

Derivative-based trapezoid rule for a special kind of Riemann-Stieltjes integral

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Abstract. This paper adopts the concept of algebraic precision to construct the derivative-based trapezoid rule for a special kind of Riemann-Stieltjes integral, which uses two derivative values at the endpoints. This kind of quadrature rule obtains an increase of two orders of precision over the trapezoid rule for the Riemann-Stieltjes integral and the error term is investigated. Finally, some numerical examples indicate the numerical superiority of the proposed approach with respect to closed Newton-Cotes formulas.

Keywords: derivative, trapezoid rules, Riemann-Stieltjes integral, numerical integration, error term.

1. Introduction

Roughly speaking, the operation of integration is the reverse of differentiation. Definite integration is one of the most important and basic concepts in mathematics. The Riemann integral of a function f provides a continuous analog of the process of summation of numerical values $f(\xi_i)$, with each such value weighted by the width Δx_i of the interval $[x_{i-1}, x_i]$ from which ξ_i is selected. There are many reasons for generalizing this concept to allow for the weighting of the numerical values $f(\xi_i)$ by numbers different from Δx_i .

In mathematics, the Riemann-Stieltjes integral is a kind of generalization of the Riemann integral, named after Bernhard Riemann and Thomas Stieltjes. It is Stieltjes [1] that first gives the definition of this integral in 1894. The Riemann-Stieltjes integral allows for the replacement of Δx_i by $\Delta g_i = g(x_i) - g(x_{i-1})$, where g is a function of bounded variation [2, 3]. There are many reasons for making such an extension of the concept of the integral. It serves as an

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instructive and useful precursor of the Lebesgue integral, and an invaluable tool in unifying equivalent forms of statistical theorems that apply to discrete and continuous probability.

The reason for introducing Riemann-Stieltjes integrals is to get a more unified approach to the theory of random variables, in particular for the expectation operator, as opposed to treating discrete and continuous random variables separately.

In probability theory, the interval $[a, b]$ might be the space of possible outcomes of a probabilistic experiment. Then $\Delta g_i = g(x_i) - g(x_{i-1})$ could represent the probability of the outcome landing in the interval $[x_{i-1}, x_i]$ of possibilities, and the function f could be the value in some sense of such an outcome [3]. In this illustration, $\int_a^b f(t)dg$ would be a probabilistically expected value to result from running the experiment [2, 3].

It is known that the Riemann-Stieltjes integral has wide applications in the field of stochastic process [4] and functional analysis [5], especially the spectral theorem for self-adjoint operators in a Hilbert space [2, 5] and in original formulation of F. Riesz's theorem [2, 5]. The Riesz's representation theorem establishes that every such bounded linear functional comes from a Riemann-Stieltjes integral with respect to a suitable function of bounded variation.

In several practical problems, we need to calculate integrals. As is known to all, as for $I = \int_a^b f(x)dx$, once the primitive function F of integrand f is known, the definite integral of f over the interval $[a, b]$ is given by Newton-Leibniz formula, i.e.,

$$(1.1) \quad \int_a^b f(x)dx = F(b) - F(a).$$

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative $F(x)$ or whose antiderivative $F(x)$ is not easy to obtain, such as $e^{\pm x^2}$, $\cos x^2$, $\frac{\sin x}{x}$, etc.

Moreover, the integrand $f(x)$ is only available at certain points x_i , $i = 1, 2, \dots, n$.

The problem of numerical evaluating definite integrals arises both in mathematics and beyond, in many areas of science and engineering. One of the most fruitful advances in the field of experimental mathematics has been the development of practical methods for very high-precision numerical integration. Beginning in the 1980s, researchers began to explore ways to extend some of the many known techniques to the realm of high precision numerical integration formulas-tens or hundreds of digits beyond the realm of standard machine precision [6].

The trapezoidal rule is the most well known numerical integration rules of this type. Trapezoidal rule for classical Riemann integral is

$$(1.2) \quad \int_a^b f(x)dx = \frac{b-a}{2} (f(a) + f(b)) - \frac{(b-a)^3}{12} f''(\xi),$$

where $\xi \in (a, b)$.

In spite of the many accurate and efficient methods for numerical integration being available in [7-9], recently Mercer [10] has obtained trapezoid rule for Riemann-Stieltjes integral which engenders a generalization of Hadamard's integral inequality. Trapezoidal rule with error term for Riemann-Stieltjes integral is

$$(1.3) \quad \int_a^b f(t)dg = [G - g(a)]f(a) + [g(b) - G]f(b) - \frac{(b-a)^3}{12}f''(\xi)g'(\eta),$$

where $G = \frac{1}{b-a} \int_a^b g(t)dt$, $\xi \in (a, b)$.

Then, Mercer develops Midpoint and Trapezoid rules for Riemann-Stieltjes integral in [11] by using the concept of relative convexity. The composite trapezoid rule for the Riemann-Stieltjes integral and its Richardson extrapolation formula is presented by Zhao, Zhang and Ye [12]. It is applied to the composite trapezoid rule to obtain high accuracy approximations with little computational cost. Burg [13] has proposed derivative-based closed Newton-Cotes numerical quadrature which uses both the function value and the derivative value on uniformly spaced intervals. Zhao and Li have proposed midpoint derivative-based closed Newton-Cotes quadrature [14] and numerical superiority has been shown. Then, the derivative-based trapezoid rule for the Riemann-Stieltjes integral is presented by Zhao and Zhang [15], which uses derivative values at the endpoints. The midpoint derivative-based trapezoid rule for the Riemann-Stieltjes integral is presented by Zhao, Zhang and Ye [16], which only uses derivative values at the midpoint. Recently, the Simpson's rule for the Riemann-Stieltjes integral is presented by Zhao and Zhang [17], which uses values instead of derivative values at the midpoint.

The exponential function is one of the most important functions in calculus. As we all know, the derivative of e^t is the exponential function e^t itself. This is one of the properties that makes the exponential function really important. Motivation for the research presented here lies in construction of derivative-based trapezoid rule for a kind of Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$, which is a generalization of the results in [10-17].

The remainder is organized into four sections. These new scheme is investigated in Section 2. Section 3 presents the error term. The numerical experiments results are shown in Section 4. Section 5 is the conclusion part.

2. Derivative-based trapezoid rule for the $\int_a^b f(t)d(e^t)$

In this section, by using the conclusions in [15], the derivative-based trapezoid rule for a kind of special Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ is presented.

Theorem 2.1. *Suppose that f' is continuous on $[a, b]$ and $g(t) = e^t$ is obviously continuously differentiable and increasing there. Let T denote the derivative-*

based trapezoid rule for a kind of Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$. Then

$$\begin{aligned}
 \int_a^b f(t)d(e^t) \approx T \triangleq & \left(\frac{6}{(b-a)^2} (e^b+e^a) - \frac{12}{(b-a)^3} (e^b - e^a) - e^a \right) f(a) \\
 & + \left(e^b - \frac{6}{(b-a)^2} (e^b+e^a) + \frac{12}{(b-a)^3} (e^b - e^a) \right) f(b) \\
 (2.1) \quad & + \left(e^a + \frac{2}{b-a} (e^b + 2e^a) - \frac{6}{(b-a)^2} (e^b - e^a) \right) f'(a) \\
 & + \left(\frac{2}{b-a} (2e^b + e^a) - \frac{6}{(b-a)^2} (e^b - e^a) - e^b \right) f'(b).
 \end{aligned}$$

Proof. First of all, it is not difficult to obtain

$$(2.2) \quad \begin{cases} \int_a^b e^t dt = e^b - e^a, \\ \int_a^b \int_a^t e^t dx dt = (e^b - e^a) - (b-a)e^a, \\ \int_a^b \int_a^t \int_a^y e^t dx dy dt = (e^b - e^a) - (b-a)e^a - \frac{1}{2}(b-a)^2 e^a, \\ \int_a^b \int_a^t \int_a^z \int_a^y e^t dx dy dz dt \\ \qquad \qquad \qquad = (e^b - e^a) - (b-a)e^a - \frac{1}{2}(b-a)^2 e^a - \frac{1}{6}(b-a)^3 e^a. \end{cases}$$

Looking for the derivative-based trapezoid rule for $\int_a^b f(t)d(e^t)$, we seek numbers a_0, a_1, b_0, b_1 such that

$$\int_a^b f(t)d(e^t) \approx a_0 f(a) + a_1 f(b) + b_0 f'(a) + b_1 f'(b)$$

is equality for $f(t) = 1, t, t^2, t^3$. That is

$$\begin{cases} \int_a^b 1 d(e^t) = a_0 + a_1, \\ \int_a^b t d(e^t) = a_0 a + a_1 b + b_0 + b_1, \\ \int_a^b t^2 d(e^t) = a_0 a^2 + a_1 b^2 + 2b_0 a + 2b_1 b, \\ \int_a^b t^3 d(e^t) = a_0 a^3 + a_1 b^3 + 3b_0 a^2 + 3b_1 b^2. \end{cases}$$

Therefore, by using the conclusions in [15] and a system of equations (2.2),

$$(2.3) \quad \begin{cases} a_0 + a_1 = e^b - e^a, \\ a_0 a + a_1 b + b_0 + b_1 = b e^b - a e^a - (e^b - e^a), \\ a_0 a^2 + a_1 b^2 + 2b_0 a + 2b_1 b \\ = b^2 e^b - a^2 e^a - 2b(e^b - e^a) + 2[(e^b - e^a) - (b-a)e^a], \\ a_0 a^3 + a_1 b^3 + 3b_0 a^2 + 3b_1 b^2 \\ = b^3 e^b - a^3 e^a - 3b^2(e^b - e^a) + 6b[(e^b - e^a) - (b-a)e^a] \\ - 6[(e^b - e^a) - (b-a)e^a - \frac{1}{2}(b-a)^2 e^a]. \end{cases}$$

Solving simultaneous equations (2.3) for a_0, a_1, b_0, b_1 , we obtain

$$\begin{cases} a_0 = \frac{6}{(b-a)^2} (e^b + e^a) - \frac{12}{(b-a)^3} (e^b - e^a) - e^a, \\ a_1 = e^b - \frac{6}{(b-a)^2} (e^b + e^a) + \frac{12}{(b-a)^3} (e^b - e^a), \\ b_0 = e^a + \frac{2}{b-a} (e^b + 2e^a) - \frac{6}{(b-a)^2} (e^b - e^a), \\ b_1 = \frac{2}{b-a} (2e^b + e^a) - \frac{6}{(b-a)^2} (e^b - e^a) - e^b. \end{cases}$$

So, we have the derivative-based trapezoid rule for the special Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ as desired. □

We shall now deduce some consequences of Theorem 2.1.

Corollary 2.1. *The degree of precision of the derivative-based trapezoid rule for the special Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ is 3. That is to say, the quadrature rule (4) is exact when f is any polynomial of degree 3 or less, but is not exact for some polynomial of degree 4.*

Proof. By looking at the construction of a_0, a_1, b_0, b_1 , we know that the derivative-based trapezoidal rule for the Riemann-Stieltjes integral has degree of precision not less than 3.

In Section 3, Theorem 3.1, we can clearly see that the quadrature is not equality for $f(t) = t^4$. So the degree of precision of this method is 3. □

Remark 2.1. An integral $\int_a^b f(x)e^{kx}dx$ ($k > 0$) over an arbitrary $[a, b]$ can be transformed into an integral over $[\frac{a}{k}, \frac{b}{k}]$ by changing the variable via $t = kx$.

This permits Theorem 2.1 to be applied to any $\int_a^b f(x)e^{kx}dx$ ($k > 0$), because

$$\int_a^b f(x)e^{kx}dx = \int_{\frac{a}{k}}^{\frac{b}{k}} \frac{1}{k} f\left(\frac{t}{k}\right)e^t dt = \frac{1}{k} \int_{\frac{a}{k}}^{\frac{b}{k}} f\left(\frac{t}{k}\right)d(e^t).$$

3. The error term for the $\int_a^b f(t)d(e^t)$

In the previous section, the derivative-based trapezoid rule for a kind of Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ is given in formula (2.1).

As is known to all, the most critical “indicator” of numerical integration, which compares the level of accuracy, is error term. In this section, we are now ready to establish the error term of the derivative-based trapezoid rule for $\int_a^b f(t)d(e^t)$.

Here, the error term for this quadrature rule has been obtained by using Generalized Rolle’s Theorem with Derivatives, the Weighted Mean Value Theorem for Integrals based on the concept of precision.

The error term is the difference between the exact value $\frac{1}{(p+1)!} \int_a^b x^{p+1}dx$ and the quadrature formula for the monomial $\frac{x^{p+1}}{(p+1)!}$, where p is the precision of the quadrature formula.

Theorem 3.1. *Suppose that $f^{(4)}$ is continuous on $[a, b]$ and $g(t) = e^t$ is obviously continuously differentiable and increasing there. The derivative-based trapezoid rule for the Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ with the error term is*

$$\begin{aligned}
 \int_a^b f(t)d(e^t) &= \left(\frac{6}{(b-a)^2} (e^b+e^a) - \frac{12}{(b-a)^3} (e^b - e^a) - e^a \right) f(a) \\
 &+ \left(e^b - \frac{6}{(b-a)^2} (e^b+e^a) + \frac{12}{(b-a)^3} (e^b - e^a) \right) f(b) \\
 &+ \left(e^a + \frac{2}{b-a} (e^b + 2e^a) - \frac{6}{(b-a)^2} (e^b - e^a) \right) f'(a) \\
 (3.1) \quad &+ \left(\frac{2}{b-a} (2e^b + e^a) - \frac{6}{(b-a)^2} (e^b - e^a) - e^b \right) f'(b) \\
 &+ \left[- \left(\frac{5(b-a)^3}{24} + \frac{(b-a)^2}{2} + \frac{11(b-a)}{12} + 1 \right) e^a \right. \\
 &\left. + \left(\frac{(b-a)^2}{12} - \frac{b-a}{12} + 1 \right) e^b \right] f^{(4)}(\xi) e^\eta,
 \end{aligned}$$

where $\xi, \eta \in (a, b)$. And the error term $R[f]$ of this method is

$$\begin{aligned}
 &\left[\left(\frac{(b-a)^2}{12} - \frac{b-a}{12} + 1 \right) e^b \right. \\
 (3.2) \quad &\left. - \left(\frac{5(b-a)^3}{24} + \frac{(b-a)^2}{2} + \frac{11(b-a)}{12} + 1 \right) e^a \right] f^{(4)}(\xi) e^\eta.
 \end{aligned}$$

Proof. Let $f(t) = \frac{t^4}{4!}$. So

$$\begin{aligned}
 \frac{1}{4!} \int_a^b t^4 d(e^t) &= \frac{1}{24} (b^4 - 4b^3 + 12b^2 - 24b - 24) e^b \\
 (3.3) \quad &- \frac{1}{24} (a^4 - 4a^3 + 12a^2 - 24a - 24) e^a.
 \end{aligned}$$

By the Theorem 2.1, we have

$$\begin{aligned}
 T &= \left(\frac{6}{(b-a)^2} (e^b+e^a) - \frac{12}{(b-a)^3} (e^b - e^a) - e^a \right) \frac{a^4}{24} \\
 &+ \left(e^b - \frac{6}{(b-a)^2} (e^b+e^a) + \frac{12}{(b-a)^3} (e^b - e^a) \right) \frac{b^4}{24} \\
 &+ \left(e^a + \frac{2}{b-a} (e^b + 2e^a) - \frac{6}{(b-a)^2} (e^b - e^a) \right) \frac{a^3}{6}
 \end{aligned}$$

$$(3.4) \quad + \left(\frac{2}{b-a} (2e^b + e^a) - \frac{6}{(b-a)^2} (e^b - e^a) - e^b \right) \frac{b^3}{6}.$$

With the help of (3.3)-(3.4), we obtain

$$\begin{aligned} & \frac{1}{4!} \int_a^b t^4 d(e^t) - T \\ &= \left[\left(\frac{(b-a)^2}{12} - \frac{b-a}{12} + 1 \right) (e^b - e^a) - \left(\frac{5(b-a)^3}{24} + \frac{5(b-a)^2}{12} + (b-a) \right) e^a \right] \\ &= \left[\left(\frac{(b-a)^2}{12} - \frac{b-a}{12} + 1 \right) e^b - \left(\frac{5(b-a)^3}{24} + \frac{(b-a)^2}{2} + \frac{11(b-a)}{12} + 1 \right) e^a \right]. \end{aligned}$$

This implies that

$$\begin{aligned} R[f] &= \left[\left(\frac{(b-a)^2}{12} - \frac{b-a}{12} + 1 \right) e^b \right. \\ &\quad \left. - \left(\frac{5(b-a)^3}{24} + \frac{(b-a)^2}{2} + \frac{11(b-a)}{12} + 1 \right) e^a \right] f^{(4)}(\xi) e^\eta. \quad \square \end{aligned}$$

Remark 3.1. The method used in Theorem 3.1 does not only apply to special cases, but that one may select the precision p to calculate the difference between the exact value $\frac{1}{(p+1)!} \int_a^b x^{p+1} dx$ and the quadrature formula for the monomial $\frac{x^{p+1}}{(p+1)!}$ and the similar conclusion will still hold.

Remark 3.2. The error term for the derivative-based trapezoid rule could also be obtained using Taylor series expansions, by making certain unverifiable assumptions about the higher order terms.

4. Numerical results

So far, we have proposed derivative-based trapezoid rule for a kind of Riemann-Stieltjes integral in Section 2 and demonstrate the error term in Section 3.

In this section, compared with the traditional Newton-Cotes quadrature, some numerical experiments are carried out to verify whether the novel methods are of high precision.

In order to compare the precision of Newton-Cotes quadrature and the proposed approach, we calculate the following integrals $\int_0^1 x^4 e^x dx$. The comparison results are shown in the following tables.

Let us define Absolute Error = |Exact value - Approximate value|.

In the following tables, the item Int. stands for the number of composite interval.

Exact value of $\int_0^1 x^4 e^x dx = 9e - 24 \approx 0.4645$.

Int.	Trapezoidal rule		Int.	Derivative-based trapezoid rule	
	Approximate value	Absolute Error		Approximate value	Absolute Error
1	1.3591	0.8946	1	0.4086	0.0559
2	0.7311	0.2666	2	0.4610	0.0035
4	0.5342	0.0697			
8	0.4822	0.0177			

Table 1: Numerical comparison of the new method with the classical method

Int.	Simpson’s rule		Int.	Derivative-based trapezoid rule	
	Approximate value	Absolute Error		Approximate value	Absolute Error
1	0.5217	0.0572	1	0.4086	0.0559
2	0.4686	0.0041	2	0.4610	0.0035

Table 2: Numerical comparison of the new method with the classical method

It can be seen from Table 1, Derivative-based trapezoid rule with Int.=1, 2 has a much higher accuracy than classical Trapezoidal rule with Int.=4, 8 respectively.

It can be seen from Table 2, Derivative-based trapezoid rule has a much higher accuracy than classical Simpson’s rule with the same number of subintervals.

The efficiency of the proposed approach has been demonstrated.

5. Conclusions

The main contributions of this paper are highlighted as follows.

- 1) By using the concept of algebraic precision, the derivative-based trapezoid rule for a kind of Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$ is presented.
- 2) This kind of quadrature rule has 3 orders of algebraic precision.
- 3) The error term for Riemann-Stieltjes Simpson’s rule is investigated. Some numerical examples are given to show the efficiency of the proposed approach. In future work, we will seriously consider the Simpson’s rule for the kind of Riemann-Stieltjes integral $\int_a^b f(t)d(e^t)$.

It is hoped that the results in this paper will stimulate further research in this direction.

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