The numerical evaluation of principal value integrals

By L. M. Delves*

This paper considers the numerical evaluation of the Principal Value of the improper integral

\[ P \int_{a}^{b} \frac{f(t)}{t - q} \, dt \]

over a region \([a, b]\) which may include \(q\). Methods of Newton–Cotes and modified Gaussian type are considered. Some of these require the evaluation of \(f(q)\), while others do not. The methods are illustrated by some numerical examples.

The Principal Value \(P(I)\) of the integral

\[ I(f) = \int_{a}^{b} \frac{f(t)}{t - q} \, dt \]  

is defined as

\[ P(I) = \lim_{\varepsilon \to 0} \left[ \int_{a}^{a+\varepsilon} \frac{f(t)}{t - q} \, dt + \int_{a+\varepsilon}^{b} \frac{f(t)}{t - q} \, dt \right] a < q < b \]  

\[ = I(f) \]  

when \(q < a\) or \(q > b\).

We do not consider in this paper the cases \(q = a\) or \(q = b\).

Integrals such as (1) often arise for instance in scattering theory. It is possible to treat the singularity by deforming the path of the integration into the complex plane (see Hetherington and Schick, 1965; Phillips, 1966); we give here a number of simpler methods involving only real \(t\).

These include methods of Newton–Cotes and modified Gaussian type.

A. Newton-Cotes methods

These methods are obtained from a truncated Taylor expansion for \(f(t)\). The derivation is simple, and we quote only the results here. In the following, \(N\) denotes the order of the rule; the rule is exact if \(f(x)\) is a polynomial in \(x\) of degree \(N\) or less; \(h\) is the mesh size used and we set

\[ k = (q - a)/h \]

\[ f_a = f(a + nh). \]  

Then the forward-difference Newton–Cotes expansion for \(I\) has the form

\[ I(p) = \int_{a}^{a+ph} \frac{f(t)}{t - q} \, dt \]

\[ = \sum_{j=0}^{\infty} \Delta f_0 \frac{A_j}{j!} C_j \]  

where

\[ C_j = P \int_{0}^{\varphi} \frac{z^j}{z - k} \, dz. \]  

From (4) we derive, in particular, the following low-order rules \(R_N\)

(i) Two-point rule, \(N = 1\)

\[ R^0(f) = (C_0 - C_1)f_0 + C_1 f_1. \]  

(ii) Three-point rule, \(N = 2\)

\[ R^2(f) = \left[ C_0 - C_1 + \frac{C_2}{2} \right] f_0 + \left[ C_1 - C_2 \right] f_1 + \frac{C_2}{2} f_2. \]  

The relevant values of the constants \(C_j\) are given by equation 8: we set

\[ A_{pk} = \ln[(p - k)/k] \]

and then

\[ C_0 = A_{pk} \]

\[ C_1 = p + k A_{pk} \]

\[ C_2 = p(k - 1 + p/2) + k(k - 1)A_{pk}. \]  

Some typical numerical values of the weights defined by eqn. (8) and (7) are given in Table 1.

Error bounds

We can obtain bounds for the error in these rules in a straightforward way from the Taylor expansion of \(f(t)\). We quote here the results for the most commonly used case; that is, we set \(p = 1\) for the two-point rule, \(p = 2\) for the three-point rule. We also set, for convenience, the lower limit \(a = 0\), and obtain the following error bounds

\[ R^1(f) - I(f) = \epsilon_1 \]

\[ R^2(f) - I(f) = \epsilon_2 \]  

where

\[ |\epsilon_1| \leq \frac{h^2 M_2}{2} \left\{ \frac{1}{2} (k^2 + (1 - k)^2) + k^2 |C_0 - C_1| \right\} \]

\[ + (1 - k)^2 |C_1| \]  

\[ \leq \frac{h^2 M_2}{2} \left[ 2k C_1 + |C_1| \right] \]  

otherwise

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Table 1

Numerical values of the weights for the rules defined by equations (6) and (7). The range $p$ has been taken to be $p = 1$ for the two-point rule (6) and $p = 2$ for rule (7).

<table>
<thead>
<tr>
<th>$k/p$</th>
<th>$f_0$</th>
<th>$f_1$</th>
<th>$f_0$</th>
<th>$f_1$</th>
<th>$f_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.10903549</td>
<td>1.27725887</td>
<td>-0.93457871</td>
<td>2.08722839</td>
<td>0.23364468</td>
</tr>
<tr>
<td>0.4</td>
<td>-0.75672094</td>
<td>1.16218604</td>
<td>-1.15134419</td>
<td>0.78924650</td>
<td>0.76756279</td>
</tr>
<tr>
<td>0.6</td>
<td>-1.16218604</td>
<td>0.75672094</td>
<td>-0.76756279</td>
<td>-0.78924650</td>
<td>1.15134419</td>
</tr>
<tr>
<td>0.8</td>
<td>-1.27725887</td>
<td>-0.10903549</td>
<td>-0.23364468</td>
<td>-2.08722839</td>
<td>0.93457871</td>
</tr>
</tbody>
</table>

Table 2

Evaluation of a principal value integral

This table gives errors in the values of the integral $P \int_0^1 f(t)/(x - \sqrt{\frac{k}{2}}) dt$ obtained from the two- and three-point rules (6) and (7) and the modified Gauss rule (12). For the latter, the number of points shown is one more than that of the underlying Gauss rule.

<table>
<thead>
<tr>
<th>FUNCTION $f(x)$</th>
<th>EXACT</th>
<th>ERROR</th>
<th>EQN. (6), $h = 0.2$</th>
<th>EQN. (6), $h = 0.05$</th>
<th>EQN. (7), $h = 0.66667$</th>
<th>EQN. (7), $h = 0.05$</th>
<th>EQN. (12), 4 point</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x^3$</td>
<td>0.87527</td>
<td>0.00118</td>
<td>0.00218</td>
<td>-0.000338</td>
<td>-0.00014</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>$x^4$</td>
<td>0.86891</td>
<td>0.01837</td>
<td>0.00437</td>
<td>-0.00944</td>
<td>-0.00041</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>$x^5$</td>
<td>0.81441</td>
<td>0.04001</td>
<td>0.00657</td>
<td>-0.01718</td>
<td>-0.00073</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>$\cos x$</td>
<td>-1.2294</td>
<td>0.0046</td>
<td>0.0000</td>
<td>-0.00004</td>
<td>0.00000</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>$e^{-x}$</td>
<td>-0.99049</td>
<td>0.00359</td>
<td>0.00001</td>
<td>0.00029</td>
<td>0.00000</td>
<td>0.00000</td>
<td></td>
</tr>
<tr>
<td>$e^{-x^2}$</td>
<td>-1.31570</td>
<td>0.00994</td>
<td>0.00071</td>
<td>-0.00183</td>
<td>-0.00009</td>
<td>-0.00003</td>
<td></td>
</tr>
<tr>
<td>No. of points</td>
<td>—</td>
<td>6</td>
<td>21</td>
<td>7</td>
<td>21</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>

and

$$\varepsilon_2 \leq \frac{h^3 M_2}{18} \{ |D| + 3|C_1 - C_2| + 12|C_3| \} 0 < k < 2$$

where

$$D = 8 + 6k(1 + k) + 3k^3 \ln(2 - k/k)$$

$$\leq \frac{h^3 M_3}{18} \{ |D'| + 3|k^2(C_0 - C_1 + C_2)| + 3|1 - k|^3(C_1 - C_2)| \} \text{ otherwise}$$

In these formulae

$$M_2 = \sup_{0 < t < h} |f''(t)|$$

$$M_3 = \sup_{0 < t < 2h} |f'''(t)|.$$
in terms of the original function \( f(x) \). This rule contains in general one more point than the corresponding Gauss rule since it contains a nonzero weight for \( f(q) \).

C. Numerical examples

The simple rules given here comprise convenient methods for evaluating the integrals (1). We illustrate these rules with the numerical examples shown in Table 2; in this table, we have set \( a = 0, b = 1, q = \sqrt{2} \), and we compare the two-point and three-point rules (6) and (7) at a number of step sizes with the modified Gaussian rule (12).

References


Book Review


Marvin Minsky is a superb teacher and his new book a marvel of lucid exposition which one can hardly recommend too highly to anybody wishing to understand the concept of computation and the abilities and disabilities of computing machinery. The technical ideas involved are simple enough and, given an average amount of patience and the capacity to follow straightforward reasoning, we cannot fail to follow where Minsky leads, impelled by such infectious enthusiasm.

Indeed, machine and computability theory is not the abstruse subject it is often made out to be, and made. If the significance of the questions at issue is not always immediately obvious, much can be done to hasten understanding. There is all the difference in the world, for instance, between presenting the fully fledged concept of finite automaton on a plate, as it were, take it or leave it, and the careful build-up of the concept as a highly reasonable object for study which we find in the opening pages of this book. Again, when we relax the finite restriction, it is no use ignoring the heckler in the back row who naturally wants to know why we are wasting our time with infinity, although to give him an adequate reply is not easy, even for Minsky.

The classical type of "infinite machine" is of course Turing's. One of the chief problems of exposition here arises from the fact that, while it is natural to define such a machine formally by means of a matrix, the matrix itself reveals nothing of the associated algorithmic structure. We need to devise some system of flow diagrams to convey what even the simplest Turing machine is doing. Minsky's neat resolution of the difficulty is to employ diagrams linking "left-moving" and "right-moving" states. (For every Turing machine there is an equivalent machine with such "directed" states.) Equally admirable is the way he then steers us through the crucial sequence of argument that shows how every action of a Turing machine may be mirrored in operations of a certain kind on the non-negative integers and precisely in what sense we may then deduce that a "universal" machine exists.

Since Turing's day, much consideration has been given to simple universal machines of quite different form from his. Some of these—Minsky terms them "program machines"—are closer to "real" computers in their types of instruction and use of separately accessible registers. Others have been developed from the symbol-manipulation systems of Emil Post. These, particularly "tag", have long been among Minsky's special research interests and their directness and simplicity which "steps around arithmetic" makes them particularly illuminating.

It is now possible to demonstrate, as Minsky does, that many of these systems are in some sense equivalent, but this very equivalence involves their sharing essential limitations which render various classes of problem for all time insoluble. The solubility status of specific problems, on the other hand, remains an unsatisfactorily "grey area" which Minsky tentatively explores in some of the most interesting sections of the book. Could, for example, Fermat's Last Theorem be actually proved insoluble? This is a field in which ingenious arguments abound but it is particularly difficult to access their logical validity.

The volume is elegantly produced, and a real pleasure to use. If printing errors are common (Why?) in no case do they handicap the reader to any serious extent except possibly in the definition and illustration of "Jump unless equal" (page 208). The author sets us problems of all grades of difficulty, includes solutions of a selection, and adds wise words on human problem-solving in general. It is all excellently carried out, though I should query the solutions of problems 4.2–1, 12.3–1 and 12.3–2.

According to the blurb, this book is "an essential tool in the hands of anyone whose professional range encompasses computers and their use". One wonders how far Minsky himself would endorse that statement. It is of course true that many of the geniuses of the computer from Turing to von Neumann have been deeply concerned with the ideas here discussed. Yet in the meantime, the art of the practical impact of these ideas is surely negligible. Only at some distant date may, as von Neumann believed, the development of computers come to depend crucially on developments in the theory of computability. Only then will the concepts of this book at last be seen to lie in the mainstream of computer development itself.

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