SUPPLEMENT B

Article: "Numerical tools to estimate the flux of a gas across the air-water interface and assess the heterogeny of its forcing functions."

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by Vasco M. N. C. S. Vieira

1. *Estimation of numerical derivatives upon Newton's formula of finite differences*

The partial derivatives of complicated functions may be estimated numerically. One way is to approximate the function by its collocation polynomial, upon which the partial derivatives are deduced. A familiar method to estimate the collocation polynomial is through *Newton's formula of finite differences*. This method is first presented for the well-known case of univariate (single variable) partial derivatives. Afterwards, it is presented the deduction of the method for the multivariate (crossed) partial derivatives.

1.1 *Univariate partial derivatives*

A function $y=f(x)$ is evaluated at each x_i, where i equals 0 to k, with equally spaced intervals ($x_{i+1}-x_i=\delta$). The y_i are recorded and its differences are estimated as $\Delta^1 y_i=y_{i+1}-y_i$ (equation B1). The subsequent higher order differences are also estimated following the same rule and thus $\Delta^m y_i=\Delta^{m-1}y_{i+1}-\Delta^{m-1}y_i$. From these rules comes that $\Delta^0 y_i=y_i$. It is important to notice that in order to estimate Δ^m it is necessary to go m steps forward ($k=m$). Hence, if $\Delta^k y_0$ is solved in order to y it yields *Newton's formula* in equation (B2), for which the column vector within brackets represents *Newton's binomial* that can be estimated as in equation (B3).

$$
\begin{array}{cccccccc}
i & x & y & \Delta^1 & \Delta^2 & \Delta^3 & \Delta^4 & \Delta^5 \\
0 & x_0 & y_0 & & & & & \\
 & & & \Delta^1 y_0 & & & & \\
1 & x_1 & y_1 & & \Delta^2 y_0 & & & \\
 & & & \Delta^1 y_1 & & \Delta^3 y_0 & & \\
2 & x_2 & y_2 & & \Delta^2 y_1 & & \Delta^4 y_0 & \\
 & & & \Delta^1 y_2 & & \Delta^3 y_1 & & \Delta^5 y_0 \\
3 & x_3 & y_3 & & \Delta^2 y_2 & & \Delta^4 y_1 & \\
 & & & \Delta^1 y_3 & & \Delta^3 y_2 & & \\
4 & x_4 & y_4 & & \Delta^2 y_3 & & & \\
 & & & \Delta^1 y_4 & & & & \\
5 & x_5 & y_5 & & & & &
\end{array} \qquad \text{(B1)}
$$

$$
\Delta^k y_0 = \sum_{i=0}^{k} (-1)^i \binom{k}{i} y_{k-i} \qquad \text{(B2)}
$$

$$
\binom{k}{i} = \frac{k!}{i!(k-i)!} = \frac{k(k-1)\dots(k-i+1)}{i!} \qquad \text{(B3)}
$$

The value of the function $y=f(x)$ is approximated by the collocation polynomial, which in its turn can be estimated from *Newton's formula of finite differences* (equation B4). This polynomial is presented for $k>5$ and written extensively until the fifth order term ($\Delta^5 y_0$) in equation (B5).

$$
y_k \approx p_K = \sum_{i=0}^{k} \binom{k}{i} \Delta^i y_0 \qquad \text{(B4)}
$$

$$
\begin{aligned}
p_K &= y_0 + k\Delta^1 y_0 + \frac{(k^2-k)}{2!}\Delta^2 y_0 + \frac{(k^3-3k^2+2k)}{3!}\Delta^3 y_0 + \\
&+ \frac{(k^4-6k^3+11k^2-6k)}{4!}\Delta^4 y_0 + \frac{(k^5-10k^4+35k^3-50k^2+24k)}{5!}\Delta^5 y_0 + \\
&+ \dots + \frac{(k^k-\dots)}{k!}\Delta^{-k} y_0
\end{aligned} \qquad \text{(B5)}
$$

The m order partial derivatives of the collocation polynomial with respect to k are taken and afterwards estimated for $k=0$ (equations B6 to B10 for m=1 to m=5). These are the m order partial derivatives of p_0 which approximate the m order partial derivatives of $y=f(x)$ at point x_0.

$$\frac{\partial y}{\partial x} \approx \left.\frac{\partial p_k}{\partial k}\right|_{k=0} = \frac{1}{\delta}\left(\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4} + \frac{\Delta^5 y_0}{5} + \ldots\right) \tag{B6}$$

$$\frac{\partial^2 y}{\partial x^2} \approx \left.\frac{\partial^2 p_k}{\partial k^2}\right|_{k=0} = \frac{1}{\delta^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \ldots\right) \tag{B7}$$

$$\frac{\partial^3 y}{\partial x^3} \approx \left.\frac{\partial^3 p_k}{\partial k^3}\right|_{k=0} = \frac{1}{\delta^3}\left(\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 + \frac{7}{4}\Delta^5 y_0 + \ldots\right) \tag{B8}$$

$$\frac{\partial^4 y}{\partial x^4} \approx \left.\frac{\partial^4 p_k}{\partial k^4}\right|_{k=0} = \frac{1}{\delta^4}\left(\Delta^4 y_0 - 2\Delta^5 y_0 + \ldots\right) \tag{B9}$$

$$\frac{\partial^5 y}{\partial x^5} \approx \left.\frac{\partial^5 p_k}{\partial k^5}\right|_{k=0} = \frac{1}{\delta^5}\left(\Delta^5 y_0 + \ldots\right) \tag{B10}$$

The equations presented above are named the *forward formulas* as they are obtained from increasing the x value by δ. Below are presented the *backward formulas* obtained from decreasing the x value by δ. The y_i are recorded and its differences are estimated as y_i-y_{i-1} (equation B11). *Newton's backward formula* is given by equation (B12). The collocation polynomial estimated from *Newton's backward formula* is presented in equation (B13). It is presented for $k>5$ and written extensively until the fifth order term in equation (B14).

$$
\begin{array}{cccccccc}
i & x & y & \nabla^{-1} & \nabla^{-2} & \nabla^{-3} & \nabla^{-4} & \nabla^{-5} \\
0 & x_0 & y_0 & & & & & \\
 & & & \nabla^{-1}y_0 & & & & \\
-1 & x_{-1} & y_{-1} & & \nabla^{-2}y_0 & & & \\
 & & & \nabla^{-1}y_{-1} & & \nabla^{-3}y_0 & & \\
-2 & x_{-2} & y_{-2} & & \nabla^{-2}y_{-1} & & \nabla^{-4}y_0 & \\
 & & & \nabla^{-1}y_{-2} & & \nabla^{-3}y_{-1} & & \nabla^{-5}y_0 \\
-3 & x_{-3} & y_{-3} & & \nabla^{-2}y_{-2} & & \nabla^{-4}y_{-1} & \\
 & & & \nabla^{-1}y_{-3} & & \nabla^{-3}y_{-2} & & \\
-4 & x_{-4} & y_{-4} & & \nabla^{-2}y_{-3} & & & \\
 & & & \nabla^{-1}y_{-4} & & & & \\
-5 & x_{-5} & y_{-5} & & & & &
\end{array}
\tag{B11}
$$

$$
\nabla^{-k} y_0 = \sum_{i=0}^{k} (-1)^i \binom{k}{i} y_{-i} \tag{B12}
$$

$$
y_{-k} \approx p_{-K} = \sum_{i=0}^{k} (-1)^i \binom{k}{i} \nabla^{-i} y_0 \tag{B13}
$$

$$
\begin{aligned}
p_{-K} = {} & y_0 - k\nabla^{-1}y_0 + \frac{\left(k^2 - k\right)}{2!}\nabla^{-2}y_0 - \frac{\left(k^3 - 3k^2 + 2k\right)}{3!}\nabla^{-3}y_0 + \\
& + \frac{\left(k^4 - 6k^3 + 11k^2 - 6k\right)}{4!}\nabla^{-4}y_0 + \\
& - \frac{\left(k^5 - 10k^4 + 35k^3 - 50k^2 + 24k\right)}{5!}\nabla^{-5}y_0 + \ldots \\
& \pm \frac{\left(k^k - \ldots\right)}{k!}\nabla^{-k}y_0
\end{aligned}
\tag{B14}
$$

The *m* order partial derivatives of $y=f(x)$ at point x_0 are approximated by first taking the *m* order partial derivatives of p_{-k} with respect to $-k$ and afterwards estimating it for $k=0$ (equations B15 to B19 for n=1 to n=5). These are the *backward formulas* for the numerical estimates of the derivatives.

$$\frac{\partial y}{\partial x} \approx \left.\frac{\partial p_{-k}}{\partial(-k)}\right|_{k=0} = \frac{1}{\delta}\left(\nabla^{-1}y_0 + \frac{\nabla^{-2}y_0}{2} + \frac{\nabla^{-3}y_0}{3} + \frac{\nabla^{-4}y_0}{4} + \frac{\nabla^{-5}y_0}{5} + \ldots\right) \quad \text{(B15)}$$

$$\frac{\partial^2 y}{\partial x^2} \approx \left.\frac{\partial^2 p_{-k}}{\partial(-k)^2}\right|_{k=0} = \frac{1}{\delta^2}\left(\nabla^{-2}y_0 + \nabla^{-3}y_0 + \frac{11}{12}\nabla^{-4}y_0 + \frac{5}{6}\nabla^{-5}y_0 + \ldots\right) \quad \text{(B16)}$$

$$\frac{\partial^3 y}{\partial x^3} \approx \left.\frac{\partial^3 p_{-k}}{\partial(-k)^3}\right|_{k=0} = \frac{1}{\delta^3}\left(\nabla^{-3}y_0 + \frac{3}{2}\nabla^{-4}y_0 + \frac{7}{4}\nabla^{-5}y_0 + \ldots\right) \quad \text{(B17)}$$

$$\frac{\partial^4 y}{\partial x^4} \approx \left.\frac{\partial^4 p_{-k}}{\partial(-k)^4}\right|_{k=0} = \frac{1}{\delta^4}\left(\nabla^{-4}y_0 + 2\nabla^{-5}y_0 + \ldots\right) \quad \text{(B18)}$$

$$\frac{\partial^5 y}{\partial x^5} \approx \left.\frac{\partial^5 p_{-k}}{\partial(-k)^5}\right|_{k=0} = \frac{1}{\delta^5}\left(\nabla^{-5}y_0 + \ldots\right) \quad \text{(B19)}$$

1.2 *Multivariate partial derivatives*

This deduction is demonstrated with more detail in the bivariate case. Its presentation is easier whereas the cases with more variables become evident once the bivariate case is understood. A function $y=f(x_1,x_2)$ is evaluated at each pair $(x_{1,i},x_{2,j})$, where i equals 0 to k while j equals 0 to l (this is minor letter ‘L’ not to make confusion with number 1), with equally spaced intervals ($x_{1,i+1}-x_{1,i}=h_1$ *and* $x_{2,j+1}-x_{2,j}=h_2$). The $y_{i,j}$ are recorded (equation B20). This matrix is the ‘ground zero’ of a pile of m order finite differences’ matrices, where m equals 0 to k. The finite differences are first taken along the x_1 dimension so that $\Delta^{1,0}y_{i,0}=y_{i+1,0}-y_{i,0}$ and generically $\Delta^{m,0}y_{i,0}=\Delta^{m-1,0}y_{i+1,0}-\Delta^{m-1,0}y_{i,0}$. So, each new floor above has a new matrix formed by subtracting from each line the preceding line in the matrix below. This results in a building of finite differences between the lines in the same horizontal plans (equations B21 to B23).

$$\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l} \\
\hline
0 & x_{1,0} & y_{0,0} & y_{0,1} & y_{0,2} & \ldots & y_{0,l} \\
1 & x_{1,1} & y_{1,0} & y_{1,1} & y_{1,2} & \ldots & y_{1,l} \\
2 & x_{1,2} & y_{2,0} & y_{2,1} & y_{2,2} & \ldots & y_{2,l} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
k & x_{1,k} & y_{k,0} & y_{k,1} & y_{k,2} & \ldots & y_{k,l}
\end{array} \quad \text{‘ground zero’} \tag{B20}$$

$$\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l} \\
\hline
0 & x_{1,0} & \Delta^{1,0} y_{0,0} & \Delta^{1,0} y_{0,1} & \Delta^{1,0} y_{0,2} & \ldots & \Delta^{1,0} y_{0,l} \\
1 & x_{1,1} & \Delta^{1,0} y_{1,0} & \Delta^{1,0} y_{1,1} & \Delta^{1,0} y_{1,2} & \ldots & \Delta^{1,0} y_{1,l} \\
2 & x_{1,2} & \Delta^{1,0} y_{2,0} & \Delta^{1,0} y_{2,1} & \Delta^{1,0} y_{2,2} & \ldots & \Delta^{1,0} y_{2,l} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
k-1 & x_{1,k-1} & \Delta^{1,0} y_{k-1,0} & \Delta^{1,0} y_{k-1,1} & \Delta^{1,0} y_{k-1,2} & \ldots & \Delta^{1,0} y_{k-1,l}
\end{array} \quad \text{‘1}^{\text{st}}\text{ floor’} \tag{B21}$$

$$\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l} \\
\hline
0 & x_{1,0} & \Delta^{2,0} y_{0,0} & \Delta^{2,0} y_{0,1} & \Delta^{2,0} y_{0,2} & \ldots & \Delta^{2,0} y_{0,l} \\
1 & x_{1,1} & \Delta^{2,0} y_{1,0} & \Delta^{2,0} y_{1,1} & \Delta^{2,0} y_{1,2} & \ldots & \Delta^{2,0} y_{1,l} \\
2 & x_{1,2} & \Delta^{2,0} y_{2,0} & \Delta^{2,0} y_{2,1} & \Delta^{2,0} y_{2,2} & \ldots & \Delta^{2,0} y_{2,l} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
k-2 & x_{1,k-2} & \Delta^{2,0} y_{k-2,0} & \Delta^{2,0} y_{k-2,1} & \Delta^{2,0} y_{k-2,2} & \ldots & \Delta^{2,0} y_{k-2,l}
\end{array} \quad \text{‘2}^{\text{nd}}\text{ floor’} \tag{B22}$$

$$\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l} \\
\hline
0 & x_{1,0} & \Delta^{k,0} y_{0,0} & \Delta^{k,0} y_{0,1} & \Delta^{k,0} y_{0,2} & \ldots & \Delta^{k,0} y_{0,l}
\end{array} \quad \text{‘k}^{\text{th}}\text{ floor’} \tag{B23}$$

Afterwards, the equivalent is done for the differences along the x_2 dimension, resulting in a building of differences between the columns in the same horizontal plans (equations B24 to B26). Nevertheless, both buildings share the same ‘ground zero’.

$$
\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l-1 \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l-1} \\
\hline
0 & x_{1,0} & \Delta^{0,1} y_{0,0} & \Delta^{0,1} y_{0,1} & \Delta^{0,1} y_{0,2} & \ldots & \Delta^{0,1} y_{0,l-1} \\
1 & x_{1,1} & \Delta^{0,1} y_{1,0} & \Delta^{0,1} y_{1,1} & \Delta^{0,1} y_{1,2} & \ldots & \Delta^{0,1} y_{1,l-1} \\
2 & x_{1,2} & \Delta^{0,1} y_{2,0} & \Delta^{0,1} y_{2,1} & \Delta^{0,1} y_{2,2} & \ldots & \Delta^{0,1} y_{2,l-1} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
k & x_{1,k} & \Delta^{0,1} y_{k,0} & \Delta^{0,1} y_{k,1} & \Delta^{0,1} y_{k,2} & \ldots & \Delta^{0,1} y_{k,l-1}
\end{array}
\qquad \text{‘1}^{\text{st}}\text{ floor’} \qquad \text{(B24)}
$$

$$
\begin{array}{cc|ccccc}
 & j & 0 & 1 & 2 & \ldots & l-2 \\
i & x_1, x_2 & x_{2,0} & x_{2,1} & x_{2,2} & \ldots & x_{2,l} \\
\hline
0 & x_{1,0} & \Delta^{0,2} y_{0,0} & \Delta^{0,2} y_{0,1} & \Delta^{0,2} y_{0,2} & \ldots & \Delta^{0,2} y_{0,l-2} \\
1 & x_{1,1} & \Delta^{0,2} y_{1,0} & \Delta^{0,2} y_{1,1} & \Delta^{0,2} y_{1,2} & \ldots & \Delta^{0,2} y_{1,l-2} \\
2 & x_{1,2} & \Delta^{0,2} y_{2,0} & \Delta^{0,2} y_{2,1} & \Delta^{0,2} y_{2,2} & \ldots & \Delta^{0,2} y_{2,l-2} \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
k & x_{1,k} & \Delta^{0,2} y_{k,0} & \Delta^{0,2} y_{k,1} & \Delta^{0,2} y_{k,2} & \ldots & \Delta^{0,2} y_{k,l-2}
\end{array}
\qquad \text{‘2}^{\text{nd}}\text{ floor’} \qquad \text{(B25)}
$$

$$
\begin{array}{cc|c}
 & j & 0 \\
i & x_1, x_2 & x_{2,0} \\
\hline
0 & x_{1,0} & \Delta^{0,l} y_{0,0} \\
1 & x_{1,1} & \Delta^{0,l} y_{1,0} \\
2 & x_{1,2} & \Delta^{0,l} y_{2,0} \\
\ldots & \ldots & \ldots \\
k & x_{1,k} & \Delta^{0,l} y_{k,0}
\end{array}
\qquad \text{‘l}^{\text{th}}\text{ floor’} \qquad \text{(B26)}
$$

From the orthogonal differences it can be deduced the oblique differences by doing first line-wise and then column-wise or vice-versa. In a first step it is presented the oblique differences along the main diagonal. Here, the first order oblique difference for $y_{0,0}$ is set by starting with the first order vertical difference. This is the finite differences between lines, or line-wise differences. Afterwards, it proceeds to the first order horizontal (column-wise) difference (equation B27). Nevertheless, the same result would be obtained if it had been started the other way around. Both ways, the final result is the algorithm essential to define bivariate oblique differences, present in the latter development of equation (B27). Starting from the origin, are identified the size one steps to all surrounding $y_{i,j}$. Then, the $y_{i,j}$ in the oblique path is added whereas the $y_{i,j}$ in the orthonormal paths are subtracted. Its general form is presented in equation (B28) and (B29) irrespective whether i equal j or not.

$$\Delta^{1,1} y_{0,0} = \Delta^{0,1}\left(\Delta^{1,0} y_{0,0}\right) = \Delta^{1,0} y_{0,1} - \Delta^{1,0} y_{0,0} = y_{1,1} - y_{0,1} - y_{1,0} + y_{0,0} \tag{B27}$$

$$\Delta^{1,1} y_{i,j} = y_{i+1,j+1} - y_{i,j+1} - y_{i+1,j} + y_{i,j} \tag{B28}$$

$$\Delta^{m+1,m+1} y_{i,j} = \Delta^{m,m} y_{i+1,j+1} - \Delta^{m,m} y_{i,j+1} - \Delta^{m,m} y_{i+1,j} + \Delta^{m,m} y_{i,j} \tag{B29}$$

Once the first order differences have been established, both the orthonormal and the oblique, the bivariate form of the first order *Newton's formula* for the collocation polynomial can be determined. This is essayed starting from $y_{0,0}$ (equation B30) and transposed to its general formula (equation B31) irrespective whether i equals j or not.

$$P_{1,1} = \Delta^{0,0} y_{0,0} + \Delta^{0,1} y_{0,0} + \Delta^{1,0} y_{0,0} + \Delta^{1,1} y_{0,0} \tag{B30}$$

$$P_{i+1,j+1} = \Delta^{0,0} y_{i,j} + \Delta^{0,1} y_{i,j} + \Delta^{1,0} y_{i,j} + \Delta^{1,1} y_{i,j} \tag{B31}$$

The second order oblique difference applied to $y_{0,0}$ is estimated applying the essential algorithm in equation (B29) to the 'first floor' with the first order oblique differences. This is in the first development of equation (B32). In the second development it is solved to the $y_{i,j}$ in the 'ground zero'. In the third development it is written in matrix algebra notation, where the $\otimes$ symbol represents the *Hadamard product*. This is the element-wise product between complementary entries in both matrices. The third development is done in order to clearly illustrate the point that takes it to the fourth and fifth developments. These latter ones are the objectives.

$$
\begin{aligned}
\Delta^{2,2} y_{0,0} &= \Delta^{1,1} y_{1,1} - \Delta^{1,1} y_{0,1} - \Delta^{1,1} y_{1,0} + \Delta^{1,1} y_{0,0} \\
&= y_{0,0} - 2y_{0,1} + y_{0,2} - 2y_{1,0} + 4y_{1,1} - 2y_{1,2} + y_{2,0} - 2y_{2,1} + y_{2,2} \\
&= sum\left(\begin{bmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{bmatrix} \otimes \begin{bmatrix} y_{0,0} & y_{0,1} & y_{0,2} \\ y_{1,0} & y_{1,1} & y_{1,2} \\ y_{2,0} & y_{2,1} & y_{2,2} \end{bmatrix}\right) \\
&= \sum_{i=0}^{2} \sum_{j=0}^{2} \left(\frac{2!}{i!(2-i)!} . \frac{2!}{j!(2-j)!} . y_{i,j} \right) \\
&= \sum_{i=0}^{2} \sum_{j=0}^{2} \left(\binom{2}{i} . \binom{2}{j} . y_{i,j} \right)
\end{aligned}
\qquad \text{(B32)}
$$

Repeating this exercise to higher order differences leads to the general formula applied to $y_{0,0}$ (equation B33) and to $y_{k,l}$ (equation B34). Notice that, comparing to the univariate situation, the sorting of the sum was reversed. Presently, it starts by the closer term and proceeds towards the term further away. Yet, results are equally valid.

$$
\Delta^{m,m} y_{0,0} = \sum_{i=0}^{m} \sum_{j=0}^{m} \left((-1)^{m-i+m-j} \binom{m}{i} . \binom{m}{j} . y_{i,j} \right) \qquad \text{(B33)}
$$

$$
\Delta^{m,m} y_{k,l} = \sum_{i=0}^{m} \sum_{j=0}^{m} \left((-1)^{m-i+m-j} \binom{m}{i} . \binom{m}{j} . y_{k+i,l+j} \right) \qquad \text{(B34)}
$$

Oblique differences do not necessarily go on a -45º angle. This is the same as saying oblique differences do not necessarily have the same order vertically and horizontally. Starting by the first floor with the $\Delta^{1,1} y_{i,j}$ finite differences and differentiating once more vertically (line-wise), it is obtained the $\Delta^{2,1} y_{i,j}$ oblique differences. This is illustrated for the $\Delta^{2,1} y_{0,0}$ in equation (B35). The same result would be obtained if the sequence was permuted to first line-wise (leading to $\Delta^{1,0} y_{i,j}$) and afterwards obliquely upon $\Delta^{1,0} y_{i,j}$ using the fundamental rule in equation (B29) (leading to $\Delta^{2,1} y_{i,j}$). The general case presented in equation 36 is for all bivariate finite differences, horizontal, vertical or oblique, equal orders or distinct orders. In equation (B37) it is extended for the general case of all multivariate finite differences with an *s* number of variables.

$$\Delta^{2,1}y_{0,0} = \Delta^{1,1}y_{1,0} - \Delta^{1,1}y_{0,0}$$
$$= -y_{0,0} + y_{0,1} + 2y_{1,0} - 2y_{1,1} - y_{2,0} + 2y_{2,1} \qquad \text{(B35)}$$
$$= sum\left(\begin{bmatrix} -1 & 1 \\ 2 & -2 \\ -1 & 1 \end{bmatrix} \otimes \begin{bmatrix} y_{0,0} & y_{0,1} \\ y_{1,0} & y_{1,1} \\ y_{2,0} & y_{2,1} \end{bmatrix}\right)$$

$$\Delta^{m_1,m_2} y_{k_1,k_2} = \sum_{j_1=0}^{m_1} \sum_{j_2=0}^{m_2} \left((-1)^{m_1-j_1+m_2-j_2} \binom{m_1}{j_1} . \binom{m_2}{j_2} . y_{k_1+j_1,k_2+j_2} \right) \qquad \text{(B36)}$$

$$\Delta^{m_1,m_2,\ldots,m_s} y_{k_1,k_2,\ldots k_s} = \sum_{j_1=0}^{m_1} \sum_{j_2=0}^{m_2} \ldots \sum_{j_s}^{m_s} \left((-1)^{\sum m_i - \sum j_i} \prod_{i=1}^{s} \binom{m_i}{j_i} . y_{k_1+j_1,k_2+j_2,\ldots,k_s+j_s} \right)$$
(B37)

Equation (B37) is the general case when all finite differences are estimated forward. Whenever the finite differences are meant to be estimated backward in a certain dimension the formula must be updated for that dimension according to equation (B38). However, for computational matters, as software do not support zero or negative indices for data arrays, the $-m_x+j_x$ entry is actually store in array's cell m_x-j_x, with $k_x=0$.

$$\Delta^{\ldots,-m_x,\ldots} y_{\ldots,k_x,\ldots} = \ldots \sum_{j_x=0}^{m_x} \ldots \left((-1)^{\sum m_i - \sum j_i} \prod_{i=1}^{s} \binom{m_i}{j_i} . y_{\ldots,k_x-m_x+j_x,\ldots} \right) \qquad \text{(B38)}$$

Setting the general rule for any bivariate finite differences is fundamental for the definition of the bivariate collocation polynomial. This polynomial, when estimated one step forward in both directions has vertical, horizontal and oblique finite differences of -45º angle (equations B30 and B31). However, when estimated more then one step forward for both of the directions it also has oblique finite differences of angles other than -45º. This is illustrated by its estimation two steps forward (equation B39). The general rule of this bivariate collocation polynomial is presented in equation (B40). It is anchored to $y_{0,0}$ and progresses m steps in the x_1 dimension and n steps in the x_2 dimension. This is upgraded to its general multivariate form (equation B41).

$$p_{2,2} = \sum_{m_1=0}^{2} \sum_{m_2=0}^{2} \binom{2}{m_1}\binom{2}{m_2} \Delta^{m_1,m_2} y_{0,0}$$

$$\begin{aligned} &= \binom{2}{0}\binom{2}{0}\Delta^{0,0} y_{0,0} + \binom{2}{0}\binom{2}{1}\Delta^{0,1} y_{0,0} + \binom{2}{0}\binom{2}{2}\Delta^{0,2} y_{0,0} + \\ &+ \binom{2}{1}\binom{2}{0}\Delta^{1,0} y_{0,0} + \binom{2}{1}\binom{2}{1}\Delta^{1,1} y_{0,0} + \binom{2}{1}\binom{2}{2}\Delta^{1,2} y_{0,0} + \\ &+ \binom{2}{2}\binom{2}{0}\Delta^{2,0} y_{0,0} + \binom{2}{2}\binom{2}{1}\Delta^{2,1} y_{0,0} + \binom{2}{2}\binom{2}{2}\Delta^{2,2} y_{0,0} \end{aligned} \tag{B39}$$

$$p_{n_1,n_2} = \sum_{m_1=0}^{n_1} \sum_{m_2=0}^{n_2} \binom{n_1}{m_1}\binom{n_2}{m_2} \Delta^{m_1,m_2} y_{0,0} \tag{B40}$$

$$p_{n_1,n_2,\ldots,n_s} = \sum_{m_1=0}^{n_1} \sum_{m_2=0}^{n_2} \cdots \sum_{m_s=0}^{n_s} \prod_{i=1}^{s} \binom{n_i}{m_i} \Delta^{m_1,m_2,\ldots,m_s} y_{0,0,\ldots,0} \tag{B41}$$

In order to demonstrate the general principle used to take the crossed partial derivatives of the polynomial above, it is first presented its development for the trivariate case (equation B42).

$$\begin{aligned} p_{n_1,n_2,n_3} &= Y_{0,0,0} + n_3\Delta^{0,0,1} y_{0,0,0} + \frac{\left(n_3^2 - n_3\right)}{2!}\Delta^{0,0,2} y_{0,0,0} + \ldots + \frac{\left(n_3^{n_3} - \ldots\right)}{n_3!}\Delta^{0,0,n_3} y_{0,0,0} + \\ &+ n_2.n_3\Delta^{0,1,1} y_{0,0,0} + n_2.\frac{\left(n_3^2 - n_3\right)}{2!}\Delta^{0,1,2} y_{0,0,0} + \ldots + n_2.\frac{\left(n_3^{n_3} - \ldots\right)}{n_3!}\Delta^{0,1,n_3} y_{0,0,0} + \\ &+ \frac{\left(n_2^2 - n_2\right)}{2!}.n_3\Delta^{0,2,1} y_{0,0,0} + \ldots + \frac{\left(n_2^2 - n_2\right)}{2!}.\frac{\left(n_3^{n_3} - \ldots\right)}{n_3!}\Delta^{0,2,n_3} y_{0,0,0} + \\ &+ \ldots + \frac{\left(n_2^{n_2} - \ldots\right)}{n_2!}.n_3\Delta^{0,n_2,1} y_{0,0,0} + \ldots + \frac{\left(n_2^{n_2} - \ldots\right)}{n_2!}.\frac{\left(n_3^{n_3} - \ldots\right)}{n_3!}\Delta^{0,n_2,n_3} y_{0,0,0} + \\ &+ n_1\Delta^{1,0,0} y_{0,0,0} + \ldots + \frac{\left(n_1^{n_1} - \ldots\right)}{n_1!}.\frac{\left(n_2^{n_2} - \ldots\right)}{n_2!}.\frac{\left(n_3^{n_3} - \ldots\right)}{n_3!}\Delta^{n_1,n_2,n_3} y_{0,0,0} \end{aligned} \tag{B42}$$

The terms of this sum may be displayed in a 3 dimensional array. Likewise, the terms of the sum of such type of polynomial with s variables may be arranged in an s-dimensional array ($p_{n_1,n_2,\ldots,n_s} = sum\left({}^{(n_1+1)\times(n_2+1)\times\ldots\times(n_s+1)}A\right)$). Notice that the A array has size $n+1$ in the each dimension because software does not allow entries with index zero. Therefore $p_{\ldots,0,\ldots}$ must be stored in $A_{\ldots,1,\ldots}$. To facilitate the calculus and the demonstration the 3 dimensional A array is rearranged to equation (B43), where ${}^{(n_1+1)\times(n_2+1)\times(n_3+1)}D$ is a matrix for which the entry d_{m_1+1,m_2+1,m_3+1} corresponds to the finite difference Δ^{m_1,m_2,m_3}. This 3D array is multiplied element-wise (*Hadamard product*) by another 3D array created by the polynomial coefficients vector (${}^{i}K$) applied to each dimension x_i and all multiplied orthogonally as to create the dimensional expansion to 3D. It is chosen the symbol Ц to represent such multiplication where ${}^{1}K$ operated by ${}^{2}K$ yields ${}^{(n_1+1)\times1\times1}K\times{}^{1\times(n_2+1)\times1}K={}^{(n_1+1)\times(n_2+1)\times1}K$. If this is operated by ${}^{3}K$ it yields ${}^{(n_1+1)\times(n_2+1)\times1}K\times{}^{1\times1\times(n_3+1)}K={}^{(n_1+1)\times(n_2+1)\times(n_3+1)}K$. Working with s variables this multiplication is repeated $s-1$ times generating an s-dimensional array ${}^{(n_1+1)\times(n_2+1)\times\ldots\times(n_s+1)}K$. At this step and further on, where n_i is meant to be variable, it is replaced by the similar k_i variable. This is done to prevent confusion later on between where n_i codes for the length of the array along dimension i and where n_i may be replaced by k_i which is coding for the point of estimate of the partial derivative. The coefficients in each ${}^{i}K$ vector are the ones already presented in equation (B5) for the forward finite differences and so, if the partial derivative is meant to be estimated forward the ${}^{i}K$ vector is given by equation 44. Otherwise, if the partial derivative is meant to be estimated backward the entries in the ${}^{i}K$ vector are taken from equation (B14), leading to the ${}^{i}K$ vector given by equation (B45).

$$ {}^{(n_1+1)\times(n_2+1)\times(n_3+1)}A={}^{(n_1+1)\times(n_2+1)\times(n_3+1)}D\otimes\coprod_{i=1}^{3}{}^{i}K \tag{B43}$$

$$ {}^{i}K_{forward}=\begin{bmatrix}1 & k_i & \dfrac{k_i^2-k_i}{2!} & \dfrac{k_i{}^3-3k_i^2+2k_i}{3!} & \dfrac{k_i{}^4-6k_i^3+11k_i^2-6k_i}{4!} & \ldots\end{bmatrix} \tag{B44}$$

$$
{}^{i}K_{backward} = \begin{bmatrix} 1 & -k_i & \dfrac{k_i^2 - k_i}{2!} & -\dfrac{k_i^3 - 3k_i^2 + 2k_i}{3!} & \dfrac{k_i^4 - 6k_i^3 + 11k_i^2 - 6k_i}{4!} & \dots \end{bmatrix}
$$

(B45)

The partial derivatives of the function may be estimated numerically by taking the partial derivatives of the multivariate collocation polynomial rearranged as the sum of all the terms in an s-dimensional A array (first line of development B46). These partial derivatives are taken in order to k. The s-dimensional D array is evaluated for $y_{0,0,\dots,0}$. Each ${}^{i}K$ vector must have size θ_i+1 in its i^{th} dimension and size 1 in every other dimension. While taking the partial derivatives the s-dimensional D array works as an array of constants and thus the process is simplified to the second line of development (B46). Each k_i only occurs in the related ${}^{i}K$ vector of coefficients. Therefore, from the basic rules of derivation the process is simplified to the third line of development (B46). Finally, $\dfrac{\partial^{\theta_i}}{\partial k_i^{\theta_i}}\,{}^{i}K$ is evaluated for $k_i=0$.

$$
\begin{aligned}
\frac{\partial^{\sum \theta_i} y_{0,0,\dots,0}}{\partial^{\theta_1} x_1 \partial^{\theta_2} x_2 \dots \partial^{\theta_s} x_s} &= \frac{\partial^{\sum \theta_i}}{\partial k_1^{\theta_1} \partial k_2^{\theta_2} \dots \partial k_s^{\theta_s}} sum\left({}^{(\theta_1+1)\times(\theta_2+1)\times\dots\times(\theta_s+1)}D \otimes K \right) \Bigg|_{\substack{\dim(i,{}^{i}K)=\theta_i \\ \dim(\neq i,{}^{i}K)=1 \\ \Delta y_{0,0,\dots,0} \\ k_i=0}} \\
&= sum\left({}^{(\theta_1+1)\times(\theta_2+1)\times\dots\times(\theta_s+1)}D \otimes \frac{\partial^{\sum \theta_i}}{\partial k_1^{\theta_1} \partial k_2^{\theta_2} \dots \partial k_s^{\theta_s}} \coprod {}^{i}K \right) \Bigg|_{\substack{\dim(i,{}^{i}K)=\theta_i \\ \dim(\neq i,{}^{i}K)=1 \\ \Delta y_{0,0,\dots,0} \\ k_i=0}} \\
&= sum\left({}^{(\theta_1+1)\times(\theta_2+1)\times\dots\times(\theta_s+1)}D \otimes \coprod \frac{\partial^{\theta_i}}{\partial k_i^{\theta_i}}\,{}^{i}K \right) \Bigg|_{\substack{\dim(i,{}^{i}K)=\theta_i \\ \dim(\neq i,{}^{i}K)=1 \\ \Delta y_{0,0,\dots,0} \\ k_i=0}}
\end{aligned}
$$

(B46)

The *forward* and *backward* vectors of coefficients for $\partial^0/\partial k_i^0({}^{i}K)$ were already presented in equation (B44) and equation (B45). The *forward* vectors of coefficients for partial derivatives of order 1 to 5 are presented in equations (B47) to (B51). The *backward* vectors of coefficients for partial derivatives of order 1 to 5 are presented in equations (B52) to (B56).

Forward vectors of coefficients

$$\frac{\partial}{\partial k_i}{}^{i}K = \frac{1}{\delta_i}\begin{bmatrix} 0 & 1 & \frac{(2k_i - 1)}{2!} & \frac{(3k_i^2 - 6k_i + 2)}{3!} & \frac{(4k_i^3 - 18k_i^2 + 22k_i - 6)}{4!} & \cdots \end{bmatrix} \tag{B47}$$

$$\frac{\partial^2}{\partial k_i{}^2}{}^{i}K = \frac{1}{\delta_i^2}\begin{bmatrix} 0 & 0 & 1 & \frac{(6k_i - 6)}{3!} & \frac{(12k_i^2 - 36k_i + 22)}{4!} & \cdots \end{bmatrix} \tag{B48}$$

$$\frac{\partial^3}{\partial k_i{}^3}{}^{i}K = \frac{1}{\delta_i^3}\begin{bmatrix} 0 & 0 & 0 & 1 & \frac{(24k_i - 36)}{4!} & \cdots \end{bmatrix} \tag{B49}$$

$$\frac{\partial^4}{\partial k_i{}^4}{}^{i}K = \frac{1}{\delta_i^4}\begin{bmatrix} 0 & 0 & 0 & 0 & 1 & \frac{(120k_i - 240)}{5!} & \cdots. \end{bmatrix} \tag{B50}$$

$$\frac{\partial^5}{\partial k_i{}^5}{}^{i}K = \frac{1}{\delta_i^5}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & \cdots. \end{bmatrix} \tag{B51}$$

Backward vectors of coefficients

$$\frac{\partial}{\partial k_i}{}^{i}K = \frac{1}{-\delta_i}\begin{bmatrix} 0 & -1 & \frac{(2k_i - 1)}{2!} & -\frac{(3k_i^2 - 6k_i + 2)}{3!} & \frac{(4k_i^3 - 18k_i^2 + 22k_i - 6)}{4!} & \cdots \end{bmatrix} \tag{B52}$$

$$\frac{\partial^2}{\partial k_i{}^2}{}^{i}K = \frac{1}{(-\delta_i)^2}\begin{bmatrix} 0 & 0 & 1 & -\frac{(6k_i - 6)}{3!} & \frac{(12k_i^2 - 36k_i + 22)}{4!} & \cdots \end{bmatrix} \tag{B53}$$

$$\frac{\partial^3}{\partial k_i^{\,3}}{}^iK = \frac{1}{(-\delta_i)3}\begin{bmatrix} 0 & 0 & 0 & -1 & \frac{(24k_i - 36)}{4!} & \ldots \end{bmatrix} \tag{B54}$$

$$\frac{\partial^4}{\partial k_i^{\,4}}{}^iK = \frac{1}{(-\delta_i)4}\begin{bmatrix} 0 & 0 & 0 & 0 & 1 & -\frac{(120k_i - 240)}{5!} & \ldots. \end{bmatrix} \tag{B55}$$

$$\frac{\partial^5}{\partial k_i^{\,5}}{}^iK = \frac{1}{(-\delta_i)5}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 & \ldots. \end{bmatrix} \tag{B56}$$

Two further upgrades may be added to the numerical solution for the partial derivatives previously shown in equation (B46). These are presented in equation (B57). One of the upgrades is that the partial derivatives may be estimated for y at $j_1,j_2,\ldots,j_s$ steps away from $y_{0,0,\ldots,0}$. In order to set where the partial derivatives are evaluated the ${}^iK$ vector of coefficients must be estimated for $k_i=j_i$. So, besides zero, k_i may also be any positive integer for the forward formula or any negative integer for the backward formula. However, computationally, as software does not support negative indices for data array entries, the negative integer for the backward formula is replaced by its absolute value. Estimating the partial derivatives at $k_i>0$ may be advantageous in the current case for which partial derivatives are intended to be used in the Taylor expansion of the model. This way, if δ_i is selected to be a fraction of h_i ($h=x_b-x_a$) j_i may be selected to be anywhere in between x_a and x_b. Nevertheless, it must be taken care not to set δ_i much lower or higher than 1 as this brings error into the numerical estimates on the account of being in a denominator raised to high powers. The other upgrade is that to estimate a partial derivative of order θ_i it must be taken at least $n_i=\theta_i$ steps. Then, the accuracy of the estimate may be increased if it is taken a number of steps n_i higher than the θ_i order of the derivative.

$$\frac{\partial^{\sum\theta_i} y_{j_1,j_2,\ldots,j_i}}{\partial^{\theta_1}x_1\partial^{\theta_2}x_2\ldots\partial^{\theta_i}x_i} = sum\left((n_1+1)\times(n_2+1)\times\ldots\times(n_i+1)_{\Delta} \otimes \coprod \frac{\partial^{\theta_i}}{\partial k_i^{\theta_i}}{}^iK\right)\Bigg\|_{\substack{\dim(i,{}^iK)=n_i\geq\theta_i \\ \dim(\neq i,{}^iK)=1 \\ \Delta y_{0,0,\ldots,0} \\ k_i=j_i}} \tag{B57}$$