# Composite Quadrature

We are interested in approximating $\int_a^b f(x)\,dx$.

We again begin with the Lagrange interpolating polynomial.

$$f(x) = P_n(x) + \frac{1}{(n+1)!} f^{(n+1)}(c(x)) \prod_{i=0}^{n} (x - x_i),$$
$$P_n(x) = \sum_{k=0}^{n} f(x_k) L_{nk}(x),$$
$$L_{nk}(x) = \prod_{i=0, i\neq k}^{n} \frac{(x - x_i)}{(x_k - x_i)}.$$

When deriving the point formulas it is standard to use points starting at $x_0$, and use equally spaced points:

$$x_0, \qquad x_1 = x_0 + h, \qquad x_2 = x_0 + 2h, \qquad \ldots, \qquad x_n = x_0 + nh.$$

Let's integrate and see what happens.

$$f(x) = \sum_{k=0}^{n} f(x_k) L_{nk}(x) + \frac{1}{(n+1)!} f^{(n+1)}(c(x)) \prod_{i=0}^{n} (x - x_i)$$
$$\int_a^b f(x)\,dx = \sum_{k=0}^{n} f(x_k) \int_a^b L_{nk}(x)\,dx + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(c(x)) \prod_{i=0}^{n} (x - x_i)\,dx$$
$$= \sum_{k=0}^{n} a_{nk} f(x_k) + E(f)$$

where

$$a_{nk} = \int_a^b L_{nk}(x)\,dx$$
$$E(f) = \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(c(x)) \prod_{i=0}^{n} (x - x_i)\,dx$$

To compute $E(f)$ we can use the two theorem:

1. **Weighted Mean Value Theorem for Integrals:** If $g(x)$ does not change sign on $[a, b]$ then there exists $c \in (a, b)$ such that $\int_a^b f(x)g(x)\,dx = f(c) \int_a^b g(x)\,dx$.
2. **Generalized Intermediate Value Theorem** Let $f$ be a continuous function on the interval $[a, b]$. Let $x_0, \ldots, x_n$ be points in $[a, b]$ and $a_0, \ldots, a_n > 0$. Then there exists a number $c$ between $a$ and $b$ such that

$$(a_1 + \cdots + a_n)f(c) = a_1 f(x_1) + \cdots + a_n f(x_n).$$

We will set everything up initially on a single partition, then use the single partition result to extend to multiple partitions.

Useful results:

$$L_{00}(x) = 1$$
$$L_{10}(x) = \frac{x - x_1}{x_0 - x_1}$$
$$L_{11}(x) = \frac{x - x_0}{x_1 - x_0}$$

*Mathematica* can help with the tedious integration:

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Integrate[(x - x1)/(x0 - x1), {x, a, b}]
% /. x0 -> a /. x1 -> a + h /. b -> a + h
Simplify[%]
```

## Case $n = 0$: $x_0 = a$ and $h = b - a$ (Left Hand Rule)

$$\int_a^b f(x)\,dx = a_{00} f(x_0) + E(f)$$
$$\begin{aligned} a_{00} &= \int_a^b L_{00}(x)\,dx = \int_a^b 1\,dx = b - a \\ &= h \end{aligned}$$

Now, since $(x - x_0)$ does not change sign in $[a, b]$, we can use the Weighted Mean Value Theorem for Integrals to simplify the error as

$$\begin{aligned} E(f) &= \int_a^b f^{(1)}(c(x))(x - x_0)\,dx \\ &= f^{(1)}(c_0) \int_a^b (x - x_0)\,dx, \qquad \text{where } c_0 \in (a, b) \\ &= f^{(1)}(c_0) \frac{(b-a)^2}{2} \\ &= f^{(1)}(c_0) \frac{h^2}{2} \end{aligned}$$

Therefore we have recovered the Left Hand Rule:

$$\int_{x_0}^{x_0+h} f(x)\,dx = h f(x_0) + h^2 \frac{f^{(1)}(c_0)}{2} \qquad \text{(Left Hand Rule)}$$

## Case $n = 1$: equally spaced nodes $x_0 = a$, $x_1 = b$, $h = b - a$ (Trapezoidal Rule)

$$\int_a^b f(x)\,dx = a_{10} f(x_0) + a_{11} f(x_1) + E(f)$$

$$a_{10} = \int_a^b L_{10}(x)\,dx = \int_a^b \frac{x - x_1}{x_0 - x_1}\,dx = \frac{h}{2}$$

$$a_{11} = \int_a^b L_{11}(x)\,dx = \int_a^b \frac{x - x_0}{x_1 - x_0}\,dx = \frac{h}{2}$$

Now, since $(x-x_0)(x-x_1)$ does not change sign in $[a,b] = [x_0, x_1]$, we can use the Weighted Mean Value Theorem for Integrals to simplify the error as

$$\begin{aligned}
E(f) &= \frac{1}{2}\int_a^b f^{(2)}(c(x))(x-x_0)(x-1)\,dx \\
&= \frac{1}{2} f^{(2)}(c_0) \int_a^b (x-x_0)(x-x_1)\,dx, \qquad \text{where } c_0 \in (a,b) \\
&= \frac{1}{2} f^{(2)}(c_0)\left(-\frac{h^3}{6}\right) \\
&= -h^3 \frac{f^{(2)}(c_0)}{12}
\end{aligned}$$

Therefore we have recovered the Trapezoidal Rule:

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}\left(f(x_0) + f(x_1)\right) - h^3 \frac{f^{(2)}(c_0)}{12} \qquad \text{(Trapezoidal Rule)}$$

## Case $n = 0$: $x_0 = a + h/2$ and $h = b - a$ (MidPoint Rule)

$$\int_a^b f(x)\,dx = a_{00} f(x_0) + E(f)$$

$$a_{00} = \int_a^b L_{00}(x)\,dx = \int_a^b 1\,dx = b - a = h$$

Now, since $(x - x_0)$ does not change sign in $[a,b]$, we can use the Weighted Mean Value Theorem for Integrals to simplify the error as

$$\begin{aligned}
E(f) &= \int_a^b f^{(1)}(c(x))(x - x_0)\,dx \\
&= f^{(1)}(c_0)\int_a^b (x - x_0)\,dx, \quad \text{where } c_0 \in (a,b) \\
&= f^{(1)}(c_0)\left(\frac{(x-x_0)^2}{2}\right)_a^b = f^{(1)}(c_0)\left(\frac{(b-x_0)^2}{2} - \frac{(a-x_0)^2}{2}\right) \\
&= f^{(1)}(c_0)\left(\frac{(h/2)^2}{2} - \frac{(-h/2)^2}{2}\right) = 0
\end{aligned}$$

Whoops. To get the correct error we just need to keep higher derivatives, or switch to a Taylor Series representation. Let's do the latter, since this would be something you could do in all cases.

$$\begin{aligned}
f(x) &= f(x_0) + f'(x_0)(x - x_0) + \frac{f^{(2)}(c(x))}{2}(x - x_0)^2 \\
\int_a^b f(x)\,dx &= f(x_0)(b-a) + \frac{1}{2}f'(x_0)(x-x_0)^2\Big|_a^b + \int_a^b \frac{f^{(2)}(c(x))}{2}(x-x_0)^2\,dx
\end{aligned}$$

Since $(x - x_0)^2$ is positive, we can use the weighted mean value theorem (also note the second integral is zero, which is what we found above).

$$\begin{aligned}
\int_a^b f(x)\,dx &= hf(x_0) + \frac{f^{(2)}(c_0)}{2}\int_a^b (x-x_0)^2\,dx \text{ where } c \in [a,b] \\
&= hf(x_0) + h^3\frac{f^{(2)}(c_0)}{24}
\end{aligned}$$

Therefore we have recovered the Midpoint Rule:

$$\int_{x_0-h/2}^{x_0+h/2} f(x)\,dx = hf(x_0) + h^3\frac{f^{(2)}(c_0)}{24} \qquad \text{(Midpoint Rule)}$$

As with derivatives, *Mathematica* can help do the algebra for you and create more formulas.

### A Note About The Error

In all of the above examples, the weighted mean value theorem applied since the quantity $\prod_{i=0}^{n}(x - x_i)$ does not change sign for $n = 0$ or $n = 1$ when $a = x_0$ and $b = x_1$. However, when we do $n = 2$, things get a bit more complicated.

## Case $n = 2$: equally spaced nodes $x_0 = a$, $x_2 = b$, $x_1 = a + h$, $h = (b - a)/2$ (Simpson's Rule)

$$\int_a^b f(x)\,dx = a_{20}f(x_0) + a_{21}f(x_1) + a_{22}f(x_2) + E(f)$$

$$a_{20} = \int_a^b L_{20}(x)\,dx = \frac{h}{3}$$

$$a_{21} = \int_a^b L_{21}(x)\,dx = \frac{4h}{3}$$

$$a_{22} = \int_a^b L_{22}(x)\,dx = \frac{h}{3}$$

Now, tackle the error. We cannot use the Weighted Mean Value Theorem for Integrals to simplify the error since $(x - x_0)(x - x_1)(x - x_2)$ changes sign on the interval $[a, b] = [x_0, x_2]$. However, if we split the integral up we can get around this.

$$\begin{aligned} E(f) &= \frac{1}{6}\int_a^b f^{(3)}(c(x))(x - x_0)(x - x_1)(x - x_2)\,dx \\ &= \frac{1}{6}\int_{x_0}^{x_1} f^{(3)}(c(x))(x - x_0)(x - x_1)(x - x_2)\,dx + \frac{1}{6}\int_{x_1}^{x_2} f^{(3)}(c(x))(x - x_0)(x - 1)(x - x_2)\,dx \end{aligned}$$

Now, on each integral we can apply the Weighted Mean Value Theorem for Integrals, so we have for $c_i \in (x_i, x_{i+1})$:

$$\begin{aligned} E(f) &= \frac{1}{6}f^{(3)}(c_0)\int_{x_0}^{x_1} (x - x_0)(x - x_1)(x - x_2)\,dx + \frac{1}{6}f^{(3)}(c_1)\int_{x_1}^{x_2} (x - x_0)(x - 1)(x - x_2)\,dx \\ &= \frac{1}{6}f^{(3)}(c_0)\left(\frac{h^4}{4}\right) + \frac{1}{6}f^{(3)}(c_1)\left(-\frac{h^4}{4}\right) \\ &= \frac{h^4}{24}\left(f^{(3)}(c_0) - f^{(3)}(c_1)\right) \end{aligned}$$

Therefore we have recovered Simpson's Rule:

$$\int_a^b f(x)\,dx = \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big) + \frac{h^4}{24}\left(f^{(3)}(c_0) - f^{(3)}(c_1)\right) \qquad \text{(Simpson's Rule)}$$

- Notice that we might expect $f^{(3)}(c_0) - f^{(3)}(c_1) \sim 0$ (this is the sort of idea we will soon use for adaptive quadrature), and if that is the case it seems like we might have an error that is better than $0(h^4)$.
- If we instead derive Simpson's Rule using Taylor series about $x_1$ one can show the error goes as $O(h^5)$. Let's do that, since it is interesting.

$$f(x) = f(x_1) + f^{(1)}(x_1)(x - x_1) + \frac{1}{2}f^{(2)}(x_1)(x - x_1)^2 + \frac{1}{6}f^{(3)}(x_1)(x - x_1)^3 + \frac{f^{(4)}(c(x))}{24}(x - x_1)^4$$

$$\int_a^b f(x)\,dx = 2hf(x_1) + 0 + \frac{h^3}{3}f^{(2)}(x_1) + 0 + \int_a^b \frac{f^{(4)}(c(x))}{24}(x - x_1)^4\,dx$$

Since $(x - x_1)^4$ is positive, we can use the weighted mean value theorem.

$$\int_a^b f(x)\,dx = 2hf(x_1) + \frac{h^3}{3} f^{(2)}(x_1) + \frac{f^{(4)}(c_0)}{24} \cdot \left(\frac{2h^5}{5}\right)$$

Notice at this point we still have $f^{(2)}$ in the formula. We can replace it with an earlier 3-point formula for derivative:

$$\begin{aligned}\int_a^b f(x)\,dx &= 2hf(x_1) + \frac{h^3}{3}\left(\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(c_1)\right) + \frac{f^{(4)}(c_0)}{24} \cdot \left(\frac{2h^5}{5}\right) \\ &= \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big) - h^5\left(\frac{1}{36} f^{(4)}(c_1) - \frac{1}{60} f^{(4)}(c_0)\right)\end{aligned}$$

This shows the error goes as $O(h^5)$. If we can assume $f^{(4)}(c_0) \sim f^{(4)}(c_1)$ $f^{(4)}(c)$, where $c \in [a, b]$ we arrive at Simpson's Rule with best error estimate:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big) - h^5 \frac{f^{(4)}(c)}{90} \qquad \text{(Simpson's Rule)}$$

See the article *Simpson's Rule is Exact for Quintics* to see a significantly more involved discussion of the error in Simpson's rule if you are interested–it is quite a good read!

**These methods are called Newton's-Cotes formulas.**

- Closed methods include the endpoints as nodes (left-hand rule, trapezoidal rule, Simpson's rule).
- Open methods do not include the endpoints as nodes (midpoint rule).

So far the formulas were on a single partition of the region $[a, b]$, or at most two partitions (Simpson's rule). We can of course use these results over multiple partitions, a process that is called composite numerical integration.

**Composite Trapezoidal Rule**

Split the region up as $a = x_0 < x_1 < x_2 \cdots < x_{m-1} < x_m = b$ where $x_{i+1} = x_i + h$. Note: In the *Mathematica* file, I just set up a module to call the single interval result. The following is useful to obtain the results you see in calculus, as well as the error term.

On interval $[x_i, x_{i+1}]$ we can use (for this example choose the Trapezoidal rule):

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}\left(f(x_i) + f(x_{i+1})\right) - h^3 \frac{f^{(2)}(c_i)}{12}$$

Sum over $m$ subintervals:

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=0}^{m-1} \int_{x_i}^{x_{i+1}} f(x)\,dx \\ &= \frac{h}{2}\sum_{i=0}^{m-1}\left(f(x_i) + f(x_{i+1})\right) - h^3 \sum_{i=0}^{m-1} \frac{f^{(2)}(c_i)}{12}\end{aligned}$$

The error term can be simplified using the generalized intermediate value theorem:

$$\begin{aligned}\sum_{i=0}^{m-1} f(x_i) &= f(x_0) + \sum_{i=1}^{m-1} f(x_i) \\ \sum_{i=0}^{m-1} f(x_{i+1}) &= \sum_{i=1}^{m} f(x_i) = f(x_m) + \sum_{i=1}^{m-1} f(x_i) \\ -h^3 \sum_{i=0}^{m-1} \frac{f^{(2)}(c_i)}{12} &= -h^3 m \frac{f^{(2)}(c)}{12} && \text{where } c \in [a,b] \\ &= -h^2(b-a)\frac{f^{(2)}(c)}{12} && \text{since } mh = b - a\end{aligned}$$

So the composite trapezoidal rule is

$$\int_a^b f(x)\,dx = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)\right) - h^2(b-a)\frac{f^{(2)}(c)}{12} \qquad \text{(Composite Trapezoidal)}$$

The composite Simpson's rule is derived in the text, following the same procedure as above.

$$\int_a^b f(x)\,dx = \frac{h}{3}\left(f(a) + f(b) + 4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i})\right) - h^4(b-a)\frac{f^{(4)}(c)}{180} \quad \text{(Composite Simpson's)}$$