Some Remarks on Mathematical Reasoning Relating to Sufficient Conditions of Theorems: A Case Study on the Quadrature Formulas of Integral

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Abstract

One issue with mathematical reasoning is that many college students do not really understand the mathematical rules underlying the conditional statement $p \to q$. 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 and then examined for cases where the sufficient conditions are fulfilled as well as cases where they are not fulfilled.

Keywords: Mathematical reasoning, sufficient condition, integral approximation, quadrature formula, error estimation, accuracy, convergence order.
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1 Introduction

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 certain to fail. This fact is at least based on the author's own real experience in mathematics 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 proposition in which the truth can be proven. The formulas in mathematics are actually a part of the theorem. The mathematical statements are generally in the form of compound sentences containing connectivities such as negation ($\neg$), disjunction ($\vee$), exclusive disjunction ($\oplus$), conjunction ($\wedge$), implication ($\to$), and bi-implication ($\leftrightarrow$). The notation implication $p \to q$ is read "if p then q" or "p implies q" or "p is a sufficient condition for q". The implication $p \to q$ is sometimes called the conditional statement where p is the antecedent and q the conclusion. Some simple and interesting illustrations of the sufficient and necessary conditions has been exposed in [10]. Greenberg in [4] claimed that almost all theorems in mathematics can be represented in the form of conditional sentences. For example, "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 $\frac{x}{y} + \frac{y}{x} > 2$".

Tab. 1.1: Truth value of implication, converse, inverse, and contrapositive

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

Tabel 1 shows the 4 possibilities of implication $p \to q$ and its variants. Let $\tau(p)$ stands for the truth value of proposition p, then the only case $\tau(p \to q) = F$ only if $\tau(p) = T$ and $\tau(q) = F$, other cases are true. The logic consideration of the implications truth value has been examined in [7, 12] and the reason fits to human cognition. A various forms of implication $p \to q$ are converse $(q \to p)$, inverse $(\neg p \to \neg q)$, and contrapositive $(\neg q \to \neg p)$. It can be verified that $p \to q \equiv \neg q \to \neg p$ and they are called equivalent. The similar fact also holds for inverse and converse.

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 is represented as $p_1 \wedge p_2 \to q$. 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. 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 can not be verified. As reported by Krantz [12] 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 [12]. 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. In the other hand, modifying the sufficient condition of theorem to make it easier to examine is an issue in mathematics research. Some well-known theorems are frequently proven in the classroom while learning mathematics. As mentioned in [15], 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. Some authors also mentioned the importance of proof in mathematics, see for instance, [1, 3, 4, 13].

The paper begins by presenting some preliminaries of integral approximation schemes. Derivation of three quadrature formulas will be presented in this part as well as the problem formulation of obtaining the error terms as a function of partition size. In the next section, some supporting theorems for solving the problems will be reviewed and commented. Hereafter, some theorems which describe the error estimation of basic quadrature formulas are presented and proved. Finally, some numerical simulations are carried over to justify the conclusion of theorem in case the sufficient fulfilled as well as unfulfilled.

2 Preliminaries of Integral Approximation

A various definitions of integral are intended to provide theoretical justification for various problems that arise from mathematics and applied sciences. The integral was theoretically de ned as an in nite process, but computing integral using de nition is not appropriate in practical application. The finite sum is built by taking the values of integrand f at finite number of points in $[a, b]$. The quadrature formula of $n + 1$ points is given by:

$$I(f) = \int_a^b f(x)\, dx = \sum_{i=0}^{n} w_i f(x_i) + R_n. \tag{2.1}$$

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 the reminder or error term. Afterwards, the definite integral $I(f)$ is approximated by the quadrature formula:

$$I(f) \approx Q(f) := \sum_{i=0}^{n} w_i f(x_i). \tag{2.2}$$

The first problem is how to choose the abscissa x_i's and to determine the weight of w_i's so that $Q(f)$ in (2.2) is a good approximation for $I(f)$ in (2.1). The next problem is how to obtain 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 $\int_a^b f(x)dx$ is approximated by $\int_a^b P_n(x)dx$. The calculation of $\int_a^b P_n(x)dx$ is trivial. 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. $P_n(x_i) = f(x_i)$, $i = 0, 1, \cdots, n$. The interpolation polynomial can be constructed by either Lagrange or divided-difference method [2, 15]. The basic quadrature formulas are built up by taking $n = 0, 1, 2$.

- for $n = 0$ take node $x_0 = \frac{a+b}{2}$, results the midpoint formula: $I(f) \approx M(f) = (b-a)f\left(\frac{a+b}{2}\right)$, the appropriate weight is $w_0 = b - a$.
- for $n = 1$ take node $x_0 = a$ and $x_1 = b$, results the trapezoidal formula: $I(f) \approx T(f) = \frac{1}{2}(b-a)\left(f(a) + f(b)\right)$, the relevant weights are $w_0 = w_1 = \frac{b-a}{2}$.
- for $n = 2$ take node $x_0 = a, x_1 = \frac{a+b}{2}$, and $x_2 = b$, results the Simpson formula: $I(f) \approx S(f) = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$, the appropriate weights are $w_0 = \frac{b-a}{6}$, $b_1 = \frac{2}{3}(b-a)$, and $w_2 = \frac{b-a}{6}$.

In order to improve the accuracy, the interval $[a, b]$ is partitioned into $x_0 := a < x_1 < x_2 < \cdots < x_n := b$, then, the basic quadrature formulas applied 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: for each three consecutive nodes $x_{k-1}, x_k, x_{k+1}, k = 1, 3, \cdots, n-1$, one has $M_k(f) = (x_{k+1} - x_{k-1})f(x_k) = 2hf(x_k)$. By summing up these terms, we obtain the midpoint (composite) formula.
$$M(f) = \sum_{k=1, k \text{ odd}}^{n-1} M_k(f) = 2h \sum_{k=1}^{n/2} f(a + (2k-1)h).$$
- Simpson: for each three consecutive nodes $x_{k-1}, x_k, x_{k+1}, k = 1, 3, \cdots, n-1$, one has $S_k(f) = \frac{h}{3}\left(f(x_{k-1} + 4f(x_k) + f(x_{k+1})\right)$ and the Simpson formula is obtained.
$$S(f) = \frac{h}{3}\left(f(a) + f(b) + 4\sum_{k=1}^{\frac{n}{2}} f(x_{2k-1}) + 2\sum_{k=1}^{\frac{n}{2}-1} f(x_{2k})\right).$$
- Trapezoidal: a single trapezoidal formula is resulted by two consecutive nodes $x_{k-1}, x_k, k = 1, 2, \cdots, n$, i.e. $T_k(f) = \frac{1}{2}(x_k - x_{k-1})\left(f(x_{k-1}) + f(x_k)\right)$. The trapezoidal formula is given by:
$$T(f) = \sum_{k=1}^{n} T_k(f) = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k)\right).$$

Recall that n must be even for midpoint and Simpson while trapezoidal could be odd. Some detail derivation of basic quadrature formulas can be read on the elementary numerical method textbooks [3, 2]. The calculating technique of definite integral using definition has been discussed in [14] while the proofs of error estimates given in [13].

The main problem in this paper is how to obtain the error term R_n as a function of h. Once this error term is known, the estimated error and the order of convergence of the approximation formula can be known. Furthermore how to understand the meaning of these two terms from the numerical simulations.

3 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 B-IVT are formally presented as follows.

Theorem 3.1. D-IVT STANDAR *Let $f : [a, b] \to \mathbb{R}$ be a continuous function α a real number between $f(a)$ and $f(b)$, then there always $c \in (a, b)$ such that $f(c) = \alpha$.*

To prove this theorem we need the Bolzano intermediate value theorem or theorem of root location (RLT) as follows: 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 $f(x) = 0$. For the proof, see [2, 8].

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 we can take $c = a$ or $c = b$. Without lost of generality, we assume $f(a) < f(b)$, as a consequence we have $f(a) < \alpha < f(b)$. Take $h(x) := f(x) - \alpha$, then we find h is continuous, $h(a) = f(a) - \alpha < 0$ and $h(b) = f(b) - \alpha > 0$. It can 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 $\lambda_i > 0$ as well as $\lambda_i f(a) < \lambda_i\alpha_i < \lambda_i f(b)$. Summing up all terms of the inequality $(i = 1, 2, \cdots, n)$ we obtain: $f(a)\sum_{i=1}^{n} \lambda_i < \sum_{i=1}^{n} \lambda_i\alpha_i < f(b)\sum_{i=1}^{n} \lambda_i$. It is known that $\sum_{i=1}^{n} \lambda_i = 1$, so we conclude that $f(a) < \sum_{i=1}^{n} \lambda_i\alpha_i < f(b)$. Formally, the extended version of D-IVT is described as follows.

Theorem 3.2. D-IVT EXTENDED *$f : [a, b] \to \mathbb{R}$ a continuous function on $[a, b]$ and $\alpha_1, \alpha_2, \cdots, \alpha_n$ are real number located 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 $f(c) = \sum_{i=1}^{n} \lambda_i\alpha_i$.*

If we take in Theorem **??**, $\alpha_1 = \alpha_2 = \cdots = \alpha_n := \alpha$ and $\lambda_i := \frac{1}{n}$ for each $i = 1, 2, \cdots, n$ then we get Theorem **??**. This is the reason why Theorem **??** is called the extended version of Theorem **??**.

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

Commentary Here, $f(c) = \frac{1}{b-a}\int_a^b f(x)dx$ is understood as the mean of f on $[a, b]$. Suppose that the continuous condition is weakened 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 on $[0, n]$, 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 nothing but the ordinary (arithmetic) mean for discrete data $y_1, y_2, \cdots, y_n$.

Proof. Since f continuous on $[a, b]$, the maximum and minimum within $[a, b]$ are reachable, say $m = \min_{x\in[a,b]} f(x)$ dan $M = \max_{x\in[a,b]} f(x)$. Therefore, the following inequality holds $m \leq f(x) \leq M$ for each $x \in [a, b]$. Integrate both sides, we obtain $m(b-a) \leq \int_a^b f(x)dx \leq M(b-a)$ or $m \leq \frac{\int_a^b f(x)dx}{b-a} \leq M$.

Let $a' := \text{argmin} f(x)$, $b' := \text{argmax} f(x)$, $x \in [a, b]$ and $\alpha = \frac{\int_a^b f(x)dx}{b-a}$ then according to Theorem **??**, there exists $c \in (a', b') \subseteq (a, b)$ such that $f(c) = \alpha = \frac{\int_a^b f(x)dx}{b-a}$ or $\int_a^b f(x)dx = f(c)(b-a)$. □

4 Error Estimation of Quadrature Formulas

As mentioned earlier that integral approximation by quadrature formula is based on polynomial interpolation. If the interpolation is applied on whole domain $[a, b]$ we obtain the basic quadrature formulas. Otherwise, if the domain is partitioned into several subdomains we obtain the composite quadrature formulas. The composite quadrature formulas depend on parameter h as the partition length (mesh) or index n representing the number of subintervals. Following are three theorems concerned with the error estimation of the basic quadrature formulas.

Theorem 4.1. *If $f \in \mathcal{C}^2[a, b]$, i.e. continuously differentiable up to second order, then there exists $\xi \in (a, b)$ such that the midpoint gives following error.*

$$I(f) - M(f) := \int_a^b f(x)\,dx - (b-a) f\left(\frac{a+b}{2}\right) = \frac{f''(\xi)}{24}(b-a)^3. \tag{4.1}$$

Proof. Apply the Taylor theorem around $x_0 = \frac{a+b}{2}$, that means for each $x \in [a, b]$ there is a $\xi(x) \in (a, b)$ such that $f(x) - f(x_0) = f'(x_0)(x - x_0) + \frac{f''(\xi(x))}{2}(x - x_0)^2$. By considering that $\int_a^b f(x_0)dx = (b-a) f\left(\frac{a+b}{2}\right) = M(f)$ we obtain

$$\begin{aligned} I(f) - M(f) &= \int_a^b \left(f(x) - f(x_0)\right) dx \\ &= \underbrace{\int_a^b f'(x_0)(x - x_0)dx}_{=0} + \int_a^b \frac{f''(\xi(x))}{2}(x - x_0)^2 dx \\ &= \frac{f''(\xi)}{6}\left[\left(\frac{b-a}{2}\right)^3 - \left(\frac{a-b}{2}\right)^3\right] = \frac{f''(\xi)}{24}(b-a)^3. \end{aligned}$$

The proof is actually already complete. For further explanation, the zero of the first term can be validated easily by using the fact that $\int_a^b (x - x_0)dx = 0$. Meanwhile, the second term is derived by Theorem **??**, that is by taking $g(x) := (x - x_0)^2 \geq 0$ and $f_1(x) := \frac{f''(\xi(x))}{2}$, and 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 $\xi \in (a, b)$. □

The error estimation derivation of the trapezoidal and Simpson's method needs the polynomial interpolation error formula as stated on following theorem. The proof can be found on [15].

Theorem 4.2. *Suppose that $f : [a, b] \to \mathbb{R}$ has continuous derivatives up to order of $n + 1$. If P_n is the interpolation polynomial of function f at nodes $x_0, x_1, \cdots, x_n \in [a, b]$ then following estimate holds,*

$$f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n) \tag{4.2}$$

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

Theorem 4.3. *If $f \in \mathcal{C}^2[a, b]$ then there exists $\xi \in (a, b)$ so that the trapezoidal method holds the following estimate.*

$$I(f) - T(f) = \int_a^b f(x)\,dx - \frac{b-a}{2}\left(f(a) + f(b)\right) = -\frac{f''(\xi)}{12}(b-a)^3. \tag{4.3}$$

Proof. Let $P_2 := L_2 f$ be the second order polynomial of f, then we have $E_1(f) = \int_a^b \left(f(x) - (L_2 f)(x)\right) dx = I(f) - T(f)$. By the error formula (4.2) for $n = 1$, then for each $x \in [a, b]$ we have $R_2(x) = f(x) - (L_2 f)(x) = \frac{f''(\xi(x))}{2}(x - a)(x - b)$ where $\xi(x) \in (a, b)$. Furthermore,

$$I(f) - T(f) = \int_a^b R_2(x)dx = \int_a^b \frac{f''(\xi(x))}{2}(x - a)(x - b)dx$$

Applying I-MVT extended, take $g(x) := (x-a)(x-b) \leq 0$ and $f_1(x) := \frac{f''(\xi(x))}{2}$, there is a number $\xi \in (a,b)$ so that

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

By elementary calculus the following is easily to do.

$$\begin{aligned}\int_a^b (x-a)(x-b)dx &= \int_a^b (x-a)(x-a+(a-b))dx \\ &= \int_a^b (x-a)^2 dx + \int_a^b (a-b)(x-a)dx \\ &= \left[\frac{1}{3}(x-a)^3 + \frac{a-b}{2}(x-a)\right]_a^b = -\frac{1}{6}(b-a)^3.\end{aligned}$$

Substituting this result into previous integral, we obtain

$$E_1(f) = I(f) - T(f) = \frac{f''(\xi)}{2}\int_a^b ((x-a)(x-b))\,dx = -\frac{f''(\xi)}{12}(b-a)^3.$$

□

Theorem 4.4. *In condition that $f \in \mathcal{C}^4[a,b]$ then there exists $\xi \in (a,b)$ so that the Simpson method satisfies the following error estimate*

$$I(f) - S(f) = \int_a^b f(x)dx - \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right) = -\frac{f^{(4)}(\xi)}{2880}(b-a)^5. \tag{4.4}$$

Proof. The proof here refers to ideas given in [15]. Let $L_2 f$ be the second order polynomial interpolation of f on nodes $x_0 = a, x_1 = \frac{1}{2}(a+b)$ and $x_2 = b$. This means, $E_2(f) := I(f) - S(f) = \int_a^b [f(x) - (L_2 f)(x)]\,dx$. Construct the following cubic polynomial: $p(x) := (L_2 f)(x) + \frac{4}{(b-a)^2}\left[(L_2 f)'(x_1) - f'(x_1)\right] q_3(x)$ where $q_3(x) = (x-x_0)(x-x_1)(x-x_2)$. We obtain the following properties for p:

- for $k = 0,1,2$ then $q_3(x_k) = 0$, so that $p(x_k) = (L_2 f)(x_k) + 0 = f(x_k)$; hence p interpolated.
- $p'(x) = (L_2 f)'(x) + \frac{4}{(b-a)^2}\left[(L_2 f)'(x_1) - f'(x_1)\right] q_3^{'}(x)$. It's easy to calculate to find $q_3^{'}(x_1) = \frac{1}{4}(b-a)^2$, we obtain $p'(x_1) = f'(x_1)$.

Similarly, we also have $\int_a^b q_3(x)\,dx = \int_a^b (x-x_0)(x-x_1)(x-x_2)dx = 0$. This fact can be understood since q_3 is an odd function with respect to $x = x_1$. Hence, the error formula $E_2 f$ can be written as $E_2(f) = \int_a^b [f(x) - p(x)]\,dx$. By taking $g(x) := (x-x_0)(x-x_1)^2(x-x_2)$ then $g(x) \leq 0$ for all $x \in [a,b]$. By applying the L'Hospital rule, it can be shown the following limit exist for $x_k = x_0, x_1$, dan x_2.

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

Let say the limit values are ℓ_0, ℓ_1, and ℓ_2, respectively. Then the function h defined below continuous on $[a,b]$, in particular at $x = x_k$, $k = 0,1,2$.

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

It now the error E_2 can be written as:

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

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

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

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 the interpolation error formula (4.2), there is a $\xi \in (a,b)$ such that $f(z)-p(z) = \frac{f^{(4)}(\xi)}{4!}(z-x_0)(z-x_1)^2(z-x_2)$. On the other hand, it is trivial to gain $\int_a^b (x-x_0)(x-x_1)^2(x-x_2)dx = -\frac{(b-a)^5}{120}$. Substituting both results into (*), we finally get $E_2(f) = -\frac{f^{(4)}(\xi)}{4!}\frac{(b-a)^5}{120} = -\frac{f^{(4)}(\xi)}{2880}(b-a)^5$. □

The error estimate of the composite quadrature formulas are derived by taking the uniform partition, i.e. $h := \frac{b-a}{n}$ where n the number of nodes.

Theorem 4.5. *Let f, f' and f'' be continuous on $[a,b]$ and given the following midpoint formula,*

$$M_n(f) = 2h\sum_{k=1}^{n/2} f(a+(2k-1)h),$$

then there exists $\xi \in (a,b)$ such that

$$I(f) - M_n(f) := \int_a^b f(x)dx - M_n(f) = \frac{(b-a)h^2}{6} f''(\xi). \qquad (4.5)$$

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

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

where $M_n^k(f) = 2hf\left(\frac{x_{2(k-1)}+x_{2k}}{2}\right) = 2hf(x_{2k-1})$, the midpoint formula on $[x_{2(k-1)}, x_{2k}]$. According to Theorem 4.1, then for each $k = 1,2,\cdots,\frac{n}{2}$ the following holds.

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

Substitute back into sigma sign we obtain: $I(f) - M_n(f) = \frac{b-a}{6}h^2\sum_{k=1}^{n/2}\left(\frac{2}{n}\right)f''(\xi_k)$. Think the coefficients $a_k = \frac{2}{n}$, $k = 1,2,\cdots,\frac{n}{2}$, we find $\sum_{k=1}^{n/2} a_k = \left(\frac{n}{2}\right)\left(\frac{2}{n}\right) = 1$. Remembering the hypothesis that f'' continuous on $[a,b]$ then by Theorem **??**, there exists $\xi \in (a,b)$ such that $\sum_{k=1}^{n/2}\left(\frac{2}{n}\right)f''(\xi_k) = f''(\xi)$. The proof is complete by substituting this result into expression of previous stage. □

Theorem 4.6. *Let f, f' and f'' be continuos functions on $[a,b]$ and $T_n(f) = \frac{h}{2}\left(f(a)+f(b)+2\sum_{k=1}^{n-1} f(x_k)\right)$ the trapezoidal formula, then there exists $\xi \in (a,b)$ such that*

$$I(f) - T_n(f) := \int_a^b f(x)dx - T_n(f) = -\frac{(b-a)h^2}{12} f''(\xi). \qquad (4.6)$$

Proof. Follow a similar idea to previous proof, let $[x_{k-1}, x_k], k = 1,2,\cdots,n$ be subintervals partitioned of $[a,b]$. By applying the additive property of integral along this partition we have

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

Here, Theorem **??** had been applied to $\sum_{k=1}^{n}\frac{1}{n}f''(\xi_k)$ by noting that $\sum_{k=1}^{n}\frac{1}{n} = 1$. □

Theorem 4.7. *Let $f, f', f'', f^{(3)}$ and $f^{(4)}$ be continuous in $[a,b]$ and*

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

is the Simpson approximation, then there exists $\xi \in (a,b)$ such that

$$I(f) - S_n(f) := \int_a^b f(x)dx - S_n(f) = -\frac{(b-a)h^4}{180} f^{(4)}(\xi).$$

Proof. Recall that Simpson formula takes n even, then the domain $[a,b]$ partitioned by $[x_{2(k-1)}, x_{2k}]$, $k = 1, 2, 3, \cdots, \frac{n}{2}$. Hence, the subinterval length is $2h$. Similar to when we decipher the composite midpoint formula before to 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 find that

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

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.

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

□

In the numerical simulation, the factors $\frac{1}{180}$ on Simpson, $\frac{1}{12}$ on trapezoidal, and $\frac{1}{6}$ on midpoint are not the critical issues. However, the power of h is significance because it affects the convergence rate of the quadrature formulas. We say the midpoint and trapezoidal have the second-order of convergence, written by $\mathcal{O}(h^2)$, while Simpson provides the fourth-order $\mathcal{O}(h^4)$. The following numerical experiments examine the significance of order convergence with respect to the approximation behavior.

5 Numerical Experiments

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

Experiment 1: $f_1(x) = xe^{-x^2}, x \in [0,4]$. The exact integral is given by $I(f_1) = \int_0^4 xe^{-x^2}dx = 0.499999943732413$. The function and all derivatives are continuously on domain $[0,4]$. The results are summarized on Table 1.

The best accuracy given by the Simpson, followed by the midpoint and trapezoidal. It is found that the convergence rate $\frac{E(h)}{E(h/2)} \approx 4 = 2^2$ for the midpoint and trapezoidal and $\frac{E(h)}{E(h/2)} \approx 16 = 2^4$ for the Simpson. The power of 2 indicates the convergence order and it provides the information of speed towards the exact. If the mesh is refined from h to $\frac{h}{2}$ then the error reduces to 25% for midpoint and trapezoidal and to 6.25% for Simpson. This means that convergence orders are maximally reached by three quadrature formulas. This is not surprisingly because the sufficient conditions are fulfilled by f_1.

Tab. 5.1: Errors and convergence rates of Experiment 1.

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

Experiment 2: $f_2(x) = \sqrt{1-x^2}, x \in [-1,1]$. The exact integral is equal to the area of a half unit-circle, i.e. $I(f_2) = \int_{-1}^{1} \sqrt{1-x^2} = \pi/2 = 1.570796326794897$. This function is continuous on $[-1,1]$ but not differentiable at boundaries $x = \pm 1$. The results are presented on Table 2.

It is found that the ratios of midpoint and trapezoidal are around 2.8 and the convergence order is derived as follows: $2^p = 2.8$ so that $p = \frac{\log 2.8}{\log 2} \approx 1.485$. That means the convergence of second-order $\mathcal{O}(h^2)$ is not reachable, but only around $\mathcal{O}(h^{1.5})$. The convergence order between 1 and 2 is sometimes called superlinear. It is also discovered that the Simpson's method only reaches superlinear $\mathcal{O}(h^{1.5})$ worse than supposed to give $\mathcal{O}(h^4)$. In this problem the sufficient conditions are not satisfied by f_2.

Tab. 5.2: Errors and convergence rates of Experiment 2.

k	n	Midpoint; Rate	Trapezoidal; Rate	Simpson; Rate
1	2	$4.2920 \times 10^{-1}; 2.66$	$5.7080 \times 10^{-1}; 2.79$	$2.3746 \times 10^{-1}; 2.87$
2	4	$1.6125 \times 10^{-1}; 2.74$	$2.0477 \times 10^{-1}; 2.81$	$8.2762 \times 10^{-2}; 2.85$
3	8	$5.8887 \times 10^{-2}; 2.78$	$7.2942 \times 10^{-2}; 2.82$	$2.8999 \times 10^{-2}; 2.84$
4	16	$2.1168 \times 10^{-2}; 2.80$	$2.5887 \times 10^{-2}; 2.83$	$1.0202 \times 10^{-2}; 2.84$
5	32	$7.5471 \times 10^{-3}; 2.82$	$9.1698 \times 10^{-3}; 2.83$	$3.5975 \times 10^{-3}; 2.83$
6	64	$2.6796 \times 10^{-3}; 2.82$	$3.2451 \times 10^{-3}; 2.83$	$1.2702 \times 10^{-3}; 2.83$
7	128	9.4937×10^{-4}; 2.83	$1.1479 \times 10^{-3}; 2.83$	$4.4879 \times 10^{-4}; 2.83$
8	256	3.3600×10^{-4}; 2.83	$4.0593 \times 10^{-4}; 2.83$	$1.5862 \times 10^{-4}; 2.83$

Experiment 3: Consider the following function:

$$f_3(x) := \begin{cases} \frac{1}{1-x}, & -2 \le x \le 0 \\ \frac{1}{1+x}, & 0 < x \le 2. \end{cases}$$

The exact solution is $I(f_3) = 2\ln 3 = 2.197224577336219$. This function is not differentiable at the interior $x = 0$. The results are displayed on Table 3.

The result is quite surprising because the convergent orders are achieved almost perfectly, i.e. $\mathcal{O}(h^2)$ for midpoint and trapezoidal and $\mathcal{O}(h^4)$ for Simpson, even though the sufficient conditions were not met by f_3.

6 Concluding Remarks

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

Tab. 5.3: Errors and convergence rates of Experiment 3.

k	n	Midpoint; Rate	Trapezoidal; Rate	Simpson; Rate
1	2	$1.8028 \times 10^{1}; 9.14$	$4.6944 \times 10^{1}; 3.44$	$9.1389 \times 10^{-1}; 36.56$
2	4	$1.9722 \times 10^{-1}; 3.09$	$1.3611 \times 10^{-1}; 3.77$	$2.4998 \times 10^{-2}; 9.01$
3	8	$6.3891 \times 10^{-2}; 3.61$	$3.6109 \times 10^{-2}; 3.93$	$2.7754 \times 10^{-3}; 12.27$
4	16	$1.7715 \times 10^{-2}; 3.87$	$9.1968 \times 10^{-3}; 4.00$	$2.2612 \times 10^{-4}; 14.58$
5	32	$4.5751 \times 10^{-3}; 3.96$	$2.3108 \times 10^{-3}; 4.00$	$1.5508 \times 10^{-5}; 15.58$
6	64	$1.1539 \times 10^{-3}; 4.00$	$5.7845 \times 10^{-4}; 4.00$	$9.9540 \times 10^{-6}; 15.89$
7	128	$2.8913 \times 10^{-4}; 4.00$	$1.4466 \times 10^{-4}; 4.00$	$6.2646 \times 10^{-7}; 15.97$
8	256	$1.8083 \times 10^{-4}; 4.00$	$3.6168 \times 10^{-5}; 4.00$	$1.5331 \times 10^{-8}; 15.99$

It should be noted that the higher demand to order of convergence, 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.

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