Newton-Cotes Formulas

In Calculus, we introduce the ideas of numerical integration in a geometric manner. We first recall the Trapezoid Rule.

Trapezoid Rule

To approximate the integral $\int_a^b f(x)dx$ for a continuous function $f(x)$,

1. Subdivide the interval into n subintervals, producing $n+1$ grid points $x_0 = 1, \dots, x_n = b$ (as opposed to n internal points for the mesh grid $t_1, \dots, t_n$ for BVP's last handout).
2. Compute the width of each interval $\Delta x = \frac{b-a}{n}$.
3. Compute $f(x_i)$ for $i = 0, \dots, n$.
4. The Trapezoid approximation is given by $T_n = \frac{\Delta x}{2}[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)]$.

Theorem 1. *If $f''(x)$ is continuous and $|f''(x)| \leq M$ for x in $[a, b]$, the error associated with the approximation T_n satisfies $|E_T| \leq \frac{M(b-a)^3}{12n^2}$.*

Example 1. Compute the Trapezoid approximation for $\int_{-1}^3 4x^3 dx$ and $n = 4$. Then compute a bound on the error.

Since $n = 4$, $\Delta x = \frac{3-(-1)}{4} = 1$. So the grid points and function values at them are as follows.

$$\begin{array}{ll} x_0 = -1 & f(x_0) = -4 \\ x_1 = 0 & f(x_1) = 0 \\ x_2 = 1 & f(x_2) = 4 \\ x_3 = 2 & f(x_3) = 32 \\ x_4 = 3 & f(x_4) = 108 \end{array}$$

So $T_4 = \frac{1}{2}(-4 + 2(0) + 2(4) + 2(32) + 108) = 88$.

Since $f''(x) = 24x \leq 72$, a bound on the error is $\frac{72(4)^3}{12(4)^2} = 24$. So we can say the real value is between 64 and 112.

We can now pose the problem in numerical analysis terms. Connecting the two values $f(x_i)$ and $f(x_{i+1})$ with a line is a degree 1 interpolation.

That is, for x in the interval $[x_i, x_{i+1}]$, we have that the interpolating polynomial is $P(x) = f(x_i)\frac{x-x_{i+1}}{x_i-x_{i+1}} + f(x_{i+1})\frac{x-x_i}{x_{i+1}-x_i}$.

Using the Taylor formula, we have that the function $f(x)$ is exactly

$$f(x) = P(x) + E(x) = f(x_i)\frac{x - x_{i+1}}{x_i - x_{i+1}} + f(x_{i+1})\frac{x - x_i}{x_{i+1} - x_i} + \frac{(x - x_i)(x - x_{i+1})}{2}f''(c)$$

for c between x_i and x_{i+1}.

Then we can find the bound formula by an examination of the error term $E(x)$. That is, in a particular subinterval, we are off by

$$\frac{1}{2}\int_{x_i}^{x_{i+1}} (x - x_i)(x - x_{i+1})f''(c)dx.$$

We have that $h = x_i - x_{i+1}$ and let $u = x - x_i$. Then

$$\begin{aligned}
\frac{f''(c)}{2}\int_{x_i}^{x_{i+1}} (x - x_i)(x - x_{i+1})dx &= \frac{f''(c)}{2}\int_0^h u(u-h)du \\
&= \frac{f''(c)}{2}\int_0^h u^2 - hu)du \\
&= \frac{f''(c)}{2}(\frac{h^3}{3} - \frac{h^3}{2}) \\
&= -\frac{f''(c)h^3}{12} \\
&= -\frac{f''(c)(b-a)^3}{12n^3}.
\end{aligned}$$

Since there are n subintervals, and assuming that $f''(c) \leq M$, we get Theorem 1.

Simpson's Rule

For the Simpson's approximation, compute $S_n = \frac{\Delta x}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 4f(x_{n-1}) + f(x_n)]$. The coefficients alternate between 4 and 2, and should end with 4. So n has to be even.

Theorem 2. *If $f^{(4)}(x)$ is continuous and $|f^{(4)}x)| \leq M_4$ for x in $[a, b]$, the error associated with the approximation S_n satisfies $|E_S| \leq \frac{M_4(b-a)^5}{180n^4}$.*

Example 2. Recompute $\int_{-1}^{3} 4x^3 dx$ using Simpson's Rule with $n = 4$. Compute the error bound.

$S_4 = \frac{1}{3}(-4 + 4(0) + 2(4) + 4(32) + 108) = \frac{240}{3} = 80$

Since $f^{(4)}(x) = 0$, $|E_S| \leq 0$ so the answer should be correct.

The Simpson's Rule formula is found by replacing the degree 1 interpolation with a degree 2. Let's start with the first three points, x_0, x_1, x_2. Then the interpolating polynomial plus error gives a function value

$$\begin{aligned}
f(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \\
+ \frac{f^{(4)}(c)}{6}(x-x_0)(x-x_1)(x-x_2) = P(x) + E(x).
\end{aligned}$$

Integrating $P(x)$ gives

$$\int_{x_0}^{x_2} f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx$$

$$= \frac{f(x_0)}{2h^2}\int_{x_0}^{x_2}(x-x_1)(x-x_2)dx - \frac{f(x_1)}{h^2}\int_{x_0}^{x_2}(x-x_0)(x-x_2)dx + \frac{f(x_2)}{2h^2}\int_{x_0}^{x_2}(x-x_0)(x-x_1)dx.$$

Then letting $u = x - x_1$ and noting that the first and third integrals have the same value, we evaluate just the first and second integrals.

$$\begin{aligned}\int_{x_0}^{x_2} (x - x_1)(x - x_2)dx &= \int_0^{2h} u(u - h)du \\ &= (\frac{u^3}{3} - h\frac{u^2}{2})\Big|_0^{2h} \\ &= \frac{2h^3}{3}\end{aligned}$$

$$\begin{aligned}\int_{x_0}^{x_2} (x - x_0)(x - x_2)dx &= \int_0^{2h} u(u - 2h)du \\ &= \int_0^{2h} u^2 - 2hudu \\ &= (\frac{u^3}{3} - hu^2)\Big|_0^{2h} \\ &= -\frac{4h^3}{3}\end{aligned}$$

Thus we have, for one interval, the interpolating formula

$$\left(\frac{f(x_0)}{2h^2}\right)\left(\frac{2h^3}{3}\right) - \left(\frac{f(x_1)}{h^2}\right)\left(-\frac{4h^3}{3}\right) + \left(\frac{f(x_2)}{2h^2}\right)\left(\frac{2h^3}{3}\right)$$

$$\frac{hf(x_0)}{3} + \frac{4hf(x_1)}{3} + \frac{hf(x_2)}{3} = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)).$$

Adding these together gives the correct formula, with error term $-\frac{h^5}{90}f^{(4)}(c)$. Noting that $b - a = 2hn$, we get the bound in Theorem 2.

Composite Newton-Cotes Formulas

As described, these "Trapezoid" and "Simpson's" Rules are actually *composite* versions of the rules, as they can be applied to many *panels*, not just a single formula using the endpoints. They are part of a larger class of approximation methods called Newton-Cotes Methods, which integrate an interpolating polynomial for a set of points from the desired function. Because they are methods that use the endpoints, they are called *closed* methods. There also exist *open* Newton-Cotes Methods, such as the midpoint rule (Riemann sums where the function value at the middle of the interval).

Definition 3. The *degree of precision* of a numerical integration method is the greatest integer k for which all degree k or less polynomials are integrated exactly by the method.

Question 4. What are the degrees of precision of the Trapezoid and Simpson's Rules?

The Trapezoid rule is degree 1, which is pretty apparent geometrically. Simpson's Rule is degree 3, which is not nearly as observable geometrically but does follow from the error term.

Question 5. Find the degree of precision of the degree 3 Newton-Cotes formula, called the *Simpson's 3/8 Rule*,

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)).$$

When you're just given an arbitrary formula, finding the degree of precision comes down to testing the polynomials of each degree, $1, x, x^2, x^3, x^4, \ldots$. I'm going to assume that this is at least degree 2 and start with x^3 - if that turns out to not be exact, then I'd go back to x^2.

Let $f(x) = x^3$, so that the correct integral on $[x_0, x_0 + 3h]$ is $\frac{(x_0+3h)^4 - x_0^4}{4}$. Then we have

$$\begin{aligned}
&\frac{3h}{8}((x_0)^3 + 3(x_0 + h)^3 + 3(x_0 + 2h)^3 + (x_0 + 3h)^3) \\
=&\frac{3h}{8}((x_0)^3 + 3(x_0^3 + 3x_0^2h + 3x_0h^2 + h^3) + 3(x_0^3 + 3(x_0^2)(2h) + 3x_0(2h)^2 + (2h)^3) \\
&+ (x_0^3 + 3x_0(3h) + 3x_0^2(3h) + (3h)^3)) \\
=&\frac{3h}{8}(8x_0^3 + (9 + 18 + 9)x_0^2h + (9 + 36 + 27)x_0h^2 + 54h^3) \\
=&\frac{1}{4}(12x_0^3h + 54x_0^2h^2 + 108x_0h^3 + 81h^4) \\
=&\frac{1}{4}(x_0^4 + 12x_0^3h + 54x_0^2h^2 + 108x_0h^3 + 81h^4 - x_0^4) \\
=&\frac{1}{4}((x_0 + 3h)^4 - x_0^4),
\end{aligned}$$

as desired.