Mathematics 30: Numerical Laplace

Many physical problems are centred upon the solution to partial differential operators involving the *Laplacian,* ∇^2. In numerical approaches space is usually discretised and then a discrete version of the laplacian operator is required. The simplest approach, 'Maths8', involves finding a quadratic approximation to the laplacian using a symmetric sum over nearest-neighbours. Improved accuracy can then be obtained by reducing the separation between grid points. Sometimes it is useful to be able to increase the accuracy be improving the *algorithm* and not by increasing the number of grid points. In this document some simple schemes for solving:

$$\nabla^2 z(x,y) = \lambda z(x,y)$$

will be developed, for the case of the two-dimensional square lattice.

The basic idea is to use *symmetric shells* of neighbours and to tune the relative contributions carefully. We elect to use:

$$\begin{aligned}
A_1 &= \sum_{\tau=\pm} z(x+\tau\delta, y) + z(x, y+\tau\delta) \\
A_2 &= \sum_{\tau_1=\pm}\sum_{\tau_2=\pm} z(x+\tau_1\delta, y+\tau_2\delta) \\
A_3 &= \sum_{\tau=\pm} z(x+2\tau\delta, y) + z(x, y+2\tau\delta)
\end{aligned}$$

symmetric sums over first to third neighbours, to assess the value of $\nabla^2 z(x,y)$, where δ is the grid-spacing. Expanding in powers of δ we find:

$$A_1 = 4z + \delta^2\nabla^2 z + \frac{\delta^4}{12}(\nabla_x^4 z + \nabla_y^4 z) + \frac{\delta^6}{360}(\nabla_x^6 z + \nabla_y^6 z) + \ldots$$

$$A_2 = 4z + 2\delta^2\nabla^2 z + \frac{\delta^4}{6}(\nabla_x^4 z + 6\delta_x^2\nabla_y^2 z + \nabla_y^4 z) + \frac{\delta^6}{180}(\nabla_x^6 z + 15\nabla_x^4\nabla_y^2 z + 15\nabla_x^2\nabla_y^4 z + \nabla_y^6 z) + \ldots$$

$$A_3 = 4z + 4\delta^2\nabla^2 z + \frac{4\delta^4}{3}(\nabla_x^4 z + \nabla_y^4 z) + \frac{8\delta^6}{45}(\nabla_x^6 z + \nabla_y^6 z) + \ldots$$

To generate an effective algorithm one might assume that the best approach is to eliminate all the higher-order terms, but this is not so. We can leave terms involving $\nabla^{2n} z$ with no ill effects. The simplest two algorithms are:

$$A_1 + \frac{1}{4}A_2 = 5z + \frac{3}{2}\delta^2\nabla^2 z + \frac{1}{8}\delta^4\nabla^4 z + O(\delta^6)$$

$$A_1 + \frac{3}{8}A_2 + \frac{1}{32}A_3 = \frac{45}{8}z + \frac{15}{8}\delta^2\nabla^2 z + \frac{3}{16}\delta^4\nabla^4 z + \frac{1}{96}\delta^6\nabla^6 z + O(\delta^8)$$

The final algorithms take the form:

$$z \mapsto \frac{A_1 + \frac{1}{4}A_2}{5 + \frac{3}{2}\delta^2\lambda + \frac{1}{8}\delta^4\lambda^2}$$

$$z \mapsto \frac{A_1 + \frac{3}{8}A_2 + \frac{1}{32}A_3}{\frac{45}{8}z + \frac{15}{8}\delta^2\lambda + \frac{3}{16}\delta^4\lambda^2 + \frac{1}{96}\delta^6\lambda^3}$$

Similar arguments for the triangular lattice provide:

$$A_1 = 6z + \frac{3}{2}\delta^2\nabla^2 z + \frac{9}{96}\delta^4\nabla^4 z + \frac{3}{11520}\delta^6(11\nabla_x^6 z + 15\nabla_x^4\nabla_y^2 z + 45\nabla_x^2\nabla_y^4 z + 9\nabla_y^6 z) + \ldots$$

$$A_2 = 6z + \frac{9}{2}\delta^2\nabla^2 z + \frac{81}{96}\delta^4\nabla^4 z + \frac{81}{11520}\delta^6(9\nabla_x^6 z + 45\nabla_x^4\nabla_y^2 z + 15\nabla_x^2\nabla_y^4 z + 11\nabla_y^6 z) + \ldots$$

and consequently:

$$z \mapsto \frac{A_1}{6 + \frac{3}{2}\delta^2\lambda + \frac{9}{128}\delta^4\lambda^2}$$

$$z \mapsto \frac{A_1 + \frac{1}{27}A_2}{\frac{56}{9} + \frac{5}{3}\delta^2\lambda + \frac{1}{8}\delta^4\lambda^2 + \frac{1}{192}\delta^6\lambda^3}$$

Similar arguments for the face-centre-cubic lattice provide:

$$A_1 = 12z + 2\delta^2\nabla^2 z + \frac{1}{12}\delta^4(\nabla_x^4 + \nabla_y^4 + \nabla_z^4 + 3\nabla_y^2\nabla_z^2 + 3\nabla_z^2\nabla_x^2 + 3\nabla_x^2\nabla_y^2)z + \ldots$$

$$A_2 = 6z + 2\delta^2\nabla^2 z + \frac{1}{3}\delta^4(\nabla_x^4 + \nabla_y^4 + \nabla_z^4)z + \ldots$$

and consequently:

$$z \mapsto \frac{A_1}{12 + 2\delta^2\lambda + \frac{2}{9}\delta^4\lambda^2}$$

$$z \mapsto \frac{A_1 + \frac{1}{8}A_2}{\frac{51}{4} + \frac{9}{4}\delta^2\lambda + \frac{1}{8}\delta^4\lambda^2}$$