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# Note

## Integration Weights for Experimental Data

### 1. Introduction

Given a set of points, $x_i$ ($i = 1, 2, \ldots, M$), with $0 \leqslant x_i \leqslant 1$, we seek a set of weights, $w_i$, such that

$$\int_0^1 f(x)\,dx = \sum_{i=1}^{M} w_i f(x_i). \tag{1}$$

The integration limits impose no restrictions as an appropriate mapping allows the formula to be applied to any finite range. The numerical values of the function, $f(x_i)$, are considered to be derivable from experimental data and as such will have standard errors, $\sigma_i$, associated with each point, $x_i$. It is the taking into account of the $\sigma_i$ that alters the standard quadrature approach somewhat. This problem arises when the experimental limitations require measurements at particular points, or more frequently, when one wishes to use data taken from the literature.

By requiring that the quadrature relation be exact for a polynomial of degree $M - 1$, the $w_i$ in (1) may be determined by solving the system of equations

$$\sum_{i=1}^{M} w_i x_i^n = \frac{1}{n+1} \qquad (n = 0, 1, 2, \ldots, M-1). \tag{2}$$

This is the usual procedure, but the weights so produced may be of such magnitudes as to be of no practical value. Numerical integration using experimental data contains two sources of error: the first is related to the accuracy of the quadrature formula itself, and the second to the accuracy of the experimentally determined values of $f(x_i)$. The standard error, $\sigma$, due to the latter is given by

$$\sigma = \left[\sum_{i=1}^{M} w_i^2 \sigma_i^2\right]^{1/2}, \tag{3}$$

which, for the case of equal $\sigma_i$, is $W\sigma_i$, where $W$ is the square root of the sum of weights squared and has a theoretical minimum value $= 1/M^{1/2}$. Clearly a small value of $W$ is desirable, but the determination of the weights from (2) leaves no freedom in this respect. To illustrate the serious nature of the problem, we consider the set of $x_i$ given by the square roots of 0, 0.1, 0.2,..., 1.0. The solutions, $w_i$, obtained from (2) and rounded off to the nearest integer are shown in Table I in Column I; the corresponding value of $W$ is 1768. Thus, while the $w_i$ are indeed correct from a



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mathematical viewpoint, they would produce in a statistical sense a huge amplification of the experimental error.

There are several reasonable approaches to this problem. The technique presented here is based on lowering the degree of the polynomial satisfied by the $x_i$ and using the resulting freedom to minimize $\sigma$.

TABLE I

| $x_i$ | I | II | $x_i$ | III | IV |
|---|---|---|---|---|---|
| 0 | 0 | 0.131502 | 0 | 0.026834 | 0.029446 |
| $0.1^{1/2}$ | 4 | 0.224142 | 0.1 | 0.177536 | 0.151414 |
| $0.2^{1/2}$ | −34 | 0.174332 | 0.2 | −0.081042 | 0.036504 |
| $0.3^{1/2}$ | 168 | 0.124001 | 0.3 | 0.454946 | 0.141487 |
| $0.4^{1/2}$ | −484 | 0.082327 | 0.4 | −0.435154 | 0.113398 |
| $0.5^{1/2}$ | 887 | 0.051744 | 0.5 | 0.713764 | 0.055001 |
| $0.6^{1/2}$ | −1071 | 0.032955 | 0.6 | −0.435154 | 0.113398 |
| $0.7^{1/2}$ | 852 | 0.026054 | 0.7 | 0.454946 | 0.141487 |
| $0.8^{1/2}$ | −430 | 0.030897 | 0.8 | −0.081042 | 0.036504 |
| $0.9^{1/2}$ | 126 | 0.047241 | 0.9 | 0.177536 | 0.151414 |
| 1 | −16 | 0.074804 | 1.0 | 0.026834 | 0.029446 |
| $W$ | 1768 | 0.365 | | 1.175 | 0.345 |

## 2. Formulation and Examples

The system of linear equations (2) is well known to be inherently ill-conditioned. To eliminate this aspect of the problem, we require (1) to be exact for the first $M$ shifted Legendre polynomials, $P^*_n(x)$. These polynomials are generated from

$$\begin{aligned} P^*_0(x) &= 1, \\ P^*_1(x) &= 2x - 1, \\ (n+1)\, P^*_{n+1}(x) &= (2n+1)(2x-1)\, P^*_n(x) - nP^*_{n-1}(x). \end{aligned} \tag{4}$$

The system of equations (2) now takes the equivalent form

$$\begin{aligned} \sum_{i=1}^{M} w_i P^*_n(x_i) &= 1, \qquad n = 0, \\ &= 0, \qquad n = 1, 2, \ldots, M-1. \end{aligned} \tag{5}$$

We require (5) to be satisfied for $n \leqslant L$, with $L \leqslant M - 1$, and proceed to minimize subject to this condition the function

$$\sum_{i=1}^{M} E_i w_i^2, \tag{6}$$

where the $E_i$ are the statistical weights which are proportional to the $\sigma_i^2$. Minimization of this function, which is equivalent to minimizing $\sigma$ of Eq. (3), leads to the linear system: Eqs. (5) with $n = 0, 1, 2,..., L$ and

$$2E_i w_i + \sum_{n=0}^{L} \lambda_n P^*_n(x_i) = 0 \qquad (i = 1, 2,..., M). \tag{7}$$

These are then solved for the $M$ values of $w_i$ and the $L + 1$ values of $\lambda_n$, the Lagrangian undetermined multipliers. The $E_i$ are introduced in (6) in place of the $\sigma_i^2$ to stress that only relative values of the $\sigma_i$ are required in (7); to find $\sigma$ from (3), a knowledge of the absolute values is necessary.

All calculations in the following examples were performed on an HP-2000 computer which employs 6 to 7 digit precision. The inherent ill-conditioning, which is due to the nature of the series (2) itself, has been removed through the use of orthogonal polynomials. It should be noted that serious ill-conditioning can nevertheless result from a poor distribution of the points, $x_i$. Consequently, it is generally advisable whenever possible to employ extended precision in this type of numerical procedure.

We consider first the problem previously cited, that is, the case where the $x_i$ are given by the square roots of 0, 0.1, 0.2,..., 1.0. We begin by setting all $E_i = 1$ and taking $L = 9$. This produces a value of $W = 190$ which is still large for a practical quadrature formula. By lowering $L$ further, the following results are obtained: $L = 8$, $W = 30$; $L = 7$, $W = 6$; $L = 6$, $W = 1.8$; $L = 5$, $W = 0.72$; $L = 4$, $W = 0.46$; and $L = 3$, $W = 0.365$. The last value of $W$ is close to the theoretical minimum, 0.302; the values of the corresponding $w_i$ are shown in Column II of Table I.

In the above example, the distribution of the quadrature points was such that the degree of the polynomial satisfied by these points had to be reduced by approximately a factor of 2 before $W$ was within an order of magnitude of the theoretical minimum and hence expected to be small enough for practical applications. In many instances, however, lowering the degree by one will produce a substantial improvement. Consider the case where the $x_i$ are 0, 0.1, 0.2,..., 1.0. Equally spaced quadrature points give rise to Newton–Cotes formulas which are popular since the weights can be expressed as a ratio of integers. These formulas are tabulated [1] and the $w_i$ for this case are listed in Column III in Table I. The corresponding value of $W$ is 1.175. By setting $L = 9$ instead of 10, the $w_i$ shown in Column IV are obtained with $W = 0.345$, which is a threefold improvement in the statistical error, $\sigma$.

The program used in these calculations is available in both HP-BASIC and FORTRAN IV. Copies may be obtained from the first author.

## References

1. "Handbook of Mathematical Functions" (NBS-1964), Dover, New York, 1965.

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