Physics 115/242; Peter Young

Slowing down of the rate of convergence in numerical integration due to a singularity at the boundary of the region of integration (and how to avoid this).

When doing numerical integration you should

always avoid singularities of the integrand INSIDE the region of integration.

If your integral has a singularity in the interior of the region, then break it up into two pieces joined at the point of singularity. Each piece then has a singularity at an end point. As discussed in this handout, singularities at an end point can be dealt with by a change of variables to remove the singularity.

As a first example of an integral with a singularity at an end point, consider

$$\boxed{I_1 = \int_0^1 \sqrt{x}\, dx\,,} \tag{1}$$

for which the exact answer is 2/3. We will verify here that the square-root singularity at $x = 0$ slows down the convergence of numerical methods.

Let us first evaluate I_1 using the **trapezium rule**. I obtain the following results for h-values which decrease by a (multiplicative) factor of 0.1 each time.

h	answer	error
0.100000	0.660509341707	0.006157324960
0.010000	0.666462947103	0.000203719564
0.001000	0.666660134394	0.000006532273
0.000100	0.666666459197	0.000000207470
0.000010	0.666666660097	0.000000006570
0.000001	0.666666666459	0.000000000208

It is seen that the error goes down by about a factor of about 10^3 when h is decreased by a factor of 10^2. This implies that the leading contribution to the error varies as $\boxed{h^{3/2}}$, compared with h^2 which is the trapezium rule result for a smooth function.

Next consider **Simpson's rule**, for which I obtain

h	answer	error
0.100000	0.664099589757	0.002567076909
0.010000	0.666585482067	0.000081184600
0.001000	0.666664099384	0.000002567283
0.000100	0.666666585482	0.000000081185
0.000010	0.666666664099	0.000000002567
0.000001	0.666666666585	0.000000000081

Again the error decreases by about 10^3 for a decrease of h by a factor of 10^2. This implies an error of order $\boxed{h^{3/2}}$, the same as for the trapezium rule, rather than h^4 error obtained in Simpson's rule for smooth integrands.

In fact, if the integrand varies as

$$f(x) \propto (x-a)^{\alpha} \tag{2}$$

near the lower limit[1] a, one can show that the error is dominated by this singularity and is of the form

$$\boxed{\text{error} \propto h^{1+\alpha}} \tag{3}$$

for both the trapezium rule and Simpson's rule. (The above example had $\alpha = 1/2$). In these circumstances Simpson's rule is not significantly better than the trapezium rule, and Romberg integration is not better either because the error does not have the expected form. As discussed below one should do a change of variables to remove the singularity, so the numerical methods then have their usual (more rapid) convergence (h^2 for trapezium, h^4 for Simpson, and faster that these for Romberg).

Next we consider a more extreme example in which the integral actually *blows up* at one end,

$$\boxed{I_2 = \int_0^1 x^{-1/2}\, dx\,,} \tag{4}$$

for which the exact answer is 2. Clearly we cannot use the trapezium or Simpson's rule because f_0 is infinite. We *can*, however, use the **midpoint rule** since this does not require evaluation of the function precisely at the end point. This gives the following results for I_2:

[1] Naturally the error has the same form if the singularity is at the upper limit.

h	answer	error
0.100000	1.808922359730	0.191077640270
0.010000	1.939512218968	0.060487781032
0.001000	1.980871446166	0.019128553834
0.000100	1.993951013774	0.006048986226
0.000010	1.998087142535	0.001912857465
0.000001	1.999395101357	0.000604898643

We see that the error goes down only by about a factor of 10, when h decreases by a factor of 100. Hence, even though using the midpoint rule avoids an infinite answer, convergence is *very slow*, and indeed corresponds to Eq. (3) with $\alpha = -1/2$. This example emphasizes even more strongly that singularities at the ends of the region of integration should be transformed away by a change of variables.

We now illustrate how to change variables to remove the singularity for the following integral,

$$\boxed{I_3 = \int_0^1 \frac{x^{1/2}}{\sin x}\, dx\,,} \tag{5}$$

which, like I_2 in Eq. (4), diverges as $x^{-1/2}$ as $x \to 0$. The transformation $x = u^2$ removes this singularity[2]. We then get the following integral

$$\boxed{I_3 = 2\int_0^1 \frac{u^2}{\sin(u^2)}\, du\,.} \tag{6}$$

The integrand now tends to a constant as $u \to 0$. However, it is actually undefined $(0/0)$ for u precisely 0. Rather than adding a separate definition of the integrand for $u = 0$ it is better to use the midpoint rule, where we do not need to evaluate the integrand at the limits.

Let us suppose that we need 6 decimal places of accuracy. In the output below I evaluated the transformed integral in Eq. (6) using the midpoint rule, doubled the number of intervals on each iteration and stopped when the difference between the last two estimates was less than 10^{-6}:

This required $n = 1/0.0015625 = 640$ intervals. We could have reduced this number by a large factor if we had used Romberg integration[3] rather than the midpoint rule.

[2] We shall show in class that the transformation which removes a power-law singularity in the integrand of the form $(x-a)^\lambda$ (where a is the lower limit) is $x - a = u^{1/(1+\lambda)}$. Here we have $\lambda = -1/2$.

[3] One can do Romberg integration, i.e. successively eliminate the leading error, starting from the midpoint rule, just as we did in class starting from the trapezium rule, see Numerical Recipes Sec. 4.4 which also discusses changing variables to eliminate singularities at the endpoints.

h	estimate for I	estimate - previous estimate
0.100000000	2.070624515078	
0.050000000	2.071152996605	0.000528481527
0.025000000	2.071285713266	0.000132716661
0.012500000	2.071318930030	0.000033216764
0.006250000	2.071327236576	0.000008306546
0.003125000	2.071329313360	0.000002076784
0.001562500	2.071329832565	0.000000519205

By comparison I show below results using the midpoint rule on the *original* integral, Eq. (5) in which I increased the number of intervals by a factor of *ten*, rather than two, at each stage:

h	estimate for I	estimate - previous estimate
0.100000000	1.880123125492	
0.010000000	2.010840872325	0.130717746833
0.001000000	2.052201438090	0.041360565764
0.000100000	2.065281019271	0.013079581181
0.000010000	2.069417148168	0.004136128898
0.000001000	2.070725106991	0.001307958823
0.000000100	2.071138719888	0.000413612897
0.000000010	2.071269515770	0.000130795882
0.000000001	2.071310877060	0.000041361290

In the last line we used no less than 10^9 intervals (i.e. 10^9 function evaluations) and we still had *not* obtained the desired accuracy of 10^{-6}. Because of the $1/\sqrt{x}$ singularity at $x = 0$ the error only decreases like $h^{-1/2}$, so we would need $n = h^{-1} \simeq 10^{12}$ intervals to get an accuracy of 10^{-6}. This is over 10^9 times more than we needed above when we transformed the singularity away. The moral is therefore

if you have a singularity AT AN END of the region of integration, transform it away by an appropriate substitution,

and then use a method, such as midpoint, which doesn't require a function evaluation precisely at the end.