right]$$

5. <u>erf from Incomplete Gamma Functions</u>: Therefore, the error function can be defined in terms of the incomplete Gamma function:

$$\operatorname{erf}(x) = 1 - \frac{1}{\sqrt{\pi}} \Gamma\left(\frac{1}{2}, x^2\right)$$

Iterated Integrals of the Complementary Error Function

1. <u>Iterated Integrals of erfc - Definition</u>: The iterated integrals of the complementary error function are defined by (Carslaw, H. S., and J. C. Jaeger (1959)):

$$i^n \operatorname{erfc}(z) = \int_{z}^{\infty} i^{n-1} \operatorname{erfc}(\zeta) d\zeta$$

$$i^0 \operatorname{erfc}(z) = \operatorname{erfc}(z)$$

$$i^{1}\operatorname{erfc}(z) = i\operatorname{erfc}(z) = \frac{1}{\sqrt{\pi}}e^{-z^{2}} - z\operatorname{erfc}(z)$$

$$i^{2}\operatorname{erfc}(z) = \frac{1}{4}\left[\operatorname{erfc}(z) - 2zi\operatorname{erfc}(z)\right]$$

2. General Recurrence Formula for erfc: The general recurrence formula is

$$2ni^n \operatorname{erfc}(z) = i^{n-2} \operatorname{erfc}(z) - 2zi^{n-1} \operatorname{erfc}(z)$$

3. Power Series Representation for Iterated erfc: These have the power series

$$i^n \operatorname{erfc}(z) = \sum_{j=0}^{\infty} \frac{(-z)^j}{2^{n-j} j! \Gamma\left(1 + \frac{n-j}{2}\right)}$$

from which follow the symmetry properties

$$i^{2m}\operatorname{erfc}(-z) = -i^{2m}\operatorname{erfc}(z) + \sum_{q=0}^{m} \frac{z^{2q}}{2^{2(m-q)-1}(2q)!(m-q)!}$$

and

$$i^{2m+1}\operatorname{erfc}(-z) = i^{2m+1}\operatorname{erfc}(z) + \sum_{q=0}^{m} \frac{z^{2q+1}}{2^{2(m-q)-1}(2q+1)!(m-q)!}$$

References

Abramowitz, M., and I. A. Stegun (2007): Handbook of Mathematics Functions
 Dover Book on Mathematics



- Andrews, L. C. (1998): Special Functions of Mathematics for Engineers SPIE Press
- Bergsma, W. (2006): <u>A New Correlation Coefficient, its Orthogonal Decomposition</u>, and Associated Tests of Independence arXiv
- Chang, S. H., P. C. Cosman, L. B. Milstein (2011): Chernoff-Type Bounds for Gaussian Error Function *IEEE Transactions on Communications* 59 (11) 2939-2944
- Chiani, M., D. Dardari, and M. K. Simon (2003): New Exponential Bounds and Approximations for the Computation of Error Probability in Fading Channels *IEEE* Transactions on Wireless Communications 2 (4) 840-845
- Cody, W. J. (1991): Algorithm 715: SPECFUN A Portable FORTRAN Package of Special Function Routines and Test Drivers ACM Transactions on Mathematical Software 19 (1) 22-32
- Craig, J. W. (1991): <u>A New, Simple, and Exact Result for Calculating the Probability</u> of Error For Two-Dimensional Signal Constellations
- Glaisher, J. W. L. (1871a): On a Class of Definite Integrals Part I London,
 Edinburgh, and Dublin Philosophical Magazine and Journal of Science 4 42 (277)
 294-302
- Glaisher, J. W. L. (1871b): On a Class of Definite Integrals Part II London,
 Edinburgh, and Dublin Philosophical Magazine and Journal of Science 4 42 (279)
 421-436
- Greene, W. H. (1993): Econometric Analysis 5th Edition **Prentice-Hall**
- Karagiannidis, G. K., and A. S. Lioumpas (2007): An Improved Approximation for the Gaussian Q-function *IEEE Communications Letters* **11 (8)** 644-646
- Nielson, N. (1906): Handbuch der Theorie der Gammafunktion B. G. Teubner
 Leipzig
- Press, W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery (2007):
 Numerical Recipes: The Art of Scientific Computing 3rd Edition Cambridge
 University Press New York
- Schopf, H. M., and P. H. Supancic (2014): On Burmann's Theorem and its

 Application to Problems of Linear and Non-linear Heat Transfer and Diffusion



- Schlomilch, O. X. (1859): Ueber Facultatenreihen Zeitschrift fur Mathematik und Physik 4 390-415
- Wikipedia (2019): Error Function
- Winitzki, S. (2008): A Handy Approximation for the Error Function and its Inverse
- Zaghloul, M. R. (2007): On the Calculation of the Voigt Line Profile: A Single Proper Integral with a Damped Sign Integrand *Monthly Notices of the Royal* Astronomical Society 375 (3) 1043-1048