Numerical Integration – Improper Integrals

Now we want to compute
\[ I(a, \infty) = \int_a^\infty f(x)\,dx \]
where \( f(x) \) has no known antiderivative. If this integral exists, then
\[
\lim_{b \to \infty} \int_b^\infty f(x)\,dx = 0.
\]

Thus for each \( \epsilon \) there is a \( b \) such that
\[
| \int_b^\infty f(x)\,dx | \leq \frac{\epsilon}{2}.
\]

Once that \( b \) is found we can simply approximate
\[
\int_a^b f(x)\,dx
\]
by a numerical integration method. If we use, say, Simpson’s rule or Romberg integration to find \( S \) such that
\[
| \int_a^b f(x)\,dx - S | \leq \frac{\epsilon}{2}
\]
then
\[
| \int_a^\infty f(x)\,dx - S | = | \int_a^b f(x)\,dx - S + \int_b^\infty f(x)\,dx | \leq | \int_a^b f(x)\,dx - S | + | \int_b^\infty f(x)\,dx | \leq \epsilon.
\]

Example 1 Different from the one in class, but those of you who have taking courses in statistics or physics may have encountered this integral.

We can compute
\[
\int_2^\infty e^{-x^2/2}\,dx.
\]
Actually, there are some tricks to do this that will reduce it to a finite integral, but let’s pretend we don’t know these!

First, we attempt to bound

\[
\int_b^\infty e^{-x^2/2}dx = e^{-b^2/2} \int_b^\infty e^{(b^2-x^2)/2}dx.
\]

Using the change of variable \( y = x - b \), we have

\[
\int_b^\infty e^{-x^2/2}dx = e^{-b^2/2} \int_0^\infty e^{-y^2/2}e^{-by}dy.
\]

Since \( e^{-y^2/2} \leq 1 \) for all \( y \), for \( b \geq 2 \) we have

\[
\int_b^\infty e^{-x^2/2}dx \leq e^{-b^2/2} \int_0^\infty e^{-by}dy = e^{-b^2/2}/2.
\]

Suppose we want to compute this integral to accuracy \( \epsilon = 10^{-8} \). Then we want \( b \) such that

\[
e^{-b^2/2}/2 \leq 5 \times 10^{-9},
\]

or

\[
b^2/2 \geq 8 \log 10.
\]

Thus we want

\[
b \geq 6.0697.
\]

We will round this up to 7.

Thus we want to approximate

\[
\int_2^7 e^{-x^2/2}dx
\]

with error \( 5 \times 10^{-9} \). I used Octave’s quad routine with this tolerance. It obtains the value

\[
\int_2^7 e^{-x^2/2}dx \approx 0.057026.
\]

Thus we may assume that this value approximates \( \int_2^\infty e^{-x^2/2}dx \) with an error \( 10^{-8} \).
Numerical Differentiation

We consider the approximation of $f'(x_0)$. First we start with the definition

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h} = \lim_{h \to 0} f[x_0 + h, x_0].$$

Thus, it makes sense to fix some small value of $h$ and compute the forward difference

$$f[x_0 + h, x_0].$$

However, if we write out the Taylor series

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + O(h^3)$$

we get that

$$f[x_0 + h, x_0] = f'(x_0) + \frac{h}{2} f''(x_0) + O(h^2).$$

This is not a very good approximation. If we instead use the expansions

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f^{(3)}(x_0) + \frac{h^4}{24} f^{(4)}(x_0) + O(h^5)$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f^{(3)}(x_0) + \frac{h^4}{24} f^{(4)}(x_0) + O(h^5)$$

then the centered difference

$$f[x_0 + h, x_0 - h] = \frac{f(x_0 + h) - f(x_0 - h)}{2h} = f'(x_0) + \frac{h^2}{6} f^{(3)}(x_0) + \frac{h^4}{120} f^{(5)}(x_0) + O(h^6)$$

yields an $O(h^2)$ approximation.

First of all, this is a much better approximation than the forward difference. Secondly, it has an even power error expansion. We can use Richardson extrapolation to improve the error quite significantly.

Let

$$D_1(h) = (4f[x_0 + h, x_0 - h] - f[x_0 + 2h, x_0 - 2h]) / 3 = f'(x_0) - \frac{h^4}{30} f^{(5)}(x_0) + O(h^6).$$

Now we have a formula with $4th$ order accuracy. An actual formula for this is given in your book, but I would choose to just compute it this way.

Second derivative approximations are also possible. We note that

$$2f[x_0 - h, x_0, x + h] = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} = f''(x_0) + \frac{h^2}{12} f^{(4)}(x_0) + \frac{h^4}{360} f^{(6)}(x_0) + O(h^6).$$

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If we let $D_0^2(h) = 2f[x_0 - h, x_0, x + h]$, a higher order approximation is given by

$$D_1^2(h) = (8f[x_0-h, x_0, x+h] - 2f[x_0-2h, x_0, x+2h])/3 = f''(x_0) - \frac{h^4}{90} f^{(6)}(x_0) + O(h^6).$$

Again, your book gives a formula for this, but I would also just compute this one this way.