Some error identities in numerical differentiation and integration

Some of you have asked about the error identity for Simpson's method and fourth order approximation of th first derivative that were not shown in the textbook. Both of them can be obtained using the integral form of Taylor's remainder formula. Here are the details for those interested.

1. Error identity for Simpson's method

Proposition 0.1. *Let $x_1 = x_0 + h$, $x_2 = x_1 + h$ and $f \in C^4([x_0, x_2])$. Then the error term of Simpson's method is given by*

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{f^{(4)}(\xi)}{90}h^5$$

for some $\xi \in (x_0, x_2)$.

Proof:

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

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

We have

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

Furthermore,

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

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

where the **error term** is

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

and

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

So, the **error term** becomes

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

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 integral equals to

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

This completes the proof.

2. Error identity for 4th order approximation of first derivative

Proposition 0.2. *Let $f \in C^5([x_0-2h, x_0+2h])$, then*

$$f^{'}(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{1}{30}f^{(5)}(\xi_1)h^4$$

for some $\xi_1 \in (x_0-2h, x_0+2h)$.

Proof:

$$f(x_0+h) = f(x_0) + f^{'}(x_0)h + \frac{f^{''}(x_0)}{2}h^2 + \frac{f^{(3)}(x_0)}{6}h^3 + \frac{f^{(4)}(x_0)}{24}h^4 + \frac{1}{24}\int_{x_0}^{x_0+h} f^{(5)}(t)(x_0+h-t)^4 dt$$

$$f(x_0-h) = f(x_0) - f^{'}(x_0)h + \frac{f^{''}(x_0)}{2}h^2 - \frac{f^{(3)}(x_0)}{6}h^3 + \frac{f^{(4)}(x_0)}{24}h^4 + \frac{1}{24}\int_{x_0}^{x_0-h} f^{(5)}(t)(x_0-h-t)^4 dt$$

We have

$$\begin{aligned} f^{'}(x_0) &= \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{f^{(3)}(x_0)}{6}h^2 \\ &\quad - \frac{1}{48h}[\int_{x_0}^{x_0+h} f^{(5)}(t)(x_0+h-t)^4 dt + \int_{x_0-h}^{x_0} f^{(5)}(t)(x_0-h-t)^4 dt] \end{aligned}$$

Also,

$$\begin{aligned} f^{'}(x_0) &= \frac{1}{4h}[f(x_0+2h) - f(x_0-2h)] - \frac{f^{(3)}(x_0)}{6}4h^2 \\ &\quad - \frac{1}{96h}[\int_{x_0}^{x_0+2h} f^{(5)}(t)(x_0+2h-t)^4 dt + \int_{x_0-2h}^{x_0} f^{(5)}(t)(x_0-2h-t)^4 dt] \end{aligned}$$

which implies that

$$\begin{aligned} f^{'}(x_0) &= \frac{2}{3h}[f(x_0+h) - f(x_0-h)] - \frac{1}{12h}[f(x_0+2h) - f(x_0-2h)] \\ &\quad - \frac{1}{36h}[\int_{x_0}^{x_0+h} f^{(5)}(t)(x_0+h-t)^4 dt + \int_{x_0-h}^{x_0} f^{(5)}(t)(x_0-h-t)^4 dt] \\ &\quad + \frac{1}{288h}[\int_{x_0}^{x_0+2h} f^{(5)}(t)(x_0+2h-t)^4 dt + \int_{x_0-2h}^{x_0} f^{(5)}(t)(x_0-2h-t)^4 dt] \\ &= \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \textbf{error term} \end{aligned}$$

where the **error term** is

$$\begin{aligned} &- \frac{1}{36h}[\int_{x_0}^{x_0+h} f^{(5)}(t)(x_0+h-t)^4 dt + \int_{x_0-h}^{x_0} f^{(5)}(t)(x_0-h-t)^4 dt] \\ &+ \frac{1}{288h}[\int_{x_0}^{x_0+2h} f^{(5)}(t)(x_0+2h-t)^4 dt + \int_{x_0-2h}^{x_0} f^{(5)}(t)(x_0-2h-t)^4 dt] \end{aligned}$$

By letting $u = x_0 + h - t$ and $u = t - x_0 + h$, respectively,
the **error term** becomes

$$-\frac{1}{36h}\int_0^h f^{(5)}(x_0+h-u)u^4du + \frac{1}{288h}\int_{-h}^h f^{(5)}(x_0+h-u)(h+u)^4du$$
$$-\frac{1}{36h}\int_0^h f^{(5)}(x_0-h+u)u^4du + \frac{1}{288h}\int_{-h}^h f^{(5)}(x_0-h+u)(h+u)^4du$$

$$= \int_0^h f^{(5)}(x_0+h-u)[-\frac{1}{36h}u^4+\frac{1}{288h}(h+u)^4]du + \int_0^h f^{(5)}(x_0-h+u)[-\frac{1}{36h}u^4+\frac{1}{288h}(h+u)^4]du \qquad (1)$$

$$+\frac{1}{288h}\int_{-h}^0 f^{(5)}(x_0+h-u)(h+u)^4du + \frac{1}{288h}\int_{-h}^0 f^{(5)}(x_0-h+u)(h+u)^4du \qquad (2)$$

$$\begin{aligned}
(1) &= \int_0^h [f^{(5)}(x_0+h-u)+f^{(5)}(x_0-h+u)][-\frac{1}{36h}u^4+\frac{1}{288h}(h+u)^4]du \\
&= \int_0^h 2f^{(5)}(\xi(u))(-\frac{1}{36h})[u^4-\frac{1}{8}(h+u)^4]du \quad \text{(By I.V.T.)} \\
&= 2f^{(5)}(\xi)(-\frac{1}{36h})\int_0^h [u^4-\frac{1}{8}(h+u)^4]du \quad \text{(By M.V.T. Note } [u^4-\frac{1}{8}(h+u)^4] < 0,\ \forall u \in [0,h].) \\
&= \frac{23}{720}f^{(5)}(\xi)h^4
\end{aligned}$$

$$\begin{aligned}
(2) &= \frac{1}{288h}\int_{-h}^0 [f^{(5)}(x_0+h-u)+f^{(5)}(x_0-h+u)](h+u)^4du \\
&= \frac{1}{288h}\int_{-h}^0 [2f^{(5)}(\eta(w))](h+u)^4du \quad \text{(By I.V.T.)} \\
&= \frac{f^{(5)}(\eta)}{144h}\int_{-h}^0 (h+u)^4du \quad \text{(By M.V.T. Note } (h+u)^4 > 0.) \\
&= \frac{1}{720}f^{(5)}(\eta)h^4
\end{aligned}$$

Thus, the **error term** is

$$\begin{aligned}
(1)+(2) &= \frac{23}{720}f^{(5)}(\xi)h^4 + \frac{1}{720}f^{(5)}(\eta)h^4 \quad \text{(By I.V.T.)} \\
&= \frac{1}{30}f^{(5)}(\xi_1)h^4 \qquad \square
\end{aligned}$$

Note that

$$\begin{aligned}
& u^4 - \frac{1}{8}(h+u)^4 \\
&= (u^2 + \frac{1}{2^{\frac{3}{2}}}(h+u)^2)\ (u^2 - \frac{1}{2^{\frac{3}{2}}}(h+u)^2) \\
&= (u^2 + \frac{1}{2^{\frac{3}{2}}}(h+u)^2)\ (u + \frac{1}{2^{\frac{3}{4}}}(h+u)\ )\ (u - \frac{1}{2^{\frac{3}{4}}}(h+u)\ ) < 0\ \forall u \in [0,h]
\end{aligned}$$

Remark: Following the same argument, one can show the following error identity holds true for the other fourth order approximation of first derivative in midterm 2:

Let $f \in C^5([x_0 - h, x_0 + 2h])$, then

$$f^{'}(x_0 + h/2) = \frac{1}{24h}[f(x_0 - h) - 27(x_0 - h) + 27f(x_0 + h) - f(x_0 + 2h)] + \frac{3}{640}f^{(5)}(\xi_1)h^4$$

for some $\xi_1 \in (x_0 - h, x_0 + 2h)$.