Putting $E = ||y(t)||$ we find on integration

$$\tfrac{1}{2}\{720E\}^2 = \frac{1}{106496} - \frac{1}{7392}\sum_{i=1}^{l} A_i s_i^6\{231 - 396s_i + 495s_i^2 - 440s_i^3 + 264s_i^4 - 96s_i^5 + 16s_i^6\} + \frac{36}{11}\sum_{i=1}^{l} A_i^2 s_i^{11} + \frac{2}{77}\sum_{\substack{j=1 \\ i>j}}^{l-1} A_i A_j s_i^6\{462s_j^5 - 330s_j^4 s_i + 165s_j^3 s_i^2 - 55s_j^2 s_i^3 + 11s_j s_i^4 - s_i^5\}. \quad (51)$$

This was minimized subject to (45) and (46) using Powell's method (1964) and the resulting points and weights will be found in **Table 6** for $m = 3, 4, 5, 6$. These formulae were then applied, together with other sixth order formulae to a wide range of functions, and the errors in the calculation are given in **Table 7**. As in the fourth order case we see that optimal formulae do give much more accurate results than any of the classical quadrature formulae. (The six point Gaussian formula used was that obtained by applying Gauss three point formula to half intervals in order to obtain sixth order formula. The formulae termed Sard's are also the Newton Cotes formulae in the cases here considered.)

11. Conclusion

We have shown a method for finding quadrature formulae that are optimal in the sense that they give much lower errors for functions of a specific class (bounded nth derivative). The method also provides an error bound for such formulae in terms of a bound on the nth derivative. Here we have only discussed the cases $n = 2, 4, 6$, since higher derivatives of the integrand are usually not convenient to handle. However, the same methods can be applied in principle to obtain optimal formulae for any value of n. The amount of computation required increases rapidly with increasing n and m, and such difficulties are discussed by Stern (1966), where a few formulae for $n = 8$ and 10 are given.

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Correspondence

To the Editor,
The Computer Journal.

Sir,

I was interested to read the paper by B. J. Allen on "An investigation into direct numerical methods for solving some calculus of variation problems", which appeared in this *Journal* in August, 1966.

However, once one accepts that the integral must be evaluated numerically it is surely better to use the Ritz method combined with a hill-climbing technique that does not require the evaluation of derivatives. This approach has been used for partial differential equations by Rosenbrock and Storey (*Computational Techniques for Chemical Engineers*, Pergamon, 1966, p. 115).

I am investigating some boundary value problems for ordinary differential equations that arise in chemical engineering by turning the problem into a variational one and using this technique, and have obtained some useful results which I hope to publish shortly.

Yours faithfully,

H. W. Pakes

University of Technology,
Loughborough,
Leics.
8 September 1966.

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