12. Singular integrals

Methods of the type previously discussed can not be used directly to evaluate singular integrals or integrals with infinite limits of integration. We now discuss some examples and possible remedies.

Example 1: $I = \int_0^1 x^{-1/2} e^x \, dx$. Since the function is infinite at the origin, we cannot apply closed Newton-Cotes formulas. One remedy is to make a change of variables. In this case, setting $x = t^2$, $dx = 2tdt$, we get an integral easily handled by Romberg integration.

$$I = \int_0^1 (1/t) e^{t^2} 2t \, dt = 2 \int_0^1 e^{t^2} \, dt.$$

Example 2: Another approach to this integral is to remove the singularity by integration by parts.

$$I = \int_0^1 x^{-1/2} e^x \, dx = 2x^{1/2} e^x |_0^1 - 2 \int_0^1 x^{1/2} e^x \, dx = 2e - 2 \int_0^1 x^{1/2} e^x \, dx$$

Although the new integral is not singular, the derivative of the integrand is singular, so to improve performance, we could first integrate by parts a few more times.

Example 3: $\int_{-\infty}^{\infty} e^{-x^2} f(x) \, dx$, where say $|f(x)| \le M$. Although the interval of integration is infinite, the integrand decays rapidly. Hence, we could break up the integral as:

$$\int_{-\infty}^{-a} e^{-x^2} f(x) \, dx + \int_{-a}^{a} e^{-x^2} f(x) \, dx + \int_{a}^{\infty} e^{-x^2} f(x) \, dx.$$

Then

$$\left| \int_{-\infty}^{-a} e^{-x^2} f(x) \, dx \right| + \left| \int_{a}^{\infty} e^{-x^2} f(x) \, dx \right| \le M \int_{-\infty}^{-a} e^{-x^2} \, dx + M \int_{a}^{\infty} e^{-x^2} \, dx \le 2M \int_{a}^{\infty} e^{-x^2} \, dx.$$

To bound $\int_a^\infty e^{-x^2} \, dx$, we can make a change of variable $t = x^2$. Then $dt = 2xdx$ so $dx = (1/2)t^{-1/2} dt$. Then

$$\int_a^\infty e^{-x^2} \, dx = \int_{a^2}^\infty e^{-t} (1/2) t^{-1/2} \, dt \le \frac{1}{2a} \int_{a^2}^\infty e^{-t} \, dt = \frac{1}{2a} e^{-a^2}.$$

Choose a so that $(M/a)e^{-a^2} < \epsilon$. For example, if $a = 4$ and $M = 1$, $(M/a)e^{-a^2} < 10^{-7}$. Then approximate the finite integral by a standard method.

Example 4: Another way of treating infinite integrals is to make a change of variables that maps the infinite interval, e.g., $(0, \infty)$ to the finite interval $(0, 1)$. For example, set $t = e^{-x}$ or $t = 1/(1 + x)$. Consider $I = \int_0^\infty (1 + x^2)^{-4/3} \, dx$. Let $t = 1/(1 + x)$. Then $x = (1 - t)/t$ so $dx = -t^{-2} dt$. Hence,

$$I = -\int_1^0 \left[1 + \left(\frac{1-t}{t} \right)^2 \right]^{-4/3} t^{-2} dt = \int_0^1 [t^2 + (1-t)^2]^{-4/3} t^{2/3} \, dt.$$

Now the integrand has an infinite derivative at the origin, so further transformation is desirable. For example, setting $t = u^3$, $u = t^{1/3}$ and $dt = 3u^2 du$, the integral becomes

$$I = \int_0^1 [u^6 + (1 - u^3)^2]^{-4/3} 3u^4 \, du.$$