

Error term of Simpson's rule

$$f(x_1 + h) = f(x_1) + hf'(x_1) + \frac{h^2}{2}f''(x_1) + \frac{h^3}{6}f^{(3)}(x_1) + \frac{1}{6} \int_{x_1}^{x_1+h} f^{(4)}(t)(x_1 + h - t)^3 dt$$

$$f(x_1 - h) = f(x_1) - hf'(x_1) + \frac{h^2}{2}f''(x_1) - \frac{h^3}{6}f^{(3)}(x_1) + \frac{1}{6} \int_{x_1}^{x_1-h} f^{(4)}(t)(x_1 - h - t)^3 dt$$

We have

$$f''(x_1) = \frac{1}{h^2} [f(x_1 - h) - 2f(x_1) + f(x_1 + h)] - \frac{1}{6h^2} \left[\int_{x_1}^{x_1+h} f^{(4)}(t)(x_1 + h - t)^3 dt - \int_{x_1-h}^{x_1} f^{(4)}(t)(x_1 - h - t)^3 dt \right] (*)$$

Furthermore,

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f^{(3)}(x_1)}{6}(x - x_1)^3 + \frac{1}{6} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt$$

$$\begin{aligned} \int_{x_0}^{x_2} f(x) dx &= \left[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 + \frac{f^{(3)}(x_1)}{24}(x - x_1)^4 \right] \Big|_{x_0}^{x_2} \\ &\quad + \frac{1}{6} \int_{x_0}^{x_2} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx \\ &= 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{1}{6} \int_{x_0}^{x_2} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx \\ &= 2hf(x_1) + \frac{h^3}{3}[f(x_0) - 2f(x_1) + f(x_2)] + \text{error term} \quad (\text{By } (*)) \\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] + \text{error term} \end{aligned}$$

where the **error term** is

$$-\frac{h}{18} \left[\int_{x_1}^{x_2} f^{(4)}(t)(x_2 - t)^3 dt - \int_{x_0}^{x_1} f^{(4)}(t)(x_0 - t)^3 dt \right] + \frac{1}{6} \int_{x_0}^{x_2} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx$$

and

$$\begin{aligned} \frac{1}{6} \int_{x_0}^{x_2} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx &= \frac{1}{6} \int_{x_0}^{x_1} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx + \frac{1}{6} \int_{x_1}^{x_2} \int_{x_1}^x f^{(4)}(t)(x - t)^3 dt dx \\ &= -\frac{1}{6} \int_{x_0}^{x_1} \int_{x_0}^t f^{(4)}(t)(x - t)^3 dx dt + \frac{1}{6} \int_{x_1}^{x_2} \int_t^{x_2} f^{(4)}(t)(x - t)^3 dx dt \\ &= \frac{1}{24} \int_{x_0}^{x_1} f^{(4)}(t)(x_0 - t)^4 dt + \frac{1}{24} \int_{x_1}^{x_2} f^{(4)}(t)(x_2 - t)^4 dt \end{aligned}$$

So, the **error term** becomes

$$\begin{aligned}
& \int_{x_1}^{x_2} f^{(4)}(t) \left[-\frac{h}{18}(x_2 - t)^3 + \frac{1}{24}(x_2 - t)^4 \right] dt + \int_{x_0}^{x_1} f^{(4)}(t) \left[\frac{h}{18}(x_0 - t)^3 + \frac{1}{24}(x_0 - t)^4 \right] dt \\
&= \int_0^h f^{(4)}(x_2 - u) \left[-\frac{h}{18}u^3 + \frac{1}{24}u^4 \right] du + \int_0^h f^{(4)}(x_0 + u) \left[-\frac{h}{18}u^3 + \frac{1}{24}u^4 \right] du \\
&= \int_0^h [f^{(4)}(u + x_0) + f^{(4)}(x_2 - u)] \left[-\frac{h}{18}u^3 + \frac{1}{24}u^4 \right] du
\end{aligned}$$

Since $[-\frac{h}{18}u^3 + \frac{1}{24}u^4] = \frac{1}{24}u^3[u - \frac{4}{3}h] < 0$ for $u \in [0, h]$, by I.V.T and M.V.T,

the above intergral equals to

$$\begin{aligned}
\int_0^h 2f^{(4)}(\xi(u)) \frac{1}{24}u^3[u - \frac{4}{3}h] du &= f^{(4)}(\xi) \int_0^h \frac{1}{12}[u^4 - \frac{4}{3}u^3h] du \\
&= \frac{f^{(4)}(\xi)}{12} \left[\frac{h^5}{5} - \frac{4}{3} \frac{h^4}{4} h \right] \\
&= -\frac{f^{(4)}(\xi)}{90} h^5 \quad \square
\end{aligned}$$