Short Note

A Note on Second Vertical Derivatives

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The calculation of second vertical derivatives has assumed some importance in gravity and magnetic interpretation, and various operators for approximating to such derivatives have been suggested. A convenient summary of the literature has been given by Fuller (1967).

The purpose of this note is to point out that the actual values of the weights involved in these operators are of very little significance. In fact, if the operator is specified by a 3 x 3 matrix, the terms of the matrix may be chosen arbitrarily, provided two conditions are satisfied, and a certain region is avoided. The fact is most easily established from finite difference theory.

Methods for calculating second vertical derivatives depend on the fact that the fields measured in gravity and magnetic surveys are harmonic, satisfying Laplace's equation.

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = 0$$

in source free regions. If such a field is known everywhere on a plane z = constant, then, providing all sources are below the plane,

$$\frac{\partial^2}{\partial z^2} = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$$

at all points on the plane. This combination of derivatives has been extensively studied in connection with the numerical solution of partial differential equations. The development of the theory is largely due to Milne, but a convenient summary is given by Buckingham (1962) (provided care is taken to allow for the numerous editorial errors contained in this book).

The notation used below is Milne's notation, which is also used by Buckingham. W is the sampling interval, which must appear as a factor in any digital estimate of a derivative, and which is assumed to be the same in both x and y directions. The derivatives required are:—

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

$$Q^4 = \frac{\partial^4}{\partial x^2 \, \partial y^2}$$

with obvious extensions to higher orders.

A first approximation to ∇^2 is the operator H defined by

$$H = \boxed{\begin{matrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{matrix}}$$

(The significance of the box notation, due originally to Hartree, is obvious.) In fact, this is obtained by mere addition of second difference operators in the x & y directions. It is easy to show that another approximation to ∇^2 of the same order of accuracy is the operator X, defined by

$$2X = \boxed{\begin{matrix} 1 & 0 & 1 \\ 0 & -4 & 0 \\ 1 & 0 & 1 \end{matrix}}$$

Using the standard expressions for differences in terms of derivatives, these operators can be expanded as follows.

$$H = W^2\nabla^2 + \frac{W^4}{2\underline{|3}}(\nabla^4 - 2Q^4) + \frac{W^6}{3\underline{|5}}(\nabla^6 - 3Q^4\nabla^2) + \ldots\ldots.$$

$$X = W^2\nabla^2 + \frac{W^4}{2\underline{|3}}(\nabla^4 + 4Q^4) + \frac{W^6}{3\underline{|5}}(\nabla^6 + 12Q^4\nabla^2) + \ldots\ldots$$

Obviously any 3 x 3 matrix which satisfies the following conditions

(1) it is completely symmetrical
(2) the sum of the weights is zero

can be expressed as a linear combination of H & X. Its expansion will have a leading term $W^2\nabla^2$ (possibly multiplied by a numerical factor). To the first order, the performance of all such operators will be identical. It is necessary to exclude cases close to (X − H), in which the term in ∇^2 cancels out, and the leading term of the expansion contains derivatives of the fourth order.

Thus the operator $N^2 = \boxed{\begin{matrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{matrix}}$

= 2X − 2H, has the expansion

$$N^2 = W^4Q^4 + \frac{W^6}{2\underline{|3}}Q^4\nabla^2 + \frac{W^8}{3\underline{|5}}(\nabla^4Q^4 + \tfrac{1}{2}Q^8) + \ldots\ldots\ldots.$$

and could be used to obtain an estimate of Q^4, if this were required.

The above process may be used to obtain operators of superior performance. Thus the operator K = 4H + 2X =

$$\boxed{\begin{matrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{matrix}}$$

has the expansion

$$\frac{1}{6}K = W^2\nabla^2 + \frac{W^4\nabla^4}{2\underline{|3}} + \frac{W^6}{3\underline{|5}}(\nabla^6 + 2Q^4\nabla^2) + \ldots\ldots\ldots$$

Here the term in W^4Q^4 has disappeared, so that in principle, the performance is superior. The advantage is appreciable in dealing with well behaved mathematical functions, but is apt to be illusory when applied to observational data, due to the sharply tuned high pass nature of differentiating or differencing processes.

In fact, a test on a particular case using a few operators written down more or less at random, showed that there was no significant difference in performance.

The theory can easily be expanded to cover operators defined by matrices of higher order. Thus, a second order approximation to ∇^2 is given by the operator Z_1, defined by

$$Z_1 = \begin{array}{|rrrrr|} \hline 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 \\ -1 & 16 & -60 & 16 & -1 \\ 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ \hline \end{array}$$

which has the expansion

$$Z_1 = 12\,W^2\nabla^2 + 0\,(W^6).$$

Similarly, another approximation of the same order of accuracy is given by Z_2, defined by

$$2Z_2 = \begin{array}{|rrrrr|} \hline -1 & 0 & 0 & 0 & -1 \\ 0 & 16 & 0 & 16 & 0 \\ 0 & 0 & -60 & 0 & 0 \\ 0 & 16 & 0 & 16 & 0 \\ -1 & 0 & 0 & 0 & -1 \\ \hline \end{array}$$

which has the same expansion as Z_1.

The expansion of any linear combination of Z_1 and Z_2 will have a leading term in $W^2\nabla^2$, with further terms involving derivatives of the sixth and higher orders. As before, it is necessary to exclude cases close to $(Z_1 - Z_2)$, since the terms in $W^2\nabla^2$ cancel. Thus the operator

$$2Z_1 - 2Z_2 = \begin{array}{|rrrrr|} \hline 1 & 0 & -2 & 0 & 1 \\ 0 & -16 & 32 & -16 & 0 \\ -2 & 32 & -60 & 32 & -2 \\ 0 & -16 & 32 & -16 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ \hline \end{array}$$

has an expansion with a leading term involving derivatives of the sixth order.

Suitable operators for obtaining second derivatives are

$$Z_1 + 2Z_2 = \begin{array}{|rrrrr|} \hline -1 & 0 & -1 & 0 & -1 \\ 0 & 16 & 16 & 16 & 0 \\ -1 & 16 & -120 & 16 & -1 \\ 0 & 16 & 16 & 16 & 0 \\ -1 & 0 & -1 & 0 & -1 \\ \hline \end{array}$$

$$= 36\,W^2\nabla^2 + 0\,(W^6)$$

or

$$2Z_2 - Z_1 = \begin{array}{|rrrrr|} \hline -1 & 0 & 1 & 0 & -1 \\ 0 & 16 & -16 & 16 & 0 \\ 1 & -16 & 0 & -16 & 1 \\ 0 & 16 & -16 & 16 & 0 \\ -1 & 0 & 1 & 0 & -1 \\ \hline \end{array}$$

$$= 12\,W^2\nabla^2 + 0\,(W^6)$$

It will be noted that, in all the operators discussed, the sum of the weights is zero. This is a necessary condition for a differentiating or differencing operator. However, in the operators $(Z_1 - Z_2)$ or N^2, in which the leading term in $W^2\nabla^2$ cancels out, not only is the overall sum of weights zero, but the sum of weights in any row or column is zero.

Study of the expansions of operators having this property may lead to interesting results. Thus a symmetrical 5 x 5 matrix of this type depends on two parameters (to within a multiplying factor), and suitable choice of these parameters might allow of obtaining an estimate of any particular sixth derivative, if this were required.

Two further points may be mentioned. If estimates of derivatives are required for the solution of differential equations, it is essential that account be taken of the W factor, and of any numerical factors which may be introduced by the operator used. For the purposes for which second derivatives are generally required in geophysics, absolute values have no significance (except possibly for the zero value), and there is no disadvantage, and often some advantage, in conducting all calculations in the units of measurement, neglecting other multiplying factors. Such derivatives are often calculated for the purpose of separating anomalies lying very close together. If the calculation is made in units of measurement, it is often possible to obtain useful estimates of the individual anomalies by applying a relaxation process to the second derivative map.

Apart from their use in estimating derivatives, operators of the type discussed are capable of providing a sensitive test for herring-boning. If such an operator is applied to magnetic contours derived from an airborne survey on a suitably chosen grid, and the results exhibited as stacked profiles on lines perpendicular to the flight direction, any line up of peaks parallel to the flight direction would be open to grave suspicion. The process may have some application in cases where it is necessary to draw conclusions involving the highest possible accuracy in the observed data.

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References

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