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Integrals with Singularities or Discontinuous Derivatives

Numerical integration algorithms such as Simpson's rule are designed to work with "smooth" integrands, because they assume that the function is locally a polynomial. If the integrand has discontinuous derivatives or poles or a branch point in the integration region, such integration rules will generally do poorly. However, one can convert the original integral into a mathematically equivalent one that *is* smooth in this sense. Here are some strategies (check *Numerical Recipes* and the Hjorth-Jensen notes for others):

- If there is a discontinuous derivative somewhere in the integrand, then split the integral into two integrals at the discontinuity. For example, if there is an absolute value, then

$$\int_{-1}^{1} |x|\, f(x)\, dx = \int_{-1}^{0} (-x)\, f(x)\, dx + \int_{0}^{1} x\, f(x)\, dx \ , \tag{1}$$

  if $f(x)$ is smooth. (One can combine the integrals after taking $x \to -x$ in the first.)

- If there is a branch point, such as $x^{1/n}$ with n an integer greater than one, a simple variable change can usually be found to convert the integrand to a smooth one. For example, the variable change $x = y^n$ yields the following equality (assume $n > 1$):

$$\int_{0}^{1} x^{1/n}\, f(x)\, dx = \int_{0}^{1} n y^n\, f(y^n)\, dy \ , \tag{2}$$

  if $f(x)$ is smooth. See *Numerical Recipes* for other transformations.

- If there is a pole (or other singularity) in the integrand, you can often subtract and add the singularity, leaving one integral that can be evaluated numerically and another that can be evaluated analytically. E.g., the principal value integral:

$$\mathcal{P}\int_{-1}^{2} \frac{f(x)}{x}\, dx = \int_{-1}^{2} \frac{f(x) - f(0)}{x}\, dx + f(0)\, \mathcal{P}\int_{-1}^{2} \frac{1}{x}\, dx \ . \tag{3}$$

  If $f(x)$ is analytic at $x = 0$, the first integral can be evaluated numerically (treating $x = 0$ carefully) while the last term is evaluated analytically as $f(0) \times \ln 2$.

- A similar "trick" lets us evaluate principal value integrals that arise frequently in integral equations (such as for quantum mechanical scattering). First we note that

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{dk}{k - k_0} = 0 \quad \Longrightarrow \quad \mathcal{P}\int_{0}^{\infty} \frac{dk}{k^2 - k_0^2} = 0 \ , \tag{4}$$

  where we changed broke the first integral in two and changed variables $k \to -k$ to get the second expression. Then we can evaluate (assuming smooth $f(k)$),

$$\mathcal{P}\int_{0}^{\infty} \frac{f(k)\, dk}{k^2 - k_0^2} = \int_{0}^{\infty} \frac{f(k) - f(k_0)}{k^2 - k_0^2}\, dk \ , \tag{5}$$

  and the second integral no longer has a singularity.

Packaged integration routines, such as those in the Gnu Scientific Library (GSL) will typically have versions designed specifically to deal with singularities such as discontinuities or poles. See the online GSL manual for descriptions of the different routines.

Here are some integrals to practice on. Compare a direct numerical calculation of the integrals as given to the numerical calculation after an appropriate transformation.

$$\int_0^1 x^{1/3}\, dx = 0.75 \;, \tag{6}$$

$$\int_0^1 x^{1/4}\, e^{-x}\, dx = 0.4769591535856598 \;, \tag{7}$$

$$\int_{-1}^{+1} |x - 0.5|\, \sin x\, dx = -0.4185487713402663 \;. \tag{8}$$

Try the following ones in Mathematica as well, comparing the results from `Integrate` and `NIntegrate` to 16 digits. (You'll need to use N[ ] to get a numerical answer from the former and NumberForm[ ] to get 16 output digits from both.) Then make the transformation (in Mathematica, if you like) and compare again.

$$\int_0^2 \frac{1}{(1+x)\sqrt{x}}\, dx = 1.910633236249019 \tag{9}$$

$$\int_0^1 \frac{\cos x}{\sqrt{x}}\, dx = 1.809048475800544 \tag{10}$$

$$\int_0^1 \sqrt{(1-x^2)(2-x)}\, dx = 0.982246183109692 \tag{11}$$

You can increase the precision from a numerical integration in Mathematica using the PrecisionGoal option (see the Help Browser).

Here's a principal value integral to try numerically:

$$\mathcal{P}\int_{-1}^2 \frac{e^{-x^2}}{x}\, dx = 0.1078022909928357 \tag{12}$$

In Mathematica, you can use `Integrate` with `PrincipalValue->True` to get the answer in terms of exponential integrals (which can then be evaluated numerically).