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Note

A Rapidly Convergent Method for the Inversion of Separable, Positive, Self-Adjoint Discrete Elliptic Operators in Three or More Dimensions

Iterative methods for inverting the linear systems that arise from finite difference approximations to partial differential equations suffer from an operation count per point that increases algebraically with the resolution. Multigrid methods correct this defect in a generic way but are not trivial to code [1]. Packaged codes employing these techniques or other sparse matrix methods frequently require storage space several times larger than the original lattice, which can be a real limitation in three dimensions, [2, 3].

When separability can be effectively exploited, memory requirements should not significantly exceed what is necessary to store the solution itself. In two dimensions, Swarztrauber [4] has extended and implemented a direct method of Buzbee *et al.* [5] which is optimal in both storage and time (i.e., order $nm \ln(n)$ operations on an nm lattice). Implementing this algorithm directly in three dimensions appears difficult. In this note we call attention to a trivial device through which to extend a routine such as Swarztrauber's to a separable, positive, self-adjoint elliptic operator in higher dimensions with proportionate efficiency. (The inversion is done in place and the operation count per point increases only as the logarithm of the resolution.) The Poisson equation in separating coordinates is probably the most important application of our method.

In three dimensions consider the problem

$$L\varphi \equiv (L_x + L_y + L_z)\varphi = \rho,$$

where (x, y, z) are the three separable directions. Iterate in the following obvious way,

$$\begin{aligned}(L_x + L_y)\varphi^1 &= \rho - L_z\varphi^0 \\ (L_y + L_z)\varphi^2 &= \rho - L_x\varphi^1 \\ (L_z + L_x)\varphi^3 &= \rho - L_y\varphi^2.\end{aligned} \tag{1}$$

Let $\lambda_{x,y,z} > 0$ be a set of eigenvalues for $L_{x,y,z}$. Then the error, $\delta\varphi$, after one complete pass decreases as

$$|\delta\varphi^3| = \left|\frac{\lambda_x\lambda_y\lambda_z}{(\lambda_x+\lambda_y)(\lambda_y+\lambda_z)(\lambda_z+\lambda_x)}\right| |\delta\varphi^0| \leqslant \frac{1}{8}\,|\delta\varphi^0|. \tag{2}$$

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The convergence is linear for any eigenfunctions of L, which taken together are complete. In contrast to conventional iterative inversion, the convergence in (2) is as rapid for small λ as for large. Note that it would be self-defeating to collect all the diagonal terms in L into the two dimensional operator that gets inverted on each pass. Also, it is not possible to promote a direct method in one dimension to two.

The algorithm (1), can be readily extended to the Poisson equation with Neumann boundary conditions where strictly speaking there is a zero eigenmode. In fact (1), then, does not fully define the iteration since one is always free to add a different constant to φ in each 2-plane. However, if the discrete equation is written in conservative form, then the average of φ over any 2-plane may be determined exactly by solving a one dimensional system in the normal direction. This fixes the additive constants in $\varphi^{1,2,3}$ in (1) to within one overall constant.

Once one has a fast three dimensional method, a four dimensional operator can be inverted by running successively over all 3-planes. Hence by induction, all dimensions are accessible to a two dimensional algorithm.

Self-adjointness is only used to provide a simple bound on the rational function of $\lambda_{x,y,z}$ in (2), so this assumption could be eliminated by a case by case check. There appears to be no general way to lift the remaining assumptions of separability and positivity. An operator such as $(-\nabla^2 - 1)\varphi = \rho$, could certainly have growing eigenmodes if iterated as in (1).

The separability property seems indispensable. Even for the Laplacian in rectangular coordinates on a nonseparable domain, a rigorous proof of convergence eludes us. To appreciate the difficulty in the case just mentioned, define $\Sigma_1 = -(\partial_x^2 + \partial_y^2)(\partial_y^2 + \partial_z^2)(\partial_z^2 + \partial_x^2)$, and $\Sigma_2 = -\partial_x^2 \partial_y^2 \partial_z^2$. Since the derivatives all commute in rectangular coordinates, we have $\Sigma_1 \delta\varphi^3 = \Sigma_2 \delta\varphi^0$ and we wish to infer $|\delta\varphi^3| < cst\, |\delta\varphi^0|$, where the constant $cst < 1$. Rewrite $\Sigma_1 = 2\Sigma_2 + (\Sigma_1 - 2\Sigma_2)$ and observe that $(\Sigma_1 - 2\Sigma_2)$ can be made self-adjoint and positive definite if suitable boundary conditions are imposed on the space of functions. One might therefore suppose the $cst \leqslant \frac{1}{2}$. However, Σ_2 is only self-adjoint and positive definite on a space of functions different from the $(\Sigma_1 - 2\Sigma_2)$ space. Hence the argument fails.

By continuity, if the deviation from separability is sufficiently small, the iteration should still converge. It is clearly the lowest modes that are most apt to cause convergence problems when separability is lost.

We have implemented this algorithm for the Poisson equation in rectangular coordinates on all of R^3 by mapping each axis onto the internal $(-\pi/2, \pi/2)$ with the inverse tangent. The convergence rate within the L^2 norm was in the range 8–10 as expected.

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