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

$$I(\alpha) \;=\; \frac{\pi}{2} - \arctan\alpha \quad \Rightarrow \quad J \;\equiv\; I(0) \;=\; \frac{\pi}{2} \quad . \tag{15}$$

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

$$I \;=\; \int_0^\infty \frac{(\log_e x)^2}{1+x^2}\,dx \;=\; \int_{-\infty}^\infty \frac{t^2\,e^t}{1+e^{2t}}\,dt \;=\; \int_0^\infty \frac{t^2\,dt}{\cosh t} \quad , \tag{16}$$

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:

$$I \;=\; \int_{-\infty}^\infty \frac{t^2\,e^{-t}}{1+e^{-2t}}\,dt \;=\; 2\sum_{n=0}^\infty (-1)^n \int_0^\infty t^2\,e^{-t}\,e^{-2nt}\,dt \quad , \tag{17}$$

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

$$I \;=\; 4\sum_{n=0}^\infty \frac{(-1)^n}{(1+2n)^3} \;=\; 8\sum_{k=0}^\infty \frac{48k^2+48k+13}{(1+4k)^3\,(3+4k)^3} \quad . \tag{18}$$

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.

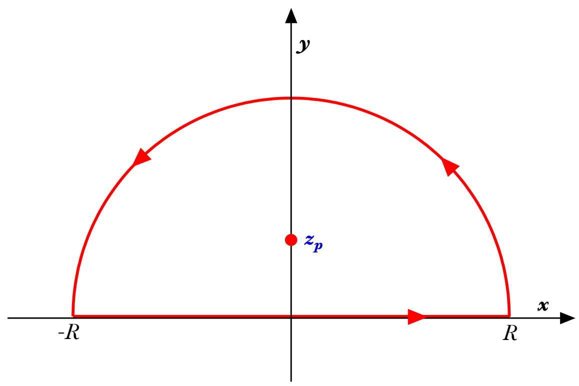

Figure 1: The semi-circular contour that is optimal for the $1/(1+z^2)$ integration. Only the simple pole at $z_p = +i$ is encircled by the contour and thus contributes a residue to the integral evaluation.

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,

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

• **Example 6:** Now, to a more complicated case, let us reconsider the integral in Example 4, for which the last form in Eq. (16) is amenable to contour integration. For $f(z) = z^2/\cosh z$, which has a simple pole at $z = i\pi/2$, the appropriate choice of contour is a rectangular one with vertices at $x = \pm R$ and $y = 0, i\pi$.

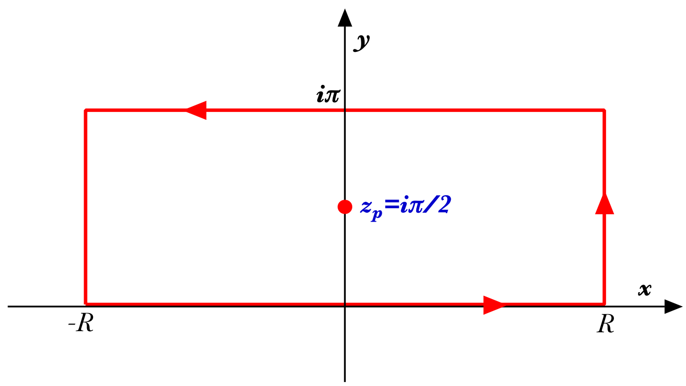

Figure 2: The rectangular contour that is optimal for the $z^2/\cosh z$ integration. Only the simple pole at $z_p = +i\pi/2$ is encircled by the contour and thus contributes a residue to the integral evaluation.

The function $f(z)$ has a simple pole at $z = i\pi/2$, so to determine the residue there, we set $z = i\pi/2 + \delta$. Then, as $\delta \to 0$,

$$\cosh z \;=\; \frac{1}{2}\left(e^{i\pi/2+\delta} + e^{-i\pi/2-\delta}\right) \;=\; \frac{i}{2}\left(e^{\delta} - e^{-\delta}\right) \;\to\; i\delta \quad . \tag{22}$$

From this, one discerns that the residue of $f(z)$ is

$$\mathrm{Res}\left(\frac{i\pi}{2}\right) \;=\; \frac{1}{i}\left(\frac{i\pi}{2}\right)^2 \;=\; i\,\frac{\pi^2}{4} \quad . \tag{23}$$

As $R \to \infty$, the contributions along the contour intervals $[R,\, R + i\pi]$ and $[-R + i\pi,\, -R]$ approach zero. Therefore, the Residue Theorem results in

$$\oint_C \frac{z^2\,dz}{\cosh z} \;=\; \int_{-\infty}^{\infty} \frac{u^2\,du}{\cosh u} - \int_{-\infty}^{\infty} \frac{(u+i\pi)^2\,du}{\cosh(u+i\pi)} \;=\; 2\pi i\,\mathrm{Res}\left(\frac{i\pi}{2}\right) \quad . \tag{24}$$

The term that is odd in u contributes zero identically, so that

$$2\int_{-\infty}^{\infty} \frac{u^2\,du}{\cosh u} - \pi^2\int_{-\infty}^{\infty} \frac{du}{\cosh u} \;=\; -\,\frac{\pi^3}{2} \quad . \tag{25}$$

The substitution $x = e^u$ then facilitates the evaluation of the remaining integral:

$$\int_{-\infty}^{\infty} \frac{du}{\cosh u} = 2\int_0^{\infty} \frac{dx}{x^2+1} = 2\Big[\arctan x\Big]_0^{\infty} = \pi \quad . \tag{27}$$

The first integral on the LHS of Eq. (26) is therefore $\pi^3/4$, twice that sought. The final analytic result is

$$I = \int_0^{\infty} \frac{(\log_e x)^2}{1+x^2}\, dx \equiv \int_0^{\infty} \frac{t^2\, dt}{\cosh t} = \frac{\pi^3}{8} \quad , \tag{28}$$

and together with Eq. (19), this yields a series evaluation for π^3.

• This examples serves to illustrate how integral manipulation, series contructs, and contour integration can be used to facilitate a variety of identities and techniques for evaluation.

• **Example 7:** As a final example of the contour integration technique, here the integral in Example 3 is reconsidered. For this, one uses a contour that is semi-circular in the upper half z plane, for the function $f(z) = e^{iz}/z$:

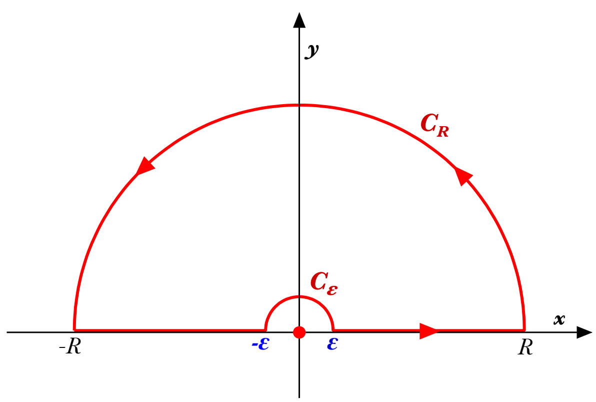

Figure 3: The indented semi-circular contour that is optimal for the e^{iz}/z integration. Only the simple pole at $z_p = 0$ is abutted by the contour and thus contributes the negative of half a residue to the integral evaluation.

Since $f(z)$ has a simple pole at $z = 0$, we can either include or exclude it, a choice that is immaterial. For simplicity, we exclude it here, using a small, semi-circular portion of the contour or radius ϵ. The Residue Theorem then gives

$$\oint_C \frac{e^{iz}}{z}\, dz \;=\; \int_{-R}^{-\epsilon} \frac{e^{ix}}{x}\, dx + \int_{C_\epsilon} \frac{e^{iz}}{z}\, dz + \int_{\epsilon}^{R} \frac{e^{ix}}{x}\, dx + \int_{C_R} \frac{e^{iz}}{z}\, dz \;=\; 0 \quad . \tag{28}$$

The integral over the semi-circular portion of radius R contributes zero as $R \to \infty$. This can be established by substituting $z \to Re^{i\theta}$ and observing that the exponential crushes the integrand except for a range of θ near zero of width $\sim 1/R$. To discern this in greater detail, develop this integral via **A & W, p. 467**

$$\int_{C_R} \frac{e^{iz}}{z}\, dz \;=\; \int_0^{\pi} e^{iR[\cos\theta + i\sin\theta]}\, \frac{i\cancel{Re^{i\theta}}\, d\theta}{\cancel{Re^{i\theta}}} \;=\; i \int_0^{\pi} d\theta\, \underbrace{e^{-R\sin\theta}}_{\text{Factor 1}}\, \underbrace{e^{iR\cos\theta}}_{\text{Factor 2}} \;. \tag{29}$$

The first highlighted factor in the integrand is exponentially suppressed unless $|\theta| \lesssim 1/R$ or $|\pi - \theta| \lesssim 1/R$, two extremely narrow windows. In these domains, $|\cos\theta| \approx 1$, implying that the second highlighted factor oscillates rapidly, and therefore causes destructive interference, so that the integral tends to zero. This result, in a form generalized to a host of weighting functions in the integrand, is known as **Jordan's lemma**.

Then, the overall contour integral reduces to two contributions:

$$\oint \frac{e^{iz}}{z}\, dz \;=\; \int_{C_\epsilon} \frac{e^{iz}}{z}\, dz + \mathcal{P} \int_{-\infty}^{\infty} \frac{e^{ix}}{x}\, dx \;=\; 0 \quad . \tag{30}$$

Here the symbol $\mathcal{P}$ denotes the **principal part**, which constitutes the limiting contribution around $x = 0$:

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{e^{ix}}{x}\, dx \;\equiv\; \lim_{\epsilon \to 0^+} \left\{ \int_{\epsilon}^{\infty} \frac{e^{ix}}{x}\, dx + \int_{-\infty}^{-\epsilon} \frac{e^{ix}}{x}\, dx \right\} \quad . \tag{31}$$

Only the imaginary part contributes to this, since the real part is odd in x.

The integral over C_ϵ can be evaluated using $z = \epsilon e^{i\theta}$, but now with the more limited range of angles $0 \leq \theta \leq \pi$. Hence, it contributes $-1/2$ of $2\pi i$ times the residue of the $z = 0$ simple pole, i.e. $-i\,\pi$ (the minus sign originates in the clockwise sense of C_ϵ). From this, we deduce

$$J \;=\; \int_0^{\infty} \frac{\sin x}{x}\, dx \;=\; \frac{\pi}{2} \quad . \tag{32}$$

Other contours can be deployed to effect the contour integration of this integral: see Problem 7.1.15 of Arfken & Weber.

3 Asymptotic Expansions

A second series technique that is generally applicable for large arguments is the generation of **asymptotic series**. These are useful, though not necessarily convergent series: convergence becomes irrelevant if an accurate approximation is achieved by truncating the series at a small number of terms.

Consider the **error function** of probability theory

$$\mathrm{erf}(x) \;\equiv\; \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt \;=\; \frac{2}{\sqrt{\pi}} \left[x - \frac{x^3}{3} + \frac{x^5}{5.2!} - \frac{x^7}{7.3!} + \ldots \right] \quad . \tag{33}$$

The Taylor series is clearly convergent for all x, but is generally only computationally useful for $x \lesssim 1$. For large arguments x, it is convenient to consider the **complementary error function**

$$\mathrm{erfc}(x) \;\equiv\; 1 - \mathrm{erf}(x) \;=\; \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt \quad . \tag{34}$$

The integral is intractable, but it can be manipulated by sequential integration by parts to generate an asymptotic series:

$$\begin{aligned} \mathrm{erfc}(x) &= \frac{2}{\sqrt{\pi}} \left\{ \left[-\frac{1}{2t}\, e^{-t^2} \right]_x^\infty - \frac{1}{2} \int_x^\infty e^{-t^2}\, \frac{dt}{t^2} \right\} \\ &= \frac{2}{\sqrt{\pi}} \left\{ \frac{e^{-x^2}}{2x} - \frac{e^{-x^2}}{4x^3} + \frac{3}{4} \int_x^\infty e^{-t^2}\, \frac{dt}{t^4} \right\} \end{aligned} \tag{35}$$

with the result (see Exercise 5.10.4 in Arfken & Weber)

$$\mathrm{erf}(x) \;=\; 1 - \frac{e^{-x^2}}{x\sqrt{\pi}} \left[1 - \frac{1}{2x^2} + \frac{3}{8x^4} - \frac{15}{8x^6} + \ldots \right] \quad . \tag{36}$$

This is useful for computation purposes when x is large, but is formally divergent when $x \lesssim 1$. This is due to the factorial nature of the coefficient of $1/x^{2n}$, a property that is easily discerned from the integrals in Eq. (35).

3.1 Laplace's Method of Steepest Descents

This method approximates the value of an integral that has a strong peaking of the integrand forced by the presence of an exponential. **A & W, Sec. 7.3**

- **Example 8:** Consider the **Gamma function**

$$\Gamma(z) \equiv \int_0^\infty t^{z-1} e^{-t}\, dt \quad . \tag{37}$$

Integrating by parts quickly gives the relation $\Gamma(z) = (z-1)\,\Gamma(z-1)$, from which we deduce that $\Gamma(n) = (n-1)!$ Accordingly, $\Gamma(z)$ is also known as the **factorial function**. We seek an asymptotic expansion for this when $z = x+1 \gg 1$. The integrand can be written

$$t^x e^{-t} = e^{-f(t,x)} \quad , \quad f(t,\, x) \equiv t - x \log_e t \quad . \tag{38}$$

Now expand the exponent in a Taylor series about its maximum, $t = x$, which is the solution of $\partial f/\partial t = 0$. This algorithm gives a much better approximation than expanding the whole integrand itself because $f(t,\, x)$ varies much more slowly than $\exp\{f(t,\, x)\}$. Then

$$f(t,\, x) \approx f(x,\, x) + \frac{1}{2} f''(x,\, x)\,(t-x)^2 + \ldots \approx x - x\, \log_e x + \frac{(t-x)^2}{2x} \tag{39}$$

Truncating at the quadratic term, this can be substituted in the exponential to yield

$$\Gamma(1+x) \approx x^x e^{-x} \int_0^\infty \exp\left[-\frac{(t-x)^2}{2x}\right] dt \quad . \tag{40}$$

Then, using the change of variables $u = (t-x)/\sqrt{2x}$, the integration reduces to a complementary error function:

$$\Gamma(1+x) \approx x^x e^{-x} \sqrt{2x} \int_{-\sqrt{x/2}}^{\infty} e^{-u^2}\, du \quad . \tag{41}$$

With minimal incursion of error, the lower limit can be replaced by $-\infty$, so that

$$\Gamma(1+x) \equiv x! \approx \sqrt{2\pi}\, x^{x+1/2}\, e^{-x} \quad . \tag{42}$$

This is the first term in **Stirling's approximation** to the Γ function.

• The technique just illustrated is called the **method of steepest descents**, and is akin to the WKB approximation. Its extension to the complex plane is entitled the **saddle-point method**, based on the fact that an analytic function $f(z)$ has no absolute maxima or minima, only saddle points, due to the harmonic nature of its (u, v) components.

• The general formalism can quickly be deduced using the same Taylor series expansion technique, where $f(t,\, x)$ is a slowly varying function of t that achieves a minimum at $t = t_0$. It quickly follows that

$$I \;=\; \int_0^\infty \exp\left\{ -f(t,\, x)\right\}\, dt \;\approx\; \sqrt{\frac{2\pi}{\vert f''(t_0,\, x)\vert}}\; \exp\Bigl\{ -f(t_0,\, x)\Bigr\} \tag{43}$$

again by changing variables and extending the Gaussian integral lower limit to negative infinity.

• **Example 9:** The modified Bessel function of the second kind, $K_\nu(x)$, which appears in the theory of synchrotron radiation and bremsstrahlung (describe), has an integral representation

$$K_\nu(x) \;=\; \frac{1}{2}\int_0^\infty \exp\biggl\{ -\frac{x}{2}\biggl(s + \frac{1}{s}\biggr)\biggr\}\, \frac{ds}{s^{1-\nu}} \quad . \tag{44}$$

This can be written in the form

$$K_\nu(x) \;=\; \frac{1}{2}\int_0^\infty \exp\Bigl\{ -f(s)\Bigr\} \quad ,\quad f(s) \;=\; \frac{x}{2}\biggl(s + \frac{1}{s}\biggr) - (\nu - 1)\, \log_e s \;\; . \tag{45}$$

Then

$$f'(s) \;=\; \frac{x}{2}\biggl(1 - \frac{1}{s^2}\biggr) - \frac{\nu - 1}{s} \quad ,\quad f''(s) \;=\; \frac{x}{s^3} + \frac{\nu - 1}{s^2} \quad , \tag{46}$$

so that as $x \to \infty$, the condition $f'(s) = 0$ is satisfied by $s = 1$. Then $f''(1) \approx x$, and the method of steepest descents yields

$$K_\nu(x) \;\approx\; \sqrt{\frac{\pi}{2x}}\, e^{-x} \quad ,\quad x \;\gg\; \nu \;\gtrsim 1 \tag{47}$$

as the asymptotic approximation. Observe that retention of the ν contribution would lead to the next order term in the asymptotic expansion.

4 Numerical Integration

The foregoing formal content is now supplemented by an exploration of numerical aspects. The focus will be two-fold: first Newton-Cotes type approaches that are more elemental in character, and then a more sophisticated technique, specifically Gaussian quadrature.

4.1 Newton-Cotes Formulae

These derived from the elemental approach of Newton's theory of integration. The agenda is to compute areas under curves with increasing accuracy and complexity of algorithm. The first method is to approximate functional behavior on a sequence of intervals $[x_i,\, x_{i+1}]$ by a piecewise linear construct, thereby formulating the **trapezoidal rule**.

$\boxed{\textbf{Plot:}}$ Trapezoidal Rule Construct

Then,

$$f(x) \;\approx\; f_i + \Big(f_{i+1} - f_i\Big)\,\frac{x - x_i}{x_{i+1} - x_i} \quad . \tag{49}$$

This then gives an integral approximation on this interval of

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \;\approx\; \frac{h_i}{2}\Big(f_{i+1} + f_i\Big) \quad , \quad h_i \;=\; x_{i+1} - x_i \quad , \tag{50}$$

with an error of the order of h_i^3. Often, the implementation is for a sequence of evenly-spaced intervals. With $h_i = h$ for all i, the total integration over two consecutive intervals becomes

$$\boxed{\int_{x_i}^{x_{i+2}} f(x)\,dx \;\approx\; \frac{h}{2}\Big(f_i + 2f_{i+1} + f_{i+2}\Big) \quad .} \tag{51}$$

The accuracy of this trapezoidal rule can clearly be improved by choosing smaller intervals, unless their is a pathological problem with the integrand, for example a singularity or sharp peak within the overall integration range.

Simpson's Rule for Numerical Integration