Numerical integration — a different approach

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In common with, I suspect, many people the author does not have access to the NAG library [1] and so, when I was asked recently to calculate the value of the integral

$$\int_{-1}^{1} \frac{\sinh^2(x/2)}{(1-x)^{0.005}(1+x)^{0.995}} \, dx$$

(1)
correct to 10 decimal places my first reaction was to try several different calculators as well as several mathematical software packages. On doing so it was disappointing to find they either gave widely differing values such as 7.9065200767, 4.1317217452 or 0.9174196842 or an error message indicating that the method had not converged.

Obviously this approach did not work and so, since the integrand in (1) has end-point singularities at ±1 and the integral itself is of the form

$$I(f) = \int_{-1}^{1} (1-x)^\alpha (1+x)^\beta f(x) \, dx, \quad \alpha, \beta > -1,$$

(2)
with $\alpha = -0.005$, $\beta = -0.995$ and $f(x) = \sinh^2(x/2)$, I decided to apply Gauss-Jacobi integration which is the accepted numerical analytical technique for approximating this type of integral. We recall that Gauss-Jacobi integration takes the form [2]

$$I(f) = \sum_{i=1}^{n} w_i f(x_i) + E_n(f)$$

(3)
where the abscissae $x_i$ are the zeros of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ of degree $n$ in $x$, the $w_i$ are the weights of the rule and $E_n(f)$ denotes the error term. Since the $x_i$ and the $w_i$ depend on $\alpha$, $\beta$ and $n$ anyone wishing to apply this rule who does not have access to the NAG library must first choose a value for $n$, then calculate the abscissae and weights and finally apply the rule. In practice, the calculation of the weights and the abscissae can be an onerous task, one in which great care must be taken [3]. Having gone through the process once the whole process must then be repeated, possibly for several values of $n$, until the approximate value of the integral is obtained to the number of decimal places required.

In this paper however, we shall describe a different approach, one in which Gauss-Jacobi integration is still used but only with $n = 2$. Then, instead of increasing $n$ and re-calculating the weights and abscissae in (3), we shall keep $n$ fixed at $n = 2$ and evaluate the error term $E_2(f)$. Thus, throughout the remainder of this paper we shall use only the Gauss-Jacobi integration rule of order 2, namely

$$I(f) = \sum_{i=1}^{2} w_i f(x_i) + E_2(f).$$

(4)
The abscissae and weights

For \( n = 2 \) the abscissae in rule (4) are the roots of

\[ p_2^{(\alpha,\beta)}(x) = 0 \]

that is, the roots of

\[(\alpha + \beta + 3)(\alpha + \beta + 4)x^2 + 2(\alpha - \beta)(\alpha + \beta + 3)x + (\alpha - \beta)^2 - (\alpha + \beta + 4) = 0\]

[4], from which we see the abscissae are given by

\[ x_i = \frac{-(\alpha - \beta)(\alpha + \beta + 3) \pm \sqrt{(\alpha + \beta + 3)(\alpha + 2)(\beta + 2)}}{(\alpha + \beta + 3)(\alpha + \beta + 4)}, \quad i = 1, 2 \quad (5) \]

where the upper sign is chosen when \( i = 1 \) and the lower sign when \( i = 2 \).

It is now easy to follow [3], for example, and deduce from (2), (4), the integral definition of the beta function [4] and the relationship between the beta and gamma functions [4] that the weights corresponding to these abscissae are given by

\[ w_i = \frac{s}{2t} \left[ \frac{(\alpha + \beta + 2)t \mp (\alpha - \beta)(\alpha + \beta + 3)}{\alpha + \beta + 2} \right], \quad i = 1, 2 \quad (6) \]

where

\[ s = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} \quad (7) \]

and

\[ t = \sqrt{(\alpha + \beta + 3)(\alpha + 2)(\beta + 2)}. \]

All that now remains is for us to evaluate the error term \( E_2(f) \) in rule (4).

The error term \( E_2(f) \)

Following Stenger [5, p. 152] it is straightforward to show that the error term \( E_2(f) \) in rule (4) may be expressed as

\[ E_2(f) = \sum_{k=4}^{\infty} a_k e_{2,k} \quad (8) \]

where the \( e_{2,k} \) are independent of \( f(x) \) and the \( a_k \) are the Chebyshev coefficients of the first kind of the function \( f(x) \) which we assume known, but if they are not, they may be approximated very easily as follows.

The evaluation of the Chebyshev coefficients [3]

When \( f(x) \) is expressed in the form

\[ f(x) = \sum_{r=0}^{N} a_r T_n(x), \quad (-1 \leq x \leq 1) \]

where \( T_n(x) \) denotes the Chebyshev polynomial of the first kind of degree \( n \) in \( x \) [4] and the double prime indicates that the first and last terms in the
summation are to be halved, then the coefficients $a_r$ are given by

$$a_r = \frac{2}{N} \sum_{s=0}^{N} f \left( \cos \left( \frac{\pi s}{N} \right) \right) \cos \left( \frac{\pi r s}{N} \right).$$

(9)

The evaluation of $e_{2,k}$

By letting $f(x) = T_k(x)$, $k \geq 4$, in rule (4) it follows from expressions (2) and (8) that $e_{2,k}$ is given by

$$e_{2,k} = \int_{-1}^{1} (1 - x)^\alpha (1 + x)^\beta T_k(x) \, dx - \sum_{i=1}^{2} w_i T_k(x_i), \quad (k = 4, 5, \ldots) \tag{10}$$

that is, $e_{2,k}$ denotes the error term in approximating the integral $I(T_k(x))$ by rule (4).

In order to evaluate the $e_{2,k}$ the following approach, using lemmas 1 and 2 below, is recommended although, if one wished, for small values of $k$, the right-hand side of expression (10) could be evaluated analytically in terms of $\alpha$ and $\beta$.

Lemma 1 [6]

Let

$$c_r = \int_{-1}^{1} (1 - x)^\alpha (1 + x)^\beta T_r(x) \, dx;$$

then the $c_r$ satisfy the recurrence relationship

$$c_0 = s, \quad c_1 = \frac{(\beta - \alpha)s}{\alpha + \beta + 2},$$

$$(\alpha + \beta + 2 + r)c_{r+1} - 2(\beta - \alpha)c_r + (\alpha + \beta + 2 - r)c_{r-1} = 0, \quad r = 1, 2, \ldots,$$

where $s$ is defined by expression (7).

Lemma 2

$$\sum_{i=1}^{2} w_i T_r(x_i) = \sum_{i=1}^{2} w_i \cos \left( r \cos^{-1}(x_i) \right), \quad r = 0, 1, 2, \ldots$$

Proof:

This follows directly from $T_r(x) = \cos \left( r \cos^{-1} x \right)$ [4].

Thus, for any given values of $\alpha$ and $\beta$, the numerical values of the $e_{2,k}$ now follow from lemmas 1, 2 and expression (10).

Before illustrating our method by evaluating the integral in expression (1) we shall list the values of those $e_{2,k}$ that we shall require (see Table 1).

<table>
<thead>
<tr>
<th>$e_{2,4}$</th>
<th>$e_{2,6}$</th>
<th>$e_{2,8}$</th>
<th>$e_{2,10}$</th>
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<td>12.205127986298</td>
<td>26.603439386049</td>
<td>40.799462498916</td>
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</tbody>
</table>

TABLE 1: Values of $e_{2,k}$ for $\alpha = -0.005, \beta = -0.995$
Numerical example

\[ J = \int_{-1}^{1} \frac{\sinh^2(x/2)}{(1 - x)^{0.005}(1 + x)^{0.995}} \, dx = 53.7554087347. \]

From [7]

\[ \sinh^2(x/2) = \frac{1}{2} \left( I_0(1) - 1 + 2 \sum_{n=1}^{\infty} I_{2n}(1) T_{2n}(x) \right), \tag{11} \]

where \( I_k \) denotes the modified Bessel function of the first kind which are tabulated in [7] or, for example, in Mathcad. Table 2 now follows from Table 1 and expressions (4), (5), (6) and (11) with \( \alpha = -0.005 \) and \( \beta = -0.995 \).

<table>
<thead>
<tr>
<th>( r )</th>
<th>The approximation of ( J ) using Gauss-Jacobi integration (with ( n = 2 ) + ( r ) terms of (8))</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>53.7454237870</td>
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<td>2</td>
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<tr>
<td>4</td>
<td>53.7554087347</td>
</tr>
</tbody>
</table>

TABLE 2: Using exact Chebyshev coefficients

Finally, the same results are obtained using expression (9) with \( N = 16 \) and \( r = 4, 6, 8 \) and 10 to calculate the Chebyshev coefficients.

References

1. The NAG Fortran Library, Numerical Algorithms Group Ltd., 256 Banbury Road, Oxford OX2 7DE.

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