Integration

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Introduction

Integration in closed form is rapidly becoming a lost art. Unlike differentiation, whose clear rules permit direct if tedious evaluation, integration often relies upon trial and error with many dead ends. In the heroic era of theoretical physics cleverness in changing variables or choosing contours was revered, but now practically any integral that can be done in closed form may be found in standard compilations, such as Gradshteyn and Ryzhik, or in mathematical software, such as *Mathematica*. Although some skill in symbolic integration is still needed for traditional examinations, for most physicists its usefulness beyond the Ph.D qualifier examination is rather limited, unless you happen to be teaching a course that still relies on the methodology of the nineteenth century. Nevertheless, compilations are not entirely complete and software packages are not perfect. Furthermore, traditional integration methods remain useful for developing insightful approximations to integrals that cannot be evaluated fully in closed form. Numerical methods provide answers but limited insight. Therefore, in this chapter we briefly present some of the most useful symbolic techniques. We also discuss integral representations of analytic functions.

Initialization

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Needs["Graphics`Master`"]
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Good tricks

Presumably integration by parts and variable transformations are too familiar to merit discussion here, but there are several other elementary methods that I have found quite valuable.

■ Parametric differentiation

Often when one integral is known, an entire family of related integrals can be developed by differentiating with respect to a parameter in the integrand. For example, given

$$I_0[\lambda] = \int_0^\infty e^{-\lambda x}\, dx = \frac{1}{\lambda}$$

the entire family

$$I_n[\lambda] = \int_0^\infty x^n e^{-\lambda x}\, dx = \left(-\frac{\partial}{\partial\lambda}\right)^n I_0[\lambda] = \frac{n!}{\lambda^{n+1}}$$

becomes available. If one needs to evaluate an integral, like $\int_{-\infty}^{\infty} x^{2n} e^{-x^2}\, dx$, that is presented without a parameter, simply insert one to obtain

$$\int_{-\infty}^{\infty} x^{2n} e^{-\lambda x^2}\, dx = \left(-\frac{\partial}{\partial\lambda}\right)^n \sqrt{\frac{\pi}{\lambda}} = \frac{(2n-1)!!}{2^n \lambda^{n+\frac{1}{2}}}$$

and then set $\lambda \to 1$. It might surprise you how often this trick is helpful.

Notice that if a parameter appears in the limits of integration, one must also include the variation of these limits using

$$\frac{\partial}{\partial\lambda} \int_{a[\lambda]}^{b[\lambda]} f[x, \lambda]\, d\lambda = \int_a^b \frac{\partial f[x, \lambda]}{\partial\lambda}\, dx + f[b, \lambda]\, \frac{\partial b}{\partial\lambda} - f[a, \lambda]\, \frac{\partial a}{\partial\lambda}$$

with the rhs evaluated for the appropriate λ.

■ Convergence factors

Sometimes when it is not obvious whether the integral of an oscillatory function over an infinite range will converge to a definite value, application of a convergence factor may help resolve the question. For example, it is not obvious, at least to me, whether $\int_0^\infty \mathrm{Sin}[k\,x]\, dx$ converges. Consider instead

$$\int_0^\infty e^{-\lambda x}\, \mathrm{Sin}[k\,x]\, dx = \mathrm{Im}\left[\int_0^\infty e^{-\lambda x} e^{i k x}\, dx\right] = \mathrm{Im}\left[\frac{1}{\lambda - i k}\right] = \frac{k}{\lambda^2 + k^2}$$

which does converge for $\lambda > 0$. The desired integral is then obtained from the limit $\lambda \to 0$, whereby

$$\int_0^\infty \mathrm{Sin}[k\,x]\, dx = \lim_{\lambda\to 0} \int_0^\infty e^{-\lambda x}\, \mathrm{Sin}[k\,x]\, dx = \frac{1}{k}$$

Admittedly, this result does appear somewhat arbitrary and some skepticism is justified. However, if this integral were encountered in a physics problem, it probably would arise from a limiting process anyway. Either a spatial or temporal variable should be limited to a finite range or a damping mechanism should be present that ensures convergence. One should then retreat a few steps in the derivation, identify the appropriate convergence factor, and evaluate the integral before that convergence factor is lost from view.

Contour integration

■ Residue theorem

Suppose that $f[z]$ is analytic throughout a domain D except for isolated singularities (poles) and that a simple closed contour C within D encircles poles $\{z_k,\ k = 1, N\}$ with residues R_k. By deforming the contour to encircle each pole, we obtain

$$\oint_C f[z]\, dz = \sum_{k=1}^{N} \oint_{C_k} f[z]\, dz$$

where each C_k is a small circle encompassing pole k. Near each z_k we can employ a Laurent expansion

$$f[z] = \sum_{n=-m_k}^{\infty} a_{n,k} (z - z_k)^n \implies \oint_{C_k} f[z]\, dz = \sum_{n=-m_k}^{\infty} a_{n,k} \oint_{C_k} (z - z_k)^n\, dz$$

to evaluate its contribution to the contour integral. Using the now familiar circular contour integration with $z - z_k = \rho\, e^{i\theta} \implies dz = \rho\, e^{i\theta}\, i\, d\theta$, we obtain

$$\oint_{C_k} (z - z_k)^n\, dz = i\, \rho^{n+1} \int_0^{2\pi} e^{i(n+1)\theta}\, d\theta = 2\pi i\, \delta_{n,-1} \implies \oint_{C_k} f[z]\, dz = 2\pi i\, a_{-1,k} = 2\pi i\, R_k$$

Therefore, we obtain the *residue theorem*:

> *Residue theorem*: If $f[z]$ is analytic on and within a simple closed counterclockwise contour C, except for interior poles $\{z_k,\ k = 1, N\}$ with residues R_k, then
> $\oint_C f[z]\, dz = 2\pi i \sum_{k=1}^{N} R_k$

This is an amazingly powerful theorem that can be used, with clever choices of contour, to evaluate a wide variety of definite integrals which might be very difficult by means of familiar antidifferentiation methods. The trick is to find a simple closed contour that contains the desired integral on one portion of the path with easier integrals on the remainder of the path (if any). The examples in following subsections will demonstrate that contour integration using the residue theorem provides some of the most versatile methods for evaluating definite integrals.

■ Definite integrals of the form $\int_0^{2\pi} f[\sin\theta, \cos\theta]\, d\theta$

We assume that $f[\sin\theta, \cos\theta]$ can be represented by a single-valued function of $z = e^{i\theta}$ in the relevant region of the complex plane. Often f is a rational function of $\sin\theta$ and $\cos\theta$. Then we use

$$z = e^{i\theta} \implies d\theta = -i\,\frac{dz}{z}, \quad \text{Sin}[\theta] = \frac{z - z^{-1}}{2i}, \quad \text{Cos}[\theta] = \frac{z + z^{-1}}{2}$$

such that

$$\int_0^{2\pi} f[\text{Sin}[\theta], \text{Cos}[\theta]]\, d\theta = -i \oint f\left[\frac{z - z^{-1}}{2i}, \frac{z + z^{-1}}{2}\right] \frac{dz}{z} = 2\pi \sum \text{residues within unit circle}$$

where the contour is the unit circle about the origin. Special handling is needed if any of the singularities of f are on the unit circle.

example: $I[a] = \int_0^{\pi} \frac{a}{a^2 + \text{Sin}[\theta]^2}\, d\theta$

Although this integral is not stated in the desired form, the integrand is even. Hence, by direct application of the recipe above, we find

$$I[a] = \frac{1}{2} \int_0^{2\pi} \frac{a}{a^2 + \text{Sin}[\theta]^2}\, d\theta = -4\, i\, a \oint \frac{z}{4 a^2 z^2 - (z^2 - 1)^2}\, dz$$

The denominator is a quadratic in z^2, so that one obtains four poles at

```
denominator = 4 a^2 z^2 - (z^2 - 1)^2;
poles = z /. Solve[denominator == 0, z]
```

$$\left\{-a - \sqrt{1 + a^2},\ a - \sqrt{1 + a^2},\ -a + \sqrt{1 + a^2},\ a + \sqrt{1 + a^2}\right\}$$

Evaluation of the residues

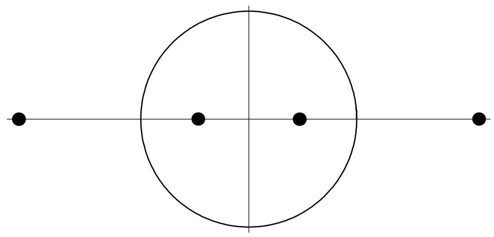
```
Map[Residue[z/denominator, {z, #}] &, poles]
```

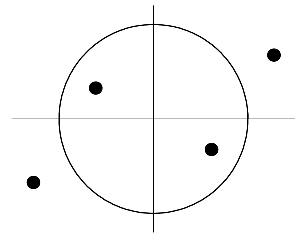
$$\left\{-\frac{1}{8 a \sqrt{1 + a^2}},\ \frac{1}{8 a \sqrt{1 + a^2}},\ \frac{1}{8 a \sqrt{1 + a^2}},\ -\frac{1}{8 a \sqrt{1 + a^2}}\right\}$$

is straightforward, even by hand. If $a > 0$ the pair of poles at $\pm\left(a - \sqrt{1 + a^2}\right)$ is inside the unit circle while the other pair is outside, while if $a < 0$ the reverse is true. In either case we have two equal contributions, such that

$$I[a] = \frac{\pi}{\sqrt{1 + a^2}}$$

The sketch below illustrates the positions of the poles relative to the unit circle. The left figure uses a real value for a, while the right figure uses a complex value. Although one typically assumes that parameters in definite integrals are real, the method is more general and does not require that assumption.





Alternatively, if we use a trigonometric identity to express the integrand as

$$\frac{\mathtt{a}}{\mathtt{a}^2+\mathtt{Sin}[\theta]^2}\ \mathtt{/.}\ \mathtt{Sin}[\theta]^2 \to \frac{1-\mathtt{Cos}[2\,\theta]}{2}\ \mathtt{//\ Simplify}$$

$$\frac{2\,\mathtt{a}}{1+2\,\mathtt{a}^2-\mathtt{Cos}[2\,\theta]}$$

we obtain a contour integral with a quadratic denominator

$$I[a] = \int_0^{2\pi} \frac{a}{1+2\,a^2-\mathrm{Cos}[\theta]}\,d\theta = 2\,i\,a \oint \frac{1}{z^2-2\,(2\,a^2+1)\,z+1}\,dz$$

for which evaluation of the residues is easier by hand.

```
denominator = z^2 - 2 (2 a^2 + 1) z + 1;
poles = z /. Solve[denominator == 0, z]
```

$$\left\{1+2\,\mathtt{a}^2-2\,\mathtt{a}\,\sqrt{1+\mathtt{a}^2},\ 1+2\,\mathtt{a}^2+2\,\mathtt{a}\,\sqrt{1+\mathtt{a}^2}\right\}$$

$$\mathtt{Map}\left[\mathtt{Residue}\left[\frac{1}{\mathtt{denominator}},\ \{\mathtt{z},\ \#\}\right]\ \&,\ \mathtt{poles}\right]$$

$$\left\{-\frac{1}{4\,\mathtt{a}\,\sqrt{1+\mathtt{a}^2}},\ \frac{1}{4\,\mathtt{a}\,\sqrt{1+\mathtt{a}^2}}\right\}$$

Notice that there are only two poles in the transformed function because the angular variable was replaced by $\theta \to \theta/2$. Recognizing that for either sign of a just one of the poles is within the unit circle, one obtains the same final result.

■ Definite integrals of the form $\int_{-\infty}^{\infty} f[x]\,dx$

We assume that $f[z]$ is analytic except for isolated singularities and vanishes faster than z^{-1} for $r \to \infty$ in either half-plane. With these conditions we can employ a semicircular contour of radius $R \to \infty$ closed in the appropriate half-plane to obtain

$$\int_{-\infty}^{\infty} f[x]\,dx = \oint f[z]\,dz = 2\,\pi\,i \sum \text{residues in half–plane}$$

To prove this result, suppose that $f[z]$ is bounded in the upper half-plane such that

$$|f[R\,e^{i\,\theta}]| \le M\,R^{-\alpha} \implies \left|\int_0^{\pi} f[R\,e^{i\,\theta}]\,d\theta\right| \le M\,R^{-\alpha}\,\pi\,R$$

where M is a positive real number. Then

$$\alpha > 1 \implies \lim_{R\to\infty} \left|\int_0^{\pi} f[R\,e^{i\,\theta}]\,d\theta\right| \le \lim_{R\to\infty} \pi\,M\,R^{1-\alpha} = 0 \implies \lim_{R\to\infty} \int_{-R}^{R} f[x]\,dx = 2\,\pi\,i \sum \text{residues in half–plane}$$

ensures that if f falls fast enough we need only evaluate the residues at isolated singularities of the analytic function $f[z]$ in the appropriate half plane. Therefore, we find

$$\lim_{R\to\infty} R\,|f[R\,e^{i\,\theta}]| = 0 \implies \lim_{R\to\infty} \int_{-R}^{R} f[x]\,dx = 2\,\pi\,i \sum \text{residues in half–plane}$$

using a *great semicircle*.

example: $I[a] = \int_{-\infty}^{\infty} \frac{1}{1+x^4}\,dx$

The integral

$$\int_{-\infty}^{\infty} \frac{1}{1+x^4}\,dx = \oint_C \frac{1}{1+z^4}\,dz$$

can be evaluated using a semicircular contour in either half plane. The integrand has poles at $z_k = \text{Exp}[i\,\pi\,\frac{2\,k+1}{4}]$ for $k = 1, 4$ of which two are found in each half plane. The residues can be evaluated using

$$f[z] = \frac{1}{q[z]} \implies R_k = \frac{1}{q'[z_k]} = \frac{1}{4\,{z_k}^3} = \frac{1}{4}\,e^{-3\,i\,\pi/4}\,i^k = -\frac{1+i}{4\,\sqrt{2}}\,i^k$$

Thus, we obtain

$$\int_{-\infty}^{\infty} \frac{1}{1+x^4}\,dx = \oint_C \frac{1}{1+z^4}\,dz = 2\,\pi\,i\left(-\frac{1+i}{4\,\sqrt{2}}\right)(1+i) = \frac{\pi}{\sqrt{2}}$$

■ Fourier integrals

Consider a Fourier integral of the form

$$\tilde{f}[k] = \int_{-\infty}^{\infty} f[x]\,e^{i\,k\,x}\,dx$$

where k is a positive real number. Integrals of this type can often be evaluated by extending f to the complex plane and using a great semicircle in the upper half-plane, provided that the contribution of the return path

$$I_R[k] = i\,R \int_0^{\pi} f[R\,e^{i\,\theta}]\,\text{Exp}[-k\,R\,(\text{Sin}[\theta] - i\,\text{Cos}[\theta])]\,d\theta$$

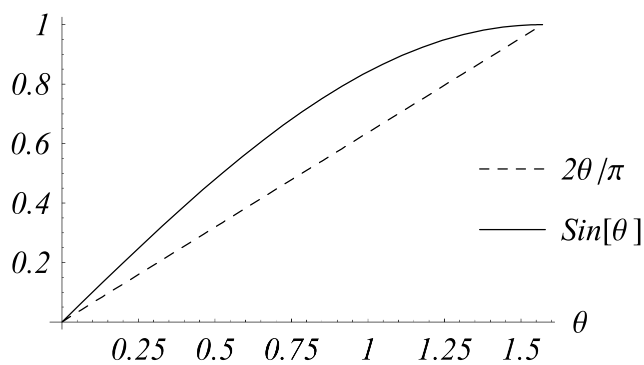
vanishes in the limit $R \to \infty$. Suppose that M_R is the maximum modulus of f on this arc, such that

$$|I_R| \le R\,M_R \int_0^{\pi} \text{Exp}[-k\,R\,\text{Sin}[\theta]\,]\,d\theta$$

Dividing this latter result into two equal contributions now gives

$$|I_R| \le 2\,R\,M_R \int_0^{\pi/2} \text{Exp}[-k\,R\,\text{Sin}[\theta]\,]\,d\theta$$

The figure below illustrates that $\text{Sin}[\theta] > 2\,\theta/\pi$ on this interval.



Thus, the integral on the great semicircle is limited by

$$|I_R| \le 2\,R\,M_R \int_0^{\pi/2} \mathrm{Exp}[-2\,k\,R\,\theta/\pi]\,d\theta$$

or

$$|I_R| \le \pi\,M_R\,\frac{1-e^{-k\,R}}{k}$$

This result is known as *Jordan's lemma*. Therefore, if $k>0$ and if $f[z]$ vanishes on an infinite semicircle, such that

$$\lim_{R\to\infty} M_R = 0 \implies |I_R| = 0$$

the contribution of the return path vanishes and we may evaluate the Fourier integral using

$$\lim_{R\to\infty} |f[R\,e^{i\,\theta}]| = 0 \implies \int_{-\infty}^{\infty} f[x]\,e^{i\,k\,x}\,dx = 2\,\pi\,i \sum \text{residues of integrand in half–plane}$$

If k happens to be a negative real number, we close in the lower half-plane instead and obtain the same result. Notice that this condition upon f is less restrictive than in the previous section due to the presence of the exponential factor, which is damping in the appropriate half plane. However, convergence for $k=0$ requires $\lim_{R\to\infty} R\,|f[R\,e^{i\,\theta}]| = 0$ as before.

example: $\int_0^\infty \frac{\mathrm{Cos}[k\,x]}{x^2+a^2}\,dx$

Consider the integral

$$\tilde{f}[k] = \int_0^\infty \frac{\mathrm{Cos}[k\,x]}{x^2+a^2}\,dx$$

where k and a are positive real numbers. Although this integral is not presented in the desired form, it is simply half the real part of

$$\tilde{g}[k] = \int_{-\infty}^{\infty} \frac{\mathrm{Exp}[i\,k\,x]}{x^2+a^2}\,dx = \oint \frac{\mathrm{Exp}[i\,k\,z]}{z^2+a^2}\,dz \implies \tilde{f}[k] = \frac{1}{2}\,\mathrm{Re}[\,\tilde{g}[k]\,]$$

and may be evaluated using a great semicircle in the upper half-plane, wherein lies one simple pole at $z = i\,a$. Therefore, we obtain

$$\tilde{g}[k] = 2\,\pi\,i\,\frac{\mathrm{Exp}[-k\,a]}{2\,i\,a} \implies \tilde{f}[k] = \frac{\pi\,e^{-k\,a}}{2\,a}$$

without further ado. The result is actually more general than this derivation — it applies equally well for complex a provided only that $\mathrm{Re}[a] \neq 0$ to ensure that the poles are not on the real axis. Be alert to generalizations! Having expended some effort to obtain a result, it is good practice to extend it to the most general conditions possible. Also notice that one cannot use $\mathrm{Cos}[a\,z]/(z^2+a^2)$ directly because $\mathrm{Cos}[a\,z]$ is not bounded on the great semicircle — it diverges exponentially for large $\mathrm{Im}[z]$ in both upper and lower half-planes.

■ Custom contours

Sometimes it is necessary to design a contour which exploits specific characteristics of the integrand. For example, when previously evaluating the integral $\int_0^\infty \mathrm{Cos}[x^2]\, dx$ we employed an arc subtending $\pi/4$ radians. Unfortunately, there are no general rules to guide one toward the optimum contour for an arbitrary integrand; one must rely on intuition and experience to minimize the amount of trial-and-error in choosing such contours. Below we give just one more example of a custom contour.

Consider the integral

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

The integral on the real axis converges because the integrand is of order $e^{a x}$ for $x \to -\infty$ or $\mathrm{Exp}[(a-1)\,x]$ for $x \to \infty$ and decreases exponentially in either limit when $0 < a < 1$. However, the function

$$f[z] = \frac{e^{a z}}{e^z + 1} \implies z_k = (2\,k+1)\,\pi\, i$$

with simple poles on the imaginary axis at odd-integer multiples of π does not satisfy the conditions needed to employ a great semicircle. Fortunately, the contour integral around a rectangular strip $(-\infty < x < \infty,\ 0 \le y \le 2\,\pi)$

$$\oint f[z]\, dz = \lim_{R\to\infty}\left(\int_{-R}^{R} f[(x,0)]\, dx + \int_0^{2\pi} f[(R,y)]\, dy + \int_R^{-R} f[(x,2\,\pi)]\, dx + \int_{2\pi}^{0} f[(-R,y)]\, dy \right)$$

can be evaluated fairly easily. This contour encloses a single pole at $z_0 = i\,\pi$ with residue $-e^{i\,\pi\,a}$, such that

$$\oint f[z]\, dz = -2\,\pi\, i\, e^{i\,\pi\,a}$$

The contributions from vertical segments

$$\lim_{R\to\infty} f[(R,y)] = \lim_{R\to\infty} \frac{\mathrm{Exp}[a\,(R+i\,y)]}{\mathrm{Exp}[R+i\,y]+1} = \lim_{R\to\infty} \mathrm{Exp}[(a-1)\,R] = 0$$

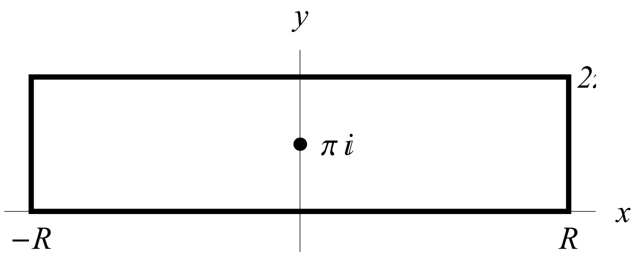
$$\lim_{R\to\infty} f[(-R,y)] = \lim_{R\to\infty} \frac{\mathrm{Exp}[a\,(-R+i\,y)]}{\mathrm{Exp}[-R+i\,y]+1} = \lim_{R\to\infty} \mathrm{Exp}[-a\,R] = 0$$

vanish in the limit $R \to \infty$, while the horizontal segments are related by

$$f[(x,2\,\pi)] = \frac{\mathrm{Exp}[a\,(x + 2\,\pi\, i)]}{\mathrm{Exp}[x + 2\,\pi\, i]+1} = \mathrm{Exp}[2\,\pi\, i\, a]\, f[(x,0)]$$

such that

$$\oint f[z]\, dz = (1 - e^{2\,\pi\, i\, a})\, I \implies I = \frac{\pi}{\mathrm{Sin}[\pi\, a]}$$



This result actually finds somewhat broader applicability because the contributions from the vertical segments vanish provided only that $0 < \mathrm{Re}[a] < 1$. Therefore, we can allow a to be complex and find

$$\int_{-\infty}^{\infty} \frac{e^{a x}}{e^x + 1} \, dx = \frac{\pi}{\mathrm{Sin}[\pi a]} \qquad \text{for } 0 < \mathrm{Re}[a] < 1$$

As always, be alert for possible generalizations.

Isolated singularities on the contour

■ Removable singularity

Often one encounters isolated singularities on the integration path. For example, the integral

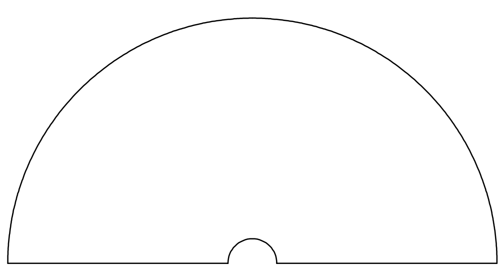
$$I = \int_{-\infty}^{\infty} \frac{\mathrm{Sin}[x]}{x} \, dx$$

is important in Fourier analysis. The integrand has a removable singularity at the origin, but that would not cause any difficulty if the integral remained in this form. However, because $\mathrm{Sin}[z]$ is divergent as $y \to \infty$, we would prefer to evaluate

$$I = \mathrm{Im} \int_{-\infty}^{\infty} \frac{e^{i x}}{x} \, dx$$

by closing the contour in the upper half plane. The penalty for this transformation is that the singularity at the origin is no longer removable. Fortunately, that problem can be avoided by also making a small semicircular detour around the origin

$$\oint \frac{e^{i z}}{z} \, dz = 0$$



such that, according to Cauchy's theorem, the integral

$$\oint \frac{e^{iz}}{z}\, dz = 0$$

vanishes on this contour because no singularities are enclosed. The contribution of the great semicircle vanishes because the integrand satisfies the requirements of Jordan's lemma. The linear segments

$$\lim_{\varepsilon \to 0} \left(\int_{-\infty}^{-\varepsilon} f[x]\, dx + \int_{\varepsilon}^{\infty} f[x]\, dx \right)$$

converge to the desired integral in the limit $\varepsilon \to 0$ because the integrand is well-behaved on the real axis. The contribution of the small semicircle of radius $\varepsilon \to 0$ is evaluated using

$$dz = i\, z\, d\theta \implies i \int_{\pi}^{0} f[z]\, z\, d\theta = i \lim_{\varepsilon \to 0} \int_{\pi}^{0} \mathrm{Exp}[i\, \varepsilon\, e^{i\theta}]\, d\theta = -i\, \pi$$

Therefore, we find

$$\int_{-\infty}^{\infty} \frac{\mathrm{Sin}[x]}{x}\, dx = \pi$$

Notice that the contribution of the semicircular detour is $\pi\, i$ times the residue of the integrand, half the value we would have obtained from the residue theorem for a complete circle around the singularity. More generally, if $f[z]$ is analytic at z_0, the detour integral

$$z - z_0 = \varepsilon\, e^{i\theta} \implies \lim_{\varepsilon \to 0} \int_{\theta}^{\theta + \Delta\theta} \frac{f[z_0 + \varepsilon\, e^{i\theta}]}{z - z_0}\, dz = f[z_0]\, i\, \Delta\theta$$

is proportional to the angle subtended. This result is easily proven by expanding $f[z]$ around z_0. Also, notice that $\Delta\theta$ is positive for counterclockwise or negative for clockwise detours.

■ Cauchy principal value

An improper integral whose integrand is singular at one of the endpoints of the integration range is defined by one of the limits

$$\int_a^b f[x]\, dx = \lim_{\varepsilon \to 0} \int_{a+\varepsilon}^{b} f[x]\, dx \quad \text{or} \quad \int_a^b f[x]\, dx = \lim_{\varepsilon \to 0} \int_a^{b-\varepsilon} f[x]\, dx$$

However, if an isolated singularity lies within the range of integration then two limits are needed

$$\int_a^c f[x]\, dx = \lim_{\varepsilon_1 \to 0} \int_a^{b-\varepsilon_1} f[x]\, dx + \lim_{\varepsilon_2 \to 0} \int_{b+\varepsilon_2}^{c} f[x]\, dx$$

and often there will be no unique value if the two limits are taken independently. For example, applying this method to

$$\int_{-1}^{1} \frac{dx}{x} = \lim_{\varepsilon_1 \to 0} \int_{-1}^{-\varepsilon_1} \frac{dx}{x} + \lim_{\varepsilon_2 \to 0} \int_{\varepsilon_2}^{1} \frac{dx}{x} = \lim_{\varepsilon_1 \to 0, \varepsilon_2 \to 0} \log\left[\frac{\varepsilon_1}{\varepsilon_2}\right]$$

does not provide an unambiguous result unless one decides to approach the singularity in a symmetric manner, such that $\varepsilon_1 = \varepsilon_2$. This particular value is designated the *Cauchy principal value* of the integral and denoted by $\mathcal{P}\int$, such that

$$\mathcal{P}\int_a^c f[x]\, dx = \lim_{\varepsilon \to 0} \left(\int_a^{b-\varepsilon} f[x]\, dx + \int_{b+\varepsilon}^{c} f[x]\, dx \right)$$

Hence, for the example above we find

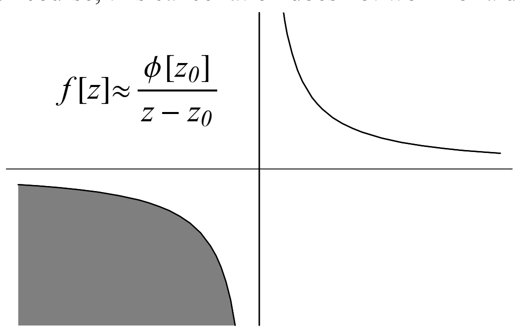
$$\mathcal{P}\int_{-1}^{1}\frac{dx}{x} = 0$$

If there are several isolated singularities on the contour, the Cauchy principal value treats each symmetrically.

The Cauchy principal value is based upon antisymmetric behavior near a simple pole, where we can write

$$f[z] = \frac{a_{-1}}{z-z_0} + g[z]$$

with $g[z]$ analytic near z_0. The two divergent contributions on either side cancel, leaving behind the background contribution g. Of course, this cancellation does not work for a double pole with symmetric divergence.

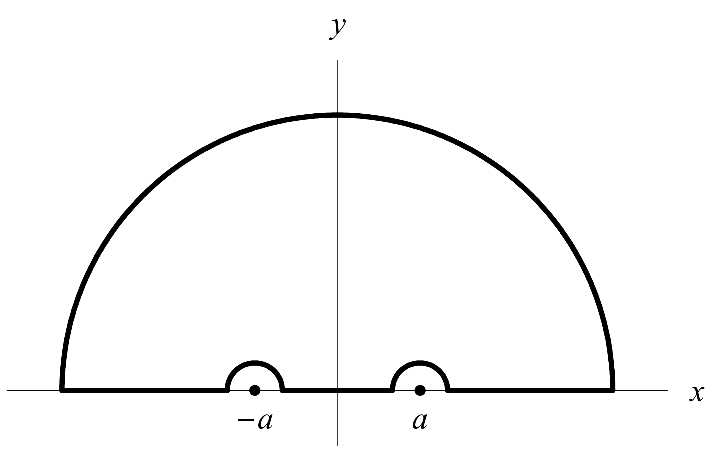


example: $\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Cos}[k\,x]}{a^2-x^2}\,dx$

Consider the integral

$$I = \mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Cos}[k\,x]}{a^2-x^2}\,dx = \mathrm{Re}\left[\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Exp}[i\,k\,x]}{a^2-x^2}\,dx\right]$$

where a and k are positive real numbers. By replacing Cos with Exp we are able to close the contour in the upper half plane and use Jordan's lemma to discard the contribution of the great semicircle. The singularities at $x=\pm a$ are avoided using small semicircular indentations, as sketched below.



The contribution from the segments along the real axis sum to the principal value, while the indentations contribute $-i\pi$ times the sum of the two residues because the semicircles are traversed in a negative sense. Thus,

$$0 = \oint_C\frac{\mathrm{Exp}[i\,k\,z]}{a^2-z^2}\,dz = \mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Exp}[i\,k\,x]}{a^2-x^2}\,dx - i\pi\left(\frac{e^{i\,k\,a}}{-2\,a}+\frac{e^{-i\,k\,a}}{2\,a}\right)$$

gives

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{\text{Exp}[i\,k\,x]}{a^2-x^2}\,dx = \frac{\pi}{a}\,\text{Sin}[k\,a] \quad\Longrightarrow\quad \mathcal{P}\int_{-\infty}^{\infty}\frac{\text{Cos}[k\,x]}{a^2-x^2}\,dx = \frac{\pi}{a}\,\text{Sin}[k\,a]$$

Notice that the principal value is the same whether we choose indentations to exclude or to include either or both poles (four possibilities) — check this for yourself!. Thus, the contribution to a principal value integral made by a simple pole on the contour is half the value it would have made if enclosed.

Integration around a branch point

If the integrand involves a multivalued function, care must be taken with any branch cuts in the integration region. Such functions often differ in phase on opposite sides of the cut, so that contours with segments on opposite sides will include contributions of equal magnitude but different phase. Often the presence of a branch cut actually assists in evaluation of an integral — branch cuts are not always monsters to be feared! While it is difficult to formulate general rules, a couple of examples should suffice to illustrate the method.

Suppose that we wish to evaluate the integral

$$\int_0^{\infty}\frac{x^a}{x+b}\,dx \quad \text{with} \quad -1<a<0\,,\; b>0$$

using contour integration. The function

$$f[z] = \frac{z^a}{z+b}$$

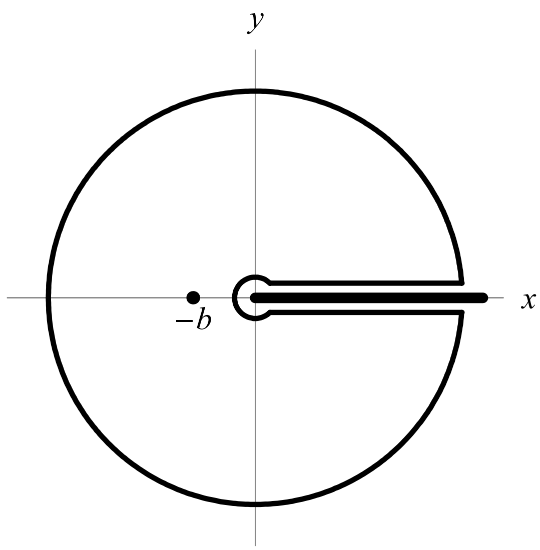
has a pole at $z=-b$ and requires a branch cut to define the phase of the numerator when a is nonintegral. This branch cut will connect singularities at $z=0$ and $z\to\infty$, but we have some freedom in choosing its orientation. Although one usually cuts such a function along the negative real axis, for this purpose it is more convenient to put the cut on the positive real axis so that the desired integral is found on one segment of the contour sketched below. For now we assume that $b>0$ so that the pole is is on the negative real axis. Thus, for this problem we will cut just below the positive real axis and define the principal branch as

$$z^a = |z|^a\,\text{Exp}[i\,a\,\text{arg}[z]\,] \qquad \text{with} \quad 0\le\text{arg}[z]<2\,\pi$$

by restricting the phase of z to the range $(0,2\pi)$. The residue of the pole is then $b^a\,\text{Exp}[i\,\pi\,a]$ such that

$$\oint_C f[z]\,dz = 2\,\pi\,i\,b^a\,\text{Exp}[i\,\pi\,a]$$

on the positive contour below, which encloses the pole without crossing the branch cut.



The contribution of the outer circle vanishes in the limit $R \to \infty$ because

$$|z| \to \infty \implies |f[z]| \longrightarrow |z|^{a-1}$$

falls more rapidly than $|z|^{-1}$ when $a < 0$. Similarly, the integral on the inner circle with radius ε vanishes in the limit $\varepsilon \to 0$. The contributions on either side of the real axis are both proportional to the desired integral but differ in phase. On the top side of the cut $z^a \to x^a$ while on the bottom side $z^a \to x^a \,\mathrm{Exp}[2\,\pi\,i\,a]$, such that

$$(1 - \mathrm{Exp}[2\,\pi\,i\,a])\int_0^\infty \frac{x^a}{x+b}\,dx = 2\,\pi\,i\,b^a\,\mathrm{Exp}[i\,\pi\,a]$$

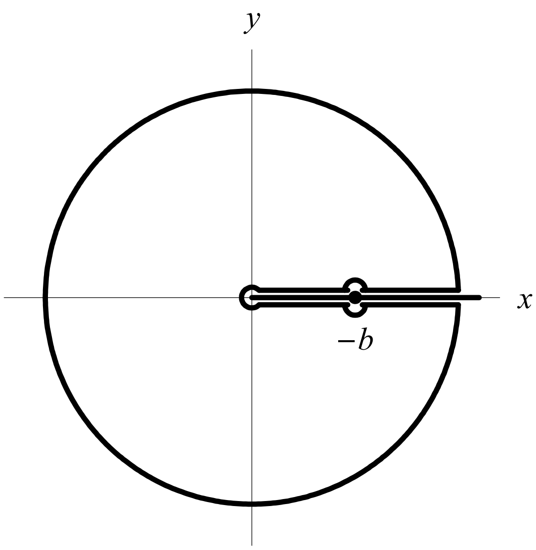
Therefore, we obtain the integral

$$\int_0^\infty \frac{x^a}{x+b}\,dx = -\frac{b^a\,\pi}{\mathrm{Sin}[\pi\,a]} \qquad \text{for } -1 < a < 0,\ b > 0$$

This result can be generalized by recognizing that we need only require $-1 < \mathrm{Re}[a] < 0$ to ensure that the contribution of the outer circle vanishes as its radius becomes infinite. The definition of $b^a = \mathrm{Exp}[a\,\mathrm{Log}[b]] = \mathrm{Exp}[a\,(\mathrm{Log}[|b|] + i\,\mathrm{Arg}[b])]$ can be extended to complex powers. Therefore, we obtain the more general result

$$\int_0^\infty \frac{x^a}{x+b}\,dx = -\frac{b^a\,\pi}{\mathrm{Sin}[\pi\,a]} \qquad \text{for } -1 < \mathrm{Re}[a] < 0 \text{ and } \mathrm{Arg}[b] \neq \pi$$

without extra work. However, this result does not apply if $\mathrm{Arg}[b] = \pi$, because then there would be a pole on the contour. To handle that situation, we employ the contour shown below for which the segments on either side of the positive real axis are proportional to the principal value of the desired integral.



This contour encloses no poles, so that

$$b < 0 \implies \oint_C \frac{z^a}{z+b}\, dz = 0$$

The integral around the great circle vanishes, as before, but we now have two small semicircular indentations to evaluate. Using $z + b = \varepsilon e^{i\theta} \implies dz = i\,\varepsilon\, e^{i\theta}\, d\theta$, both contributions take the form

$$\lim_{\varepsilon\to 0} \int_{\theta_1}^{\theta_2} \frac{(-b+\varepsilon\, e^{i\theta})^a}{\varepsilon\, e^{i\theta}}\, i\,\varepsilon\, e^{i\theta}\, d\theta = i\,(-b)^a\, e^{i a \phi}\, (\theta_2 - \theta_1) = i\,(-b)^a\, e^{i a\phi}\, \Delta\theta$$

where on the upper semicircle $\phi = 0$ and $\theta_1 = \pi$, $\theta_2 = 0 \implies \Delta\theta = -\pi$ while on the lower semicircle we must choose $\phi = 2\pi$ and $\theta_1 = 2\pi$, $\theta_2 = \pi \implies \Delta\theta = -\pi$ for the selected branch of z^a. The integrals along the real axis on either side of the branch cut are both principal-value integrals with different phase factors because on the upper side $z^a = x^a$ while on the lower side $z^a = x^a\, e^{2\pi i a}$. Thus, we obtain

$$(1 - e^{2\pi i a})\, \mathcal{P}\int_0^\infty \frac{x^a}{x-b}\, dx = i\,\pi\,(-b)^a\,(1 + e^{2\pi i a})$$

and conclude

$$b < 0 \implies \mathcal{P}\int_0^\infty \frac{x^a}{x+b}\, dx = -(-b)^a\,\pi\,\mathrm{Cot}[\pi\, a]$$

Notice that *Mathematica* provides the expected result for Arg[b] ≠ π, but does not automatically assume that the principal value is meant when the singularity is on the contour. Consequently,

$$\int_0^\infty \frac{\mathbf{x^a}}{\mathbf{x+b}}\, d\mathbf{x}$$

```
Integrate::gener : Unable to check convergence. More…
```

```
If[Re[a] < 0 && 1 + Re[a] > 0 && Re[b] > 0 && Re[b] ≥ 0 ||
   Im[b] ≠ 0 && Re[a] < 0 && 1 + Re[a] > 0 && Re[b] > 0, -b^a π Csc[a π],
  Integrate[x^a/(b + x), {x, 0, ∞}, Assumptions → Re[a] ≥ 0 || 1 + Re[a] ≤ 0 || Re[b] ≤ 0]]
```

returns a result with warnings about possible convergence issues and the conditions for validity. Unfortunately, version 5.0 is still not able to determine that the following conditions are sufficient to ensure the convergence of this definite integral.

$$\texttt{Integrate}\left[\frac{x^a}{x+b}, \{x, -\infty, \infty\}, \texttt{Assumptions} \to \{-1 < \texttt{Re}[a] < 0, \texttt{Re}[b] \neq 0, \texttt{Arg}[b] \neq \pi\}\right]$$

```
Integrate::gener : Unable to check convergence. More…
```

$$\texttt{If}\left[\texttt{Im}[b] \neq 0 \,\&\&\, \texttt{Re}[b] > 0,\ \left(-\frac{1}{b^2}\right)^{-a} \left(-\left(-\frac{1}{b}\right)^{a} + (-1)^a b^{-a}\right) \pi\,\texttt{Csc}[a\,\pi],\right.$$
$$\texttt{Integrate}\left[\frac{x^a}{b+x}, \{x, -\infty, \infty\}, \texttt{Assumptions} \to\right.$$
$$\left.\left.\texttt{Re}[a] > -1 \,\&\&\, \texttt{Re}[a] < 0 \,\&\&\, \texttt{Arg}[b] \neq \pi \,\&\&\, \texttt{Re}[b] \neq 0 \,\&\&\, (\texttt{Im}[b] == 0 \,||\, \texttt{Re}[b] \leq 0)\right]\right]$$

Using the option PrincipalValue→True, together with specific assumptions about the parameters, provides the desired result

$$\texttt{Integrate}\left[\frac{x^a}{x+b}, \{x, 0, \infty\},\right.$$
$$\left.\texttt{Assumptions} \to \{-1 < \texttt{Re}[a] < 0, b < 0\}, \texttt{PrincipalValue} \to \texttt{True}\right]$$

$$-(-b)^a\, \pi\, \texttt{Cot}[a\,\pi]$$

without cautions about convergence or conditions for validity.

Reduction to tabulated integrals

Some integrals that cannot be evaluated in terms of elementary functions occur sufficiently frequently to merit naming as special functions. Among the most useful are the *gamma function*

$$\Gamma[x] = \int_0^\infty t^{x-1}\, e^{-t}\, dt\,, \quad x > 0$$

and its cousins the *incomplete gamma function*

$$\Gamma[x, a] = \int_a^\infty t^{x-1}\, e^{-t}\, dt\,, \quad x > 0,\ a \geq 0$$

and the *beta function*

$$B[r, s] = \frac{\Gamma[r]\,\Gamma[s]}{\Gamma[r+s]} = \int_0^1 t^{r-1}\,(1-t)^{s-1}\, dt$$

Also important are the *sine* and *cosine integrals*

$$\text{Si}[x] = \int_0^x \frac{dt}{t}\,\text{Sin}[t] \qquad \text{Ci}[x] = -\int_x^\infty \frac{dt}{t}\,\text{Cos}[t]$$

and the *exponential integrals*

$$E_n[x] = \int_1^\infty \frac{dt}{t^n} e^{-x t} \qquad \text{Ei}[x] = \mathcal{P}\int_{-\infty}^x \frac{dt}{t} e^t$$

The *error function* $\text{Erf}[x]$ and *complementary error function* $\text{Erfc}[x] = 1 - \text{Erf}[x]$ are defined by

$$\text{Erf}[x] = \frac{2}{\sqrt{\pi}} \int_0^x dt\, e^{-t^2} \qquad \text{Erfc}[x] = \frac{2}{\sqrt{\pi}} \int_x^\infty dt\, e^{-t^2}$$

while their trigonometric cousins are the *Fresnel sine* and *cosine functions*

$$S[x] = \int_0^x dt\,\text{Sin}\left[\frac{\pi t^2}{2}\right] \qquad C[x] = \int_0^x dt\,\text{Cos}\left[\frac{\pi t^2}{2}\right]$$

Once an integral has been reduced to one of these special functions, it can be considered done because these functions have been studied and tabulated extensively and are also available in many mathematical software packages.

■ example: $\int_{-\infty}^{\infty} e^{-x^4}\, dx$

The integral

$$I = \int_{-\infty}^\infty e^{-x^4}\, dx = 2\int_0^\infty e^{-x^4}\, dx$$

can be expressed in terms of a gamma function using the variable transformation

$$y = x^4 \quad dy = 4x^3\, dx \Longrightarrow dx = \frac{1}{4} y^{-3/4}\, dy$$

whereby

$$I = \frac{1}{2}\int_0^\infty y^{-3/4} e^{-y}\, dy = \frac{1}{2}\Gamma\left[\frac{1}{4}\right]$$

is obtained directly.

■ example: $\int_0^\infty \frac{\omega^n}{e^{\alpha\omega}-1}\, d\omega$

Integrals of this form appear in the statistical mechanics of Bose systems. Here we assume that $\alpha > 0$ and that n is a nonnegative integer. The integrand can be expanded as a power series in the small quantity $e^{-\alpha\omega}$, such that

$$\int_0^\infty \frac{\omega^n}{e^{\alpha\omega}-1}\, d\omega = \int_0^\infty \frac{\omega^n e^{-\alpha\omega}}{1-e^{-\alpha\omega}}\, d\omega = \sum_{m=1}^\infty \int_0^\infty \omega^n\, \text{Exp}[-m\,\alpha\,\omega]\, d\omega$$

We evaluated the integrals on the right-hand side using parametric differentiation at the beginning of this chapter. Using that result, we write

$$\int_0^\infty \frac{\omega^n}{e^{\alpha\omega}-1}\, d\omega = \frac{n!}{\alpha^{n+1}} \sum_{m=1}^\infty \frac{1}{m^{n+1}} = \frac{n!}{\alpha^{n+1}} \zeta[n+1]$$

where the *Riemann zeta function* is defined by

$$\zeta[z] = \sum_{m=1}^\infty \frac{1}{m^z}$$

for $\text{Re}[z] > 1$. Special values for integer arguments can be expressed in terms of the Bernoulli numbers and evaluated in closed form, but for our purposes we can consider the problem solved because the properties of the Riemann zeta function are well established and one can find numerical values in standard tables or mathemetical software.

More generally, we combine the same expansion with variable transformations to write

$$\int_0^\infty \frac{\omega^\beta}{e^{\alpha\omega}-1}\,d\omega = \alpha^{-\beta-1}\int_0^\infty \frac{t^\beta e^{-t}}{1-e^{-t}}\,dt = \alpha^{-\beta-1}\sum_{m=1}^\infty \int_0^\infty t^\beta \,\text{Exp}[-m\,t]\,dt = \alpha^{-\beta-1}\int_0^\infty s^\beta\,\text{Exp}[-s]\,ds \sum_{m=1}^\infty m^{-\beta-1}$$

Thus, we identify

$$\text{Re}[\alpha] > 0,\ \text{Re}[\beta] > 0 \implies \int_0^\infty \frac{\omega^\beta}{e^{\alpha\omega}-1}\,d\omega = \alpha^{-\beta-1}\,\Gamma[\beta+1]\,\zeta[\beta+1]$$

with much less restrictive conditions upon the parameters.

Integral representations for analytic functions

Special functions motivated by integrals for real variables can usually be extended into a portion of the complex plane simply by replacing the argument by a complex variable and employing a contour through the domain of analyticity of the integrand. Thus, one can define the complex sine integral by

$$\text{Si}[z] = \int_0^z \frac{dt}{t}\,\text{Sin}[t]$$

where the contour is any path between the indicated endpoints in the complex t-plane. This case is particularly simple because the integrand is entire — there is no danger of encountering singularities or branch cuts during integration. Similarly, the error function can be extended to the entire complex plane simply by using a complex argument

$$\text{Erf}[z] = \frac{2}{\sqrt{\pi}}\int_0^z dt\, e^{-t^2} \qquad \text{Erfc}[z] = \frac{2}{\sqrt{\pi}}\int_z^\infty dt\, e^{-t^2}$$

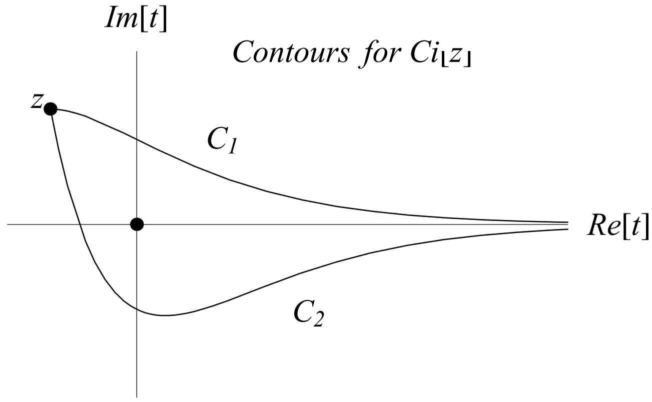
where an upper limit of ∞ is interpreted as a path that asymptotically approaches the positive real axis such that $t \to (R, 0)$ where $R \to \infty$. It is also useful to define the *imaginary error function* $\text{Erfi}[z] = -i\,\text{Erf}[i\,z]$, such that

$$\text{Erfi}[z] = \frac{2}{\sqrt{\pi}}\int_0^{i\,z} dt\, e^{t^2}$$

Conversely, if the integrand is multivalued or has singularities, the definition of a function by means of an *integral representation* must constrain the contour enough to produce a unique value for the integral. For example, the integrand of the complex cosine integral

$$\text{Ci}[z] = -\int_z^\infty \frac{dt}{t}\,\text{Cos}[t]$$

has a simple pole at the origin with unit residue. Suppose that z is found in the second quadrant, as shown. The integral along contour C_2 that dips below the real axis for $\text{Re}[t] < 0$ and then approaches the positive real axis from below differs by $2\pi i$ from the integral for contour C_1 that remains in the upper half-plane and approaches the positive real axis from above. (Imagine closing the contour for large Re[t] where the integrand is vanishingly small.) Contours which circle the origin several times differ by multiples of $2\pi i$, representing various branches of a multivalued function. The principal branch for this function is defined by the requirement that the positive real axis is approached from above without encircling the origin; this requirement is sufficient to provide a single-valued definition while still leaving considerable flexibility in the choice of contour.



The domain of analyticity will often be limited by requirements for the convergence of the defining integral. For example, the present definition for $\Gamma[x]$ is limited to $x > 0$, suggesting that straightforward extension to the complex plane would be limited to $\mathrm{Re}[z] > 0$. However, we must still be wary of the branch cut needed to establish a unique value for the integrand when z is not an integer. Thus, for $\mathrm{Re}[z] > 0$ we could use

$$\Gamma[z] = \int_0^\infty t^{z-1} e^{-t} \, dt, \quad \mathrm{Re}[z] > 0$$

with the contour in the left side of the figure below, where the positive real axis is approached from above. A more general definition can be made by using a theorem of *analytic continuation* that we will derive and discuss more thoroughly in a later chapter which states that if the functions $f_1[z]$ and $f_2[z]$ are analytic in domains D_1 and D_2 and if $f_1[z] = f_2[z]$ for all $z \in D_1 \cap D_2$, then f_1 and f_2 are representations of the same analytic function $f[z]$ within their respective domains and $f[z]$ is analytic throughout $D_1 \cup D_2$. Therefore, if we can design an integral representation that provides identical values for $\mathrm{Re}[z] > 0$ while avoiding the singularity in the integrand, we would be able to extend the definition of $\Gamma[z]$ to the entire complex plane. Consider the function

$$f[z] = \int_C t^{z-1} e^{-t} \, dt = \int_C \mathrm{Exp}[-t + (z-1)\,\mathrm{Log}[t]] \, dt$$

for the inner keyhole contour around a branch cut on the positive real axis that is shown on the right side of the figure below and is navigated in a counterclockwise sense. The small circle about the origin does not contribute when $\mathrm{Re}[z] > 0$. The contributions from either side of the branch cut differ in phase according to

$$t = x + i\varepsilon \implies \mathrm{Log}[t] = \mathrm{Log}[x]$$
$$t = x - i\varepsilon \implies \mathrm{Log}[t] = \mathrm{Log}[x] + 2\pi i$$

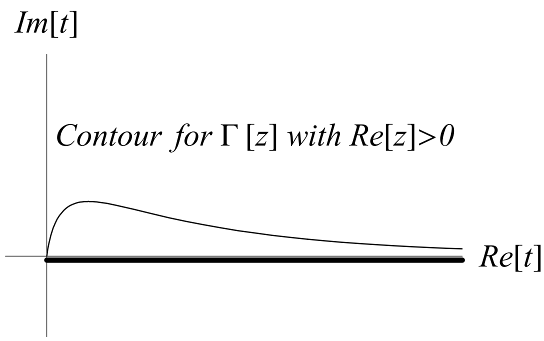
such that

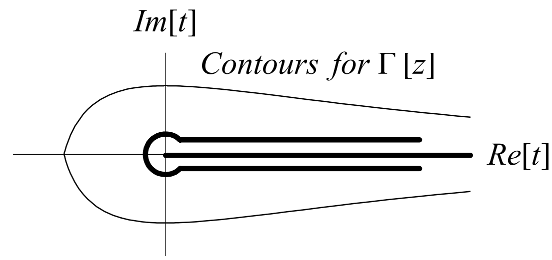
$$f[z] = (\mathrm{Exp}[2\pi i z] - 1) \int_0^\infty t^{x-1} e^{-t} \, dt$$

Thus, we obtain a definition of the gamma function

$$\Gamma[z] = \frac{1}{\mathrm{Exp}[2\pi i z] - 1} \int_C t^{z-1} e^{-t} \, dt$$

that can be used for complex variables with positive real parts. The keyhole contour can now be deformed into the outer contour in the same figure without encountering any singularities and without altering the value of the integral. We simply require that C enters from $+\infty$ just above the real axis and exits toward $+\infty$ just below the real axis without crossing the positive real axis. Therefore, the proposed integral representation extends the definition of the gamma function to the entire complex plane. When $\mathrm{Re}[z] < 0$, one simply avoids the immediate vicinity of the origin.





It might appear that this integral representation for $\Gamma[z]$ has singularities for any integer value of z, but the singularities for positive integers are illusory (removable). When $z = n$ is an integer, t^{n-1} does not require a branch cut such that the contributions from the segments of the keyhole contour above and below the real axis cancel, leaving only the small circle about the origin. Alternatively, in the absence of a branch cut the contour can be deformed into a closed circle about the origin. (We imagine that the original contour is closed across the real axis so far out that the integrand is vanishingly small.) When $n > 0$ the integrand is analytic and the integral vanishes, leaving a $0/0$ situation that suggests a removable singularity whose value should be determined by a limiting process that ensures continuity. Although we expect that the appropriate value is $\Gamma[n] = (n-1)!$, it is instructive to demonstrate that this results emerges from a suitable limiting process. Performing Taylor series expansions around $z = n$,

$$t^{z-1} \approx t^{n-1}\,\mathrm{Log}[t]\,(z-n)\,, \quad \mathrm{Exp}[2\pi i z] - 1 \approx 2\pi i\,(z-n)$$

we find

$$z \approx n \implies \Gamma[z] \approx \frac{1}{2\pi i}\int_C t^{n-1}\,e^{-t}\,\mathrm{Log}[t]\,dt$$

and can employ the keyhole contour for $n > 0$ without obtaining any contribution from the small circle aroung the origin because

$$n > 0 \implies \lim_{\varepsilon\to 0} \varepsilon^n\,\mathrm{Log}[\varepsilon] = 0$$

Placing the branch cut for $\mathrm{Log}[t]$ immediately below the positive real axis, the contributions from $\mathrm{Log}[|t|]$ on opposite sides cancel, leaving the contribution from the phase of $\mathrm{Log}[t - i\varepsilon] = \mathrm{Log}[|t|] + 2\pi i$ to give

$$\Gamma[z] \approx \frac{1}{2\pi i}\int_0^\infty t^{n-1}\,e^{-t}\,(2\pi i)\,dt = (n-1)!$$

as expected. When $n < 0$, we use

$$\oint dt\,\frac{e^{-t}}{t^{n-1}} = (-)^n\,\frac{2\pi i}{n!}$$

for a circle about the origin to discover that the residue for a simple pole at $z = -n$ is $(-)^n/n!$. Therefore, the integral representation teaches us that $\Gamma[z]$ is a meromorphic function with simple poles at negative integers and determines its residues. Although further analysis of the properties of this function is postponed to a later chapter, it should be clear that the new integral representation offers much more detailed information than the original definition on the real axis.

Many special functions have several different integral representations, with one or another being most useful under differing circumstances or for various purposes. These integral representations often provide the simplest or most general derivations for the properties of a function. For example, in the chapter on *Asymptotic Series* we will use integral representations to study the properties of several useful functions when $|z|$ is large. There we take advantage of the flexibility of the contour to concentrate upon a segment which dominates the integral. However, one must be careful when deforming contours of infinite length because the Cauchy-Goursat theorem on the path-independence of integrals of analytic functions was derived for finite contours. When one or both of the endpoints is at infinity, it can matter whether the approach toward infinity is along the real axis, the imaginary axis, or some intermediate direction. Penalty-free movement of a "free end" requires that the contribution of an arc of radius R subtending the angle through which the free end is moved must vanish as $R \to 0$. Although this requirement should be obvious by now from the care with which we studied the return paths for closing a contour of infinite length, it still bears some repetition. The contours used for integral representations offer considerable but not unlimited flexibility.

Using *Mathematica* to evaluate integrals

■ Symbolic integration

Integrals can be entered in typeset form using the BasicInput palette, but if you wish to modify any options you will need to use the command line. The basic syntax for an indefinite integral is **`Integrate[`***f[x],x***`]`**. Indefinite integrals like

$$\mathbf{ans1} = \int \mathbf{x^n\, a^x\, dx}$$

$$-x^{1+n}\,\text{Gamma}[1+n, -x\,\text{Log}[a]]\,(-x\,\text{Log}[a])^{-1-n}$$

are returned without constants of integration and can be checked easily by differentiation

```
D[ans1, x] // Simplify
```

$$a^x\, x^n$$

The integral above is expressed in terms of the incomplete gamma function. *Mathematica* makes no *a priori* assumptions about the variable of integration or the constants, so that the result applies to either real or complex variables and parameters. However, it also makes no assumption regarding the values of parameters, returning results for generic values that are not always valid for special values of the parameters. Thus, the simple integral

$$\int \mathbf{x^a\, dx}$$

$$\frac{x^{1+a}}{1+a}$$

is not valid if a happens to have the value -1.

The basic syntax for a definite integral is **Integrate[***f[x],{x,a,b}***]**. The limits of integration may be numerical, symbolic, or infinite. In early versions any symbolic parameters or limits would also be interpreted in a generic sense. Thus, one would obtain a result for

$$\int_a^b x^n \, dx = \frac{b^{n+1} - a^{n+1}}{n+1}$$

that would valid for most choices of parameters, but fails for $n = -1$, while

$$\int_a^b x^{-1} \, dx = \text{Log}[b] - \text{Log}[a]$$

would fail for negative limits of integration. In more recent versions *Mathematica* usually returns conditional results

$$\int_0^1 \mathbf{x^n \, dx}$$

$$\texttt{If}\left[\texttt{Re[n]} > -1,\ \frac{1}{1+\texttt{n}},\ \texttt{Integrate}[\texttt{x}^\texttt{n}, \{\texttt{x}, 0, 1\}, \texttt{Assumptions} \to \texttt{Re[n]} \le -1]\right]$$

$$\int_a^b \mathbf{x^n \, dx}$$

$$(-\texttt{a}+\texttt{b})\ \texttt{If}\left[(\texttt{Im[a]} - \texttt{Im[b]})\ (-\texttt{Im[b] Re[a]} + \texttt{Im[a] Re[b]}) > 0 \,||\, \frac{\texttt{Im[b]}}{\texttt{Im[a]} - \texttt{Im[b]}} \ge 0 \,||\, \frac{\texttt{Im[a]}}{-\texttt{Im[a]} + \texttt{Im[b]}} \ge 0,\ \frac{\texttt{a}^{1+\texttt{n}} - \texttt{b}^{1+\texttt{n}}}{(\texttt{a}-\texttt{b})\ (1+\texttt{n})},\ \texttt{Integrate}\left[(\texttt{a} + (-\texttt{a}+\texttt{b})\ \texttt{x})^\texttt{n}, \{\texttt{x}, 0, 1\}, \texttt{Assumptions} \to\ !\left((\texttt{Im[a]} - \texttt{Im[b]})\ (-\texttt{Im[b] Re[a]} + \texttt{Im[a] Re[b]}) > 0 \,||\, \frac{\texttt{Im[b]}}{\texttt{Im[a]} - \texttt{Im[b]}} \ge 0 \,||\, \frac{\texttt{Im[a]}}{-\texttt{Im[a]} + \texttt{Im[b]}} \ge 0\right)\right]\right]$$

$$\int_a^b \mathbf{x^{-1} \, dx}$$

$$\texttt{If}\left[\texttt{Im[b]} == 0\ \&\&\ \texttt{Im[a]} > 0 \,||\, \texttt{Im[b]} == 0\ \&\&\ \texttt{Im[a]} < 0 \,||\, \texttt{Im[b]} > 0\ \&\&\ \texttt{Im[a]} \ge 0 \,||\, \texttt{Im[b]} < 0\ \&\&\ \texttt{Im[a]} \le 0 \,||\, \texttt{Im[a]} > 0\ \&\&\ \texttt{Re[a]} > \frac{\texttt{Im[a] Re[b]}}{\texttt{Im[b]}}\ \&\&\ \texttt{Im[b]} < 0 \,||\, \texttt{Im[b]} > 0\ \&\&\ \texttt{Re[a]} > \frac{\texttt{Im[a] Re[b]}}{\texttt{Im[b]}}\ \&\&\ \texttt{Im[a]} < 0,\ -\texttt{Log[a]} + \texttt{Log[b]},\ \texttt{Integrate}\left[\frac{1}{\texttt{x}}, \{\texttt{x}, \texttt{a}, \texttt{b}\}, \texttt{Assumptions} \to \texttt{Im[a]} > 0\ \&\&\ \texttt{Im[b]} < 0\ \&\&\ \frac{\texttt{Im[a] Re[b]}}{\texttt{Im[b]}} \ge \texttt{Re[a]} \,||\, \texttt{Im[a]} == 0\ \&\&\ \texttt{Im[b]} == 0 \,||\, \texttt{Im[a]} < 0\ \&\&\ \texttt{Im[b]} > 0\ \&\&\ \frac{\texttt{Im[a] Re[b]}}{\texttt{Im[b]}} \ge \texttt{Re[a]}\right]\right]$$

that test any parameters that appear either in the integrand or the limits of integration. Although such results are less attractive and the conditions are often expressed in unnecessarily complicated forms, there is less chance of obtaining incorrect answers due to careless unstated assumptions about the parameters. Although one can use the option Generate-Conditions→False

$$\mathbf{Integrate[x^n, \{x, a, b\}, GenerateConditions \to False]}$$

$$\frac{-\texttt{a}^{1+\texttt{n}} + \texttt{b}^{1+\texttt{n}}}{1+\texttt{n}}$$

to obtain a simple expression instead of a conditional statement, we strongly discourage that reckless practice and recommend instead that one supply the assumptions that apply to the parameters in your integrand directly, as follows.

```
Integrate[x^n, {x, a, b}, Assumptions → {Re[n] > -1}]
```

$$\frac{-a^{1+n} + b^{1+n}}{1 + n}$$

Mathematica claims to be able to produce practically any integral in standard compilations, such as the massive compilation by Gradshteyn and Ryzhik. Thus, one finds that many seemingly unpromising integrals can be evaluated in terms of recognizable functions even if the output appears complicated. However, despite its impressive versatility, there remains a nontrivial error rate in the symbolic integration package. We decline to present specific examples here because each revision of the program seems to correct some errors while introducing new ones. Nevertheless, investigation of most (but not all) disagreements you find with *Mathematica* will eventually show that you have made a mistake. *The software is good, but not perfect!* Therefore, it remains useful to be able to perform such integrals independently. Furthermore, any result that is important should be checked. A very useful method for checking a symbolic integral is to compare with numerical evaluation for representative choices of the parameters. This technique cannot prove that a result is valid for all parameters satisfying the requisite conditions, but it will sometimes find errors.

Moral: trust but verify!

■ Numerical integration

The basic syntax for numerical integration is **`NIntegrate`[*f[x],{x,a,b}*]** where the limits must be numerical and the integrand must evaluate to a number when given a numerical value for *x*. Numerical integration is generally more reliable than symbolic integration. Symbolic integration requires a vast library of pattern-matching rules for which it is difficult to ensure that all special cases are handled properly, while numerical integration is much more mechanical. The basic technique for numerical integration is to sample the integrand at strategically located positions, construct an interpolating polynomial, and then integrate the polynomial. The accuracy of the integral can be tested by subdividing the interval and applying the method to smaller parts. One can also sample more points where the integrand changes most rapidly. Many reliable algorithms have been developed and the one used by *Mathematica* is quite good. If it does encounter trouble with a particular integrand, there are options that can often be used to overcome those difficulties. If the difficulties persist, one should examine the integrand and handle its singularities more carefully.

■ Further information

More information about integration using *Mathematica*, including multiple integrals and symbolic and numerical contour integration, can be found in *calculus.nb* at EssentialMathematica.

Problems

You may use *Mathematica* to check your work, but do not trust its symbolic integration too much. When evaluating integrals, you must specify the contour, convincingly justify neglect of any vanishing portions, and define phases near any branch cuts carefully. Be sure to consider special cases and be alert to possible generalizations.

▼ some related trigonometric integrals

Evaluate

$$\int_0^{2\pi} \frac{d\theta}{a + b\,\mathrm{Cos}[\theta]} \quad \text{for} \quad a > b > 0$$

using contour integration and then deduce

$$\int_0^{2\pi} \frac{d\theta}{(a + b\,\mathrm{Cos}[\theta])^2} \quad \text{and} \quad \int_0^{2\pi} \frac{\mathrm{Cos}[\theta]\;d\theta}{(a + b\,\mathrm{Cos}[\theta])^2}$$

by more elementary means.

▼ trigonometric integrals on unit circle

a) $\displaystyle\int_0^{2\pi} \frac{\mathrm{Sin}[\theta]^2}{1 + a\,\mathrm{Cos}[\theta]}\,d\theta$ for $-1 < a < 1$

b) $\displaystyle\int_0^{2\pi} \mathrm{Exp}[\mathrm{Cos}[\theta]]\,\mathrm{Cos}[n\,\theta - \mathrm{Sin}[\theta]]\,d\theta$ for integer n

▼ magnetic flux through circle from coplanar wire

An infinitely long wire carries current I. Compute the magnetic flux through a coplanar circle of radius a that is at a distance d from the wire, where $d \geq a$. Compare the limits $d \gg a$ and $d \gtrsim a$.

▼ average power radiated by charged harmonic oscillator

The power radiated by a charge in simple harmonic motion with amplitude a and frequency ω is given by

$$\frac{dP}{d\Omega} = K\,\mathrm{Sin}[\theta]^2 \frac{\mathrm{Cos}[\omega\,t]^2}{(1 + \beta\,\mathrm{Cos}[\theta]\,\mathrm{Sin}[\omega\,t])^5}$$

where $\beta = a\,\omega / c$ is the amplitude for the velocity oscillation (relative to lightspeed) and $K = e^2\,a^2\,\omega^4 / 4\,\pi\,c^3$. Evaluate the power averaged over a period.

▼ assorted integrals on infinite range

Use contour integration to evaluate the following integrals.

a) $\displaystyle\int_0^{\infty} \frac{1}{1 + x^n}\,dx$ where $n > 1$ is a positive integer. Hint: try an arc subtending $2\,\pi / n$ radians.

b) $\displaystyle\int_{-\infty}^{\infty} \frac{\mathrm{Cos}[p\,x] - \mathrm{Cos}[q\,x]}{x^2}\,dx$ with p, q real

c) $\mathcal{P}\int_{-\infty}^{\infty} \frac{\text{Cos}[k\,x]}{1+x^3}\, dx$ with k real

d) $\int_0^{\infty} \frac{\text{Cos}[a\,x]}{(x^2+b^2)^2}\, dx$ for real a, b, $|b|>0$

e) $\int_0^{\infty} \frac{\text{Sin}[a\,x]}{x\,(x^2+b^2)}\, dx$ for real a, b, $|b|>0$

f) $\int_{-\infty}^{\infty} \frac{x\,\text{Sin}[2\,\theta]}{(1+x^2)\,(1-2\,x\,\text{Cos}[\theta]+x^2)}\, dx$ for $0 \le \theta \le 2\,\pi$

g) $\int_{-\infty}^{\infty} \frac{dx}{\text{Cosh}[k\,x]}$ with k real and nonzero

▼ an integral from diffraction theory

Evaluate

$$\int_{-\infty}^{\infty} \frac{\text{Sin}^2[x]}{x^2}\, dx$$

▼ integrals used in Fourier transform of oscillator wave functions

a) Evaluate

$$\int_0^{\infty} e^{-a\,x^2}\,\text{Cos}[b\,x]\, dx$$

for a, $b > 0$.

b) Produce a general method for evaluating integrals of the form

$$\int_0^{\infty} e^{-a\,x^2}\,x^{2\,n+1}\,\text{Sin}[b\,x]\, dx$$

with a, $b > 0$ and integer $n \ge 0$. Display explicit results for $n = 0, 1$.

Integrals of this type arise in the Fourier transform of oscillator wave functions.

▼ integration around branch cuts

a) Evaluate

$$\int_{-1}^{1} \frac{dx}{(a+b\,x)\,\sqrt{1-x^2}} \quad \text{with } a > b > 0$$

using a suitable contour. (Hint: put the branch cut on the integration interval and define phases carefully.)

b) Evaluate

$$\int_0^\infty \frac{\ln x}{1+x^2}\, dx$$

using a suitable branch of Log[z].

c) Evaluate

$$\int_0^\infty \frac{(\ln x)^2}{1+x^2}\, dx$$

using a suitable branch of Log[z].

d) Evaluate

$$\int_0^1 \frac{x^{1/4}(1-x)^{3/4}}{(1+x)^3}\, dx$$

using a suitable contour. (Hint: put the branch cut on the integration interval and define phases carefully.)

e) Evaluate

$$\int_0^\infty \frac{x^{-a}}{1+x^4}\, dx$$

for complex a and specify the conditions required for convergence.

f) Evaluate

$$\int_0^\infty \frac{x^{-a}}{1+x^n}\, dx$$

for complex a and integer n and specify the conditions required for convergence.

g) Evaluate

$$\int_0^1 x^{a-1}(1-x)^{-a}\, dx$$

for complex $0 < a < 1$. (Hint: try a large circular contour and then deform the contour to snugly embrace the branch cut.)

▼ reduction to standard functions

Express the following integrals in terms of standard functions.

a) $\int_0^\infty x^m e^{-x^n}\, dx$ for $n > 0$

b) $\int_0^\infty e^{-a x^2}\,\mathrm{Sin}[b\,x]\, dx$ with $a,\ b > 0$

c) $\int_0^\infty \frac{e^\omega \omega^\alpha}{(e^\omega - 1)^2}\, d\omega$ with $\alpha > 1$