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Numerical Simulations to Illuminate the Sufficient Condition for the Convergence Order Attainable of Quadrature Formulas

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Abstract. One of the crucial issue in the mathematical reasoning is that many students do not really understand the mathematical rules underlying the conditional statement $p \rightarrow q$, whereas most of mathematical theorems are of this pattern. They believe that the falsity of p implies the falsity of q. This is tantamount to presuming that implication is equivalent to the inverse, but that's not the case. This fact suggests that students have not been able in distinguishing the sufficient and the necessary conditions of a conditional statement. This article is concerned with this problem by investigating the sufficient conditions on the basic quadrature formulas of integral approximation and their implication to the convergence order attainable. In order to instill students' critical thinking skills, theorems relating to the convergence orders of three basic methods are proven. Furthermore, the cases where the sufficient conditions are fulfilled as well as cases where they are not satisfied are examined by a series of numerical simulation. It is concluded that the quadrature formula with a high convergence order does not provide the better results than the lower order of convergence if the sufficient conditions are not met properly.

Keywords: Mathematical reasoning; sufficient condition; quadrature formula; error estimation; convergence order.

INTRODUCTION

Once I asked students in my class to imagine a shop displayed an advertisement "if your purchase is more than IDR 100,000,- then you will get a 10% discount". What can be concluded if a customer's purchase is IDR 99,000,-? All students answered: "the customer will not get any discount". This is of course a premature conclusion. The ability to discern between the necessary and sufficient conditions of mathematical statements is a hardship for many college students when learning mathematics. For instance, students typically believed that the zeros of the first derivative of a function was a sufficient condition for an optimum, but in fact it is a necessary condition. When they are asked to determine the maximum or minimum of $f(x) = x^3$ or $f(x) = |x|$, they typically employ the standard procedure for specifying derivative zeros, which is absolutely fail. This fact is at least based on the author's classroom experience when teaching at undergraduate level.

Mathematics involves various types of statements such as axioms, postulates, definitions, undefined terms, lemmas, theorems, corollaries and conjectures. A proposition is a statements which has a definite truth value, either true or false. A theorem in mathematics is a kind of proposition in which the truth can be proven by the rule of logic. The formulas in mathematics are actually a part of the theorem. The mathematical statements are generally in the form of compound sentences involving connectivities such as negation ($\neg$), disjunction ($\vee$), exclusive disjunction ($\oplus$), conjunction ($\wedge$), implication ($\rightarrow$), and bi-implication ($\leftrightarrow$). The implication notation $p \rightarrow q$ is read "if p then q" or "p implies q" or "p is a sufficient condition for q". The implication $p \rightarrow q$ is also sometimes called the conditional statement where p is the antecedent and q is the conclusion. Some simple and interesting illustrations of the sufficient and necessary conditions has been exposed in [11, 13, 22]. As mentioned in [6] that almost all theorems in mathematics can be represented in the conditional sentences. For examples, "if a triangle has two sides congruent then it also has two opposite angles that are congruent", as well as "if x dan y positive with $x \neq y$ then $\frac{x}{y} + \frac{y}{x} > 2$.

Tabel 1 shows four possibilities of implication $p \rightarrow q$ and its variants. Let $\tau(p)$ stands for the truth value of proposition p, then the only case $\tau(p \rightarrow q) = F$ only if $\tau(p) = T$ and $\tau(q) = F$, other cases are true. From this fact, it can be understood that $p \rightarrow q \equiv \neg p \vee q$. The logic consideration of the implications truth value the reason fits to human cognition has been examined in [11, 12, 16]. Three modifications of a conditional sentence $(p \rightarrow q)$ are converse $(q \rightarrow p)$, inverse $(\neg p \rightarrow \neg q)$, and contrapositive $(\neg q \rightarrow \neg p)$. It can be verified that $p \rightarrow q \equiv \neg q \rightarrow \neg p$ and they are called equivalent. The similar fact also holds for inverse and converse.

Tabel 1. Truth value of implication, converse, inverse, and contrapositive

					implication	converse	inverse	contrapositive
Rows	p	q	$\neg p$	$\neg q$	$p \rightarrow q$	$q \rightarrow p$	$\neg p \rightarrow \neg q$	$\neg q \rightarrow \neg p$
1	T	T	F	F	T	T	T	T
2	T	F	F	T	F	T	T	F
3	F	T	T	F	T	F	F	T
4	F	F	T	T	T	T	T	T

The sufficient condition or premise of an implication might be a compound statement with some connectivities. For example, the sufficient condition of statement "if x and y positive with $x \neq y$ then $\frac{x}{y} + \frac{y}{x} > 2$$ composed of two sentences, i.e. "p_1: x and y are positive", and p_2: $x \neq y$. They are related by the connectivity $\wedge$. Symbolically, it can be represented as $p_1 \wedge p_2 \rightarrow q$. Both propositions must be true in order to get the conclusion $\frac{x}{y} + \frac{y}{x} > 2$ true. For example, $x = 2$ and $y = 3$ satisfy both conditions and we find $\frac{2}{3} + \frac{3}{2} = \frac{13}{6} > 2$ is a true statement. In case one of them is not fulfilled then the conclusion could be false. For example, $x = y = 2$ satisfies the first but not for the second. In this case we find $\frac{x}{y} + \frac{y}{x} = \frac{2}{2} + \frac{2}{2} = 2 > 2$ is a false statement. Otherwise, for $x = -2$ and $y = -3$ then the sufficient condition is not satisfied but $\frac{x}{y} + \frac{y}{x} = \frac{-2}{-3} + \frac{-3}{-2} = \frac{13}{6} > 2$ is true statement. This means that a non-fulfillment of sufficient conditions does not imply the falsity of the conclusion. In a true implication, the true of conclusion does not necessarily the result of a true premise, while the true of premise must lead to a true of conclusion.

The critical problem on the conditional sentence is when the sufficient condition or antecedent cannot be verified. As reported by Krantz [16] that one of Aristotle's rules of logic was that every sensible statement, that is clear and succinct and does not contain logical contradictions, is either true or false. There is no “middle ground” or “undecided status” for such a statement. Thus the assertion "if there is life as we know it on Mars, then fish can fly" is either true or false. We do know that fish cannot fly, but we cannot determine the truth or falsity of this statement because we do not know whether there is life as we know it on Mars.

Many cases in applied mathematics employed a heuristic approach where the conclusion was not based on the fulfillment of sufficient conditions, but only rely on the data or numerical simulations. The conclusions obtained through this approach tend to be weak and not universally true. Regretfully, a lot of people have mistakenly believed that mathematics is just a set of formulas for dealing with and calculating numbers without taking into account the necessary conditions. This reality cannot be avoided as it becomes easier to solve mathematical problems without having to study mathematics in depth, such as through various machine learning packages that are easily and inexpensively available, even for free.

In the other hand, modifying the sufficient condition of theorem to make it easier to examine is a concern in mathematics research. As computing technology advances, many students lose interest in studying theorems and proofs, as well as checking for sufficiency conditions. This might be the corner stone for the development of a new branch of mathematical logic known as reverse mathematics. Reverse mathematics is a program in mathematical logic that seeks to give precise answers to the question of which axioms are necessary in order to prove theorems of "ordinary mathematics", e.g. see [4, 19]. One question should be also considered in the reverse mathematics is how likely it is that the theorem's conclusion will be optimally unreachable if sufficient conditions are not met perfectly. This question might also relates to the philosophy of mathematics.

According to Ruben Hers in [14], philosophy of mathematics should be examined against five kinds of mathematical practice: research, application, teaching, history, and computing. Computers are increasingly being used in mathematical studies, not just in applied mathematics, but also in pure mathematical research, such as making conjectures. Proof is sometimes completed using a computer when it requires calculations that cannot be done by hand;

for example, "the four-color conjecture". Ruben Hers in his book entitled "What is Mathematics Really" noticed an ironic that for decades philosopher said the valid mathematical proofs should be checkable by machine, i.e. computer, but on the other hand when part of a proof is done on a machine, some say, "That's not a proof" [14].

Some well-known theorems are frequently proven in the classroom while learning mathematics. As mentioned in [12, 16] and many others, there are numerous advantages to learning mathematics through proving theorems, such as to establish a fact with certainty, to gain understanding, to communicate an idea to others, for challenge, to create something beautiful, to construct a large mathematical theory. Nevertheless there are some drawbacks to this learning approach because it is thought to be more complicated than using mathematics tools that already installed on computer, such as various Python libraries. A personal experience when teaching theorems in the vector calculus course with precedence some numerical and graphical simulation by GeoGebra, students become more interested in understanding the proof of theorems in depth. The acquisition of mathematics through a computational thinking approach is highly advantageous for adapting to the current state of AI advancements, see [3]. This approach is characterized by the use of numerical simulations to clarify mathematical concepts. This article is presented in light of these considerations.

For numerical simulation purposes, this paper employs a classic and simple topics on numerical analysis course, in particular the error analysis of quadrature formulas for integral approximation. For simplicity, the quadrature formula of equidistant is taken for simulation. This simplest kind of this quadrature formula had been discussed in many classical books of numerical method and it's necessary and sufficient conditions of the equidistant was introduced [25]. Despite its simplicity, the concept of the quadrature formula serves as the basis for the creation of numerical integral schemes and has been extended to more complicated integral, for instance, Riemann-Liouville fractional integral [9], fractional integral in Hilbert space [10], curvilinear integral of first kind [24], and Gauss quadrature formula [21]. So far, textbooks widely used for teaching this problem have focused solely on cases where sufficient conditions are met without paying attention on cases where sufficient conditions are not fulfilled, e.g. [2, 5, 17].

The paper begins by restating the idea of basic quadrature formulas and rewriting the midpoint, trapezoidal, and Simpsons' quadrature formulas. Furthermore, various supporting theorems from elementary real analysis are presented to prove various theorems regarding error estimation of integral approximation with the quadrature formula. The theorems and proofs presented here are already well-known; yet some reviews are included to highlight some key points. Finally, some numerical simulations are demonstrated to justify the conclusion of theorem in which the sufficient condition is fulfilled as well as not fulfilled.

MATERIALS AND METHODS

There is no spesific material used in this research except a personal computer/laptop and the software MATLAB version 2020a running on MacBook Air Intel Core i5 4GB of RAM with 128GB storage for conducting some numerical simulation. In meanwhile, the method is quite similar to literature review research in mathematics; it consists of definitions and supporting theorems.

Preliminaries on Integral Approximation

A various definitions of integral are intended to provide theoretical justification for various problems that arise from mathematics and applied sciences. Theoretically, the integral is defined as a limit of infinite sum but in practice it must be implemented by a computer that works only to the finite sums. Such a restriction which might have inspired the quadrature formula, i.e. taking only values of integrand f on some finite number of points in $[a,b]$. Let $x_i,\ i = 0,1,\cdots,n$ be $n+1$ points in $[a,b]$ and assume the integral $\int_a^b f(x)\,dx$ is given by

$$I(f) = \int_a^b f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i) + R_n. \qquad (1)$$

The points in $\{x_i : i = 0,1,\cdots,n\}$ where f evaluated are called the abscissas or nodes, the coefficients $\{w_i : i = 0,1,\cdots,n\}$ are called the weights, and R_n is the reminder or error term. The definite integral (1) is approximated by the quadrature formula, i.e.

$$I(f) \approx \int_a^b f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i). \qquad (2)$$

The first issue is how to select the abscissa x_i's and determine the weight of w_i's so that $Q(f)$ in (2) is a good approximation for $I(f)$ in (1). The second problem is how to obtain the upper bound of the remainder term R_n that specifies the approximation accuracy.

The idea for approximating the integral $\int_a^b f(x)\,dx$ is to construct an interpolation polynomial P_n for f, then $\int_a^b P_n(x)\,dx$ is taken as approximation for $\int_a^b f(x)\,dx$. This idea is based on the fact that calculating the integral of a polynomial is much easier than calculating the integral of any function in general. Let $x_0, x_1, \cdots, x_n$ be distinct nodes in $[a,b]$ and f be a continuous function on $[a,b]$, then there is a unique interpolation polynomial P_n of degree less than or equal to n, i.e. $P_n(x_i) = f(x_i)$, $i = 0, 1, \cdots, n$ and the such interpolation polynomial can be constructed by either Lagrange or divided-difference method [5, 17]. The basic quadrature formulas are according to $n = 0, 1, 2$.

- $n = 0$ and the node $x_0 = \frac{a+b}{2}$ results the midpoint formula $I(f) \approx M(f) = (b-a)f\left(\frac{a+b}{2}\right)$ where the appopriate weight is $w_0 = b - a$.
- $n = 1$ and two nodes $x_0 = a$ and $x_1 = b$ provides the trapezoidal formula $I(f) = T(f) = \frac{1}{2}(b-a)\big(f(a) + f(b)\big)$ with corresponding weights are $w_0 = w_1 = \frac{b-a}{2}$.
- $n = 2$ and three nodes $x_0 = a$, $x_1 = \frac{a+b}{2}$, and $x_2 = b$ gives the Simpson formula $I(f) \approx S(f) = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$ where the weights in this case are $w_0 = \frac{b-1}{6}$, $b_1 = \frac{2}{3}(b-a)$, $w_2 = \frac{b-a}{6}$.

In order to improve the accuracy, the interval $[a,b]$ is partitioned smaller into $x_0 := a < x_1 < x_2 < \cdots < x_n := b$, then the basic quadrature formulas defined on each subinterval. For simplification, the partition is taken to be uniform, i.e. $x_k - x_{k-1} := h$ so that $x_k = x_{k-1} + h$ for $k = 1, 2, \cdots, n$. Using the additive property of integral, the following composite quadrature formulas are obtained.

- Midpoint formula: Consider that each three consecutive nodes x_{k-1}, x_k, x_{k+1}, $k = 1, 3, \cdots, n-1$ generates one midpoint formula, i.e. $M_k(f) = (x_{k+1} - x_{k-1})f(x_k) = 2hf(x_k)$. By summing up these terms the composite midpoint formula is obtained as follows:

$$M_n(f) = \sum_{k=1, k \text{ odd}}^{n-1} M_k(f) = 2h \sum_{k=1}^{\frac{n}{2}} f(a + (2k-1)h).$$

- Simpson formula: Consider that each three consecutive nodes x_{k-1}, x_k, x_{k+1}, $k = 1, 3, \cdots, n-1$ generates one Simpson formula, i.e. $S_k(f) = \frac{h}{3}\big(f(x_{k-1}) + 4f(x_k) + f(x_{k+1})\big)$. By summing up these terms the composite Simpson formula is obtained as follows:

$$S_n(f) = \frac{h}{3}\left(f(a) + f(b) + 4\sum_{k=1}^{\frac{n}{2}} f(x_{2k-1} + 2\sum_{k=1}^{\frac{n}{2}-1} f(x_{2k}) \right).$$

- Trapezoidal formula: Consider that each two consecutive nodes x_{k-1}, x_k, $k = 1, 2, \cdots, n$ generates one Trapezoidal formula, i.e. $T_k(f) = \frac{1}{2}(x_k - x_{k-1})\big(f(x_{k-1}) + f(x_k)\big)$. By summing up these terms the composite trapezoidal formula is obtained as follows:

$$T_n(f) = \sum_{k=1}^{n} T_k(f) = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k) \right).$$

Recall that n must be even for midpoint and Simpson while trapezoidal could be odd. Some detail derivation of basic quadrature formulas, technique to calculate the approximation of integral, and derivation of the error estimation can be found on the elementary numerical method textbooks, e.g. [5, 8, 17, 23]. In addition to the quadrature formula, the error term R_n as a function of h will be formulated in order to evaluate the quality of approximation. Once this error term is known, the estimated error and the order of convergence of the approximation can be determined. Significancy of these two terms will be simulated by numerical simulations. Through numerical simulations the effect of sufficient condition on the order convergence will be examined.

Supporting Theorems

In the real analysis course, the Darboux Intermediate Value Theorem (D-IVT) states that a continuous function on interval $[a,b]$ always has pre-image for each $\alpha \in \mathbb{R}$ lying between $f(a)$ and $f(b)$. Two versions of D-IVT are formally presented as follows.

Theorema 1 [D-IVT Standard] Let $f: [a, b] \to \mathbb{R}$ be a continuous function and α a real number between $f(a)$ and $f(b)$, then there always $c \in (a, b)$ such that $f(c) = \alpha$.

The proof requires the Bolzano intermediate value theorem which is also knows as the root location theorem (RLT), i.e. if $f: [a, b] \to \mathbb{R}$ be continuous and $f(a)f(b) < 0$ then some $c \in (a, b)$ exists so that $f(c) = 0$, i.e. c is the root of $f(x) = 0$.

Proof. It is enough to assume that $f(a) \neq f(b)$, since if $f(a) = f(b)$ then it must be satisfied that $\alpha = f(a) = f(b)$ so that it can be taken $c = a$ or $c = b$. Without lost of generality, we assume $f(a) < f(b)$, there is α in between, i.e. $f(a) < \alpha < f(b)$. Take $h(x) := f(x) - \alpha$, then we find h is continuous where $h(a) = f(a) - \alpha < 0$ and $h(b) = f(b) - \alpha > 0$. It can be verified easily that $h(a)h(b) < 0$. According to RLT, it can be concluded there exists $c \in (a, b)$ such that $h(c) = 0$, i.e. $h(c) = f(c) - \alpha = 0$ or $f(c) = \alpha$. ■

Furthermore, the D-IVT is extended by allowing several numbers $\alpha_1, \alpha_2, \cdots, \alpha_n$ located between $f(a)$ and $f(b)$. Observe the convex linear combination $\sum_{i=1}^{n} \lambda_i \alpha_i$ where $0 < \lambda_i < 1$ and $\sum_{i=1}^{n} \lambda_i = 1$. Hence, $f(a) < \alpha_i < f(b)$ and $\lambda_i > 0$ implying $\lambda_i f(a) < \lambda_i \alpha_i < \lambda_i f(b)$. Summing up all these terms $f(a) \sum_{i=1}^{n} \lambda_i < \sum_{i=1}^{n} \lambda_i \alpha_i < f(b) \sum_{i=1}^{n} \lambda_i$. Since it is known that $\sum_{i=1}^{n} \lambda_i = 1$ then one obtains $f(a) < \sum_{i=1}^{n} \lambda_i \alpha_i < f(b)$. Formally, the extended version of D-IVT is described as follows.

Theorem 2 [D-IVT Extended] Let $f: [a, b] \to \mathbb{R}$ be a continuous function on $[a, b]$ and $\alpha_1, \alpha_2, \cdots, \alpha_n$ are real numbers between $f(a)$ and $f(b)$. If $0 < \lambda_i < 1$ where $\sum_{i=1}^{n} \lambda_i = 1$ then there exists $c \in (a, b)$ such that $f(c) = \sum_{i=1}^{n} \lambda_i \alpha_i$.

Theorem 1 is a special case of Theorem 2 in which $\alpha_1 = \alpha_2 = \cdots = \alpha_n := \alpha$ and $\lambda_i := \frac{1}{n}, i = 1, 2, \cdots, n$. This is the reason why Theorem 2 is regardes as the extended version of Theorem 1.

In the differential calculus, it's well-known the Mean Value Theorem (MVT) that asserts the existence a point $c \in (a, b)$ where the curve tangent $y = f(x)$ at $x = c$ is parallel to secant line connecting point $(a, f(a))$ and $(b, f(b))$, written by $f'(c) = \frac{f(b) - f(a)}{b - a}$. In the integral calculus the similar theorem is known as the the integral mean value theorem (I-MVT).

Theorem 3 [I-MVT Standard] If $f: [a, b] \to \mathbb{R}$ continuous on $[a, b]$ then there exists $c \in (a, b)$ such that $\int_a^b f(x)\, dx = f(c)(b - a)$.

Proof. Since f continuous on $[a, b]$, it reaches maximum and minimum on $[a, b]$. Let $m = \min_{x \in [a,b]} f(x)$ and $M = \max_{x \in [a,b]} f(x)$, the inequality holds: $m \leq f(x) \leq M$ for each $x \in [a, b]$. Integrating both sides we obtain $m(b - a) \leq \int_a^b f(x)\, dx \leq M(b - a)$ or $m \leq \frac{\int_a^b f(x)\, dx}{b - a} \leq M$. According to Theorem 1, there exists $c \in (a', b') \subseteq (a, b)$ such that $f(c) = \alpha = \frac{\int_a^b f(x)\, dx}{b - a}$, i.e. $\int_a^b f(x)\, dx = f(c)(b - a)$. ■

Mean of function versus arithmetic mean. The quantity $f(c) = \frac{1}{b - a} \int_a^b f(x)\, dx$ is considered as the mean of function f on $[a, b]$. Suppose that the continuous condition is relaxed just to be integrable and $[a, b] = [0, n]$. Set a partition $a := 0 < 1 < 2 < \cdots < n =: b$ and f is piece-wise constant $[0, n]$, i.e. $f(x) := y_i\, \chi_{[i-1,\ i)}(x)$ where $y_i \in \mathbb{R}$, $i = 1, 2, \cdots, n$ then $\frac{1}{b - a} \int_a^b f(x)\, dx = \frac{1}{n} \sum_{i=1}^{n} y_i := \bar{y}$, which is exactly the ordinary (arithmetic) mean for discrete data $y_1, y_2, \cdots, y_n$.

Error Estimation of Quadrature Formulas

As mentioned earlier that the quadrature formula is determined through polynomial interpolation defined on domain $[a, b]$. The basic quadrature formulas are obtained when the interpolation applied on whole domain. Composite quadrature formulas are obtained by partitioning the domain into a number subdomains. The composite quadrature formulas depend on parameter h indicating the partition mesh or natural number n representing the number of subintervals. The following three theorems deal with the error estimate of the basic quadrature formulas.

Theorem 4. If $f \in C^2[a,b]$, i.e. continuously differentiable up to second order, then there exists $\xi \in (a,b)$ such that the midpoint formula gives the following error.

$$I(f) - M(f) = \frac{f''(\xi)}{24}(b-a)^3. \qquad (3)$$

Proof. Apply the Taylor theorem around $x_0 = \frac{a+b}{2}$ then for each $x \in [a,b]$ there is a $\xi_x \in (a,b)$ such that $f(x) - f(x_0) = f'(x_0)(x-x_0) + \frac{f''(\xi_x)}{2}(x-x_0)^2$. Consider that $\int_a^b f(x_0)\,dx = (b-a)f\left(\frac{a+b}{2}\right) = M(f)$ and $\int_a^b (x - x_0)\,dx = 0$, the following derivation is obtained,

$$\begin{aligned} I(f) - M(f) &= \int_a^b \big(f(x) - f(x_0)\big)\,dx \\ &= \int_a^b f'(x_0)(x-x_0)\,dx + \int_a^b \frac{f''(\xi_x)}{2}(x-x_0)^2\,dx \\ &= \frac{f''(\xi)}{6}\left[\left(\frac{b-a}{2}\right)^3 - \left(\frac{a-b}{2}\right)^3\right] = \frac{f''(\xi)}{24}(b-a)^3. \end{aligned}$$

The proof is actually finish. The supplementary explanation that zero on the first term is because of $\int_a^b (x-x_0)\,dx = 0$ and the second term is a consequnce of Theorem 2 by taking $g(x) \coloneqq (x-x_0)^2 \geq 0$ and $f_1(x) \coloneqq \frac{f''(\xi_x)}{2}$. Thus, $\int_a^b \frac{f''(\xi_x)}{2}(x-x_0)^2\,dx = \frac{f''(\xi)}{2}\int_a^b (x-x_0)^2\,dx$ for some $\xi \in (a,b)$. This explanation is crucial for students who might be confusing to the change from existence of ξ_x depending on x becomes ξ a constant independent of x. ■

Before deriving the error estimate trapezoidal and Simpson formula, the following polynomial interpolation theorem is required, see Kress [17] for detail.

Theorem 5. Suppose that $f : [a,b] \to \mathbb{R}$ has continuous derivatives up to order $n+1$. If P_n is the interpolation polynomial of function f at nodes $x_0, x_1, \cdots, x_n$ in $[a,b]$ then the following estimate holds,

$$f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n), \qquad (4)$$

where ξ some point in (a,b) depends on x.

Theorem 6. If $f \in C^2[a,b]$ then there exists $\xi \in (a,b)$ so that the trapezoidal formula holds the following estimate.

$$I(f) - T(f) = \frac{f''(\xi)}{12}(b-a)^3. \qquad (5)$$

Proof. Let $P_1 \coloneqq L_1 f$ be the first order polynomial interpolation of f with nodes $x_0 = a$ dan $x_1 = b$. A fairly complete discussion about polynomial interpolation can refer to various numerical methods textbooks, for example see [5, 13a]. It can be understood the error $E_1(f) \coloneqq \int_a^b \big(f(x) - L_1 f(x)\big)\,dx = I(f) - T(f)$. Using (4) for $n = 1$, we find for each $x \in [a,b]$ there exists $\xi_x \in (a,b)$ such that the following holds: $R_1(x) = f(x) - L_1 f(x) = \frac{f''(\xi_x)}{2}(x-a)(x-b)$. Furthermore, consider

$$I(f) - T(f) = \int_a^b R_1(x)\,dx = \int_a^b \frac{f''(\xi_x)}{2}(x-a)(x-b)\,dx.$$

Apply the I-MVT extended for $g(x) \coloneqq (x-a)(x-b) \leq 0$ and $f(x) \leftarrow f_1(x) \coloneqq \frac{f''(\xi_x)}{2}$, there exists $\xi \in (a,b)$ so that

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

The last step can be verified by elementary calculus. ■

Theorem 7. Assuming that $f \in C^4[a,b]$ then there exists $\xi \in (a,b)$ so that the Simpson formula provide the following error estimate

$$I(f) - S(f) = -\frac{f^{(4)}(\xi)}{2880}(b-a)^3. \qquad (6)$$

Proof. Similar to the proof of Theorem 6, let $L_2 f$ be the second order polynomial interpolation of f with nodes $x_0 = a$, $x_1 = \frac{1}{2}(a+b)$, and $x_2 = b$. We have the error $E_2(f) := \int_a^b [f(x) - L_2 f(x)]\,dx = I(f) - S(f)$. Define the cubic polynomial $p(x) := L_2 f(x) + \frac{4}{(b-a)^2}[(L_2 f)'(x_1) - f'(x_1)]\, q_3(x)$, where $q_3(x) = (x-x_0)(x-x_1)(x-x_2)$. Observe that for $k = 0,1,2$ it satisfies $q_3(x_k) = 0$ so that $p(x_k) = L_2 f(x_k) + 0 = f(x_k)$; hence p interpolated. The derivative of p is obtained as $p'(x) = (L_2 f)'(x) + \frac{4}{(b-a)^2}[(L_2 f)'(x_1) - f'(x_1)]q_3'(x)$. It easy to verify that $q_3'(x_1) = \frac{1}{4}(b-a)^2$, thus $p'(x_1) = f'(x_1)$. Pay attention q_3 is an odd function with respect $x = x_1$ so that $\int_a^b q_3(x)\,dx = \int_a^b (x-x_0)(x-x_1)(x-x_2)dx = 0$. Now, the error formula can be written as $E_2(f) := \int_a^b [f(x) - p(x)]\,dx$. Take $g(x) := (x-x_0)(x-x_1)^2(x-x_2)$ then it holds $g(x) \le 0$ for all $x \in [a,b]$. Applying the L'Hospital rule, it can shown the following limit exists for each $x_k = x_0, x_1$, and x_2.

$$\lim_{x \to x_k} \frac{f(x) - p(x)}{(x-x_0)(x-x_1)^2(x-x_2)}.$$

Suppose that limits corresponding to $x_k = x_0, x_1$, and x_2 are ℓ_0, ℓ_1, and ℓ_2 repectively. Define the function h as

$$h(x) := \begin{cases} \dfrac{f(x) - p(x)}{(x-x_0)(x-x_1)^2(x-x_2)} & if\ x \ne x_0, x_1, x_2, \\ \ell_k & if\ x = x_k, k = 0,1,2. \end{cases}$$

It easy to check that h is continuous on $[a,b]$, in particular at $x = x_k, k = 0,1,2$. The error E_2 can be written as follows

$$E_2(f) = \int_a^b (x-x_0)(x-x_1)^2(x-x_2)\left[\frac{f(x) - p(x)}{(x-x_0)(x-x_1)^2(x-x_2)}\right] dx = \int_a^b g(x)h(x)\,dx.$$

Since h continuous and g does not change the sign on $[a,b]$ then by Theorem 2, there exists $z \in [a,b]$ such that

$$E_2(f) = \left[\frac{f(z) - p(z)}{(z-x_0)(z-x_1)^2(z-x_2)}\right]\int_a^b (x-x_0)(x-x_1)^2(x-x_2)\,dx. \qquad (*)$$

Observe that p is the third degree interpolation polynomial for f involving 4 nodes, namely x_0, x_1, x_1, and x_2. According to (4) there exists $\xi \in (a,b)$ such that $f(z) - p(z) = \frac{f^{(4)}(\xi)}{4!}(z-x_0)(z-x_1)^2(z-x_2)$. It is straighforward to get

$$\int_a^b (x-x_0)(x-x_1)^2(x-x_2)\,dx = -\frac{(b-a)^5}{120}.$$

Substituting the last result into the previous term (*), it is obtained that

$$E_2(f) = -\frac{f^{(4)}(\xi)}{4!}\frac{(b-a)^5}{120} = -\frac{f^{(4)}(\xi)}{2880}(b-a)^5. \qquad \blacksquare$$

It can be seen that this proof is not straightforward, but that is the challenge of studying mathematics. Learning mathematics is more than just memorizing formulas; you must also comprehend where they originate from. For further references regarding this discussion, see Kress [17].

The error estimate of the composite quadrature formulas are derived by taking the uniform partition, i.e. $h := \frac{b-a}{n}$ where n is the number of nodes. Now, we are going to discuss the derivation of the error estimation formula of composite quadrature formulas.

Theorem 8. Let f, f', and f'' be continuos on $[a,b]$ and $M_n(f)$ is the midpoint formula, i.e. $M_n(f) = 2h\sum_{k=1}^{\frac{n}{2}} f(a + (2k-1)h)$, then there exists $\xi \in (a,b)$ such that

$$I(f) - M_n(f) = \frac{(b-a)h^2}{6} f''(\xi). \qquad (7)$$

Proof. Divide interval $[a,b]$ into subintervals $[x_{2(k-1)}, x_{2k}]$, $k = 1,2,\cdots,\frac{n}{2}$ to form

$$I(f) - M_n(f) = \sum_{k=1}^{n/2}\left[\int_{x_{2(k-1)}}^{x_{2k}} f(x)\,dx - M_n^k(f)\right],$$

where $M_n^k(f) = 2h f\left(\frac{x_{2(k-1)}+x_{2k}}{2}\right) = 2hf(x_{2k-1})$. This is nothing but the midpoint formula on $[x_{2(k-1)}, x_{2k}]$. By using Theorem 4, for each $k = 1, 2, \cdots, n/2$ the following holds.

$$\int_{x_{2(k-1)}}^{x_{2k}} f(x)\,dx - M_n^k(f) = \frac{f''(\xi_k)}{24}\left(x_{2k} - x_{2(k-1)}\right)^3 = \frac{f''(\xi_k)}{24}(2h)^3 = \frac{f''(\xi_k)}{6}\frac{2(b-a)}{n}h^2.$$

Substitute this expression into summing for all k as previous, the following are obtained.

$$I(f) - M_n(f) = \frac{b-a}{6}h^2 \sum_{k=1}^{n/2}\left(\frac{2}{n}\right) f''(\xi_k).$$

Observe the coefficients $a_k = \frac{2}{n}$, $k = 1, 2, \cdots, n/2$, so that $\sum_1^{n/2} a_k = \sum_1^{n/2}\left(\frac{2}{n}\right) = \left(\frac{n}{2}\right)\left(\frac{2}{n}\right) = 1$. Since it is known that f'' is continuous on $[a, b]$ then by Theorem 2 there exists $\xi \in (a, b)$ such that $\sum_1^{n/2}\left(\frac{2}{n}\right) f''(\xi) = f''(\xi)$. Substitute it into previous expression, the proof is complete. ■

Theorem 9. Let f, f', and f'' be continuos on $[a, b]$ and $T_n(f)$ is the trapezoidal formula, i.e. $T_n(f) = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k)\right)$, then there exists $\xi \in (a, b)$ such that

$$I(f) - M_n(f) = -\frac{(b-a)h^2}{12} f''(\xi). \qquad (8)$$

Proof. The idea similar to prior proof, let $[x_{k-1}, x_k]$, $k = 1, 2, \cdots, n$ be subintervals partitioned of $[a, b]$. Using the additive property of integral on the partition, the following holds.

$$I(f) - T_n(f) = \sum_{k=1}^{n}\left[\int_{x_{k-1}}^{x_k} f(x)\,dx - T_n^k(f)\right] = \sum_{k=1}^{n} -\frac{(x_k - x_{k-1})^3}{12} f''(\xi_k)$$
$$= -\frac{h^2}{12}(b-a)\sum_{k=1}^{n}\frac{1}{n} f''(\xi_k) = -\frac{(b-a)h^2}{12} f''(\xi).$$

Theorem 2 has been applied on this derivation to term $\sum_{k=1}^{n}\frac{1}{n} f''(\xi_k)$ by noting that $\sum_{k=1}^{n}\frac{1}{n} = 1$. ■

Theorem 9. Let $f, f', f'', f^{(3)}$, and $f^{(4)}$ be continuos on $[a, b]$ and $S_n(f)$ is the Simpson formula, i.e. $S_n(f) = \frac{h}{3}\left(\left(f(a) + f(b) + 4\sum_{k=1}^{n/2} f(x_{2k-1}) + 2\sum_{k=1}^{n/2-1} f(x_{2k})\right)\right)$, then there exists $\xi \in (a, b)$ such that

$$I(f) - S_n(f) = -\frac{(b-a)h^4}{180} f^{(4)}(\xi). \qquad (9)$$

Proof. Recall that Simpson formula takes n even and the domain $[a, b]$ is partitioned by $[x_{2(k-1)}, x_{2k}]$, $k = 1, 2, \cdots, \frac{n}{2}$. Hence the subintervals is $2h$. Similar to when deriving the composite midpoint error formula we obtain $I(f) - S_n(f) = \sum_{k=1}^{n/2}\left[\int_{x_{2(k-1)}}^{x_{2k}} f(x)\,dx - S_n^k(f)\right]$ where $S_n^k(f)$ is the basic Simpson formula on $[x_{2(k-1)}, x_{2k}]$. For each $k = 1, 2, \cdots, \frac{n}{2}$, it can be found that

$$\int_{x_{2(k-1)}}^{x_{2k}} f(x)\,dx - S_n^k = -\frac{f^{(4)}(\xi_k)}{2880}\left(x_{2k} - x_{2(k-1)}\right)^5 = -\frac{f^{(4)}(\xi_k)}{2880}(2h)^5.$$

Splitting $h^5 = h^4\left(\frac{b-a}{n}\right)$ and using the fact $\sum_{k=1}^{n/2}\frac{2}{n} = 1$, the following is obtained.

$$\sum_{k=1}^{n/2}\left[\int_{x_{2(k-1)}}^{x_{2k}} f(x)\,dx - S_n^k(f)\right] = -\frac{(b-a)h^4}{180}\sum_{k=1}^{\frac{n}{2}}\left(\frac{2}{n}\right) f^{(4)}(\xi_k) = -\frac{(b-a)h^4}{180} f^{(4)}(\xi). \ ■$$

In the numerical simulation, the factors $\frac{1}{180}$ on Simpson, $\frac{1}{12}$ on trapezoidal, and $\frac{1}{6}$ on midpoint do not play significant role, meanwhile the power of h is extremely crucial because it affects the convergence rate of the quadrature formulas. In this case, the midpoint is called has the second-order of convergence, written by $\mathcal{O}(h^2)$ and trapezoidal has the fourth-order $\mathcal{O}(h^4)$. The influence of order convergence to the approximation behavior will be examined in the following numerical simulations.

RESULTS AND DISCUSSION

This section discusses some possibilities concerning with the sufficient conditions fulfillment and their corresponding with the convergence order attainable of several basic quadrature formulas. The methods were implemented by Matlab for $n = 2^k$, or $h = \frac{b-a}{2^k}$, $k = 1, 2, \cdots, 8$.

Simulation 1. $f_1(x) = xe^{-x^2}, x \in [0,4]$. The exact integral up to 16-digit accuracy is given by $I(f_1) = \int_0^4 f_1(x)\,dx = 0.499999943732413$. In this case, the function f and all its derivatives are continuous on domain $[0,4]$. The results are summarized on Table 2. The best accuracy is provided by Simpson, followed by midpoint and trapezoidal. It is found that the convergence rate $\frac{E(h)}{E(h/2)} \approx 4 = 2^2$ for midpoint and trapezoidal and $\frac{E(h)}{E(h/2)} \approx 16 = 2^4$ for Simpson. The power of 2 indicates the convergence order and it provides the information of approximation speed towards the exact. If the mesh is refined from h to $h/2$, the error reduces up to 25% for midpoint and trapezoidal and up to 6.25% for Simpson. This means that the convergence orders are perfectly attainable by three quadrature formulas. This is not surprising since f_1 satisfies the sufficient conditions properly. This perfect situation is rarely found in the applied sciences; some conditions are frequently flawed.

Table 2. Errors and convergence rates of Simulation 1.

k	n	Midpoint; Rate	Trapezoidal: Rate	Simpson; Rate
1	2	3.5347×10^{-1}; 1.49	4.2673×10^{-1}; 4.47	4.0231×10^{-1}; 26.08
2	4	2.3650×10^{-1}; 4.52	9.5119×10^{-2}; 4.45	1.5421×10^{-2}; 4.84
3	8	5.2342×10^{-2}; 4.79	2.1388×10^{-2}; 4.08	3.1885×10^{-3}; 22.63
4	16	1.0906×10^{-2}; 4.14	5.2414×10^{-3}; 4.02	1.4090×10^{-4}; 16.99
5	32	2.6331×10^{-3}; 4.03	1.3041×10^{-3}; 4.00	8.2927×10^{-6}; 16.23
6	64	6.5283×10^{-4}; 4.00	3.2565×10^{-4}; 4.00	5.1099×10^{-7}; 16.06
7	128	1.6287×10^{-4}; 4.00	8.1388×10^{-5}; 4.00	3.1825×10^{-8}; 16.00
8	256	4.0697×10^{-5}; 4.00	2.0346×10^{-5}; 4.00	1.9873×10^{-9}; 16.00

Simulation 2. $f_2(x) = \sqrt{1-x^2}$, $x \in [-1, 1]$. The exact value of integral is the area of a half unit-circle, i.e. $I(f_2) = \int_{-1}^{1} \sqrt{1-x^2}\ dx = \frac{\pi}{2} \approx 1.570796326794897$. This function is continuous on $[-1, 1]$, differentiable in interior but not differentiable at boundaries $x = \pm 1$. The numerical sumulation results are exhibited on Table 3.

Table 3. Errors and convergence rates of Simulation 2.

k	n	Midpoint; Rate	Trapezoidal: Rate	Simpson; Rate
1	2	4.2920×10^{-1}; 2.66	5.7080×10^{-1}; 2.79	2.3746×10^{-1}; 2.87
2	4	1.6125×10^{-1}; 2.74	2.0477×10^{-1}; 2.81	8.2762×10^{-2}; 2.85
3	8	5.8887×10^{-2}; 2.78	7.2942×10^{-2}; 2.82	2.8999×10^{-2}; 2.84
4	16	2.1168×10^{-2}; 2.80	2.5887×10^{-2}; 2.83	1.0202×10^{-2}; 2.84
5	32	7.5471×10^{-3}; 2.82	9.1698×10^{-3}; 2.83	3.5976×10^{-3}; 2.83
6	64	2.6796×10^{-3}; 2.82	3.2451×10^{-3}; 2.83	1.2702×10^{-3}; 2.83
7	128	9.4937×10^{-4}; 2.83	1.1479×10^{-3}; 2.83	4.4879×10^{-4}; 2.83
8	256	3.3600×10^{-4}; 2.83	4.0593×10^{-4}; 2.83	1.5862×10^{-4}; 2.83

It is found that the ratios for midpoint and trapezoidal are around 2.8 and the convergence order is derived as follows: $2^p = 2.8$ implies $p = \frac{\log 2.8}{\log 2} \approx 1.485$. It means that the second-order $\mathcal{O}(h^2)$ convergence is not reachable, but it's only around $\mathcal{O}(h^{1.5})$ which is often called superlinear convergence order. Special attention on Simpson performance that is not better than others in the accuracy as well as the convergence order. It is also discovered that the Simpson's reaches only a superlinear order $\mathcal{O}(h^{1.5})$ much lower than supposed $\mathcal{O}(h^4)$. In fact, the Simpson formula requires computational cost twice as much than two others. This is not surprising since f_2 failed to meet the sufficient condition.

Simulation 3. Consider the following function.

$$f(x) = \begin{cases} \dfrac{1}{1-x}, & -2 \le x \le 0 \\ \dfrac{1}{1+x}, & 0 < x \le 2. \end{cases}$$

The exact value up to 16-digit accuracy is $I(f_3) = 2\ln 3 = 2.197224577336219$. This function is not differentiable only at the interior $x = 0$ yet differentiable at points other than zero. The results are displayed on Table 4.

Table 3. Errors and convergence rates of Simulation 3.

k	n	Midpoint; Rate	Trapezoidal: Rate	Simpson; Rate
1	2	1.8028×10^{1}; 9.14	4.6944×10^{1}; 3.44	9.1389×10^{-1}; 36.56
2	4	1.9722×10^{-1}; 3.09	1.3611×10^{-1}; 3.77	2.4998×10^{-2}; 9.01
3	8	6.3891×10^{-2}; 3.61	3.6109×10^{-2}; 3.93	2.7754×10^{-3}; 12.27
4	16	1.7715×10^{-2}; 3.87	9.1968×10^{-3}; 4.00	2.2612×10^{-4}; 14.58
5	32	4.5751×10^{-3}; 3.96	2.3108×10^{-3}; 4.00	1.5508×10^{-5}; 15.58
6	64	1.1539×10^{-3}; 4.00	5.7845×10^{-4}; 4.00	9.9540×10^{-6}; 15.89
7	128	2.8913×10^{-4}; 4.00	1.4466×10^{-4}; 4.00	6.2646×10^{-7}; 15.97
8	256	1.8083×10^{-4}; 4.00	3.1668×10^{-5}; 4.00	1.5331×10^{-8}; 15.99

According to simulation results the convergence orders are achieved very well by three formulas eventhough the sufficient conditions were not satisfied. The midpoint and trpezoidal formula attain the second-order $O(h^2)$ anda the Simpson formula reaches the fouth-order $O(h^4)$. This confirm than a failure to satisfy the sufficient condition does not make invalid the theorem conclusion. Returning to the illustration of the store advertisement at the beginning of the background, no conclusions can be drawn for consumers who spend less than IDR100,000,-.

CONCLUSION

The numerical implementation had been conducted for three distinct examples. The first example represents the case where all the conditions of the theorem are satisfied and the order of convergence is reached perfectly. The second example deputizes the case where the sufficient conditions are not met only at the boundary points and the order of convergence is not achieved maximally. The third example shows the case where the sufficient conditions are not fulfilled at single interior point but order of convergence is well-achieved. From those numerical simulations it can be concluded that non-fulfillment of sufficient conditions does not imply unattainable the order of convergence. In case all sufficient conditions are fulfilled, the Simpson method is much better than other two.

It should be noted that the higher demand to the convergence order, the higher computational complexity and, without a doubt, the more sensitive to computer rounding errors. The incompatibility between theoretical background and computer output could be caused by such factors, especially when computer rounding errors dominate over approximation errors. Hence, it should take into consideration a trade-off between the expected accuracy and the computational effort. In addition to the rounding error issue, scientists who use mathematics directly through the computer programs are suggested to consider the possibility that the computational results are not optimal because of unfulfilled the sufficient conditions.

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