

On Optimal Quadrature Formulae

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A procedure to construct quadrature formulae which are exact for solutions of linear differential equations and are optimal in the sense of Sard is discussed. We give necessary and sufficient conditions under which such formulae do exist. Several formulae obtained by applying this method are considered and compared with well known formulae.

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1. INTRODUCTION

Let $[a, b]$ be a bounded, closed interval of the real axis and let n be a positive integer. Consider the following integral

$$\int_a^b u(x)g(x) \, dx \quad (1.1)$$

where $u \in C^n([a, b])$ and $g(x) \in L^1(a, b)$. $g(x)$ is the weight function and is supposed to be non-zero on a set of positive measure.

Denote by x_1, \dots, x_m m different points of the interval $[a, b]$ such that

$$a = x_0 \leq x_1 < \dots < x_m \leq x_{m+1} = b \quad (1.2)$$

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and denote by E a linear differential operator of order n :

$$E = \frac{d^n}{dx^n} + \sum_{k=1}^n a_k(x) \frac{d^{n-k}}{dx^{n-k}} \quad (1.3)$$

where $a_k(x) \in C^{n-k}([a, b])$, $k = 1, \dots, n$.

In [4] Ghizzetti and Ossicini consider the following general quadrature formula:

$$\int_a^b u(x)g(x) dx = \sum_{h=1}^n \sum_{i=1}^m A_{hi} u^{(h-1)}(x_i) + R[u], \quad (1.4)$$

relevant to the integral (1.1), to the nodes (1.2) and to the differential operator (1.3), with the following condition:

$$E[u] = 0 \Rightarrow R[u] = 0 \quad (1.5)$$

that is (1.4) is exact when u is solution of the linear differential equation $E[u] = 0$.

Fixed the weight $g(x)$, the nodes x_1, \dots, x_m and the operator E , in [4] a method to determine all the quadrature formulae of type (1.4), which satisfy condition (1.5), is given. In order to do that, consider the adjoint operator of E :

$$E^* = (-1)^n \frac{d^n}{dx^n} + \sum_{k=1}^n (-1)^{n-k} \frac{d^{n-k}}{dx^{n-k}} a_k(x)$$

and the reduced operators

$$E_r = \frac{d^r}{dx^r} + \sum_{k=1}^r a_k(x) \frac{d^{r-k}}{dx^{r-k}}, \quad r = 0, \dots, n-1$$

with their adjoint operators

$$E_r^* = (-1)^r \frac{d^r}{dx^r} + \sum_{k=1}^r (-1)^{r-k} \frac{d^{r-k}}{dx^{r-k}} a_k(x), \quad r = 0, \dots, n.$$

Let $\varphi_0(x)$ and $\varphi_m(x)$ be the solutions of the equation

$$E^*[\varphi] = g \quad (1.6)$$

which satisfy, respectively, the initial condition

$$\varphi_0^{(h)}(a) = 0, \quad \varphi_m^{(h)}(b) = 0, \quad h = 0, \dots, n-1$$

and let $\varphi_1(x), \dots, \varphi_{m-1}(x)$ be $m-1$ arbitrary solutions of (1.6).

By assuming in (1.4)

$$A_{hi} = E_{n-h}^*[\varphi_i - \varphi_{i-1}]_{x=x_i}, \quad h = 1, \dots, n; \quad i = 1, \dots, m \quad (1.7)$$

and

$$R[u] = \sum_{i=0}^m \int_{x_i}^{x_{i+1}} \varphi_i(x) E[u(x)] dx \quad (1.8)$$

the quadrature formula (1.4) satisfies condition (1.5). Conversely, if (1.4) and (1.5) hold true, then there are uniquely determined $\varphi_1, \dots, \varphi_{m-1}$, solutions of (1.6), such that, together with φ_0 and φ_m , make valid (1.7) and (1.8) [4, pp. 27–32].

Appropriately choosing the weight function $g(x)$, the nodes x_1, \dots, x_m , the differential operator E and the functions $\varphi_1, \dots, \varphi_{m-1}$ many of the known quadrature formulae can be found as particular cases (see [4, pp. 80–147]).

Since (1.4) depends on $(m-1)n$ free parameters, it is natural to try to determine these parameters in such a way quadrature formula (1.4) is optimal in some sense.

This problem has been investigated by many authors, see e.g. [1,2,5,6,8,11,12,19,20]. The first result of the present paper is that there is one and only one way of making (1.4) optimal in Sard's sense [11, p. 38, 16, p. 176] by choosing in a suitable way all the free parameters. This is shown by Theorem 2.I.

Moreover in Section 2 we consider the quadrature formula

$$\int_a^b u(x)g(x) dx = \sum_{h=1}^{n-p} \sum_{i=1}^m A_{hi}u^{(h-1)}(x_i) + R[u],$$

$$(E[u] = 0 \Rightarrow R[u] = 0), \quad (1.9)$$

for a fixed $p: 1 \leq p \leq n - 1$, and we investigate the existence and uniqueness of the best quadrature formula in the sense of Sard. This problem has already been discussed by several authors, mainly concerning the operator $E = d^n/dx^n$ (see [11,13–15,18] and their references).

We remark that formula (1.9) is interesting in the applications, especially if we require only the knowledge of the function's values at given points.

In Theorem 2.III we give necessary and sufficient conditions under which it is possible to make (1.9) optimal in Sard's sense. This theorem contains some previous results: if $p = n - 1$ and $m \geq n$, in [7] it has been proved that the optimal quadrature formula in Sard's sense can be written, in one and only one way, if the differential operator E has the property W in the sense of Polya (see [5,6,10]). In [17], the author extends this result to the case of the operator E of type (1.3) under the following hypothesis:

$$\begin{aligned} \text{the only solution of the equation } Eu = 0 \\ \text{vanishing at the nodes is } u \equiv 0. \end{aligned} \quad (1.10)$$

As far as our result is concerned, it must be remarked that if conditions (2.12) are not satisfied, it is not possible to write a quadrature formula of type (1.9). Therefore this paper provides a complete solution to the problem of constructing quadrature formulae of type (1.9), optimal in Sard's sense. Moreover by means of our method it is possible to obtain several new quadrature formulae.

The proofs of Theorems 2.I and 2.III lead to the explicit construction of quadrature formulae useful in the applications. In Section 3 several examples are given. In Examples (e)–(g) we consider equidistant nodes and the operator $E = d^n/dx^n$ because we want to compare the new formulae with the classical ones. Moreover we construct other formulae by choosing different operators and different nodes.

2. MAIN RESULTS

Let $\{v_1(x), \dots, v_n(x)\}$ be a fundamental system of solutions of the homogeneous equation

$$E^*v = 0 \quad (2.1)$$

and let $v_p(x)$ be a particular solution of (1.6). The solutions $\varphi_i(x)$, $i = 1, \dots, m - 1$ of (1.6) can be written as

$$\varphi_i(x) = v_p(x) + \sum_{h=1}^n c_h^{(i)} v_h(x), \quad i = 1, \dots, m - 1 \quad (2.2)$$

where $\{c_h^{(i)}\}$ ($h = 1, \dots, n, i = 1, \dots, m - 1$) denote $(m - 1)n$ arbitrary constants.

Define the function $\Phi(x)$ as

$$\Phi(x) = \varphi_i(x), \quad x \in (x_i, x_{i+1}], \quad i = 0, \dots, m.$$

Φ is called the “influence function” or the “Peano kernel”.

From (1.8) we deduce that

$$R[u] = \int_a^b \Phi(x) E[u(x)] dx.$$

The remainder $R[u]$ can be estimated in different ways.

By applying Cauchy–Schwarz inequality we deduce

$$|R[u]| \leq \|E[u]\|_2 \left(\int_a^b [\Phi(x)]^2 dx \right)^{1/2} = \|E[u]\|_2 \left(\sum_{i=0}^m \int_{x_i}^{x_{i+1}} [\varphi_i(x)]^2 dx \right)^{1/2} \quad (2.3)$$

where

$$\|E[u]\|_2 = \left(\int_a^b [E[u]]^2 dx \right)^{1/2}.$$

We say that (1.4), (1.5) is “optimal” in the sense of Sard [11,16] if the $(m - 1)n$ constants $\{c_h^{(i)}\}$ are chosen in such a way to minimize

$$\int_a^b [\Phi(x)]^2 dx.$$

Of course we may also write

$$|R[u]| \leq \|E[u]\|_\infty (b-a)^{1/2} \left(\int_a^b [\Phi(x)]^2 dx \right)^{1/2} \quad (2.4)$$

where

$$\|E[u]\|_\infty = \max_{[a,b]} |E[u]|.$$

The estimate (2.4) permits us to compare our quadrature formulae with the classical ones, where the following appraisal for $R[u]$ is used:

$$|R[u]| \leq \|E[u]\|_\infty \int_a^b |\Phi(x)| dx = \|E[u]\|_\infty \sum_{i=0}^m \int_{x_i}^{x_{i+1}} |\varphi_i(x)| dx. \quad (2.5)$$

Unfortunately in many cases it is not easy to study the sign of the function Φ that is to apply the estimate (2.5).

THEOREM 2.1 *There exists a unique quadrature formula of type (1.4)–(1.5) that is optimal in Sard's sense.*

Set, for $i = 1, \dots, m-1$,

$$\mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)}) = \int_{x_i}^{x_{i+1}} [\varphi_i(x)]^2 dx. \quad (2.6)$$

The $m-1$ terms $\mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)})$ are independent. Therefore to minimize $\int_a^b [\Phi(x)]^2 dx$ it is sufficient to minimize each term.

If the function $\varphi_i(x)$ is zero a.e. in (x_i, x_{i+1}) (i.e. $g(x)$ is zero a.e. in (x_i, x_{i+1})) then $\mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)}) = 0$. Otherwise $\mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)}) > 0$. In this case, from (2.2), we deduce that

$$\begin{aligned} \mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)}) &= \sum_{h,k}^{1,n} c_h^{(i)} c_k^{(i)} \int_{x_i}^{x_{i+1}} v_h(x) v_k(x) dx \\ &+ 2 \sum_{h=1}^n c_h^{(i)} \int_{x_i}^{x_{i+1}} v_p(x) v_h(x) dx + \int_{x_i}^{x_{i+1}} [v_p(x)]^2 dx. \end{aligned}$$

It is well known that such a polynomial has a positive minimum in \mathbb{R}^n and, denoting by $\hat{c}^{(i)} = (\hat{c}_1^{(i)}, \dots, \hat{c}_n^{(i)})$ the solution of the following system of n linear equations[†]

$$\sum_{h=1}^n c_h^{(i)} \int_{x_i}^{x_{i+1}} v_h(x)v_k(x) dx = - \int_{x_i}^{x_{i+1}} v_p(x)v_k(x) dx, \quad k = 1, \dots, n,$$

we have

$$\mathcal{F}_i(\hat{c}_1^{(i)}, \dots, \hat{c}_n^{(i)}) = \min_{\mathbb{R}^n} \mathcal{F}_i(c_1^{(i)}, \dots, c_n^{(i)}).$$

By choosing the constants $\{c_h^{(i)}\}$ in (2.2) equal to $\{\hat{c}_h^{(i)}\}$ we uniquely determine the functions $\varphi_i(x)$, $i = 1, \dots, m - 1$, solutions of (1.6) and, by means of (1.7) and (1.8), we uniquely determine a quadrature formula which is exact for the solutions of the equation $E[u] = 0$. It is the “optimal” quadrature formula in the sense of Sard.

Since

$$\mathcal{F}_i(\hat{c}_1^{(i)}, \dots, \hat{c}_n^{(i)}) = \sum_{h=1}^n \hat{c}_h^{(i)} \int_{x_i}^{x_{i+1}} v_p(x)v_h(x) dx + \int_{x_i}^{x_{i+1}} [v_p(x)]^2 dx$$

from (2.3) we obtain

$$\begin{aligned} |R[u]| \leq \|E[u]\|_2 & \left(\int_{x_0}^{x_1} [\varphi_0(x)]^2 dx + \sum_{i=1}^{m-1} \sum_{h=1}^n \hat{c}_h^{(i)} \int_{x_i}^{x_{i+1}} v_p(x)v_h(x) dx \right. \\ & \left. + \int_{x_1}^{x_m} [v_p(x)]^2 dx + \int_{x_m}^{x_{m+1}} [\varphi_m(x)]^2 dx \right)^{1/2}. \end{aligned} \tag{2.7}$$

In this way it is possible to construct a lot of new quadrature formulae (see, e.g., Examples (a)–(c) in Section 3). Formulae obtained in this way have the disadvantage that the derivatives up to the order $n - 1$ of the integrand function appear in the nodes. The choice of the $(m - 1)n$ arbitrary constants in the classical formulae is based on the requirement that the derivatives of u have not to appear in (1.4). In the following we will see how it is possible, by virtue of the arbitrary choice of the

[†] Since $\{v_h\}_{h=1, \dots, n}$ is a system of linearly independent solutions of (2.1) in $[a, b]$ then $\{v_h\}_{h=1, \dots, n}$ are linearly independent functions in $[x_i, x_{i+1}]$, $\forall i = 1, \dots, m - 1$.

functions $\{\varphi_i\}_{i=1, \dots, m-1}$, to avoid the presence of the derivatives of $u(x)$ in the nodes and, at the same time, to "optimize" the quadrature formula.

Suppose that we have fixed a differential operator (1.3), the nodes (1.2) and the weight function $g(x)$ in the interval $[a, b]$. Consider the quadrature formula (1.4), together with (1.7) and (1.8). Let us fix an integer $1 \leq p \leq n-1$. In [4] the authors give necessary and sufficient conditions in order to write a quadrature formula where the values $u^{(h)}(x_i)$ of the derivatives of order higher than $n-p-1$ are dropped, that is a quadrature formula of the following kind:

$$\int_a^b u(x)g(x) dx = \sum_{h=1}^{n-p} \sum_{i=1}^m A_{hi} u^{(h-1)}(x_i) + R[u],$$

$$(E[u] = 0 \Rightarrow R[u] = 0). \quad (2.8)$$

If some conditions are satisfied, the functions $\varphi_1, \dots, \varphi_{m-1}$ (solutions of (1.6)) can be determined in such a way

$$A_{hi} = E_{n-h}^*[\varphi_i - \varphi_{i-1}]_{x=x_i} = 0, \quad h = n-p+1, \dots, n; \quad i = 1, \dots, m \quad (2.9)$$

that is to say we can write a quadrature formula of type (2.8).

Let $(u_1(x), \dots, u_n(x))$ be n linearly independent functions, solutions of $Eu = 0$. Assume $u = u_j$, ($j = 1, \dots, n$) in (2.8):

$$\sum_{h=1}^{n-p} \sum_{i=1}^m A_{hi} u_j^{(h-1)}(x_i) = \int_a^b u_j(x)g(x) dx, \quad j = 1, \dots, n. \quad (2.10)$$

It is possible to write a quadrature formula of type (2.8) if and only if the n linear system (2.10) with $m(n-p)$ unknowns $\{A_{hi}\}$ has solutions. In order to discuss this system, consider the transposed homogeneous system

$$\sum_{j=1}^n c_j u_j^{(h-1)}(x_i) = 0, \quad h = 1, \dots, n-p; \quad i = 1, \dots, m. \quad (2.11)$$

If the rank of the matrix $(u_j^{(h-1)}(x_i))$ (with n rows and $m(n-p)$ columns) is equal to n (it must be $m(n-p) \geq n$) then (2.11) has no non-trivial

solutions and the linear system (2.10) has $m(n-p) - n$ linearly independent solutions. Then a quadrature formula of type (2.8) depends on $m(n-p) - n$ free parameters.

If the rank of the matrix $(u_j^{(h-1)}(x_i))$ is less than n , that is $n - q$, $q \geq 1$ (it must be $m(n-p) \geq n - q$) then (2.11) has q linearly independent solutions $C_r = (C_{r1}, \dots, C_{rm})$, $(r = 1, \dots, q)$. In this case (2.10) has solutions if and only if the following compatibility conditions are satisfied:

$$\sum_{j=1}^n C_{rj} \int_a^b u_j(x)g(x) dx = 0, \quad r = 1, \dots, q. \quad (2.12)$$

Then it is possible to write a quadrature formula of the type (2.8) in $\infty^{m(n-p)-(n-q)}$ different ways.

Consider the following homogeneous boundary value problem

$$\begin{cases} E[u] = 0, \\ u^{(h)}(x_i) = 0, \quad h = 0, \dots, n-p-1; \quad i = 1, \dots, m. \end{cases} \quad (2.13)$$

The general solution of the equation $Eu = 0$ is given by $u(x) = \sum_{j=1}^n c_j u_j(x)$, (c_1, \dots, c_n) denoting arbitrary parameters. By imposing the boundary conditions we obtain exactly the system (2.11). In [4] the authors proved the following.

THEOREM 2.II *If problem (2.13) admits only the solution $u(x) \equiv 0$, it is possible to write a quadrature formula of the type (2.8) in $\infty^{m(n-p)-n}$ different ways (it must be $n \leq m(n-p)$). If problem (2.13) has q ($q \geq 1$) linearly independent solutions $v_r(x) = \sum_{j=1}^n C_{rj} u_j(x)$, $(r = 1, \dots, q)$, formula (2.8) can be written only if the conditions (2.12) are satisfied. Then we may get a quadrature formula (2.8) in $\infty^{m(n-p)-n+q}$ different ways and it must be $n-p \leq n-q \leq m(n-p)$.*

Set $s = m(n-p) - n + q$, where we assume $q = 0$ if (2.13) has only the solution $u \equiv 0$.

Suppose that it is possible to write quadrature formula of type (2.8).

If $q = 0$ it is sufficient to assume the number of the nodes $m \geq n/(n-p)$. If $q > 0$ this is possible if and only if conditions (2.12) are satisfied and it must be $m \geq (n-q)/(n-p)$.

From Theorem 2.II, a quadrature formula of type (2.8) can be written in ∞^s different ways. Then it is possible to find $\varphi_1, \dots, \varphi_{m-1}$, solutions of (1.6), which satisfy the system (2.9).

If $s=0$, $\varphi_1, \dots, \varphi_{m-1}$ are uniquely determined and a quadrature formula of type (2.8) can be written in a unique way.

Suppose $s > 0$. Since the quadrature formula (2.8) can be written in ∞^s different ways, the $m-1$ functions $\varphi_1, \dots, \varphi_{m-1}$ depend altogether on s arbitrary parameters: C_1, \dots, C_s . These constants C_1, \dots, C_s can be uniquely determined such that the quadrature formula (2.8) is "optimal" that is $\int_a^b [\Phi(x)]^2 dx$ has a minimum. Therefore

THEOREM 2.III *Suppose that one of the following two conditions holds true:*

- (i) (2.13) has only the solution $u \equiv 0$;
- (ii) (2.13) has q linearly independent solutions and the compatibility conditions (2.12) are satisfied.

Then there exists a unique quadrature formula of type (2.8) that is optimal in the sense of Sard.

If (2.13) has eigensolutions and conditions (2.12) are not satisfied then quadrature formulae of type (2.8) do not exist.

We know already that if $s=0$ we have only one quadrature formula of type (2.8).

Let now $s > 0$. Because of Theorem 2.II, there exist $\varphi_1, \dots, \varphi_{m-1}$, defined as in (2.2), satisfying system (2.9). (2.9) is a linear system with $n(m-1)$ unknowns $\{c_j^{(i)}\}$ and mp equations and it has s linearly independent solutions (it must be $n(m-1) - s \geq 0$). Then it is possible to assume

$$c_j^{(i)} = \alpha_0^{ij} + \sum_{h=1}^s C_h \alpha_h^{ij}, \quad \alpha_h^{ij} \in \mathbb{R}, \quad i = 1, \dots, m-1; \quad j = 1, \dots, n.$$

The rank of the matrix $\{\alpha_h^{ij}\}$ of order $(m-1)n \times s$ is equal to s (we have $s \leq (m-1)n$).

It follows that the functions $\{\varphi_i\}_{i=1, \dots, m-1}$, which satisfy conditions (2.9), can be written as

$$\varphi_i(x) = \tilde{v}_i(x) + \sum_{h=1}^s C_h w_h^{(i)}(x), \quad i = 1, \dots, m-1 \quad (2.14)$$

where $w_h^{(i)}(x) = \sum_{j=1}^n \alpha_h^{ij} v_j(x)$, $h = 1, \dots, s$; $i = 1, \dots, m - 1$, are solutions of (2.1) and $\{\tilde{v}_i\}$ are solutions of (1.6).

Set $w_h(x) = w_h^{(i)}(x)$, $x \in (x_i, x_{i+1}]$, $i = 1, \dots, m - 1$; $h = 1, \dots, s$.

$\{w_h(x)\}_{h=1, \dots, s}$ is a system of linearly independent functions in $[a, b]$. Otherwise there exist $(d_1, \dots, d_s) \neq (0, \dots, 0)$ such that

$$\sum_{h=1}^s d_h w_h(x) = 0, \quad \forall x \in [a, b].$$

Then

$$\sum_{h=1}^s d_h w_h^{(i)}(x) = 0, \quad \forall x \in (x_i, x_{i+1}), \quad i = 1, \dots, m - 1$$

that is

$$\sum_{j=1}^n \left(\sum_{h=1}^s \alpha_h^{ij} d_h \right) v_j(x) = 0, \quad \forall x \in (x_i, x_{i+1}), \quad i = 1, \dots, m - 1.$$

Since $\{v_h(x)\}_{h=1, \dots, n}$ are linearly independent functions in (x_i, x_{i+1}) , $i = 1, \dots, m - 1$, it must be

$$\sum_{h=1}^s \alpha_h^{ij} d_h = 0, \quad i = 1, \dots, m - 1, \quad j = 1, \dots, n. \quad (2.15)$$

(2.15) is a linear homogeneous system with $n(m - 1)$ equations and s unknowns whose matrix has rank equal to s . Then $d_1 = \dots = d_s = 0$.

Define

$$F(C) = \sum_{i=1}^{m-1} \int_{x_i}^{x_{i+1}} [\varphi_i(x)]^2 dx, \quad (2.16)$$

where $C = (C_1, \dots, C_s)$. We have $F(C) > 0$ because $g(x)$ is not zero on a set of positive measure.

From (2.3) it follows that

$$\|R[u]\| \leq \|E[u]\|_2 \left(\int_{x_0}^{x_1} [\varphi_0(x)]^2 dx + F(C) + \int_{x_m}^{x_{m+1}} [\varphi_m(x)]^2 dx \right)^{1/2}.$$

Set

$$A_{kr} = \sum_{i=1}^{m-1} \int_{x_i}^{x_{i+1}} w_k^{(i)}(x) w_r^{(i)}(x) dx = \int_a^b w_k(x) w_r(x) dx, \quad k, r = 1, \dots, s;$$

$$B_k = \sum_{i=1}^{m-1} \int_{x_i}^{x_{i+1}} w_k^{(i)}(x) \tilde{v}_i(x) dx, \quad k = 1, \dots, s$$

and

$$D = \sum_{i=1}^{m-1} \int_{x_i}^{x_{i+1}} [\tilde{v}_i(x)]^2 dx.$$

Therefore we have

$$F(C) = \sum_{k,r}^{1,s} A_{kr} C_k C_r + 2 \sum_{k=1}^s B_k C_k + D.$$

The function $F(C)$ has a positive minimum in \mathbb{R}^s . Consider the system $\partial F / \partial C_h = 0$, $h = 1, \dots, s$ which corresponds to the following linear system:

$$\sum_{r=1}^s A_{hr} C_r + B_h = 0, \quad h = 1, \dots, s. \quad (2.17)$$

Since the matrix $\{A_{hr}\}_{h,r=1,\dots,s}$ is positive definite then (2.17) has one and only one solution $\tilde{C} = \{\tilde{C}_1, \dots, \tilde{C}_s\}$ which corresponds to the minimum of F :

$$F(\tilde{C}) = \min_{\mathbb{R}^s} F(C).$$

In this case we assume in (2.14): $C_i = \tilde{C}_i$, $i = 1, \dots, s$.

3. EXAMPLES OF OPTIMAL QUADRATURE FORMULAE

In this Section we shall give some examples of quadrature formulae of type (1.4) (see Examples (a)–(d)) and (1.9) (see Examples (e)–(i), (l))

obtained by applying the methods of Section 2. Observe that if $x_1 = a$, from (1.7) and (1.8) it follows that the function φ_0 must not be considered. Analogously if $x_m = b$ it is not necessary to consider the function φ_m .

Example (a) Let us assume in (1.4) $g(x) = 1/\sqrt{x-a}$, $n=2$, $E = d^2/dx^2$, $m=2$, $x_1 = a$, $x_2 = b$. A quadrature formula of type (1.4) can be written in ∞^2 different ways. The "optimal" one is:

$$\int_a^b \frac{u(x)}{\sqrt{x-a}} dx = \frac{2}{35} \sqrt{b-a} [24u(x_1) + 11u(x_2)] \\ + \frac{4}{105} (b-a)^{3/2} [4u'(x_1) - u'(x_2)] + R[u].$$

By applying (2.3) we deduce

$$|R[u]| \leq \|E[u]\|_2 \frac{2}{35} (b-a)^2.$$

Example (b) For the sake of simplicity consider the interval $[a, b] = [0, 1]$. Let us apply the general rule by assuming $g(x) = 1/\sqrt{x}$, $n=2$, $E = d^2/dx^2$, $m=3$ and the nodes: $x_1 = 0$, x_2 an arbitrary point of the interval $(0, 1)$, $x_3 = 1$. Then

$$\int_0^1 \frac{u(x)}{\sqrt{x}} dx = \frac{2}{35} \left[24\sqrt{x_2} u(0) + 8 \frac{3 + 6\sqrt{x_2} + 2x_2}{(1 + \sqrt{x_2})^3} u(x_2) \right. \\ \left. + (1 - \sqrt{x_2}) \frac{11 + 44\sqrt{x_2} + 61x_2 + 24\sqrt{x_2^3}}{(1 + \sqrt{x_2})^3} u(1) \right] \\ + \frac{4}{105} \left[4\sqrt{x_2^3} u'(0) + 4 \frac{1 + 2\sqrt{x_2} - 4x_2 - 2\sqrt{x_2^3}}{(1 + \sqrt{x_2})^2} u'(x_2) \right. \\ \left. - (1 - \sqrt{x_2})^2 \frac{3 + 12\sqrt{x_2} + 16x_2 + 4\sqrt{x_2^3}}{(1 + \sqrt{x_2})^2} u'(1) \right] + R[u].$$

From (2.3)

$$|R[u]| \leq \|E[u]\|_2 \frac{2}{105} \sqrt{\frac{\tau(\sqrt{x_2})}{(1 + \sqrt{x_2})^3}}$$

where

$$\begin{aligned} \tau(\xi) = & 9 + 27\xi - 37\xi^2 - 183\xi^3 + 128\xi^4 + 448\xi^5 \\ & - 448\xi^6 - 128\xi^7 + 192\xi^8 + 64\xi^9. \end{aligned}$$

Example (c) Assume $n=2$, $E = d^2/dx^2 - 3(d/dx) + 2$, $m=2$, $x_1=0$, $x_2=1$, $g(x)=1$ in $[a, b]=[0, 1]$. Then

$$\begin{aligned} \int_0^1 u(x) dx = & \frac{3(e^2 - 1)}{2(e^2 + 4e + 1)} (u(0) + u(1)) + \left(\frac{1}{2} - \frac{3e}{e^2 + 4e + 1} \right) \\ & \times (u'(0) + u'(1)) + R[u]; \quad |R[u]| \leq \|E[u]\|_2 K \end{aligned}$$

where

$$K = \sqrt{\frac{2 + 2e - e^2}{2(1 + 4e + e^2)}} \leq 0.03512.$$

Example (d) Let E , $[a, b]$ and $g(x)$ be the one considered in the Example (c).

Assume $m=3$, $x_1=0$, $x_2=1/2$, $x_3=1$. Then

$$\begin{aligned} \int_0^1 u(x) dx = & \frac{3(e-1)}{2(e+4\sqrt{e}+1)} (u(0) + 2u(1/2) + u(1)) \\ & + \left(\frac{1}{2} - \frac{3\sqrt{e}}{e+4\sqrt{e}+1} \right) (u'(0) - u'(1)) + R[u]; \\ & |R[u]| \leq \|E[u]\|_2 K. \end{aligned}$$

where

$$K = \sqrt{\frac{7 + 4\sqrt{e} - 5e}{4(1 + 4\sqrt{e} + e)}} \leq 0.009184.$$

Assume $n \geq 2$, $m \geq 2$ and

$$E = \frac{d^n}{dx^n}. \quad (3.1)$$

We investigate if there can exist quadrature formulae of the following type:

$$\int_a^b u(x)g(x) dx = \sum_{i=1}^m A_{1i}u(x_i) + R[u], \quad (E[u] = 0 \Rightarrow R[u] = 0); \quad (3.2)$$

this is equivalent to consider (2.8) with $p = n - 1$.

In the case we are considering, the homogeneous boundary value problem (2.13) becomes

$$\begin{cases} \frac{d^n}{dx^n} u(x) = 0, \\ u(x_i) = 0, \quad i = 1, \dots, m. \end{cases} \quad (3.3)$$

If $m \geq n$, problem (3.3) has no non-trivial solutions that is condition (1.10) is satisfied. It follows that it is possible to write a quadrature formula of type (3.2) in ∞^{m-n} different ways.

If $n \geq 3$, consider (2.8) with $p = n - 2$. We investigate if it is possible to write a quadrature formula of type

$$\begin{aligned} & \int_a^b u(x)g(x) dx \\ &= \sum_{i=1}^m [A_{1i}u(x_i) + A_{2i}u'(x_i)] + R[u] \quad (E[u] = 0 \Rightarrow R[u] = 0). \end{aligned} \quad (3.4)$$

If $n \leq 2m$ the homogeneous boundary value problem

$$\begin{cases} \frac{d^n}{dx^n} u(x) = 0, \\ u(x_i) = u'(x_i) = 0, \quad i = 1, \dots, m \end{cases}$$

has no non-trivial solutions. Therefore we may get a quadrature formula of the type (3.4) in ∞^{2m-n} different ways.

In the following we give several examples of quadrature formulae obtained by applying the method given in Section 2 to these particular

cases, for different values of n and m and for different choices of the weight function $g(x)$. In the Examples (h), (i) and (l) we consider more general cases. The optimal quadrature formula can be written in one and only one way. Of course it is possible to find a lot of other formulae.

Example (e) Assume, in (3.1), $n=2$ and let $g(x) \equiv 1$ in $[a, b]$. Consider the following equidistant nodes x_i of the interval $[a, b]$:

$$x_i = a + (i-1)h, \quad i = 1, \dots, m, \quad h = \frac{b-a}{(m-1)}. \quad (3.5)$$

These particular formulae (with $m \leq 19$) were already obtained by Sard in [10].

By assuming, in (3.5), $m=2$ we may get a quadrature formula of the type (3.2) in only one way: we obtain the classical *trapezoidal rule*.

If $m=3$ the optimal quadrature formula of the type (3.2) is

$$\int_a^b u(x) dx = \frac{b-a}{16} \left[3u(a) + 10u\left(\frac{a+b}{2}\right) + 3u(b) \right] + R[u].$$

From (2.3) and (2.4) we get

$$|R[u]| \leq \|E[u]\|_2 \frac{(b-a)^{5/2}}{32\sqrt{5}} \leq \|E[u]\|_\infty \frac{(b-a)^3}{32\sqrt{5}}. \quad (3.6)$$

Now assume $m=4$ in (3.5). By applying the general rule we obtain the following optimal quadrature formula:

$$\int_a^b u(x) dx = \frac{b-a}{30} \left[4u(a) + 11u\left(\frac{2a+b}{3}\right) + 11u\left(\frac{a+2b}{3}\right) + 4u(b) \right] + R[u].$$

(2.3) and (2.4) give the following estimates for the remainder:

$$|R[u]| \leq \|E[u]\|_2 \frac{(b-a)^{5/2}}{54\sqrt{10}} \leq \|E[u]\|_\infty \frac{(b-a)^3}{54\sqrt{10}}. \quad (3.7)$$

Assume, in (3.5), $m = 5$. We may get the quadrature formula (3.2) in ∞^3 different ways. The optimal one is

$$\int_a^b u(x) dx = \frac{b-a}{112} \left[11u(a) + 32u\left(\frac{3a+b}{4}\right) + 26u\left(\frac{a+b}{2}\right) + 32u\left(\frac{a+3b}{4}\right) + 11u(b) \right] + R[u]$$

with

$$|R[u]| \leq \|E[u]\|_2 \frac{(b-a)^{5/2}}{32\sqrt{105}} \leq \|E[u]\|_\infty \frac{(b-a)^3}{32\sqrt{105}}. \quad (3.8)$$

Finally assume, in (3.5), $m = 6$. We have the optimal formula:

$$\int_a^b u(x) dx = \frac{b-a}{190} \left[15u(a) + 43u\left(\frac{4a+b}{5}\right) + 37u\left(\frac{3a+2b}{5}\right) + 37u\left(\frac{2a+3b}{5}\right) + 43u\left(\frac{a+4b}{5}\right) + 15u(b) \right] + R[u]$$

with

$$|R[u]| \leq \|E[u]\|_2 \frac{(b-a)^{5/2}}{50\sqrt{114}} \leq \|E[u]\|_\infty \frac{(b-a)^3}{50\sqrt{114}}. \quad (3.9)$$

Now we compare all the formulae obtained up to now with the classical *composite trapezoidal rule* [3, pp. 40–42]:

$$\int_a^b u(x) dx = \frac{h}{2} \left[u(x_1) + 2 \sum_{i=2}^{m-1} u(x_i) + u(x_m) \right] + R[u];$$

$$|R[u]| \leq \|E[u]\|_\infty \frac{(b-a)^3}{12(m-1)^2}. \quad (3.10)$$

(3.6), (3.7), (3.8) and (3.9) give better estimates for $R[u]$ than (3.10) for $m = 3, 4, 5, 6$, respectively. In fact, estimates (3.6), (3.7), (3.8) and (3.9) give:

$$\begin{aligned} m = 3: & \quad |R[u]| \leq \|E[u]\|_\infty (b-a)^3 \cdot 0.01398; \\ m = 4: & \quad |R[u]| \leq \|E[u]\|_\infty (b-a)^3 \cdot 0.00586; \\ m = 5: & \quad |R[u]| \leq \|E[u]\|_\infty (b-a)^3 \cdot 0.00305; \\ m = 6: & \quad |R[u]| \leq \|E[u]\|_\infty (b-a)^3 \cdot 0.00188, \end{aligned}$$

while (3.10) gives, respectively,

$$m = 3: \quad |R[u]| \leq \|E[u]\|_{\infty} (b-a)^3 \cdot 0.02084;$$

$$m = 4: \quad |R[u]| \leq \|E[u]\|_{\infty} (b-a)^3 \cdot 0.00926;$$

$$m = 5: \quad |R[u]| \leq \|E[u]\|_{\infty} (b-a)^3 \cdot 0.00521;$$

$$m = 6: \quad |R[u]| \leq \|E[u]\|_{\infty} (b-a)^3 \cdot 0.00334.$$

Example (f) Assume, in (3.1), (3.2), $n=4$, $g(x) \equiv 1$ in $[a, b]$ and the nodes (3.5).

Consider the quadrature formula (3.4). If $m > 2$ then we may get a quadrature formula in ∞^{2m-4} different ways. If $m=3$, among the ∞^2 different quadrature formulae the “optimal” one is the following:

$$\int_a^b u(x) \, dx = \frac{b-a}{624} \left[149u(a) + 326u\left(\frac{a+b}{2}\right) + 149u(b) \right] \\ + \frac{15}{832} (b-a)^2 [u'(a) - u'(b)] + R[u]$$

with

$$|R[u]| \leq \|E[u]\|_2 \sqrt{\frac{11}{91} \frac{(b-a)^{9/2}}{4608}} \leq \|E[u]\|_{\infty} \sqrt{\frac{11}{91} \frac{(b-a)^5}{4608}} \quad (3.11)$$

Compare the last formula with the *trapezoidal rule with “end correction”* (see [3, p. 105; 21, p. 66]):

$$\int_a^b u(x) \, dx = \frac{b-a}{4} \left[u(a) + 2u\left(\frac{a+b}{2}\right) + u(b) \right] \\ + \frac{(b-a)^2}{48} [u'(a) - u'(b)] + R[u]; \\ |R[u]| \leq \|E[u]\|_{\infty} \frac{(b-a)^5}{11 \, 520}. \quad (3.12)$$

(3.11) provides better estimate for $R[u]$ than (3.12) because (3.11) gives

$$|R[u]| \leq \|E[u]\|_{\infty} (b-a)^5 \cdot 7.5451 \times 10^{-4}$$

while (3.12) gives

$$|R[u]| \leq \|E[u]\|_{\infty} (b-a)^5 8.6856 \times 10^{-4}.$$

By assuming in (2.8) $m=3$ ($m=4$) and $p=3$ the functions $\{\varphi_i\}_{i=1,2,3}$ such that (2.9) holds are uniquely determined and we obtain the classical *Cavalieri–Simpson’s rule* ($3/8$ rule).

Now assume in (3.2) $m=5$. It is possible to write this quadrature formula in ∞^1 different ways. The optimal one is

$$\int_a^b u(x) dx = \frac{b-a}{2416} \left[\frac{783}{4} u(x_1) + \frac{2483}{3} u(x_2) + \frac{2215}{6} u(x_3) + \frac{2483}{3} u(x_4) + \frac{783}{4} u(x_5) \right] + R[u].$$

By applying (2.3)

$$|R[u]| \leq \|E[u]\|_2 \frac{(b-a)^{9/2}}{24\,576} \sqrt{\frac{6557}{15\,855}}.$$

Assume, in (3.2), $m=6$. By applying the general method described in Section 2 we obtain the following optimal quadrature formula:

$$\int_a^b u(x) dx = \frac{b-a}{54\,105} \left[3674(u(x_1) + u(x_6)) + \frac{110\,209}{8}(u(x_2) + u(x_5)) + \frac{76\,819}{8}(u(x_3) + u(x_4)) \right] + R[u].$$

From (2.3)

$$\begin{aligned} |R[u]| &\leq \|E[u]\|_2 \frac{(b-a)^{9/2}}{50\,000} \sqrt{\frac{61\,633}{151\,494}} \\ &\leq \|E[u]\|_{\infty} \frac{(b-a)^5}{50\,000} \sqrt{\frac{61\,633}{151\,494}}. \end{aligned} \quad (3.13)$$

If we apply the $3/8$ rule to the interval $[x_1, x_4]$ and the *Cavalieri–Simpson’s rule* to $[x_4, x_6]$, we obtain the following estimate for the remainder:

$$|R[u]| \leq \|E[u]\|_{\infty} \frac{(b-a)^5}{64\,285} \leq \|E[u]\|_{\infty} (b-a)^5 1.5556 \times 10^{-4}$$

that is worse than (3.13) because (3.13) gives

$$|R[u]| \leq \|E[u]\|_\infty (b-a)^5 1.2757 \times 10^{-4}.$$

For $m=7$ the optimal quadrature formula is

$$\begin{aligned} \int_a^b u(x) dx &= \frac{b-a}{1\,645\,007} \left[\frac{360\,937}{4} (u(x_1) + u(x_7)) + \frac{734\,991}{2} (u(x_2) + u(x_6)) \right. \\ &\quad \left. + \frac{741\,681}{4} (u(x_3) + u(x_5)) + 358\,707 u(x_4) \right] + R[u]. \end{aligned}$$

From (2.3) and (2.4)

$$\begin{aligned} |R[u]| &\leq \|E[u]\|_2 \frac{(b-a)^{9/2}}{36\,288} \sqrt{\frac{210\,047}{7\,050\,030}} \\ &\leq \|E[u]\|_\infty \frac{(b-a)^5}{36\,288} \sqrt{\frac{210\,047}{7\,050\,030}}. \end{aligned} \quad (3.14)$$

Consider the *compound 3/8 rule*:

$$\begin{aligned} \int_a^b u(x) dx &= \frac{b-a}{8} [u(x_1) + 3u(x_2) + 3u(x_3) + 2u(x_4) \\ &\quad + 3u(x_5) + 3u(x_6) + u(x_7)] + R[u]; \\ |R[u]| &\leq \|E[u]\|_\infty \frac{(b-a)^5}{103\,680} \leq \|E[u]\|_\infty (b-a)^5 9.6451 \times 10^{-6}. \end{aligned} \quad (3.15)$$

(3.14) gives better estimates than (3.15) because (3.14) gives

$$|R[u]| \leq \|E[u]\|_\infty (b-a)^5 4.7567 \times 10^{-6}.$$

Assume $m=9$ and, for brevity, $[a, b] = [0, 1]$. The quadrature formula (3.2) depends on five arbitrary parameters. The “optimal” one is

$$\begin{aligned} \int_0^1 u(x) dx &= 0.041393[u(x_1) + u(x_9)] + 0.165878[u(x_2) + u(x_8)] \\ &\quad + 0.0898962[u(x_3) + u(x_7)] + 0.151826[u(x_4) + u(x_6)] \\ &\quad + 0.102004u(x_5) + R[u]; \\ |R[u]| &\leq \|E[u]\|_2 1.35792 \times 10^{-6}. \end{aligned}$$

If $m = 11$, among the ∞^7 quadrature formulae of type (3.2), the “optimal” one is:

$$\begin{aligned} \int_0^1 u(x) \, dx &= 0.033182[u(x_1) + u(x_{11})] + 0.132281[u(x_2) + u(x_{10})] \\ &+ 0.073287[u(x_3) + u(x_9)] + 0.118285[u(x_4) + u(x_8)] \\ &+ 0.087894[u(x_5) + u(x_7)] + 0.110141u(x_6) + R[u]; \\ |R[u]| &\leq \|E[u]\|_2 5.04696 \times 10^{-7} \leq \|E[u]\|_\infty 5.04696 \times 10^{-7}. \end{aligned} \quad (3.16)$$

Compare the last quadrature formula with the composite *Cavalieri–Simpson’s rule*. In the classical formula we have the following estimate for $R[u]$:

$$|R[u]| \leq \frac{\|E[u]\|_\infty}{180(m-1)^4}. \quad (3.17)$$

For $m = 11$, (3.17) gives worst estimate $R[u]$ than (3.16) because (3.17) gives

$$|R[u]| \leq \|E[u]\|_\infty 5.55556 \times 10^{-7}.$$

Example (g) Let us assume in (3.1) $n = 6$ and, for the sake of simplicity, $[a, b] = [0, 1]$. Let $g(x) = 1$ in $[0, 1]$ and assume the nodes (3.5). For $m = 5$ ($m = 6$), (3.2) is the classical *Boole’s rule (Newton–Cotes 6-point rule)* [3, p. 63]. By assuming $m = 7$ in (3.5), formula (3.2) can be written in ∞^1 different ways. The “optimal one” is the following:

$$\begin{aligned} \int_0^1 u(x) \, dx &= \frac{522\,593}{10\,482\,832}[u(x_1) + u(x_7)] + \frac{6\,574\,999}{26\,207\,080}[u(x_2) + u(x_6)] \\ &+ \frac{2\,504\,563}{52\,414\,160}[u(x_3) + u(x_5)] + \frac{3\,969\,777}{13\,103\,540}u(x_4) + R[u]. \end{aligned}$$

From (2.3)

$$|R[u]| \leq \|E[u]\|_2 4.7703 \times 10^{-8}.$$

If $m = 8$, the quadrature formula (3.2) depends on two free parameters. The “optimal one” is

$$\begin{aligned} \int_0^1 u(x) dx &= 0.0441851[u(x_1) + u(x_8)] + 0.20338[u(x_2) + u(x_7)] \\ &\quad + 0.0830825[u(x_3) + u(x_6)] \\ &\quad + 0.169352[u(x_4) + u(x_5)] + R[u]; \\ |R[u]| &\leq \|E[u]\|_2 2.6128 \times 10^{-8}. \end{aligned}$$

By assuming, in (3.2), $m = 9$ we may get a quadrature formula in ∞^3 different ways. The “optimal” one is

$$\begin{aligned} \int_0^1 u(x) dx &= 0.0374541[u(x_1) + u(x_9)] + 0.187974[u(x_2) + u(x_8)] \\ &\quad + 0.0341871[u(x_3) + u(x_7)] + 0.23889[u(x_4) + u(x_6)] \\ &\quad + 0.0299175u(x_5) + R[u]; \\ |R[u]| &\leq \|E[u]\|_2 7.8991 \times 10^{-9} \leq \|E[u]\|_\infty 7.8991 \times 10^{-9}. \quad (3.18) \end{aligned}$$

Compare (3.18) with the estimate for $R[u]$ in the *composite Boole’s rule* with nine nodes:

$$|R[u]| \leq \|E[u]\|_\infty 8.073 \times 10^{-9}. \quad (3.19)$$

(3.18) is better than (3.19).

Example (h) By assuming $n = 2$, $m = 3$ and $[a, b] = [0, 2\pi]$, consider the operator $E = d^2/dx^2 + 1$, the nodes $x_1 = 0$, $x_2 = \pi$, $x_3 = 2\pi$ and the weight function $g(x) \equiv 1$ in $[0, 2\pi]$. We investigate if there exists a quadrature formula of type (2.8) with $p = 1$. The homogeneous boundary value problem (2.13) has the solution $v(x) = \sin(x)$. Then $q = 1$ and the compatibility condition (2.12) is satisfied. Then it is possible to write a quadrature formula (2.8) in ∞^2 different ways.

By assuming $\varphi_1(x) = -\cos(x) - (4/\pi)\sin(x) + 1$; $\varphi_2(x) = -\cos(x) + (4/\pi)\sin(x) + 1$ we obtain the “optimal” one:

$$\begin{aligned} \int_0^{2\pi} u(x) dx &= \left(1 - \frac{4}{\pi}\right)u(0) - \frac{8}{\pi}u(\pi) - \left(1 + \frac{4}{\pi}\right)u(2\pi) + R[u], \\ |R[u]| &\leq \|E[u]\|_2 \sqrt{\left(3\pi - \frac{16}{\pi}\right)}. \end{aligned}$$

Example (i) Let be $n=4$, $m=3$, $[a, b]=[0, 2\pi]$, $E=(d^2/dx^2+1)(d^2/dx^2+9)$, the nodes $x_1=0$, $x_2=\pi$, $x_3=2\pi$ and the weight function $g(x)\equiv 1$ in $[0, 2\pi]$. Consider the quadrature formula (2.8) with $p=3$. The homogeneous boundary value problem (2.13) has three linearly independent solutions ($q=3$) and the compatibility conditions (2.12) are satisfied. A quadrature formula (2.8) with $p=3$ can be written in ∞^2 different ways. The "optimal" one can be written in one and only in one way, by assuming

$$\begin{aligned}\varphi_1(x) &= \frac{1}{9} - \frac{\cos(x)}{8} + \frac{\cos(3x)}{72} - \frac{16}{45\pi}\sin(x) + \frac{16}{135\pi}\sin(3x); \\ \varphi_2(x) &= \frac{1}{9} - \frac{\cos(x)}{8} + \frac{\cos(3x)}{72} + \frac{16}{45\pi}\sin(x) - \frac{16}{135\pi}\sin(3x).\end{aligned}$$

Then

$$\begin{aligned}\int_0^{2\pi} u(x) dx &= \frac{128}{45\pi} [u(0) + 2u(\pi) + u(2\pi)] + R[u]; \\ |R[u]| &\leq \|E[u]\|_2 K\end{aligned}$$

where

$$K = \sqrt{\frac{35\pi}{864} - \frac{512}{3645\pi}} \leq 0.28732.$$

Let us note that in Examples (h) and (i) the hypothesis (1.10) is not satisfied.

Example (l) Assume $[a, b]=[0, 1]$, $n=2$, $E=d^2/dx^2-3(d/dx)+2$, $g(x)=1$, $m=3$, $x_1=0$, $x_2=\log(2e/3)$, $x_3=1$ and $p=1$. A quadrature formula of type (2.8) can be written in ∞^1 different ways. The optimal one can be written in a unique way, that is:

$$\begin{aligned}\int_0^1 u(x) dx &= \frac{12e^2 - 35e + 24}{4(e+4)(2e-3)} u(0) \\ &+ \frac{9(4e^3 - 10e^2 + 7e - 1)}{8e(e+4)(2e-3)} u(\log(2e/3)) \\ &+ \frac{-2e^2 + 12e - 9}{4e(e+4)} u(1) + R[u]; \quad |R[u]| \leq \|E[u]\|_2 K\end{aligned}$$

where

$$K = \sqrt{\frac{-63 + 483e + 952e^2 - 412e^3}{768e^2(e + 4)}} \leq 0.01543.$$

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