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Abstract

The n-point Gauss quadrature rule states that

$$\int_{-1}^{1} f(x)\omega(x)dx = \sum_{j=1}^{n} w_i f(z_i) + R_n(f)$$

where $z_1, z_2, \ldots, z_n$ are n zeros of the nth degree orthogonal polynomial of degree n over $[-1,1]$ with respect to a positive weight function $\omega(x)$. Moreover,

$$\lim_{n \to \infty} R_n(f) = 0, \quad \forall f \in C[-1,1]$$

and

$$R_n(f) = 0, \quad \forall f \in \pi_{2n-1}.$$

In this report an extension of Gauss rule is presented which has the end points of the interval $[-1,1]$, i.e., $x = -1$ and $x = 1$ as preassigned nodes of preassigned order n_1 and n_2 respectively. We construct interpolating orthogonal polynomials which makes the suggested rule capable of utilizing the maximum information related to the derivatives of f at the endpoints of the $[-1,1]$. Some theoretical and computational aspects of the rule are also narrated.

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1. Introduction

In applied problems, most of the mathematical models involve definite integrals, which at a glance appear to be very simple but cannot be evaluated analytically. To cope with this type of situations, we require numerical techniques to approximate a given definite integral. The development of these techniques usually depends on the nature of complexity of the integrand and also on the acceptable error of approximation. One of the techniques widely used for the numerical evaluation of definite integrals is the "Gaussian Quadrature Rule". Our aim in this report is to present a review of this technique. We also propose an extension of this rule that deals with interpolating orthogonal functions.

2. Gaussian Quadrature Rule

We recall that an n-point Newton-Cotes rule is an n-point interpolatory quadrature formula where equidistant nodes $x_{i,n}, i = 1,\ldots,n,$ in the interval[3] $[-1,1]$ are fixed [H1, R1]. The degree of exactness for this rule, which is at most $n,$ is related to n parameters, the weights $w_{i,n}, i = 1,\ldots,n$ of the formula [H1, R1]. These weights may be determined by solving the system of linear equations [K1]:

$$\int_{-1}^{1} x^k \omega(x)dx = \sum_{i=1}^{n} w_{i,n}(x_{i,n})^k, \ \ k = 1,\ldots,n,$$

where ω is a nonnegative weight function defined on $[-1,1]$. If both the nodes $z_{i,n}, i = 1,\ldots,n,$ and the weights $w_{i,n}, i = 1,\ldots,n$ are kept free in an n-point interpolatory quadrature formula:

$$\int_{-1}^{1} f(x)\omega(x)dx \approx \sum_{i=1}^{n} w_{i,n} f(z_{i,n}), \tag{2.1}$$

one may expect to have an increase in the degree of exactness of the resulting quadrature rule up to $2n - 1$. This interesting point was initially noticed by Carl Gauss (1777-1855). Considering $2n$ parameters, Gauss [G1] found that the necessary condition for

$$\int_{-1}^{1} p(x)\omega(x)dx = \sum_{i=1}^{n} w_{i,n} p(z_{i,n}), \quad \forall p \in \pi_{2n-1}, \tag{2.2}$$

to hold is that

$$\int_{-1}^{1} \prod_{i=1}^{n} (x - z_{i,n}) q(x)\omega(x)dx = 0, \ \forall q \in \pi_{n-1} \tag{2.3}$$

This condition is known as orthogonality condition[4] and characterizes the Legendre polynomials [C1] if $\omega(x) = 1$ on $[-1,1]$. The resulting formula, in this case, is known as Gauss-Legendre quadrature rule.

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[3] For the sake of simplicity, we shall consider the interval of integration $[-1,1]$ in this report.

[4] Two functions f and g are orthogonal w.r.t. the weight function $\omega(x)$ over $[-1,1]$ if $\int_{-1}^{1} f(x)g(x)\omega(x)dx = 0$.

The Gauss quadraure rule is regarded as a revolutionary step towards the numerical evaluation of definite integrals. Many researchers till now are working on its modifications, extensions, and error analysis. A large amount of material is available on algorithms that are designed for its implementation.

3. Computation of Gaussian Nodes and Weights

As noticed above, the nodes $z_{i,n}, i = 1,\ldots,n,$ of the Gauss quadrature formula arise from the polynomial

$$\psi_n(x) = \prod_{i=1}^{n} (x - z_{i,n}) \tag{3.1}$$

Because of the orthogonality condition, the polynomial $\psi_n(x)$ is known as orthogonal polynomial w.r.t. the weight function $\omega(x)$ over the interval $[-1,1]$. It can be determined by the 3-term recurrence relation which is usually referred as to Stieltjes procedure [G2]. The relation is explained in the following theorem and may be found in the standard texts on approximation theory and numerical analysis, e.g., [P1]:

Theorem 3.1: The polynomials $\psi_n(x)$, $n = 1,2,3,\ldots$ satisfy the 3-term relation

$$\left.\begin{array}{c} \psi_{n+1}(x) = (x - \alpha_n)\psi_n(x) - \beta_n \psi_{n-1}(x), \quad n = 0,1,2,\ldots \\ \psi_{-1}(x) \equiv 0, \psi_0(x) \equiv 1 \end{array}\right\} \tag{3.2}$$

and

$$\left.\begin{array}{l} \alpha_n = \dfrac{\langle x\psi_n, \psi_n \rangle}{\langle \psi_n, \psi_n \rangle}, n = 0,1,2,\ldots \\[2ex] \beta_n = \dfrac{\langle \psi_n, \psi_n \rangle}{\langle \psi_{n-1}, \psi_{n-1} \rangle}, n = 1,2,\ldots \end{array}\right\} \tag{3.3}$$

where the notation $\langle .,. \rangle$ stands for the inner product and is defined by

$$\langle f, g \rangle = \int_{-1}^{1} f(x)g(x)\omega(x)dx \text{ and } \beta_0 := \langle 1,1 \rangle = \int_{-1}^{1} \omega(x)dx .$$

Remark (3.1): The relations (3.2) are due to Christoffel [C2] who had different expressions for α_n, β_n. These expressions are also referred to as the Christoffel numbers in the literature. The formulas for α_n, β_n given in (3.3) were presented by Stieltjes [S2] and Darbous [D1] independently. Stieltjes, in fact, pointed out how (3.2) and (3.3) can be used to successively generate the orthogonal polynomials $\psi_1, \psi_2, \psi_3,\ldots\ldots$ See [G2].

Remark (3.2): The orthogonal polynomials $\psi_n(x), n = 1,2,\ldots$, have some interesting properties which are as follows [C1]:

1. The numbers $\beta_n, n = 1, 2, \dots$, are positive and $\|\psi_n\|^2 = \beta_n \beta_{n-1} \dots \beta_1 \beta_0$.

2. All the zeros of the orthogonal polynomials are simple, real and lie in the interior of $[-1,1]$.

3. The n+1 zeros of $\psi_{n+1}(x)$ alternate with the n zeros of $\psi_n(x)$, i.e., if $\{z_{i,n+1}\}_{i=1}^{n+1}$ and $\{z_{i,n}\}_{i=1}^{n}$ are respectively the set of zeros of ψ_{n+1} and ψ_n, both written in descending order then

$$z_{1,n+1} < z_{1,n} < z_{2,n+1} < z_{2,n} < z_{3,n+1} \dots < z_{n,n} < z_{n+1,n+1} .$$

4. Error Term for Gauss Quadrature Formula

Counting each Gaussian node $w_{i,n}, i = 1, 2, \dots, n$, as a double node, Andrei Markoff (1856-1922) [M1], [G3, p. 165] noted that the Gaussian quadrature formula could be obtained by $H_{2n-1}(., f)$, the Hermite interpolant polynomial to *f* of degree 2*n* – 1 defined by $H_{2n-1}(z_{i,n}, f) = f(z_{i,n})$ and $H'_{2n-1}(z_{i,n}, f) = f'(z_{i,n}), i = 1, 2, \dots, n$. Since $H_{2n-1}(., f)$ is a polynomial of degree 2*n* – 1, using the degree of exactness of the Gauss rule we obtain

$$I(H_{2n-1}(., f)) = \sum_{i=1}^{n} w_{i,n} f(z_{i,n}) \approx \int_{-1}^{1} f(x)\omega(x)dx .$$

As noted above, an exclusive computation of weights $w_{i,n}$ is avoided by the use of the Hermite interpolation polynomial. This polynomial also helps in the determination of error $R_n(f)$ due to Gauss rule:

Theorem 5.1 [H2, S1]**:** If $f \in C^{2n}[-1,1]$, then for each $x \in [-1,1]$, there exists a point $\xi_x \in (-1,1)$ such that

$$f(x) - H_{2n-1}(x, f) = \frac{f^{2n}(\xi_x)}{(2n)!} (\psi_n(x))^2 .$$

Remark 5.1: The above equation together with the mean value theorem of calculus leads to the relation

$$R_n(f) = I(f - H_{2n-1}(., f)) = \frac{f^{2n}(\xi)}{(2n)!} \|\psi_n\|_2^2$$

for some $\xi \in (-1,1)$ where $\|\psi_n\|_2^2 = \int_{-1}^{1} (\psi_n(x))^2 \omega(x)dx$.

5. An Extension to *s+n*-Point Formula

It may be noted that the Lobatto, Radau, Kronrod rules [E1, H1, K1, L1, R1, G…]may be regarded as *n*+2-point, *n*+1-point and 2*n*+1-point rules respectively

with the degree of exactness as $2n - 1$, $2n$, and $3n+1$. This section deals with a different kind of extension of the Gauss Quadrature Rule. Here, we intend to consider the end points of the interval $[a,b]$ as preassigned nodes of higher multiplicity for the modified Quadrature Rule. We briefly summarize the structure of the respective orthogonal polynomials, their properties and finally the corresponding Quadrature Rule.

A. *Structure of Orthogonal Polynomials*: For fixed nonnegative integers n_1 and n_2, we set

$$(i)\, s = n_1 + n_2 \qquad\qquad (ii)\, W_s(x) = (x-a)^{n_1}(x-b)^{n_2} \qquad\qquad (5.1)$$

and generate the polynomials $\psi_{k,s}$, $k = 0,1,2,\ldots$, with respect to a given weight function $\omega(x)$ by using the standard $3-$Term Recurrence Relation :

$$\psi_{k+1,s}(x) = (x-\alpha_k)\psi_{k,s}(x) - (x-\beta_k)\psi_{k-1,s}(x)$$

where

$$\psi_{0,s}(x) = W_s(x),$$
$$\psi_{1,s}(x) = (x-\alpha_1)W_s(x)$$

and α_k and β_k are Gauss Cristoffel Numbers , i.e.,

$$\alpha_n = \left.\left\langle x\psi_{n,s},\psi_{n,s}\right\rangle \middle/ \left\langle \psi_{n,s},\psi_{n,s}\right\rangle\right., n = 0,1,2,\ldots;$$

$$\beta_n = \left.\left\langle \psi_{n,s},\psi_{n,s}\right\rangle \middle/ \left\langle \psi_{n-1,s},\psi_{n-1,s}\right\rangle\right., n = 1,2,\ldots$$

B. *Some Properties of Orthogonal Polynomials* $\psi_{k,s}$.

    a) $\psi_{n,s}(x)$ has $n_1 + n_2 +n$ zeros, namely,

        i. a is a Zero of Order n_1

        ii. b is a Zero of Order n_2

        iii. n Distinct Real Zeros in the open interval (a,b): $z_1, z_2,\ldots, z_n$

    b) If we set $\pi^*_{n-1,s} = \{W_s(.)p(.): p \in \pi_{n-1}\}$ then $\pi^*_{n-1,s}$ is a subspace of π_{n-1+s}.

    Moreover, $\psi_{n,s} \in \pi^*_{n,s}$ and $\psi_{n,s} \perp \pi^*_{n-1,s}$.

C. *The Integrand f and its Hermite Interpolant.*
In order to have a simpler expression for our proposed quadrature rule, we modify an s times differentiable integrand $f:[a,b]\to R$ to

$$f_H(x) = f(x) - H_{s-1}(x,f),$$

where $H_{s-1}(x, f)$ denotes the polynomial of degree s $-$ 1, which interpolates f at the s zeros of $W_s(x)$ in the sense of Hermite (cf (5.1)), i.e.,

$$f_H^{(j)}(a) = 0,\ \ j = 0,1,\ldots,n_1 - 1\ \&\ f_H^{(j)}(b) = 0,\ \ j = 0,1,\ldots,n_2 - 1.$$

D. *Structure of Interpolation Polynomial to f_H at the Zeros of $\psi_{n,s}$.*

In order to describe an interpolatory quadrature rule for the functions of the form f_H, we concentrate to the structure of the interpolation polynomial of degree $s + n$, which interpolates f at the $s + n$ zeros of $\psi_{n,s}$ in the sense of Hermite. If we denote this polynomial by $\Im_{n+s-1}(x, f_H)$, then it may be described as follows:

$$\Im_{n+s-1}(x, f_H) = \sum_{j=1}^{n_1-1} f_H^{(j)}(a) h_{j,a}(x) + \sum_{k=1}^{n_2-1} f_H^{(j)}(b) h_{k,b}(x) + \sum_{i=1}^{n} f_H(z_i) h_i(x)$$

where

a) $z_i, i = 1, 2, \ldots, n$ are the n simple zeros of $\psi_{n,s}$,

b) h_i are the Fundamental Polynomials of $\Im_{n+s-1}(x, f_H)$ corresponding to each simple node $z_i, i = 1, 2, \ldots, n$.

c) $h_{j,a}$ are the Fndamental Polynomials of $\Im_{n+s-1}(x, f_H)$ corresponding to the node "a of mutiplicity n_1".

d) $h_{k,b}$ are the Fndamental Polynomials of $\Im_{n+s-1}(x, f_H)$ corresponding to the node "b of mutiplicity n_2".

In addition,

$$h_i(x) = \frac{W_s(x)}{W_s(z_i)} l_{i,n}(x) \quad \text{with} \quad l_{i,n}(x) = \prod_{\substack{k=1 \\ k \neq i}}^{n} \frac{x - z_k}{z_i - z_k}.$$

Since

$$\Im_{n+s-1}^{(j)}(a, f_H) = f_H^{(j)}(a) = 0, \quad j = 0, 1, \ldots, n_1 - 1,$$

$$\Im_{n+s-1}^{(j)}(b, f_H) = f_H^{(j)}(b) = 0, \quad j = 0, 1, \ldots, n_2 - 1,$$

$$\Im_{n+s-1}(z_i, f_H) = f_H(z_i), \quad i = 1, \ldots, n,$$

we deduce from the above explanation that

$$\Im_{n+s-1}(x, f_H) = \sum_{i=1}^{n} f_H(z_i) \frac{W_s(x)}{W_s(z_i)} l_{i,n}(x).$$

E. *Main Result*

Keeping in view all the notations described above, we have the following Quadrature Rule:

Theorem (Main Result): Suppose that $f \in C^m[a,b]$, $m = \max(n_1, n_2)$ and let

$$\omega_{i,n} = \int_a^b w(x) \frac{W_s(x)}{W_s(z_i)} l_{i,n}(x) dx, \quad i = 1, 2, \ldots, n.$$

Then the quadrature rule

$$\int_a^b w(x) f_H(x) dx \approx \sum_{i=1}^{n} \omega_{i,n} f_H(z_i) \tag{5.2}$$

has the following convergence property:

$$\sum_{i=1}^{n} \omega_{i,n} f_H(z_i) \xrightarrow{L_2} \int_a^b w(x) f(x) dx + I_{H,w} \text{ as } n \to \infty,$$

where the wighted integral

$$I_{H,w} = \int_a^b w(x) H_{s-1}(x, f) dx$$

with polynomial integrand can be directly evaluated by using the quadrature formula.

E. *Some Remarks*

i. The Quadrature rule (cf (5.2)) is an n-point interpolatory formula having n weights $\omega_{i,n}, i = 1, 2, \ldots, n$.

ii. The degree of exactness for this rule is $2n - 1$.

iii. When $s = 0$, the polynomial interpolation at the end points will not be involved in the structure of the Quadrature Rule stated above. In this case, $W_s(x) \equiv 1$ and the resultant rule will be the Ordinary Gauss Quadrature formula.

6. Computational Aspects

In this section we present the numerical algorithm for the method proposed in the previous section.

A. *Numerical Algorithm*

- Input
  - f function to be integrated over $[a, b]$
  - $[a, b]$ interval
  - n_1 where the desired derivatives of f at a will be of order $0, 1, \ldots, n_1 - 1$
  - n_2 where the desired derivative of f at b will be of order $0, 1, \ldots, n_2 - 1$
  - n number of quadrature points beside the end points a, b
- generate $W_s(x) = (x-a)^{n_1}(x-b)^{n_2}$, $(s = n_1 + n_2)$
- generate the orthogonal polynomials $\psi_{k,s}$ $k = 0, 1, \ldots, n$
- compute $z = roots(\psi_{k,s}/Ws)$
- generate H_{s-1}
- set $f_H = f - H_{s-1}$
- generate $l_{i,n}(x) = \prod_{k=1, k \neq i}^{n} \frac{(x-z_k)}{(z_i - z_k)}$
- generate $h_i(x) = \frac{W_s(x)}{W_s(z_i)} l_{i,n}(x)$
- compute $\omega_{i,n} = \int_a^b w(x) h_i(x) dx$
- compute $T_1 = \sum_{i=1}^{n} \omega_{i,n} f_H(z_i)$
- compute $T_2 = \int_a^b w(x) H_{s-1}(x, f) dx$

- output $\quad T_1 + T_2 \approx \int_a^b w(x) f(x) dx$

B. *Examples*

To test the performance of the algorithm we apply it to the following examples:

Example 1:

The error function is defined as:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

We would like to evaluate

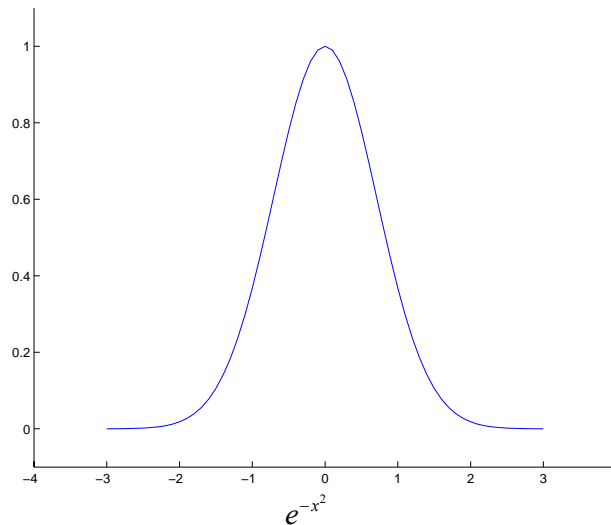$$\mathrm{erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2} dx$$

For convenience, let

$$I = \int_0^1 e^{-x^2} dx,$$

so that

$$\mathrm{erf}(1) = \frac{2I}{\sqrt{\pi}}.$$

Therefore we compute the numerical value of I.

e^{-x^2}

Numerical Results

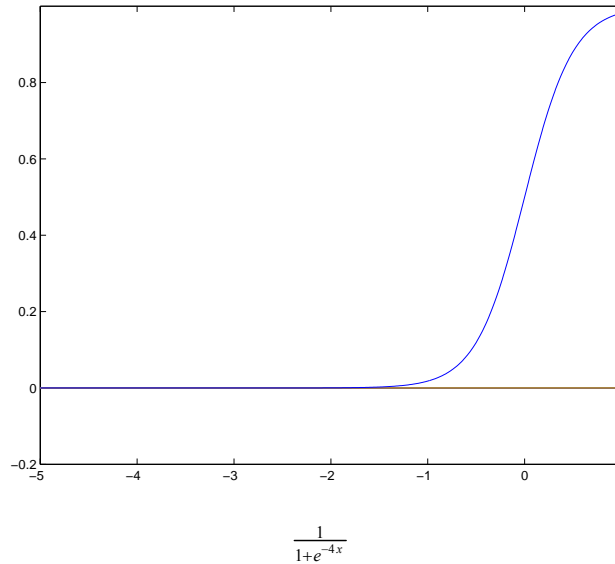The following table shows the error in the numerical computation compared with MATLAB value for erf(1).

n_1, n_2	n=1	n=2	n=3	n=4
0	0.842701	0.036082	2.589004×10^{-4}	1.077446×10^{-5}
1	0.070957	4.02037110^{-4}	1.270461×10^{-4}	5.474581×10^{-6}
2	0.001773	3.29458810^{-5}	1.123385×10^{-5}	4.830643×10^{-7}

Table 1.

Example 2
On this example we use two panels are used to numerically evaluate the integral:

$$I = \int_{-5}^{1} \frac{1}{1 + e^{-4x}} dx$$

$$\frac{1}{1+e^{-4x}}$$

Numerical Results
Using two panels, $[-5, -1]$ and $[-1, 1]$

The following table shows the error in the numerical computation compared with MATLAB "Quad" which uses adaptive Simpson quadrature

n_1, n_2	n=3	n=5
0	0.0032929	2.454541×10^{-4}
1	0.003653	4.434673×10^{-4}
2	0.0029947	2.0788489×10^{-4}

Table 2. Error Example 2

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