Computing Second Derivatives for a Padé Scheme

Consider computing the second derivative of a smooth function, f, in a domain as shown alongside. For simplicity, let $f \in \mathbb{R}^1$. Let us assume that the spatial derivative (second-order) of f, at a point 'j' can be expressed as the following linear combination:

$$b_{-1} f''_{j-1} + f''_j + b_1 f''_{j+1} + a_{-1} f_{j-1} + a_0 f_j + a_1 f_{j+1} = \epsilon. \quad (A)$$

where b_{-1}, b_1, a_{-1}, a_0 and a_1 are unknown coefficients which are to be determined. Since (A) represents discrete function values & its derivatives, the sum results in an approximation error, ϵ.

We can write Taylor's expansions for the terms in eqⁿ (A) as:

$$f''_{j-1} = f''_j - \Delta x f'''_j + \frac{\Delta x^2}{2!} f^{iv}_j - \frac{\Delta x^3}{3!} f^{v}_j + \frac{\Delta x^4}{4!} f^{vi}_j - \frac{\Delta x^5}{5!} f^{vii}_j + O(\Delta x^6) \quad (1)$$

$$f''_{j+1} = f''_j + \Delta x f'''_j + \frac{\Delta x^2}{2!} f^{iv}_j + \frac{\Delta x^3}{3!} f^{v}_j + \frac{\Delta x^4}{4!} f^{vi}_j + \frac{\Delta x^5}{5!} f^{vii}_j + O(\Delta x^6) \quad (2)$$

$$f_{j-1} = f_j - \Delta x f'_j + \frac{\Delta x^2}{2!} f''_j - \frac{\Delta x^3}{3!} f'''_j + \frac{\Delta x^4}{4!} f^{iv}_j - \frac{\Delta x^5}{5!} f^{v}_j + O(\Delta x^6) \quad (3)$$

$$f_{j+1} = f_j + \Delta x f'_j + \frac{\Delta x^2}{2!} f''_j + \frac{\Delta x^3}{3!} f'''_j + \frac{\Delta x^4}{4!} f^{iv}_j + \frac{\Delta x^5}{5!} f^{v}_j + O(\Delta x^6) \quad (4)$$

Eqⁿs (1) - (4) can be substituted in eqⁿ (A) ~~to~~ and rewritten as a Taylor Table:

Taylor table for $b_{-1} f''_{j-1} + f''_j + b_1 f''_{j+1} + a_{-1} f_{j-1} + a_0 f_j + a_1 f_{j+1} = \epsilon$

	f_j	f'_j	f''_j	f'''_j	f^{iv}_j	f^{v}_j	f^{vi}_j
$b_{-1} f''_{j-1}$	0	0	b_{-1}	$-b_{-1}\Delta x$	$b_{-1}\frac{\Delta x^2}{2}$	$-b_{-1}\frac{\Delta x^3}{6}$	$b_{-1}\frac{\Delta x^4}{24}$
$b_1 f''_{j+1}$	0	0	b_1	$b_1 \Delta x$	$b_1\frac{\Delta x^2}{2}$	$b_1\frac{\Delta x^3}{6}$	$b_1\frac{\Delta x^4}{24}$
$a_{-1} f_{j-1}$	a_{-1}	$-\Delta x\, a_{-1}$	$a_{-1}\frac{\Delta x^2}{2}$	$-a_{-1}\frac{\Delta x^3}{6}$	$a_{-1}\frac{\Delta x^4}{24}$	$-a_{-1}\frac{\Delta x^5}{120}$	$a_{-1}\frac{\Delta x^6}{720}$
$a_0 f_j$	a_0	0	0	0	0	0	0
$a_1 f_{j+1}$	a_1	$a_1 \Delta x$	$a_1\frac{\Delta x^2}{2}$	$a_1\frac{\Delta x^3}{6}$	$a_1\frac{\Delta x^4}{24}$	$a_1\frac{\Delta x^5}{120}$	$a_1\frac{\Delta x^6}{720}$
f''_j	0	0	1	0	0	0	0

The above table can be used to solve for the unknown coefficients by rewriting it as the following system:

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & -\Delta x & 0 & \Delta x \\ 1 & 1 & \Delta x^2/2 & 0 & \Delta x^2/2 \\ -\Delta x & \Delta x & -\Delta x^3/6 & 0 & \Delta x^3/6 \\ \Delta x^2/2 & \Delta x^2/2 & \Delta x^4/24 & 0 & \Delta x^4/24 \end{bmatrix} \begin{Bmatrix} b_{-1} \\ b_1 \\ a_{-1} \\ a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ -1 \\ 0 \\ 0 \end{Bmatrix}$$

Solving this system yields: $b_{-1} = 0.1$, $b_1 = 0.1$, $a_{-1} = a_1 = -\frac{1.2}{\Delta x^2}$, $a_0 = \frac{2.4}{\Delta x^2}$

Thus, our compact (Padé) scheme formulation is:

$$\frac{1}{10}\left[f''_{j-1} + 10 f''_j + f''_{j+1}\right] = \frac{12}{10}\left[\frac{f_{j-1} - 2f_j + f_{j+1}}{\Delta x^2}\right]$$