Integrals with Singularities or Discontinuous Derivatives

Numerical integration algorithms such as Simpson's rule are designed to work with "smooth" integrands. If the integrand has discontinuous derivatives or poles or a branch point in the integration region, these integration rules will generally do a poor job. However, one can convert the original integral into a mathematically equivalent one (or more than one) that *is* smooth in this sense. Here are some strategies (check *Numerical Recipes* for others):

- If there is a discontinuous derivative somewhere in the integrand, such as when there is an absolute value, then split the integral into two integrals at the discontinuity. For example:
$$\int_{-1}^{1} |x|\, f(x)\, dx = \int_{-1}^{0} (-x)\, f(x)\, dx + \int_{0}^{1} x\, f(x)\, dx \tag{1}$$
if $f(x)$ is smooth.

- 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 add and subtract the singularity, leaving one integral that is smooth and can be evaluated numerically and another that has the singularity but which can be evaluated analytically. For example:
$$\mathcal{P}\int_{-1}^{2} \frac{f(x)}{x}\, dx = \mathcal{P}\int_{-1}^{2} \frac{f(x)}{x}\, dx = \int_{-1}^{2} \frac{f(x) - f(0)}{x}\, dx + f(0)\,\mathcal{P}\int_{-1}^{2} \frac{1}{x}\, dx\ . \tag{3}$$
The last term is just $f(0) \times \ln 2$ and the first integral, if $f(x)$ is analytic at $x = 0$, will have a non-singular integrand.

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.

$$\int_{0}^{1} x^{1/3}\, dx = 0.75 \tag{4}$$

$$\int_0^2 \frac{1}{(1+x)\sqrt{x}}\,dx = 1.910633236249019 \tag{5}$$

$$\int_0^1 \frac{\cos x}{\sqrt{x}}\,dx = 1.809048475800544 \tag{6}$$

$$\int_0^1 \sqrt{(1-x^2)(2-x)}\,dx = 0.982246183109692 \tag{7}$$

$$\mathcal{P}\int_{-1}^2 \frac{e^{-x^2}}{x}\,dx = 0.1078022909928357 \tag{8}$$