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Letter to the Editor

On a Conjecture in Multidimensional Quadrature*

In a short note [1] published in this journal in 1973, Isenberg has suggested a conjecture about the nature of the asymptotic expansion for the error functional relating to multidimensional quadrature when the integrand function is singular at a point. Recent work by one of us and numerous experiments by the other have confirmed that this conjecture is incorrect in general.

The main purpose of this note is simply to set the record straight, for the benefit of readers of Isenberg's note who plan to use methods based on an invalid conjecture, with the consequent unnecessary expense. In passing we draw attention to some other errors in the note and to the misleading manner in which some of the numerical results are presented. A derivation of the correct results is presented elsewhere (Lyness [3]) and a discussion of the computational aspects of methods based on these results is published [5]. Consequently, this letter is of immediate interest only to readers familiar with Isenberg's note. It could well be ignored by other readers.

Isenberg denotes by $I(\infty)$ the value of an exact d-dimensional integral over a hypercube and defines $I(n)$ to be the approximation to $I(\infty)$ obtained by dividing the hypercube into n^d subregions and applying the same quadrature formula to each subregion. He states his conjecture as follows: "The asymptotic form of the behavior of $I(n)$ is

$$I(n) = I(\infty) + \sum_{r=0}^{\infty} A_r/n^{\alpha+r} + \text{other terms}. \tag{1}$$

For large n the 'other terms' are negligible compared with $\sum_{r=0}^{\infty} A_r/n^{\alpha+r}$. The value of α is determined by estimating the contribution to the integral of a subregion surrounding the singular point."

This conjecture is immediately implausible as it does not reduce to standard results, see e.g., Lyness and Ninham [2] in the one-dimensional case. In fact, we have now shown that the true expansion for a wide class of functions which includes those considered by Isenberg whose singularity is at a vertex is

$$I(n) \sim I(\infty) + \sum_{r\geqslant 0} A_r/n^{\alpha+r} + \sum_{s\geqslant 1} C_s \ln n/n^s + \sum_{s\geqslant 1} B_s/n^s, \tag{2}$$

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the order of the remainder coinciding with that of the first omitted term. However

$$C_s = 0, \qquad \alpha \neq \text{integer}, \tag{3}$$

and if the quadrature rule is symmetric and of polynomial degree p

$$\begin{aligned} B_s = C_s = 0, &\qquad s \text{ odd}, \\ B_s = C_s = 0, &\qquad s \leqslant p. \end{aligned} \tag{4}$$

The class of integrand functions for which (2) is valid includes those with singularities at a vertex of type r^β, where r is a distance measured from that vertex. Logarithmic singularities such as $r^\beta \ln \beta$ give rise to additional terms $D_s(\ln n)^2/n^s$ when β is an integer. The overall situation is further complicated by the occasional vanishing of some coefficients C_s and D_s when the integrand function has certain properties some of which are related to symmetry. A full discussion of the error functional expansion when these singularities are algebraic or logarithmic in nature is included in Lyness [3]. The corresponding situation with regard to essential singularities is not known to the authors.

The value of an expansion of this type is that after computing $I(n)$ for several values of n, the results can be extrapolated to produce an estimate for $I(\infty)$, which is much more accurate than any of the individual approximations $I(n)$. This is done by successively eliminating the low-order terms in the expansion for the error, $I(n) - I(\infty)$, by means of linear combinations of the $I(n)$'s. To do this, it is only necessary to know the powers of n that occur with nonzero coefficients in the expansion. It is not necessary to know the numerical values of these coefficients. Romberg Integration consists of doing this on the basis of the Euler Maclaurin asymptotic expansion.

Isenberg illustrates his conjecture with the following two examples:

$$\text{(1)} \quad I_2 = \int_0^1 \int_0^1 \frac{dx\,dy}{(2 - x^2 - y^2)^{1/2}}, \tag{5}$$

$$\text{(2)} \quad I_3 = \int_0^1 \int_0^1 \int_0^1 \left(1 - \frac{3z^2}{x^2 + y^2 + z^2}\right)^2 dx\,dy\,dz. \tag{6}$$

Application of his conjecture leads to the asymptotic expansions given in his paper, namely,

$$I_2(n) = I_2(\infty) + \sum_{r=0}^{\infty} \frac{A_r}{n^{3/2+r}} + \cdots, \tag{7}$$

$$I_3(n) = I_3(\infty) + \sum_{r=0}^{\infty} \frac{A_r}{n^{3+r}} + \cdots. \tag{8}$$

The numerical results show rather good convergence of the extrapolated values.

The given asymptotic expansion (7) is correct for I_2. The reason is that this function possesses some unusual symmetry properties that cause the terms B_s in the usual asymptotic expansion (2) to drop out. Seemingly minor changes to this integrand function (5) such as changing 2 to 3, or $\frac{1}{2}$ to $\frac{1}{3}$, or multiplying by x destroy these symmetry properties invalidating asymptotic expansion (7). We have searched for other integrand functions for which asymptotic expansion (7) is valid. The only ones we have found are trivially related to (5). This situation leads us to believe that Isenberg tested his conjecture using only an extremely limited class of integrand functions.

The correct expansion for $I_3(n)$ is

$$I_3(n) = I_3(\infty) + \frac{A_3}{n^3} + \sum_{r=3}^{l-1} \frac{A_{2r}}{n^{2r}} + O(n^{-2l}). \tag{9}$$

The expansion (8) conjectured for $I_3(n)$ is not incorrect. It contains all of the correct terms. This is the reason the numerical results appear quite good. But it also contains extra terms A_4n^{-4}, A_5n^{-5}, A_7n^{-7},... whose coefficients are actually zero. The first extrapolated value $I_{2,10}(\infty)$, which corresponds to the elimination of A_3 from the error expansion with $n = 10$ and $n = 9$ is accurate to 4 more decimal places than $I_{1,10}(\infty)$. This happens because the error in $I_{1,10}(\infty)$ is $O(n^{-3})$ and the error in $I_{2,10}(\infty)$ is $O(n^{-6})$ instead of $O(n^{-4})$ as conjectured. The elimination of the non-existent terms A_4n^{-4} and A_5n^{-5} leading to extrapolants $I_{3,10}(\infty)$ and $I_{4,10}(\infty)$ does not diminish the accuracy of these estimates for the integral, however, it also does not improve the accuracy very much. Use of the correct expansion would allow equally accurate estimates for I_3 to be computed at significantly lower cost.

The results of the numerical experiments on I_2 and I_3 are presented in the form of three tables. The notation used for these tables is correctly explained in the text, but is grossly misleading in one respect. For example, in [1, Table II], the third extrapolated value listed, i.e., $I_{3,10}(\infty)$ is accurate to nine decimal places. The number of function values required to compute $I_{3,10}(\infty)$ is not listed, but a cursory glance would leave the impression that it might be 4104 or perhaps 4104 + 2325 + 1216. In fact it is 19,000 + 13,831 + 9728. The reason is that these results refer not to extrapolation in a natural order but to a situation in which one chooses $n = 10, 9, 8, \ldots$ successively. Perhaps the results would have been more easily interpreted if the columns labeled n, $I(n)$ and n_l had been inverted.

There is also a discrepancy concerning which quadrature rule was used to obtain the results reported in [1, Table II]. The text [1, p. 420] claims that it was a 19 point quadrature formula due to Hammer and Stroud. The reference given is to C_n : 5–3 on p. 231 of Stroud (see our [4]). In fact, C_n : 5–3 is on p. 232, [4], is due to Stroud only, and uses 37 points. A 19 point rule due to Hammer and Stroud is on p. 231 [4], and is denoted C_n : 5–2. Our calculations using this rule did not duplicate the results reported. After some testing we found that the numbers given in [1, Table II] were generated using $C_n : 5\text{–}9$ in [4, p. 234]. This is a 27 point rule, and therefore all function value counts in [1, Table II] are incorrect and should be increased by a factor 27/19, i.e., the counts listed are about 30% low.

In conclusion, we should like to emphasize that these errors in [1] while significant, are errors in detail. As such they can cause endless trouble. For example a prospective user, finding that a method based on the previously conjectured expansion is inefficient and finding that the numerical results given in [1] are incorrect, may well be tempted to abandon altoghether the use of extrapolation in his problem. This might be a pity. In our opinion the underlying concept of the paper, namely, there exist expansions of this general nature that can be used to great advantage in multidimensional numerical quadrature, is quite valid. We urge users with these types of problems not to overlook the possibility of employing this type of approach simply because some vital details were presented incorrectly. The basic purpose of this letter is simply to pinpoint these errors, so that prospective users may use this approach where valid with confidence.

References

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