3 Improvement of Convergence

For efficient numerical evaluation of series, it is often important to accelerate the rate of convergence. There are several standard tools of the trade to effect such; here we will highlight **three**: Kummer's method, development of rational approximations, and Euler's transformation.

3.1 Kummer's Technique

The essence of **Kummer's method** is to form convenient linear combinations between the series in question, and slowly converging series with known sums. These combinations are chosen such that resulting combined series possess a faster rate of convergence. While there is no unique choice of comparison series, Kummer opted for the convenient (i.e. broadly useful) set

A & W, pp. 334–5

$$\begin{aligned}
\alpha_1 &= \sum_{n=1}^{\infty} \frac{1}{n(n+1)} = 1 \quad , \\
\alpha_2 &= \sum_{n=1}^{\infty} \frac{1}{n(n+1)(n+2)} = \frac{1}{4} \quad , \\
&\vdots \\
\alpha_p &= \sum_{n=1}^{\infty} \frac{1}{n(n+1)\dots(n+p)} = \frac{1}{p\,(p!)} \quad .
\end{aligned} \tag{26}$$

The first of these can be proven by appropriate partial fractions, and grouping and relabelling of series terms

$$\sum_{n=1}^{\infty} \frac{1}{n(n+1)} = \sum_{n=1}^{\infty} \left(\frac{1}{n} - \frac{1}{n+1} \right) = \lim_{N\to\infty} \left\{ 1 + \sum_{n=2}^{N} \frac{1}{n} - \sum_{n=2}^{N} \frac{1}{n} \right\} = 1 \quad . \tag{27}$$

The general result can be proven by mathematical induction.

• We first apply Kummer's technique to Riemann's zeta function $\zeta(3)$, which converges at a rate similar to α_2. Form the linear combination

$$\zeta(3) + \frac{\kappa}{4} \ = \ \sum_{n=1}^{\infty} \frac{1}{n^3} + \kappa\,\alpha_2 \quad . \tag{28}$$

This rearranges to the identity

$$\zeta(3) + \frac{\kappa}{4} \ = \ \sum_{n=1}^{\infty} \left(\frac{1}{n^3} + \frac{\kappa}{n(n+1)(n+2)} \right) \quad . \tag{29}$$

Clearly, the choice $\kappa = -1$ accelerates the convergence of the resultant series, leading to

$$\zeta(3) \ = \ \frac{1}{4} + \sum_{n=1}^{\infty} \frac{3n+2}{n^3(n+1)(n+2)} \quad , \tag{30}$$

so that convergence now goes as $1/n^4$. Using the `Mathematica` operation `Sum[f(n), {n, 1, N}]`, summing this to 10 terms gives 1.20132 and the sum to 30 yields 1.20202, very close to the precise value $\zeta(3) \approx 1.20206$.

Plot: Accelerating Riemann $\zeta(3)$ Series

• **Example 6:** Consider the functional series

$$S(x) \ = \ \sum_{n=1}^{\infty} \frac{1}{(1+2n)^2 - x^2} \ \equiv \ \frac{\pi}{4x} \tan\frac{\pi x}{2} - \frac{1}{1-x^2} \ , \quad |x| \ < \ 1 \quad . \tag{31}$$

Now subtract $\alpha_1/4$ from the series to form

$$\begin{aligned} S(x) - \frac{1}{4} \ &= \ \sum_{n=1}^{\infty} \left\{ \frac{1}{(1+2n)^2 - x^2} - \frac{1}{4n(n+1)} \right\} \\ &= \ -\frac{1-x^2}{4} \sum_{n=1}^{\infty} \frac{1}{n(n+1)\left[(1+2n)^2 - x^2\right]} \quad . \end{aligned} \tag{32}$$

This now converges more rapidly, as $1/n^4$. For this particular case, the acceleration is exceedingly efficient, increase rapidity by two orders, not the usual single order improvement enabled by Kummer's technique. Only around 20 terms are now required to obtain precision to one part in 10^6!

$*$ Using the identity in Eq. (31) affords a path to obtaining rational approximations for π. We choose $x = 1/2$ to give $S(1/2) = \pi/2 - 4/3$. Rearranging then gives

$$\begin{aligned} \pi &= \frac{8}{3} + \frac{1}{2} - \frac{3}{2} \sum_{n=1}^{\infty} \frac{1}{n(n+1)\left[4(1+2n)^2 - 1\right]} \\ &= \frac{19}{6} - \frac{3}{2} \sum_{n=1}^{\infty} \frac{1}{n(n+1)\left[3 + 16n + 16n^2\right]} \quad . \end{aligned} \tag{33}$$

This then yields the following sequence of rational approximations to π, employing just a handful of terms:

$$\begin{aligned} n = 1: \quad & \pi \approx \frac{1321}{420} \quad (0.1\% \text{ accuracy}) \\ n = 2: \quad & \pi \approx \frac{21779}{630} \quad (0.04\% \text{ accuracy}) \\ n = 5: \quad & \pi \approx \frac{4205393539}{1338557220} \quad (0.005\% \text{ accuracy}) \end{aligned} \tag{34}$$

Series such as this for trigonometric functions can yield a myriad of rational approximations to π.

3.2 Rational Approximation

Another technique is to form a rational function approximation to a series expansion to effect an acceleration of convergence. This approach is essentially to form a Padé approximation, and is best illustrated by example.

- **Example 1:** Consider the logarithmic series

$$\log_e(1+x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n} \quad . \tag{35}$$

Form

$$\begin{aligned} (1+\kappa x)\log_e(1+x) &= \sum_{n=1}^{\infty} (-1)^{n-1} (1+\kappa x) \frac{x^n}{n} \\ &= x + \sum_{n=2}^{\infty} (-1)^{n-1} \left(\frac{1}{n} - \frac{\kappa}{n-1} \right) x^n \quad . \end{aligned} \tag{36}$$

To improve the convergence of the series, we set $\kappa = 1$, giving

$$(1+x)\,\log_e(1+x) \;=\; x + \sum_{n=2}^{\infty} \frac{(-1)^n\,x^n}{n\,(n-1)} \quad , \tag{37}$$

and then relabel the series via $n \to n+1$. The result is

$$\log_e(1+x) \;=\; \frac{x}{1+x}\left\{1 - \sum_{n=1}^{\infty} \frac{(-1)^n\,x^n}{n\,(n+1)}\right\} \quad . \tag{38}$$

There is no need to stop here. The series in Eq. (38) can similarly have its convergence accelerated. Setting

$$g(x) \;=\; \log_e(1+x) - \frac{x}{1+x} \quad , \tag{39}$$

one forms

$$\begin{aligned} (1+\lambda x)\,g(x) \;&=\; \frac{x}{1+x}\sum_{n=1}^{\infty} \frac{(-1)^{n+1}\,x^n}{n\,(n+1)}\,(1+\lambda x) \\ &=\; \frac{x^2}{2(1+x)} + \frac{x^2}{1+x}\sum_{n=1}^{\infty} \frac{(-1)^n\,x^n}{n+1}\left(\frac{1}{n+2} - \frac{\lambda}{n}\right) \quad . \end{aligned} \tag{40}$$

Then choosing $\lambda = 1$ effects the acceleration, leading to

$$\log_e(1+x) \;=\; \frac{x\,(2+3x)}{2\,(1+x)^2} + \frac{2x^2}{(1+x)^2}\,S(x) \quad , \tag{41}$$

where the remaining series is

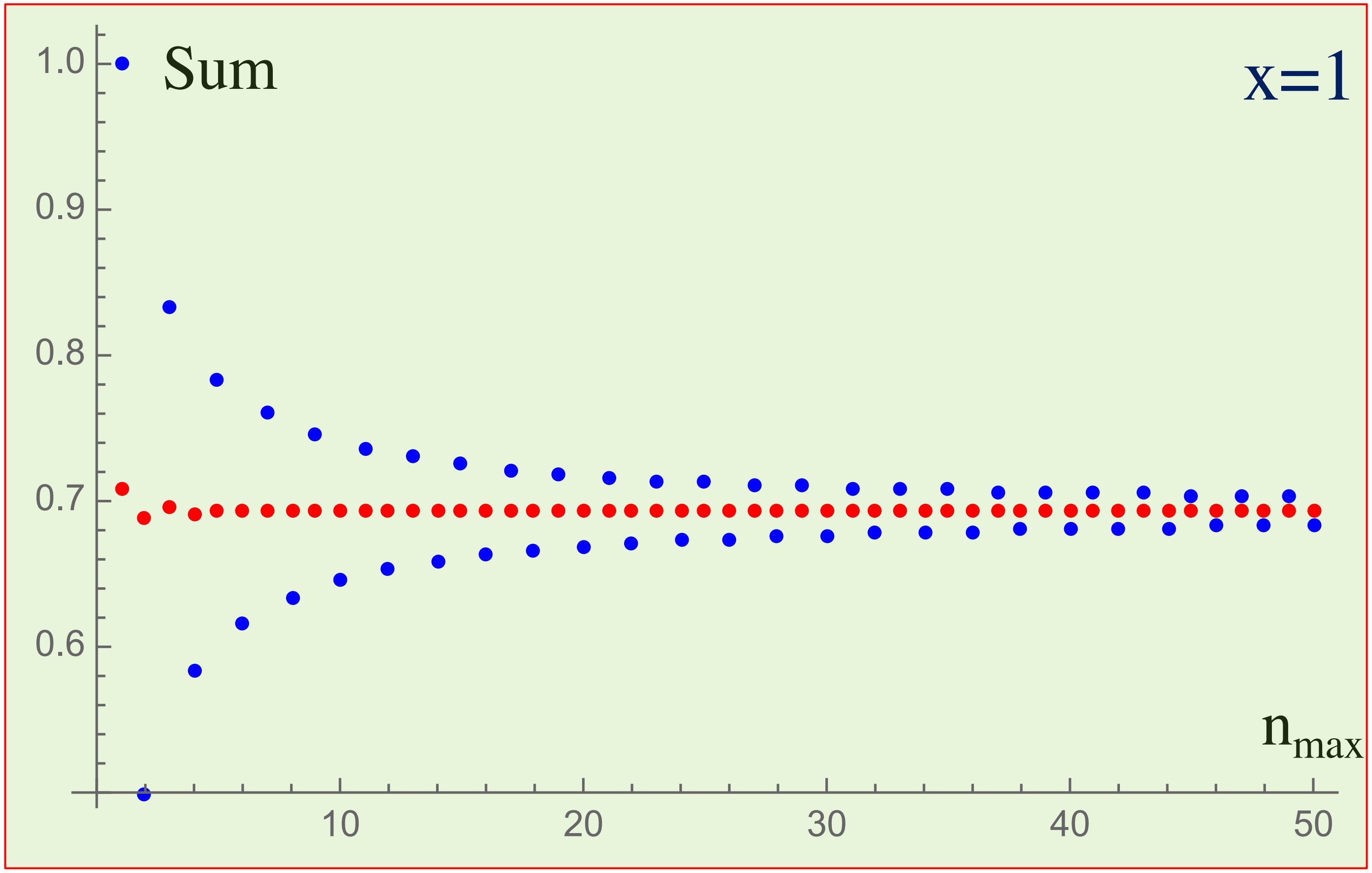
$$S(x) \;=\; \sum_{n=1}^{\infty} \frac{(-1)^{n+1}\,x^n}{n\,(n+1)\,(n+2)} \quad , \tag{42}$$

which converges quite rapidly when $|x| \leq 1$. Series expansions of both sides of Eq. (41) using `Mathematica` verify the validity of the identity.

Plot: Accelerating the $\log_e(1+x)$ Series

• The leading term in Eq. (41), plus the first term of the series contribution, clearly constitutes a **Padé approximation** involving low order polynomials (a cubic divided by a quadratic). This acceleration of convergence technique could be continued for a couple more iterations to improve the accuracy of such a rational function approximation considerably.

Accelerating the $\log_e(1+x)$ Series



- Comparison of the cumulative sum $-\Sigma_n(-1)^n/n$ for the $\log_e 2 = 0.693147\ldots$ series (blue dots), as a function of n_{max}, and the accelerated form (red dots) using the Pade approximant technique given in the lecture, illustrating the dramatic improvement of convergence.

3.3 Euler's Transformation

For alternating series, **Euler's transformation**, which is derived using binomial theory and is connected to transformations of hypergeometric functions, can be a powerful tool. This can be cast as the identity

$$\sum_{s=0}^{\infty}(-1)^s\, u_s \;=\; u_0 - u_1 + u_2 \ldots - u_{n-1} + \sum_{s=0}^{\infty}\frac{(-1)^s}{2^{s+1}}\,\Delta^s u_n \qquad (44)$$

The new coefficients in the series are **forward difference operators**:

$$\begin{aligned} \Delta u_n &= u_{n+1} - u_n \\ \Delta^2 u_n &= u_{n+2} - 2u_{n+1} + u_n \\ \Delta^3 u_n &= u_{n+3} - 3u_{n+2} + 3u_{n+1} - u_n\ , \quad \text{etc.} \end{aligned} \qquad (45)$$

These difference operators trace higher order "derivatives" of the functional form of the series terms, and are generally rapidly-declining functions of s, so that the new series in Eq. (44) is rapidly convergent. In general,

$$\Delta^s u_n \;=\; \sum_{m=0}^{s}(-1)^{s-m}\binom{s}{m}\,u_{n+m} \quad . \qquad (46)$$

∗ In practice, one sums a modest number of terms first, before applying the transformation to a domain where the asymptotic character of the series terms is well-established.

• The powerful Euler technique cannot be applied to a series of positive terms. However, **Van Wijngaarden** developed a transformation that could morph a series of positive terms into an alternating one:

$$\sum_{r=1}^{\infty} v_r \;=\; \sum_{r=1}^{\infty}(-1)^{r-1}\,w_r \quad , \quad w_r \;\equiv\; 1 + \sum_{k=1}^{\infty} 2^k\, v_{2^k r} \quad . \qquad (47)$$

These two tools provide a third, and computationally elegant method for accelerating the convergence of series.

5. INTEGRATION

Matthew Baring — Lecture Notes for PHYS 516, Fall 2022

This Chapter will outline techniques for evaluating **definite integrals** whose indefinite integrals are not known. The focus will include:

∗ **exact analytical methods**, specifically special tricks for special cases, contour integration in the complex plane, and exploitation of symmetry arguments;

∗ **approximate analytic methods**, namely asymptotic series, and the method of steepest descents (saddle-point methods);

∗ **numerical approaches**, emphasizing Newton-Cotes formulae such as Simpson's rule, and Gaussian quadrature.

1 Special Devices for Particular Cases

The tools outlined here can be very specific to the particular integral, and will be illustrated by example. Two devices of more general applicability will be highlighted, namely differentiation under the integral sign, and employment of series expansions to render the integral in tractable form.

- **Example 1:** First consider the pair of integrals

$$\mathcal{J}_R \;=\; \int_0^\infty e^{-\alpha x} \cos \lambda x \, dx \quad , \quad \mathcal{J}_I \;=\; \int_0^\infty e^{-\alpha x} \sin \lambda x \, dx \quad . \tag{1}$$

The presence of exponentials and trigonometric functions in the integrands suggests the employment of complex exponentials. Hence, form

$$\mathcal{J}_R + i\,\mathcal{J}_I \;=\; \int_0^\infty e^{-\alpha x}\, e^{i\,\lambda x}\, dx \;=\; \frac{1}{\alpha - i\lambda} \;=\; \frac{\alpha + i\lambda}{\alpha^2 + \lambda^2} \quad , \tag{2}$$

from which can be deduced

$$\mathcal{J}_R \;=\; \frac{\alpha}{\alpha^2 + \lambda^2} \quad , \quad \mathcal{J}_I \;=\; \frac{\lambda}{\alpha^2 + \lambda^2} \quad . \tag{3}$$

Accordingly, two birds are killed with one stone.

- **Example 2:** Consider now the case of the area under a Gaussian function:

$$I \;=\; \int_0^\infty e^{-t^2}\, dt \quad . \tag{4}$$

This can be squared to form

$$I^2 \;=\; \int_0^\infty e^{-x^2}\, dx \int_0^\infty e^{-y^2}\, dy \quad . \tag{5}$$

Recognizing this as an area integration in Cartesian coordinates, one can transform to the more convenient polar coordinates via $x = r\,\cos\theta$ and $y = r\,\sin\theta$. Then the square of the integral becomes

$$I^2 \;=\; \int_0^\infty r\, e^{-r^2}\, dr \int_0^{\pi/2} d\theta \quad , \tag{6}$$

since the area element is $dA = dx\, dy = r\, dr\, d\theta$. These integrals are trivially evaluated, and lead to a result $\pi/4$, from which we find

$$I \;\equiv\; \int_0^\infty e^{-t^2}\, dt \;=\; \frac{\sqrt{\pi}}{2} \quad . \tag{7}$$

This is a particularly unique manipulation in that in order to successfully apply the transformation to polar coordinates and generate separable integrals in r and θ , it is necessary for the original integral to possess a simple quadratic dependence in the argument of the exponential.

1.1 The Power of Differentiation

The first moment of the Gaussian was derived in passing in the previous example. The n^{th} **moment** is defined via the integral

$$I_n(a) \;=\; \int_0^\infty t^n\, e^{-a\,t^2}\, dt \quad . \tag{8}$$

Clearly, by simple change of variables, this is proportional to $a^{-(n+1)/2}$. Having established

$$I_0(a) \;=\; \frac{1}{2}\sqrt{\frac{\pi}{a}} \quad , \quad I_1(a) \;=\; \frac{1}{2a} \quad , \tag{9}$$

routine differentiation under the integral sign in the variable a quickly establishes the "recurrence relation"

$$I_{n+2} \;=\; -\,\frac{dI_n}{da} \quad , \tag{10}$$

which serves to determine all higher order moments given the first two in Eq. (9). This illustrates the power of differentiation with respect to some parametric variable. One finds

$$\begin{aligned} I_{2k}(a) &= (-1)^k\,\frac{d^k I_0}{da^k} \;=\; (-1)^k\,\frac{(2k-1)!!}{2^{k+1}}\,\frac{\sqrt{\pi}}{a^{(2k+1)/2}} \quad , \\ I_{2k+1}(a) &= (-1)^k\,\frac{d^k I_1}{da^k} \;=\; (-1)^k\,\frac{k!}{2a^{k+1}} \quad . \end{aligned} \tag{11}$$

• **Example 3:** Adding extraneous weighting functions can facilitate evaluation when they collapse to constants in limiting cases. Consider

$$J \;=\; \int_0^\infty \frac{\sin x}{x}\, dx \quad . \tag{12}$$

This can be treated as a special case $I(0)$ of the parametric function

$$I(\alpha) \;=\; \int_0^\infty e^{-\alpha x}\,\frac{\sin x}{x}\, dx \quad . \tag{13}$$

Differentiation then yields

$$I'(\alpha) \;=\; -\int_0^\infty e^{-\alpha x}\,\sin x\, dx \;=\; -\,\frac{1}{1+\alpha^2} \quad , \tag{14}$$

using the result of **Example 1**. This is routinely integrated to yield

$$I(\alpha) \;=\; C - \arctan\alpha \quad . \tag{15}$$

The constant of integration is determined by letting $\alpha \to \infty$, for which $I(\alpha) \to 0$ due to the precipitous reduction of the exponential factor in the integrand. Hence, $C = \pi/2$, and the final evaluation is

$$I(\alpha) \;=\; \frac{\pi}{2} - \arctan\alpha \quad \Rightarrow \quad J \;\equiv\; I(0) \;=\; \frac{\pi}{2} \quad . \tag{16}$$

1.2 Series Expansions

Exploiting the potential for series expansions of the integrand can also expedite evaluation, at least numerically. Again, we proceed via example.

- **Example 4:** Consider the integral

$$I \;=\; \int_0^\infty \frac{(\log_e x)^2}{1+x^2}\,dx \;=\; \int_{-\infty}^\infty \frac{t^2\,e^t}{1+e^{2t}}\,dt \;=\; \int_0^\infty \frac{t^2\,dt}{\cosh t} \quad , \tag{17}$$

where the change of variables $x = e^t \Rightarrow dx = e^t\,dt$ has been employed. Multiplying the integrand of the middle integral top and bottom by e^{-2t} suggests a geometric series expansion in e^{-2t} to rewrite the denominator:

$$I \;=\; \int_{-\infty}^\infty \frac{t^2\,e^{-t}}{1+e^{-2t}}\,dt \;=\; 2\sum_{n=0}^\infty (-1)^n \int_0^\infty t^2\,e^{-t}\,e^{-2nt}\,dt \quad , \tag{18}$$

The integrals are now simply evaluated to yield an alternating series, for which consecutive terms can be grouped together to accelerate convergence,

$$I \;=\; 4\sum_{n=0}^\infty \frac{(-1)^n}{(1+2n)^3} \;=\; 8\sum_{k=0}^\infty \frac{48k^2+48k+13}{(1+4k)^3\,(3+4k)^3} \quad . \tag{19}$$

This can quickly be summed to yield $I \approx 3.8758$.

2 Contour Integration

The principal attribute of the Residue Theorem is that it facilitates integral evaluation. The trick is to find a contour C that contains the desired integral as one of its segments, while all other segments are easily calculated. **A & W, Sec. 7.1**

- **Example 5:** Consider the trivial example

$$I \;=\; \int_0^\infty \frac{dx}{1+x^2} \;=\; \frac{\pi}{2} \quad , \tag{19}$$

which is analytically tractable. With $f(z) = 1/(1+z^2) = 1/(z-i)/(z+i)$, which has simple poles at $z = \pm i$. The preferred choice of contour is a semicircle of radius R that captures the entire upper half of the complex plane when $R \to \infty$. Only the pole at $z = +i$ is enclosed by the contour.

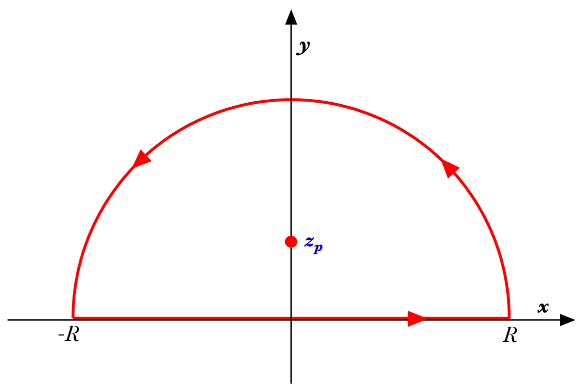


Figure 1: The semi-circular contour that is optimal for the $1/(1+z^2)$ integration. Only the simple pole at $z_p = +i$ is encircled by the contour and thus contributes a residue to the integral evaluation.

With the straight portion of the contour coinciding with the real axis, this portion generates twice the integral in Eq. (19). The integral along the semi-circular portion is

$$\int_0^\pi \frac{iR\,e^{i\theta}\,d\theta}{1+R^2\,e^{2i\theta}} \;\to\; 0 \quad \text{as} \quad R \;\to\; \infty \quad . \tag{20}$$

Accordingly,

$$2I \;=\; 2\pi i\,\text{Res}(z=+i) \;=\; 2\pi i\left(\frac{1}{2i}\right) \;=\; \pi \quad \Rightarrow \quad I \;=\; \frac{\pi}{2} \quad . \tag{21}$$