MAKING ESTIMATES IN NUMERICAL INTEGRATION

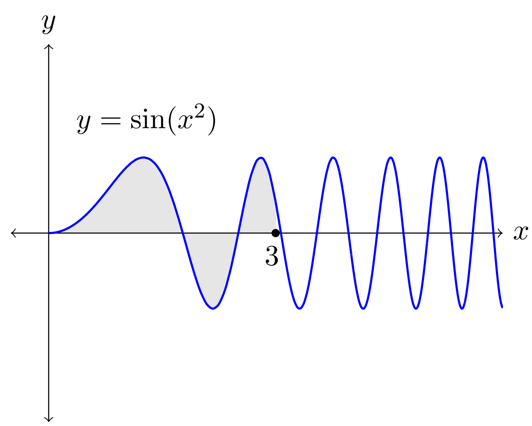
KEITH CONRAD

1. Introduction

A definite integral such as

$$\int_0^3 \sin(x^2)\, dx,$$

corresponding to the shaded region below, can't be computed exactly. Methods of approximating it, like the midpoint rule or trapezoid rule, depend on the number of subintervals chosen (the value of n). As n grows, the approximation generally improves.



If you want to approximate the integral to within a specified error[1], say .01 or .001, then you need to determine what choice of n gives an estimate within the desired error. This depends on which approximation method is used.

Midpoint Rule: If $\int_a^b f(x)\, dx$ is approximated by the midpoint rule with n subintervals, then

$$\left|\int_a^b f(x)\, dx - M_n\right| \leq \frac{K_2(b-a)^3}{24n^2}, \tag{1.1}$$

where K_2 is an upper bound on $|f''(x)|$ over $[a,b]$: $|f''(x)| \leq K_2$ for $a \leq x \leq b$.

Trapezoid Rule: If $\int_a^b f(x)\, dx$ is approximated by the trapezoid rule with n subintervals, then

$$\left|\int_a^b f(x)\, dx - T_n\right| \leq \frac{K_2(b-a)^3}{12n^2}, \tag{1.2}$$

where K_2 is an upper bound on $|f''(x)|$ over $[a,b]$: $|f''(x)| \leq K_2$ for $a \leq x \leq b$.

[1] It makes no sense to insist on an exact error in the approximation, since that is tantamount to computing the value exactly by adding the exact error to the approximation. Only *bounds* on error are practical. This is similar to the use of confidence *intervals* in statistics.

Simpson's Rule: If $\int_a^b f(x)\,dx$ is approximated by Simpson's rule with n subintervals (recall n must be even), then

$$\left|\int_a^b f(x)\,dx - S_n\right| \leq \frac{K_4(b-a)^5}{180n^4}, \tag{1.3}$$

where K_4 is an upper bound on $|f^{(4)}(x)|$ over $[a,b]$: $|f^{(4)}(x)| \leq K_4$ for $a \leq x \leq b$.

We want to discuss two aspects of applying these error bounds:

(1) Finding *reasonable* values for K_2 and K_4: how do you figure out an upper bound on $|f''(x)|$ or $|f^{(4)}(x)|$ over an interval?
(2) Converting the upper bounds on the desired error into lower bounds on the n to be used in the approximation, *e.g.*, if we want to find $\int_a^b f(x)\,dx$ to within .001 using the trapezoid rule, *at least how many* subintervals are needed in the trapezoid rule?

2. Upper Bounds on Functions

To find reasonable upper bounds for second and fourth derivatives of functions, we will use combinations of the following five ideas:

B1) **Triangle inequality**: for any numbers a and b, $|a \pm b| \leq |a| + |b|$. For three numbers $|a \pm b \pm c| \leq |a| + |b| + |c|$, and so on.
B2) Absolute values of sine and cosine are at most 1: $|\sin t| \leq 1$ and $|\cos t| \leq 1$ for all t.
B3) If $h(x)$ is monotonic (always increasing or always decreasing) and positive on a closed interval, then the largest value of $|h(x)|$ is at an endpoint: the right endpoint if it's increasing and left endpoint if it's decreasing. If $h(x)$ is monotonic on an interval but possibly negative, then the largest value of $|h(x)|$ is at one of the endpoints.
B4) If $0 \leq g(x) \leq m$ and $0 \leq h(x) \leq M$, then $g(x)h(x) \leq mM$.
B5) To make a ratio of positive numbers a/b larger, make a larger or b smaller (or both).

Example 2.1. (B3) On the interval $[0,3]$, $e^x \leq e^3$ since e^x is increasing.

Example 2.2. (B5) On the interval $[0,3]$, $\frac{1}{2x^2+3} \leq \frac{1}{3}$ since we can make $\frac{1}{2x^2+3}$ go up by making $2x^2+3$ go down, and the least value of $2x^2+3$ on $[0,3]$ is 3.

Example 2.3. On the interval $[0,3]$, $|x^3 - x + 5| \leq |x|^3 + |x| + 5 \leq 3^3 + 3 + 5 = 35$.

You may notice one "obvious" method missing from our list of methods to bound a function: differential calculus. While differential calculus provides a standard technique for finding the exact maximum value of a function, the simple ideas above, which don't need calculus, are usually sufficient for what we want to do here.

Let's consider $\int_0^3 \sin(x^2)\,dx$. Here $f(x) = \sin(x^2)$, whose first few derivatives are

$$f'(x) = 2x\cos(x^2), \qquad f''(x) = -4x^2\sin(x^2) + 2\cos(x^2),$$
$$f'''(x) = -8x^3\cos(x^2) - 12x\sin(x^2), \qquad f^{(4)}(x) = (16x^4 - 12)\sin(x^2) - 48x^2\cos(x^2).$$

To bound the error in approximating with the trapezoid rule, we seek a K_2 such that

$$|-4x^2\sin(x^2) + 2\cos(x^2)| \leq K_2 \text{ for } 0 \leq x \leq 3, \tag{2.1}$$

while for Simpson's rule we seek a K_4 such that

$$|(16x^4 - 12)\sin(x^2) - 48x^2\cos(x^2)| \leq K_4 \text{ for } 0 \leq x \leq 3. \tag{2.2}$$

Let's see how our estimation methods are used to find good values of K_2 and K_4.

Bounding the second derivative: On the left side of (2.1), by the triangle inequality

$$|-4x^2\sin(x^2)+2\cos(x^2)| \le |-4x^2\sin(x^2)| + |2\cos(x^2)|.$$

Since the absolute value is multiplicative[2] we have

$$|-4x^2\sin(x^2)| = |-4||x^2||\sin(x^2)| = 4|x|^2|\sin(x^2)| \le 4|x|^2.$$

Similarly, $|2\cos(x^2)| = |2||\cos(x^2)| \le 2$. Therefore

$$|-4x^2\sin(x^2)+2\cos(x^2)| \le 4|x|^2+2.$$

Since $0 \le x \le 3$, $|x|^2$ is at most 9, so our final estimate is

$$|-4x^2\sin(x^2)+2\cos(x^2)| \le 4\cdot 9+2 = 36+2 = 38.$$

This is **not** saying 38 is the biggest value of the left side for $0 \le x \le 3$, but only that 38 is an upper bound on the left side. The actual maximum value of $|-4x^2\sin(x^2)+2\cos(x^2)|$ for $0 \le x \le 3$ is around 32, so the bound we found with the triangle inequality is not super sharp, but it's not that far off either. As basic techniques go, the triangle inequality does a good job. We can use

$$K_2 = 38.$$

Bounding the fourth derivative: For the left side of (2.2), the triangle inequality tells us

$$|(16x^4-12)\sin(x^2) - 48x^2\cos(x^2)| \le |(16x^4-12)\sin(x^2)| + |48x^2\cos(x^2)|.$$

From multiplicativity of the absolute value,

$$|(16x^4-12)\sin(x^2)| = |16x^4-12||\sin(x^2)| \le |16x^4-12| \le |16x^4|+12 = 16|x|^4+12.$$

and

$$|48x^2\cos(x^2)| = |48||x|^2|\cos(x^2)| \le 48|x|^2.$$

Therefore

$$|(16x^4-12)\sin(x^2) - 48x^2\cos(x^2)| \le 16|x|^4+12+48|x|^2.$$

For $0 \le x \le 3$, $|x|^2$ is at most 9, so

$$|(16x^4-12)\sin(x^2) - 48x^2\cos(x^2)| \le 16|x|^4+12+48|x|^2 = 16\cdot 81+12+48\cdot 9 = 1740.$$

As before, 1740 is *not* the biggest value of the left side of the inequality; it's just an upper bound on the left side. (The actual maximum value of the left side is around 1164, which would need techniques more sophisticated than the triangle inequality to find.) We will use

$$K_4 = 1740.$$

Putting these values for K_2 and K_4 into (1.1), (1.2), and (1.3), we have

$$\left|\int_0^3 \sin(x^2)\,dx - M_n\right| \le \frac{38(3-0)^3}{24n^2} = \frac{1026}{24n^2}, \tag{2.3}$$

$$\left|\int_0^3 \sin(x^2)\,dx - T_n\right| \le \frac{38(3-0)^3}{12n^2} = \frac{1026}{12n^2}, \tag{2.4}$$

$$\left|\int_0^3 \sin(x^2)\,dx - S_n\right| \le \frac{1740(3-0)^4}{180n^2} = \frac{422820}{180n^4}, \tag{2.5}$$

[2] That is, $|ab| = |a||b|$ for all a and b.

3. Lower Bounds on n

In equations (2.3)–(2.5) we have simple expressions in n that bound the error (the difference between the integral and the estimate M_n, T_n, or S_n) from above: the expressions are each bigger than the error. Therefore if we want to make the error small, *make the upper bounds on the error that small.*

Question: For which n does M_n estimate $\displaystyle\int_0^3 \sin(x^2)\,dx$ to within .001?

This is asking for which n we can be sure that the error $|\int_0^3 \sin(x^2)\,dx - M_n|$ is $\leq .001$. By (2.3), the way to guarantee the error doesn't exceed .001 is to make sure the larger value $1026/(24n^2)$ doesn't exceed .001. That is, the inequality $1026/(24n^2) \leq .001$ is *sufficient* to be sure the error by .001.

Using some algebra,

$$\frac{1026}{24n^2} \leq .001 \iff \frac{1026}{24n^2} \leq \frac{1}{1000} \iff \frac{1026(1000)}{24} \leq n^2 \iff n \geq \sqrt{(1026)(1000)/24} \approx 206.7$$

so we can use $n = 207$ (or higher).

Question: For which n does T_n estimate $\displaystyle\int_0^3 \sin(x^2)\,dx$ to within .001?

Using (2.4), we can answer the question using n that makes $1026/(12n^2) \leq .001$:

$$\frac{1026}{12n^2} \leq .001 \iff \frac{1026}{12n^2} \leq \frac{1}{1000} \iff \frac{1026(1000)}{12} \leq n^2 \iff n \geq \sqrt{(1026)(1000)/12} \approx 292.4,$$

so use $n = 293$ (or higher).

Question: For which (even!) n does S_n estimate $\displaystyle\int_0^3 \sin(x^2)\,dx$ to within .001?

Using (2.5) we want to pick n that makes $422820/(180n^4) \leq .001$:

$$\frac{422820}{180n^4} \leq .001 \iff \frac{422820 \cdot 1000}{180} \leq n^4 \iff n \geq \sqrt[4]{422820 \cdot 1000/180} \approx 39.1,$$

so use $n = 40$ (or higher even integers).

While n at or above the bounds in each answer are guaranteed to lead to approximations within .001 of the integral, we are *not* saying for smaller values of n that the approximations don't estimate the integral to within .001. What we are after here are sufficient conditions for an approximation to be close, and the bounds in each answer give us such n.