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CRISTIAN B. JETOMO
MATH 174 - B2L

Problem Set 2.2

In this problem, we wish to derive a five-point forward formula of order four for $f'(x)$. Note that by Taylor's theorem, the expansion for $f(x+h), f(x+2h), f(x+3h), f(x+4h)$ are given below.

$$\begin{cases} f(x+h) &= f(x) + hf'(x) + \frac{h^2 f''(x)}{2!} + \frac{h^3 f'''(x)}{3!} + \frac{h^4 f^{(4)}(x)}{4!} + \frac{h^5 f^{(5)}(x)}{5!} + \cdots \\ f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2 f''(x)}{2!} + \frac{8h^3 f'''(x)}{3!} + \frac{16h^4 f^{(4)}(x)}{4!} + \frac{32h^5 f^{(5)}(x)}{5!} + \cdots \\ f(x+3h) &= f(x) + 3hf'(x) + \frac{9h^2 f''(x)}{2!} + \frac{27h^3 f'''(x)}{3!} + \frac{81h^4 f^{(4)}(x)}{4!} + \frac{243h^5 f^{(5)}(x)}{5!} + \cdots \\ f(x+4h) &= f(x) + 4hf'(x) + \frac{16h^2 f''(x)}{2!} + \frac{64h^3 f'''(x)}{3!} + \frac{256h^4 f^{(4)}(x)}{4!} + \frac{1024h^5 f^{(5)}(x)}{5!} + \cdots \end{cases}$$

Since we wish to find an order four formula, then we want to find the constants A, B, C, and D such that the $f'', f''', f^{(4)}$ terms in $Af(x+h) + Bf(x+2h) + Cf(x+3h) + Df(x+4h)$ are eliminated. From this, we have the following system of equations:

$$\begin{cases} A + 4B + 9C + 16D = 0 \\ A + 8B + 27C + 64D = 0 \\ A + 16B + 81C + 256D = 0 \end{cases}$$

Solving the given system in Symbolab[1], we obtain the solution set $\{-16D, 12D, -\frac{16}{3}D, D | D \in \mathbb{R}\}$. Suppose we wish to force the coefficient of $f(x+2h)$ to be 11, then $B = 12D = 11 \implies D = \frac{11}{12}$. From this, we obtain further that $A = -\frac{44}{3}$ and $C = -\frac{44}{9}$. Hence,

$$\begin{aligned} -\frac{44}{3}f(x+h) + 11f(x+2h) - \frac{44}{9}f(x+3h) + \frac{11}{12}f(x+4h) &= \left(-\frac{44}{3} + 11 - \frac{44}{9} + \frac{11}{12}\right) f(x) + \\ &\quad \left(-\frac{44}{3} + 22 - \frac{44}{3} + \frac{11}{3}\right) hf'(x) + \\ &\quad \left(-\frac{44}{3} + 352 - 1188 + \frac{2816}{3}\right) \frac{h^5 f^{(5)}(x)}{5!} + \cdots \\ &= -\frac{275}{36}f(x) - \frac{11}{3}hf'(x) + \frac{88h^5 f^{(5)}(x)}{5!} + \cdots \end{aligned}$$

which implies that

$$\frac{11}{3}hf'(x) = -\frac{275}{36}f(x) + \frac{44}{3}f(x+h) - 11f(x+2h) + \frac{44}{9}f(x+3h) - \frac{11}{12}f(x+4h) + \frac{88h^5 f^{(5)}(x)}{5!} + \cdots$$

Consequently

$$f'(x) = \frac{-3}{11h}\left[\frac{275}{36}f(x) - \frac{44}{3}f(x+h) + 11f(x+2h) - \frac{44}{9}f(x+3h) + \frac{11}{12}f(x+4h)\right] + \frac{h^4 f^{(5)}(\xi)}{5} \quad (2.3.1)$$

for some $\xi \in (x, x+4h)$. Notice that the obtained formula is of order $\mathcal{O}(h^4)$.

[1] https://www.symbolab.com/solver/system-of-equations-calculator/

Now, we want to find a bound for the total error incurred when the obtained formula in Equation 2.3.1 is implemented in a computer with machine epsilon $\epsilon = 10^{-16}$. For this, we let y_k be the truncated value read and understood by machine and e_k be the error of this truncation. This implies that $f(x+kh) = y_k + e_k$ is the actual function value. Therefore, if $\tilde{f}'(x)$ is the value that the machine actually computes, then the total error becomes

$$\begin{aligned}
E(h) &= f'(x) - \tilde{f}'(x) \\
&= f'(x) + \frac{3}{11h}\left[\frac{275}{36}y_0 - \frac{44}{3}y_1 + 11y_2 - \frac{44}{9}y_3 + \frac{11}{12}y_4\right] \\
&= \left(f'(x) + \frac{3}{11h}\left[\frac{275}{36}(y_0+e_0) - \frac{44}{3}(y_1+e_1) + 11(y_2+e_2) - \frac{44}{9}(y_3+e_3) + \frac{11}{12}(y_4+e_4)\right]\right) \\
&\qquad\qquad - \frac{3}{11h}\left[\frac{275}{36}e_0 - \frac{44}{3}e_1 + 11e_2 - \frac{44}{9}e_3 + \frac{11}{12}e_4\right] \\
&= \frac{h^4 f^{(5)}(\xi)}{5} - \frac{3}{11h}\left[\frac{275}{36}e_0 - \frac{44}{3}e_1 + 11e_2 - \frac{44}{9}e_3 + \frac{11}{12}e_4\right]
\end{aligned}$$

for some $\xi \in (x, x+4h)$. We need to find a bound for $|E(h)|$. By Triangle Inequality Theorem and some properties of absolute values, we have

$$|E(h)| \leq \left|\frac{h^4 f^{(5)}(\xi)}{5}\right| + \frac{3}{11h}\left(\frac{275}{36}|e_0| + \frac{44}{3}|e_1| + 11|e_2| + \frac{44}{9}|e_3| + \frac{11}{12}|e_4|\right)$$

Let $M = \max_{x\in[x,x+4h]}\left|f^{(5)}(x)\right|$ and $\max_{k\in\{0,1,2,3,4\}}|e_k| = \epsilon = 10^{-16}$. Hence, we obtain the total error bound given by

$$\begin{aligned}
|E(h)| &\leq \frac{h^4 M}{5} + \frac{3}{11h}\cdot\frac{352}{9}\epsilon \\
&= \frac{h^4 M}{5} + \frac{32\epsilon}{3h}
\end{aligned}$$

Now, we wish to find the near-optimal step size that minimizes the total error bound above. That is, minimizing $\alpha(h) = \frac{h^4 M}{5} + \frac{32\epsilon}{3h}$. Taking its first derivative, we have

$$\alpha'(h) = \frac{4h^3 M}{5} - \frac{32\epsilon}{3h^2} = \frac{12h^5 M - 160\epsilon}{15h^2}$$

Applying Extreme Value Theorem, we obtain that

$$\begin{aligned}
\alpha'(h) &= 0 \\
\frac{12h^5 M - 160\epsilon}{15h^2} &= 0 \\
12h^5 M - 160\epsilon &= 0 \\
12h^5 M &= 160\epsilon \\
h^5 &= \frac{160\epsilon}{12M} \\
h &= \sqrt[5]{\frac{40\epsilon}{3M}}
\end{aligned}$$

Using the generated formula for h and noting that $\epsilon = 10^{-16}$, we obtain that the near-optimal step size for our five-point forward formula in Equation 2.3.1 is

$$h \approx \frac{0.001059223841}{\sqrt[5]{M}}$$

where $M = \max_{x\in[x,x+4h]}\left|f^{(5)}(x)\right|$. This implies that the near-optimal step size depends on the given function, particularly the behavior of its 5^{th} order derivative over the interval of its abscissas.