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# Numerical Integration Through Concavity Analysis

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# Numerical Integration Through Concavity Analysis

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**Abstract.** We introduce a relationship between the concavity of a $C^2$ function and the area bounded by its graph and secant line. We utilize this relationship to develop a method of numerical integration. We then bound the error of the approximation, and compare to known methods, finding an improvement in error bound over methods of comparable computational complexity.

## 1 Introduction

Calculating the area underneath a curve is the motivating problem of integral calculus. Even as far back as 50 BC, the Babylonians did this numerically to approximate planetary orbits, using data collected on the planets' velocities [1]. Much later, Newton and Leibniz independently developed theorems for performing this task analytically to achieve an exact result [2]. These powerful theorems are useful for a variety of basic functions, however, most functions do not have closed form antiderivatives. Some well-known examples of these include the Gaussian distribution, Fresnel functions, and certain exponential functions [3]. Similarly, real-world applications often involve measurements in the form of discrete points rather than continuous functions that can be integrated analytically. Thus, some mathematicians began to put more focus on the development of numerical methods.

We develop a numerical method that uses derivative information about the function to improve accuracy. In Section 2 we review existing numerical integration methods. In Section 3 we present the foundation for how our novel rule was initially discovered. In Section 4 we show how this foundation can be used to create a numerical integration rule. In Section 5 we show some examples of this rule in practice, as well as compare it to other methods. Lastly, Section 6 will outline the author's planned future work on this topic.

*Mathematics Subject Classification.* 65D30
*Keywords.* Numerical Integration, Integration, Numerical Analysis, Calculus, Derivative, Concavity

## 2 Existing Quadrature Methods

A quadrature rule is a method of approximating a definite integral, typically expressed as a weighted summation. When performing this summation, the interval $[a,b]$ may be broken into $n$ subintervals, and the function $f(x)$ is sampled at various $\{x_i \in \mathbb{R} \mid a \leq x_i \leq b\}$, and combined with weights $w_i$ such that

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i).$$

Placement of $x_i$ can vary between methods, but a common choice is to equally space them throughout $[a,b]$. Undergraduate students are typically introduced to quadrature rules in their second semester of Calculus through various well known numerical integration algorithms such as:

The Trapezoid Rule:

$$x_i = a + i\left(\frac{b-a}{n}\right)$$

$$w_i = \begin{cases} \frac{b-a}{2n} & i = 0 \\ \frac{b-a}{n} & 0 < i < n \\ \frac{b-a}{2n} & i = n \end{cases}$$

This rule was used by the Babylonians too, in one of the earliest known instances of numerical integration [1]. Other well-known methods include the Midpoint Rule and Simpson's Rule [4]. We state the weights for these rules now.

The Midpoint Rule

$$x_i = a + \frac{b-a}{2n} + i\left(\frac{b-a}{n}\right)$$

$$w_i = \frac{b-a}{2n}$$

Simpson's Rule

$$x_i = a + i\left(\frac{b-a}{n}\right)$$

$$w_i = \begin{cases} \frac{b-a}{3n} & i = 0 \\ \frac{4(b-a)}{3n} & 0 < i < n,\ i \text{ is odd} \\ \frac{2(b-a)}{3n} & 0 < i < n,\ i \text{ is even} \\ \frac{b-a}{3n} & i = n \end{cases}$$

In many cases there will be some error in these approximations as portions of the curve are either overestimated or underestimated. The error for each of these methods over a single interval of with R can be bounded by the following:

| Method | \|E\| |
|---|---|
| Trapezoid | $R^3/12$ |
| Midpoint | $R^3/24$ |
| Simpsons | $R^5/180$ |

Table 1: Error for Numerical Methods

If a more accurate result is needed for a given method, one can generally be achieved by increasing the number of subdivisions. For each method mentioned thus far, we have

$$\int_a^b f(x)dx = \lim_{n\to\infty} \sum_{i=0}^{n} w_i f(x_i).$$

It is instructive to look at a simple example of these methods. Table 2 shows these methods used to compute the integral of $f(x) = \sin(x)$ over the interval $x \in (0,1)$ with $n$ subintervals. In this example, the exact solution is $\int_0^1 \sin(x)dx = 1-\cos(1) \approx 0.459697\ldots$

| Method | $n=1$ | $n=2$ | $n=4$ | $n=10$ |
|---|---|---|---|---|
| Trapezoid | 0.4207 | 0.4501 | 0.4573 | 0.4593 |
| Midpoint | 0.4794 | 0.4645 | 0.4609 | 0.4599 |
| Simpson's | N/A | 0.4599 | 0.4597 | 0.4597 |

Table 2: $\int_0^1 \sin x\, dx$ computed using known numerical methods

All of these fall under the category of 'Newton-Cotes' methods [5, 6], and work by "mimicking" the curve using polynomials over small intervals. The general strategy for these methods is to increase the accuracy over each subinterval by taking a higher order polynomial approximation of the curve. Figure 1 shows how this polynomial approximation becomes more accurate on $f(x) = xe^{-x}$ over the interval $x \in [1,5]$ for polynomials of degree 1-4.

We see that as the number of points taken over the interval increases, the polynomial more closely fits $f(x)$, and thus our integral approximation becomes more accurate.

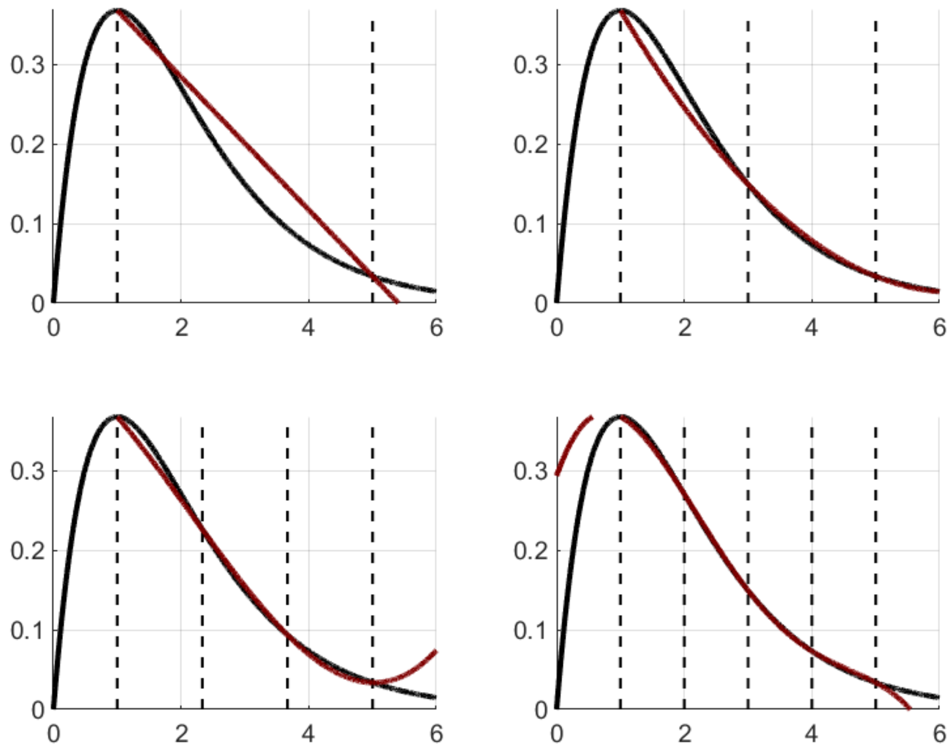


Figure 1: Polynomial Interpolation of $xe^{-x}$

In contrast to these methods, we develop an approach which augments the Trapezoid Rule by incorporating information about the derivatives of the function. Such methods have shown to provide more accurate results by accounting for curvature in the function over the period of integration, such as the technique described by Burg in 2012 [7]. Unlike methods which look at derivative values at the integration bounds, we develop a technique that instead requires concavity values at the center of the integration interval.

## 3 The Concavity-Area Connection

We begin with an observation: the area bounded by a parabola and its secant line over some interval depends only on the width of the interval.

**Proposition 1.** Let $f(x)$ denote a second degree polynomial in the form $f(x) = ax^2 + bx + c$. Let A be the area bounded by $y = f(x)$ and its secant line on the interval $(x_0 - r, x_0 + r)$. Then A is independent of $x_0$.

*Proof.* Let $f(x) = ax^2 + bx + c$. Let $\mathrm{I} = (x_0 - r, x_0 + r)$. The area of the region bounded by $y = f(x)$ and its secant line on I is

$$\int_{x_0-r}^{x_0+r} \left( \frac{f(x_0+r) - f(x_0-r)}{2r}(x - (x_0 - r)) + f(x_0 - r) - f(x) \right) dx = \frac{4r^3}{3} a.$$

□

Another way of phrasing Proposition 1 is this: if A is the area bounded by the graph of a quadratic and its secant line on an interval of positive radius $r$ centered at $x_0$, then

$$f''(x_0) = \frac{3}{2r^3}\mathrm{A}. \tag{1}$$

Allowing $r$ to approach 0, equation 1 is true of any function with continuous first and second derivatives. We prove this result now. Recall that $\mathscr{C}^2$ denotes the set of all functions with continuous first and second derivatives.

Let $r > 0$, $\mathrm{L}(x) = \frac{f(x_0+r)-f(x_0-r)}{2r}(x - (x_0 - r)) + f(x_0 - r)$, and $\mathrm{A} = \int_{x_0-r}^{x_0+r} \left(\mathrm{L}(x) - f(x)\right) dx$.

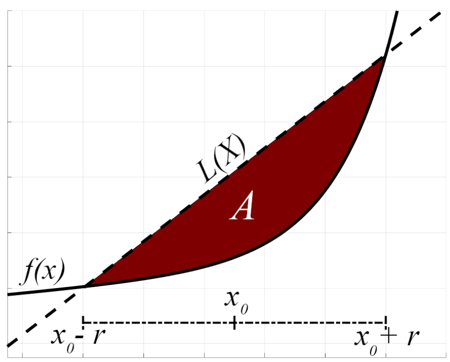


Figure 2: $f(x)$, $\mathrm{L}(x)$, and A

**Proposition 2.** Suppose $f$ is $\mathscr{C}^2$ on the interval $\mathrm{I} = (x_0 - r, x_0 + r)$. Then $\lim_{r\to 0} \frac{3}{2r^3}\mathrm{A} = f''(x_0)$.

*Proof.* Let $g(x) = f(x + x_0)$. We compute A:

$$\begin{aligned}
\mathrm{A} &= \frac{g(r) + g(-r)}{2} \cdot 2r - \int_{-r}^{r} g(x)\,dx \\
&= r(g(r) + g(-r)) - \left[\int_0^r g(x)\,dx + \int_{-r}^0 g(x)\,dx\right] \\
&= r(g(r) + g(-r)) - \left[\int_0^r g(x)\,dx - \int_0^{-r} g(x)\,dx\right] \\
&= r(g(r) + g(-r)) - \mathrm{G}(r) + \mathrm{G}(-r)
\end{aligned}$$

where $G(u) = \int_0^u f(x)\,dx$. Now applying L'Hôpital's rule we have

$$\begin{aligned}
\lim_{r\to 0} \frac{A}{r^3} &= \lim_{r\to 0} \frac{r(g(r)+g(-r)) - G(r) + G(-r)}{r^3} \\
&= \lim_{r\to 0} \frac{g(r)+g(-r)+rg'(r)-rg'(-r)-G'(r)-G'(-r)}{3r^2} \\
&= \lim_{r\to 0} \frac{g(r)+g(-r)+rg'(r)-rg'(-r)-g(r)-g(-r)}{3r^2} \\
&= \lim_{r\to 0} \frac{rg'(r)-rg'(-r)}{3r^2} \\
&= \lim_{r\to 0} \frac{g'(r)-g'(-r)}{3r} \\
&= \lim_{r\to 0} \frac{g''(r)+g''(-r)}{3} \\
&= \frac{2g''(0)}{3}
\end{aligned}$$

so that

$$\lim_{r\to 0} \frac{3}{2r^3} A = g''(0) = f''(x_0).$$

□

## 4 Numerical Integration Using Concavity

We now utilize Proposition 2 in order to develop a method of numerically approximating the definite integral of a function which is $\mathscr{C}^2$ on the domain of integration.

Suppose $f$ is $\mathscr{C}^2$ on a neighborhood $(-r,r)$ of 0. Let $L(x)$ be the secant line to $f(x)$ on $(-r,r)$. We have seen that $\frac{3}{2r^3}\int_{-r}^{r} L(x) - f(x)\,dx \approx f''(0)$ for small $r$. To approximate the integral, we solve for $\int_{-r}^{r} f(x)\,dx$.

**Lemma 4.1.** *Let $f$ be $\mathscr{C}^2$ on $I = (-r,r)$. Then*

$$\int_I f(x)\,dx \approx r(f(r)+f(-r)) - \frac{2r^3}{3} f''(0).$$

*Should $|f^{(4)}(x)| \le K$ on $I$, then the error $E$ in the estimate is bounded by*

$$|E| \le \frac{Kr^5}{15}.$$

*Proof.* We apply integration by parts several times, choosing integration constants that make odd derivative terms disappear from the final result. Because we are working with indefinite integrals, this is acceptable as long as we include these terms in the new integral at every step. When we finally switch to a definite integral, the end result of these constants will not affect the final result.

$$\begin{aligned}\int f(x)\,dx &= xf(x)-\int xf'(x)\,dx\\ &= xf(x)-\frac{1}{2}(x^2-r^2)f'(x)+\int\left(\frac{x^2}{2}-\frac{r^2}{2}\right)f''(x)\,dx\\ &= xf(x)-\frac{1}{2}(x^2-r^2)f'(x)+\left(\frac{x^3}{6}-\frac{r^2x}{2}\right)f''(x)\\ &\quad -\int\left(\frac{x^3}{6}-\frac{r^2x}{2}\right)f'''(x)\,dx\\ &= xf(x)-\frac{1}{2}(x^2-r^2)f'(x)+\left(\frac{x^3}{6}-\frac{r^2x}{2}\right)f''(x)\\ &\quad -\left(\frac{x^4}{24}-\frac{r^2x^2}{4}+\frac{5r^4}{24}\right)f'''(x)+\int\left(\frac{x^4}{24}-\frac{r^2x^2}{4}+\frac{5r^4}{24}\right)f^{(4)}(x)\,dx.\end{aligned}$$

Evaluating,

$$\begin{aligned}\int_{\mathrm{I}} f(x)\,dx &= r(f(r)+f(-r))-\frac{r^3}{3}(f''(r)+f''(-r))\\ &\quad+\int_{\mathrm{I}}\left(\frac{x^4}{24}-\frac{r^2x^2}{4}+\frac{5r^4}{24}\right)f^{(4)}(x)\,dx.\end{aligned}\tag{2}$$

We now work with the second term on the right side of (2):

$$\begin{aligned}f''(r)+f''(-r) &= 2f''(0)+\int_0^r f'''(x)\,dx+\int_0^{-r} f'''(x)\,dx\\ &= 2f''(0)+(x-r)f'''(x)\Big|_0^r-\int_0^r(x-r)f^{(4)}(x)\,dx\\ &\quad+(x+r)f'''(x)\Big|_0^{-r}-\int_0^{-r}(x+r)f^{(4)}(x)\,dx\\ &= 2f''(0)-\int_0^r(x-r)f^{(4)}(x)\,dx-\int_0^{-r}(x+r)f^{(4)}(x)\,dx.\end{aligned}\tag{3}$$

Substituting (3) into (2), we have

$$\int_{-r}^{r} f(x)\,dx = r(f(r)+f(-r))-\frac{2r^3}{3}f''(0)+\mathrm{E}$$

where $\mathrm{E} = \mathrm{E}_1 + \mathrm{E}_2 + \mathrm{E}_3$, and

$$\mathrm{E}_1 = \frac{r^3}{3}\int_0^r (x-r) f^{(4)}(x)\, dx$$
$$\mathrm{E}_2 = \frac{r^3}{3}\int_0^{-r} (x+r) f^{(4)}(x)\, dx$$
$$\mathrm{E}_3 = \int_{\mathrm{I}} \left(\frac{x^4}{24} - \frac{r^2x^2}{4} + \frac{5r^4}{24}\right) f^{(4)}(x)\, dx.$$

Computing, $|\mathrm{E}| = |\mathrm{E}_1 + \mathrm{E}_2 + \mathrm{E}_3| \le \frac{\mathrm{K}r^5}{15}$. □

Having the error bound on a single interval, we now split an interval of integration using a regular partition, that is a set of partitions of equal width, give our main estimation result, and bound the error of our numerical estimate accordingly. It is a modification of the Trapezoid Rule which improves accuracy by accounting for concavity information.

**Theorem 3.** Let $f(x)$ be $\mathscr{C}^2$ on $\mathrm{I} = [a, b]$. Let $\{a_i\}_{i=0}^n$ be a regular partition of I, with $a = a_0$ and $b = a_n$, and let $r = \frac{b-a}{2n}$. Then

$$\int_a^b f(x)\, dx \approx \sum_{i=0}^{n-1} \left[ r(f(a_i) + f(a_{i+1})) - \frac{2r^3}{3} f''(a_i + r)\right].$$

Should $|f^{(4)}(x)| \le \mathrm{K}$ on I, then the error E in the estimate is bounded by

$$|\mathrm{E}| \le \frac{\mathrm{K}(b-a)^5}{480n^4}.$$

*Proof.* Using the partition of I and invoking Lemma 4.1, we have

$$\begin{aligned}
&\left| \int_{\mathrm{I}} f(x)\, dx - \sum_{i=0}^{n-1} \left[ r(f(a_i) + f(a_{i+1})) - \frac{2r^3}{3} f''(a_i + r)\right]\right| \\
&\le \sum_{i=0}^{n-1} \left| \int_{a_i}^{a_{i+1}} f(x)\, dx - \left[ r(f(a_i) + f(a_{i+1})) - \frac{2r^3}{3} f''(a_i + r)\right]\right| \\
&\le \sum_{i=0}^{n-1} \left| \frac{\mathrm{K}r^5}{15} \right| = \frac{n\mathrm{K}(b-a)^5}{15(2n)^5} = \frac{\mathrm{K}(b-a)^5}{480n^4}.
\end{aligned}$$

□

It is instructive to compare the error bound to other well-known methods of numerical approximation of definite integrals. The Midpoint Rule and Trapezoid Rule have errors at most $|\mathrm{E_M}| \le \frac{\mathrm{K}(b-a)^3}{24n^2}$ and $|\mathrm{E_T}| \le \frac{\mathrm{K}(b-a)^3}{12n^2}$ respectively, where $|f''(x)| \le |\mathrm{K}|$ on $(a, b)$ [4]. Simpson's Rule has error at most $|\mathrm{E_S}| \le \frac{\mathrm{K}(b-a)^5}{180n^4}$.

## 5 Examples

We use Theorem 3 to estimate some definite integrals. We compare the errors arising from the estimate of Theorem 3, to the errors arising from some methods of comparable computational complexity; namely, the Midpoint, Trapezoid, and Simpson's Rules. The error for each of these four methods will be denotes as $\mathrm{E_C}$, $\mathrm{E_M}$, $\mathrm{E_T}$, and $\mathrm{E_S}$ respectively. The reader will recall that Simpson's Rule requires evenly many subintervals.

| | $n=1$ | $n=2$ | $n=4$ | $n=10$ |
|---|---|---|---|---|
| $\mathrm{E_C}$ | $9.90\cdot10^{-4}$ | $6.03\cdot10^{-5}$ | $3.75\cdot10^{-6}$ | $9.85\cdot10^{-8}$ |
| $\mathrm{E_M}$ | $0.02\cdot10^{-2}$ | $4.82\cdot10^{-3}$ | $1.20\cdot10^{-3}$ | $1.92\cdot10^{-4}$ |
| $\mathrm{E_T}$ | $0.04\cdot10^{-2}$ | $9.62\cdot10^{-3}$ | $2.40\cdot10^{-3}$ | $3.83\cdot10^{-4}$ |
| $\mathrm{E_S}$ | N/A | $1.64\cdot10^{-4}$ | $1.01\cdot10^{-5}$ | $2.57\cdot10^{-7}$ |

Table 3: Comparison of errors for $\int_0^1 \sin x\,dx$ using numerical methods

| | $n=1$ | $n=2$ | $n=4$ | $n=10$ |
|---|---|---|---|---|
| $\mathrm{E_C}$ | $4.49\cdot10^{-2}$ | $4.96\cdot10^{-3}$ | $3.97\cdot10^{-4}$ | $1.12\cdot10^{-5}$ |
| $\mathrm{E_M}$ | $6.94\cdot10^{-2}$ | $2.22\cdot10^{-2}$ | $6.08\cdot10^{-3}$ | $1.00\cdot10^{-3}$ |
| $\mathrm{E_T}$ | $1.63\cdot10^{-1}$ | $4.69\cdot10^{-2}$ | $1.24\cdot10^{-2}$ | $2.01\cdot10^{-3}$ |
| $\mathrm{E_S}$ | N/A | $8.14\cdot10^{-3}$ | $8.54\cdot10^{-4}$ | $2.84\cdot10^{-5}$ |

Table 4: Comparison of errors for $\int_0^1 \tan x\,dx$ using numerical methods

| | $n=1$ | $n=2$ | $n=4$ | $n=10$ |
|---|---|---|---|---|
| $\mathrm{E_C}$ | $1.08\cdot10^{-1}$ | $3.83\cdot10^{-2}$ | $1.35\cdot10^{-2}$ | $3.42\cdot10^{-3}$ |
| $\mathrm{E_M}$ | $4.04\cdot10^{-2}$ | $1.64\cdot10^{-2}$ | $6.31\cdot10^{-3}$ | $1.71\cdot10^{-3}$ |
| $\mathrm{E_T}$ | $1.67\cdot10^{-1}$ | $6.31\cdot10^{-2}$ | $2.34\cdot10^{-2}$ | $6.15\cdot10^{-3}$ |
| $\mathrm{E_S}$ | N/A | $2.86\cdot10^{-2}$ | $1.01\cdot10^{-2}$ | $2.56\cdot10^{-3}$ |

Table 5: Comparison of errors for $\int_0^1 \sqrt{x}\,dx$ using numerical methods

The concavity method performs comparatively well in cases where the $4^{\text{th}}$ derivative of the function is bounded over the interval. For contrast see the case of $\sqrt{x}$ in which the derivatives are unbounded near 0. In cases such as these, this method becomes less attractive than methods based on polynomial interpolation. In addition to these cases, the method can be more difficult to implement on real world numerical data where the derivatives of the function are not explicitly known. Attempts to approximate derivatives off of real world data can often times add significant noise to data [8], and as such it is often more accurate to use methods that do not rely on derivatives.

## 6 Future Work

The author plans on generalizing this rule, where additional even derivatives are taken at the midpoint of each interval. A generalization for the coefficients in this rule has been found and error bounds have been conjectured.

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