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1 The Three Main Error Bound Theorems

When you're trying to approximate the value of an integral, it's natural that you want to know how close your answer is to the correct answer. If the function you are integrating has an easy-to-calculate antiderivative, you can find the precision of your estimate by calculating the exact value of the integral and seeing how far away the exact and estimated answer are from each other; however, when integrating a function whose antiderivative you can't take, such as $f(x) = e^{-x^2/2}$, you don't have this luxury. Knowing absolutely anything - even a crude equality that bounds the precision of your answer - about the error is better than knowing nothing in this case.

This is where the **error bound** theorems come into play. For each of the major numerical integration techniques you've learned, there is a theorem that gives the error bound. First, we'll state the theorems, and then explain what they mean.

Error Bound for the Midpoint Rule: Suppose that $|f''(x)| \leq K$ for some $k \in \mathbb{R}$ where $a \leq x \leq b$. Then

$$|E_M| \leq k\frac{(b-a)^3}{24n^2}$$

Error Bound for the Trapezoid Rule: Suppose that $|f''(x)| \leq K$ for some $k \in \mathbb{R}$ where $a \leq x \leq b$. Then

$$|E_T| \leq k\frac{(b-a)^3}{12n^2}$$

Error Bound for Simpson's Rule: Suppose that $|f^{(IV)}(x)| \leq K$ for some $k \in \mathbb{R}$ where $a \leq x \leq b$. Then

$$|E_S| \leq k\frac{(b-a)^5}{180n^4}$$

I have used the symbol E_S to denote the error bound for Simpson's rule, E_T the error bound for the Trapezoid Rule, and so on.

For this class, it's best that you **memorize** these formulas, and **understand** how to use them. Since these formulas have lots of inequalities, it's easy to remember what they are but be completely lost as to how to use them on final exam day. The purpose of these notes is to do some illustrative examples that will (slowly, but certainly) demystify what the big deal with all the inequalities and absolute value bars are, and acquaint you with how powerful of a tool error analysis is.

Let's start by demystifying (well, to some extent) the absolute value bars. For example, take the assumption that $|f''(x)| \leq K$ in the Trapezoid Rule formula. What this is stating is that the magnitude of the second derivative must always be less than a number K. For example, suppose that the second derivative of a function took all of the values in the set $[-9, 8]$ over a closed interval. Then $|f''(x)| \leq 9$ for all x in the interval, since -9 has the largest absolute value. However, it's also true that $|f''(x)| \leq 20$ since no numbers in $[-9, 8]$ have magnitude 20; however, we will want the smallest value K that we can get, because it will ensure a **sharper** error bound - in other words, one that is as close to the actual error as possible.

In general, we'll get the smallest value of K by finding the **largest absolute value** of the second derivative over the interval. Sometimes, this will be easy; other times, we will have to use calculus to find the critical numbers, relative maxima, and relative minima.

Now we'll explain $|E_T|$; the idea behind this can be generalized to the other numerical techniques. $|E_T|$ specifies how far the trapezoidal approximation **actually** is from the real interval. In other words,

$$|E_T| = |\int_a^b f(x)dx - T_n| = |T_n - \int_a^b f(x)dx|$$

However, we almost never know what $|E_T|$ is when solving integrals approximately. The error bound inequalities give us an interval of the real numbers where we are guaranteed to find the actual value of the integral. With the Trapezoid Rule,

$$|T_n - \int_a^b f(x)dx| \leq k\frac{(b-a)^3}{12n^2}$$

If you're adept at converting absolute value inequalities to compound inequalities, you'll see that this means that if you know T_n, then somewhere between $T_n - k\frac{(b-a)^3}{12n^2}$ and $T_n + k\frac{(b-a)^3}{12n^2}$, you'll find the real value of the integral.

2 Precision of Numerical Estimates

In this section, we'll do some examples that will hopefully show you that there isn't much to these inequalities.

Example 1: By the Fundamental Theorem of Calculus, you can see that

$$\int_1^2 \frac{1}{x}dx = \ln(2) - \ln(1) = \ln(2)$$

Using the Midpoint Rule with $n = 2$, we get that $\ln(2) \approx .68571$. With the Trapezoid Rule, we get $\ln(2) \approx .708333$. With Simpson's Rule, we get $\ln(2) \approx .69444$. Which is the best approximation?

Let's do the Midpoint Rule and the Trapezoid Rule, and you should try to use the same steps to get the error bound for Simpson's Rule. Taking the second derivative, we have that

$$f''(x) = \frac{2}{x^3}$$

Now we need to find a K such that $|f''(x)| \leq K$ for all $x \in [1, 2]$. There are two ways we can do this: First, we can find the absolute minimum and maximum of $f''(x)$ over the interval, and take the one with the larger absolute value. You should try this yourself and verify that you get the same answer as the way we'll do, which is by manipulating inequalities.

$$\begin{aligned} 1 \leq x \leq 2 &\implies 1 \leq x^3 \leq 8 \\ &\implies 1 \geq \frac{1}{x^3} \geq \frac{1}{8} \\ &\implies 2 \geq \frac{2}{x^3} \geq \frac{1}{4} \end{aligned}$$

The symbol $\implies$ should be read as "implies". The second step of this argument is the more difficult one, and will need some explaining. What we did was first multiply both sides by x^{-3}, and then solve so x^{-3} was by itself.
The bigger of the two endpoints is 2, so $K = 2$ is the best choice to make. Then,

$$|E_T| = \frac{2(1)^3}{12(2)^2} = \frac{2}{48} = \frac{1}{24} \text{ and } |E_M| = \frac{2(1)^3}{24(2)^2} = \frac{1}{48}$$

In other words, if you used the Trapezoid Rule, you would know the real value of the integral would be between $.708333 - .0417$ and $.708333 + .0417$. If you used the midpoint rule, you would know the real value is between $.68571 - .0208$ and $.68571 + .0208$.

Suppose you knew in advance that you only needed an estimate to a certain precision. The error bound formulas are especially powerful here, since they will tell you how many subintervals you need, and they will do it without ever computing the antiderivative.

Example 2: How many subintervals do you need to approximate the integral $\int_1^2 1/x dx$ to a precision of .0001 using Simpson's Rule?
If you take the fourth derivative, you will find that $f^{IV}(x) = 24/x^5$, which has a maximum magnitude of 24. Then, we know that

$$|E_S| \leq \frac{24(1)^5}{180(n)^4}$$

but we want

$$|E_S| \leq .0001$$

To get both of these to be true, we take

$$\frac{24(1)^5}{180(n)^4} < .0001$$

Note that $|E_S|$ is guaranteed to be less than the error bound, so it most certainly will be less than .0001. Here, all we need to do now is solve the equation. Multiplying by n^4 and dividing by .0001, we will get that $n^4 > 4000/3$, or $n > 6.043$. However, the number of subintervals used in Simpson's Rule is always even, so we need at least 8 subintervals.

To see if you get the idea of how to do problems like this, try answering the same question for the Trapezoid Rule and the Midpoint Rule. You should find that with the Midpoint Rule, you need 29 subintervals, and with the Trapezoid Rule, you need 41.

The amazing thing about Simpson's Rule is that computationally, it isn't that more difficult than any of the other rules. Usually, in computing, if you want a more precise answer to a numerical problem, you need to make the computer do significantly more work. If you learn how to approximate the solutions to differential equations, you will see this tradeoff between complexity and precision: if you want a more precise answer, be prepared for the computer to do twice as many calculations. Yet with Simpson's Rule, you get far more precision for the same amount of calculations.

3 Consequences of the Error Bound

Since Simpson's Rule is so accurate, it would make sense to ask if it's ever exact. Since Simpson's Rule uses parabolas to approximate the function, it would make sense to say that it will be exact when approximating the integral of a quadratic function. However, Simpson's Rule is also exact with cubic polynomials.

Example 3: Construct a proof that shows that if $f(x)$ is a cubic polynomial, then no matter how many subintervals we divide $[a, b]$ into, the integral

$$\int_a^b f(x)dx$$

is always exact.

To do this, we appeal to the error bound for Simpson's Rule. In turn, the error bound requires that we get the number K from the fourth derivative. If $f(x)$ is cubic, then there are coefficients a, b, c, d such that $f(x) = ax^3 + bx^2 + cx + d$. Taking derivatives:

$$\begin{aligned} f'(x) &= 3ax^2 + 2bx + c \\ f''(x) &= 6ax + 2b \\ f'''(x) &= 6a \\ f^{(IV)}(x) &= 0 \end{aligned}$$

since a is held constant. Therefore,

$$|E_s| \leq 0\frac{(b-a)^5}{180n^4} = 0$$

Since the error is less than or equal to 0, it must be 0 because it is an absolute value. Therefore, Simpson's Rule is always exact with cubic polynomials.