Numerical Integration

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1 Trapezoidal Rule

We derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$
using the **Lagrange polynomial** method, with the linear Lagrange polynomial.
Let $x_0 = a$, $x_1 = b$, and $h = b - a$.

$$\begin{aligned}
\int_{a=x_0}^{b=x_1} f(x)\,dx &= \int_{x_0}^{x_1} P_1(x)\,dx \;+\; \frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)\,dx \\
&= \int_{x_0}^{x_1} \left[\frac{x-x_1}{x_0-x_1}f(x_0) + \frac{x-x_0}{x_1-x_0}f(x_1)\right]dx \;+\; \frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)\,dx \\
&= \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1} + \frac{1}{2}f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx \\
&= -\frac{(x_0-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x_1-x_0)^2}{2(x_1-x_0)}f(x_1) + \frac{1}{2}f''(\xi)\Big(-\frac{h^3}{6}\Big) \\
&= \frac{h}{2}\Big[f(x_0)+f(x_1)\Big] - \frac{h^3}{12}f''(\xi).
\end{aligned}$$

Thus, the Trapezoidal rule is

$$\boxed{\int_a^b f(x)\,dx \;=\; \frac{h}{2}\Big[f(a)+f(b)\Big] - \frac{h^3}{12}f''(\xi) \;\approx\; \frac{b-a}{2}\Big[f(a)+f(b)\Big].}$$

Since the error term for the Trapezoidal rule involves f'', the rule gives the exact result when applied to any function whose second derivative is identically zero. That is, the Trapezoidal rule gives the exact result for polynomials of degree up to or equal to one.

2 Composite Trapezoidal Rule

We define $h = \frac{b-a}{n} \;=\; x_j - x_{j-1}$.

$$\begin{aligned}
\int_{a=x_0}^{b=x_n} f(x)\,dx &= \sum_{j=1}^{n}\int_{x_{j-1}}^{x_j} f(x)\,dx \;=\; \sum_{j=1}^{n}\left(\frac{h}{2}\Big[f(x_{j-1})+f(x_j)\Big] \;-\; \frac{h^3}{12}f''(\xi_j)\right) \\
&= \sum_{j=1}^{n}\frac{h}{2}\Big[f(x_{j-1})+f(x_j)\Big] \;-\; \frac{h^3}{12}\sum_{j=1}^{n}f''(\xi_j) \\
&= \sum_{j=1}^{n}\frac{h}{2}\Big[f(x_{j-1})+f(x_j)\Big] \;-\; \frac{h^2}{12}(b-a)f''(\xi). \qquad \text{(since } nh = b-a\text{)}
\end{aligned}$$

Thus, the Composite Trapezoidal rule is

$$\boxed{\int_a^b f(x)\,dx \;=\; \sum_{j=1}^{n}\frac{x_j-x_{j-1}}{2}\Big[f(x_{j-1})+f(x_j)\Big] \;-\; \frac{h^2}{12}(b-a)f''(\xi).}$$

3 Simpson's Rule

Simpson's rule can be derived by integrating the second Lagrange polynomial. However, this derivation gives only an $O(h^4)$ error term involving $f^{(3)}$. To get a better error term, we use **Taylor polynomial** to derive the Simpson's rule.
Let $x_0 = a$, $x_2 = b$, and $x_1 = \frac{a+b}{2} = a + \frac{b-a}{2} = a + h$. That is, $x_1 - x_0 = h$ and $x_2 - x_1 = h$.

$$\begin{aligned}
\int_{a=x_0}^{b=x_2} f(x)\,dx &= \int_{x_0}^{x_2} \Bigg[f(x_1) \ + \ f'(x_1)(x-x_1) \ + \ \frac{f''(x_1)}{2}(x-x_1)^2 \\
&\quad + \frac{f'''(x_1)}{6}(x-x_1)^3 \ + \ \frac{f^{(4)}(\xi)}{24}(x-x_1)^4 \Bigg] dx \\
&= \Bigg[f(x_1)x + \frac{f'(x_1)}{2}(x-x_1)^2 \ + \ \frac{f''(x_1)}{6}(x-x_1)^3 \\
&\quad + \frac{f'''(x_1)}{24}(x-x_1)^4 \ + \ \frac{f^{(4)}(\xi)}{120}(x-x_1)^5 \Bigg]_{x_0}^{x_2} \\
&= f(x_1)(x_2-x_0) + \frac{f'(x_1)}{2}\Big[(x_2-x_1)^2 - (x_0-x_1)^2\Big] + \frac{f''(x_1)}{6}\Big[(x_2-x_1)^3 - (x_0-x_1)^3\Big] \\
&\quad + \frac{f'''(x_1)}{24}\Big[(x_2-x_1)^4 - (x_0-x_1)^4\Big] \ + \ \frac{f^{(4)}(\xi)}{120}\Big[(x_2-x_1)^5 - (x_0-x_1)^5\Big] \\
&= 2hf(x_1) + \frac{f'(x_1)}{2}\Big[h^2 - h^2\Big] + \frac{f''(x_1)}{6}\Big[h^3 + h^3\Big] \\
&\quad + \frac{f'''(x_1)}{24}\Big[h^4 - h^4\Big] \ + \ \frac{f^{(4)}(\xi)}{120}\Big[h^5 + h^5\Big] \\
&= 2hf(x_1) \ + \ h^3\frac{f''(x_1)}{3} \ + \ h^5\frac{f^{(4)}(\xi)}{60} \\
&= 2hf(x_1) \ + \ \frac{h^3}{3}\left[\frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi)\right] \ + \ \frac{h^5}{60}f^{(4)}(\xi) \\
&= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{90}f^{(4)}(\xi).
\end{aligned}$$

Thus, the Simpson's rule is

$$\boxed{\int_a^b f(x)\,dx \ = \ \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] - \frac{h^5}{90}f^{(4)}(\xi) \ \approx \ \frac{b-a}{6}\Big[f(a) + 4f\Big(\frac{a+b}{2}\Big) + f(b)\Big].}$$

4 Composite Simpson's Rule

In order to obtain the formula for the Composite Simpson's rule that agrees with professor's formula, we need to make the change of notation. To avoid confusion, we just list the formula without its derivation. The Composite Simpson's rule is

$$\boxed{\int_a^b f(x)\,dx \ \approx \ \sum_{j=1}^{n} \frac{x_j - x_{j-1}}{6}\Big[f(x_{j-1}) + 4f\Big(\frac{x_{j-1}+x_j}{2}\Big) + f(x_j)\Big].}$$