

Theorem 1. *Error formula for the Simpson's Rule*

If $f \in \mathcal{C}^4$, error in the Simpson's rule is $-\frac{(b-a)^5}{180n^4}f^{(4)}(\eta)$ where $\eta \in (a, b)$

Proof. With usual notation, let $p(x)$ be the degree two Lagrange polynomial of $f(x)$ agreeing with it on three points x_0, x_1, x_2 which are distance h apart.

Consider error on the first two intervals, $\int_{x_0}^{x_2} (f(x) - p(x)) dx$

We define a degree three polynomial as follows

$$q(x) = p(x) + \frac{1}{h^2} (p'(x_1) - f'(x_1)) w(x) \text{ where } w(x) = (x - x_0)(x - x_1)(x - x_2)$$

We notice that $q(x_k) = p(x_k) = f(x_k)$ for $k = 0, 1, 2$ and $q'(x_1) = f'(x_1)$

First we claim that $f(x) = q(x) + \frac{f^{(4)}(\zeta_1)}{4!}u(x)$ where $u(x) = (x - x_0)(x - x_1)^2(x - x_2)$ and $\zeta_1 \in (x_0, x_2)$. To prove this define $g(y) = f(y) - q(y) - u(y)\frac{f(x)-p(x)}{u(x)}$

Now $g(y) = 0$ for $y = x_0, x_1, x_2, x$ and $g'(x_1) = 0$

This implies, by the Mean Value Theorem that there is $\zeta_1 \in (x_0, x_2)$ such that $g^{(4)}(\zeta_1) = f^{(4)}(\zeta_1) - 0 - 4!\frac{f(x)-p(x)}{u(x)} = 0$ or $f(x) = q(x) + \frac{f^{(4)}(\zeta_1)}{4!}u(x)$ for some $\zeta_1 \in (x_0, x_2)$ as desired.

Now we notice that

$$\begin{aligned} & \int_{x_0}^{x_2} w(x) dx \\ &= \int_{x_0}^{x_2} (x - x_0)(x - x_1)(x - x_2) dx \\ &= \int_{-h}^h (t + h)(t)(t - h) dt = \int_{-h}^h (t^3 - h^2t) dt = 0 \end{aligned}$$

This implies that

$$\int_{x_0}^{x_2} (f(x) - p(x)) dx = \int_{x_0}^{x_2} (f(x) - q(x)) dx = \int_{x_0}^{x_2} \frac{f^{(4)}(\zeta_1)}{4!}u(x) dx = \frac{f^{(4)}(\eta_1)}{4!} \int_{x_0}^{x_2} u(x) dx$$

since $u(x)$ does not change sign on (x_0, x_2) and because $f^{(4)}(\eta_1(x))$ is a continuous function.

Now

$$\begin{aligned} & \int_{x_0}^{x_2} u(x) dx \\ &= \int_{x_0}^{x_2} (x - x_0)(x - x_1)^2(x - x_2) dx \\ &= \int_{-h}^h (t + h)(t)^2(t - h) dt = \int_{-h}^h (t^4 - h^2t^2) dt = \left[\frac{t^5}{5} - h^2\frac{t^3}{3} \right]_{-h}^h = 2 \left[\frac{h^5}{5} - \frac{h^5}{3} \right] = -\frac{4}{15}h^5 \end{aligned}$$

So the error on $[x_0, x_2]$ is

$$\frac{f^{(4)}(\eta_1)}{4!} \int_{x_0}^{x_2} u(x) dx = \frac{f^{(4)}(\eta_1)}{4!} \left(-\frac{4}{15}h^5 \right) = -\frac{h^5}{90}f^{(4)}(\eta_1)$$

We notice here that n needs to be even in order to cover $[a, b]$ by non-overlapping intervals similar to $[x_0, x_2]$ and we need $\frac{n}{2}$ of such intervals. Now adding error terms in each interval we have the total error,

$$\sum_{j=1}^{\frac{n}{2}} -\frac{h^5}{90}f^{(4)}(\eta_j) = -\frac{h^5}{90} \sum_{j=1}^{\frac{n}{2}} f^{(4)}(\eta_j) = -\frac{h^5}{90} \frac{n}{2} f^{(4)}(\eta) = -\frac{nh^5}{180} f^{(4)}(\eta) \text{ for } \eta \in (a, b)$$

using Extremum and Intermediate Value Theorems for $f \in \mathcal{C}^4$ ie. for $f^{(4)} \in \mathcal{C}$. Using $h = \frac{b-a}{n}$, the total error is also equal to $-\frac{(b-a)h^4}{180} f^{(4)}(\eta) = -\frac{(b-a)^5}{180n^4} f^{(4)}(\eta)$

□

Theorem 2. *Newton-Kantorovich Theorem*

1. Let $f : [a, b] \rightarrow \mathbb{R}$
2. f' is Lipschitz continuous with constant γ
3. $f'(x) \neq 0$ and $\frac{1}{|f'(x)|} \leq \beta$
4. $x_0 \in [a, b]$ and $\left| \frac{f(x_0)}{f'(x_0)} \right| = \alpha$
5. $q = \alpha\beta\gamma < \frac{1}{2}$
6. $[x_0 - 2\alpha, x_0 + 2\alpha] \subset [a, b]$
7. $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, k \geq 0$

Then

1. $\lim_{k \rightarrow \infty} x_k = z \in [x_0 - 2\alpha, x_0 + 2\alpha]$.
2. $f(z) = 0$ and z is a unique root of f
3. $|x_k - z| \leq 2\alpha q^{2^k - 1}$

Proof. By definition we have, $|x_{k+1} - x_k| = \left| \frac{f(x_k)}{f'(x_k)} \right| \leq \beta |f(x_k)| = \beta |f(x_k) - f(x_{k-1}) - (x_k - x_{k-1})f'(x_{k-1})| = \beta \left| \int_{x_{k-1}}^{x_k} f'(t) dt - f'(x_{k-1}) \int_{x_{k-1}}^{x_k} dt \right| \leq \beta \left| \int_{x_{k-1}}^{x_k} |f'(t) - f'(x_{k-1})| dt \right| \leq \beta \gamma \left| \int_{x_{k-1}}^{x_k} |t - x_{k-1}| dt \right| = \frac{1}{2} \beta \gamma |x_k - x_{k-1}|^2 = p |x_k - x_{k-1}|^2$

Also by using the formula k times, $|x_{k+1} - x_k| \leq p |x_k - x_{k-1}|^2 \leq p(p |x_{k-1} - x_{k-2}|^2)^2 = p^{1+2^1} |x_{k-1} - x_{k-2}|^{2^2} \leq p^{1+2^1+2^2+\dots+2^{k-1}} |x_1 - x_0|^{2^k} = p^{\frac{2^k-1}{2-1}} |x_1 - x_0|^{2^k} = \frac{1}{p} (p\alpha)^{2^k} = \frac{\alpha}{\alpha\beta\gamma} (\alpha\beta\gamma)^{2^k} = \alpha q^{2^k - 1}$

So we have $|x_{k+1} - x_k| \leq \alpha q^{2^k - 1}$

Now a general difference,

$$\begin{aligned} |x_{k+j} - x_k| &= |x_{k+j} - x_{k+j-1} + x_{k+j-1} - x_{k+j-2} + \dots + x_{k+1} - x_k| \leq |x_{k+j} - x_{k+j-1}| + |x_{k+j-1} - x_{k+j-2}| + \dots + |x_{k+1} - x_k| \leq \alpha q^{2^{k+j-1}-1} + \alpha q^{2^{k+j-2}-1} + \dots + \alpha q^{2^k-1} \\ &= \alpha q^{2^k-1} \left(q^{2^k} + q^{2^{k+1}} + \dots + q^{2^{k+j-1}} \right) \leq \alpha q^{2^k-1} \left(q^{2^k} + (q^{2^k})^2 + (q^{2^k})^4 + \dots \right) = \alpha q^{2^k-1} \left(1 + (q^{2^k}) + (q^{2^k})^3 + \dots \right) \leq \alpha q^{2^k-1} \left(1 + (q^{2^k}) + (q^{2^k})^2 + \dots \right) \\ &\leq \alpha q^{2^k-1} (1 + q + q^2 + \dots) = \alpha q^{2^k-1} \frac{1}{1-q} \leq \alpha q^{2^k-1} \frac{1}{1-\frac{1}{2}} = 2\alpha q^{2^k-1} \text{ since } 0 \leq q < \frac{1}{2} < 1 \end{aligned}$$

Finally we have $|x_{k+j} - x_k| \leq 2\alpha q^{2^k-1} (1)$

Note that by $k = 0$ in (1) we have $|x_j - x_0| \leq 2\alpha q^{2^0-1} = 2\alpha$ so $x_k \in [x_0 - 2\alpha, x_0 + 2\alpha]$

Also by (1) and $0 \leq q < 1$, x_k is a Cauchy sequence and converges to $z \in [x_0 - 2\alpha, x_0 + 2\alpha]$.

By taking $j \rightarrow \infty$ in (1), we have $|z - x_k| \leq 2\alpha q^{2^k-1}$.

Note that f' is continuous with $f'(x) \neq 0$. Taking $k \rightarrow \infty$ in $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$, we get $z = z - \frac{f(z)}{f'(z)}$ or $f(z) = 0$, so z is a root of f .

Now assume that the root z is not unique, i.e. there exists $w \neq z$ with $f(w) = 0$. By MVT, for some ζ between z, w we have $f'(\zeta) = \frac{f(z) - f(w)}{z - w} = \frac{0}{z - w} = 0$ or $f'(\zeta) = 0$ which is a contradiction. Therefore $z = w$ and the root is unique. \square