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Short note

Modal preconditioning of Galerkin spectral methods: Dual bookkeeping for the Delves–Freeman iteration

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ABSTRACT

Fourier–Galerkin discretizations of PDEs can often be preconditioned by a matrix that is the union of a dense $M \times M$ matrix plus a large matrix that is either diagonal or banded with small bandwidth. This was suggested forty years ago by L.M. Delves. For our two-dimensional example, the preconditioned iteration converges geometrically fast to machine precision in less than ten iterations. If the residual of the partial differential equation is evaluated by Fast Fourier Transform (FFT), the cost scales almost linearly in the number of unknowns. On a 6144×6144 grid, the computation needed less than an hour in Matlab on a laptop. The dense block requires a total degree ordering; the FFT evaluation of the residual requires speedometer ordering of the Fourier coefficient matrix. We show that this dual bookkeeping is essential but not difficult.

1. Introduction

Single domain spectral methods are very accurate but generate dense discretization matrices that are expensive to form and factor, and are ill-conditioned for high degree N and/or high order differential equations. Preconditioned iterative methods have been order-of-magnitude cost-reducers. Both finite difference and finite element nodal preconditioners are very useful, but are not inexpensive for multidimensional problems [1].

Forty years ago, L.M. Delves proposed an alternative that generalizes easily to multiple dimensions except for the issue of ordering the unknowns [2,3]. This operates in "modal space" (that is, on the Galerkin matrix) rather than on the nodal basis and the pseudospectral collocation matrix. Galerkin approximations are usually not "diagonally dominant" in the sense that is so valuable in iterations for finite difference matrices. However, in many cases, the diagonal element of the j-th row of the Galerkin matrix does become larger and larger relative to the other elements in the same row and column as $j \to \infty$. In this sense, the Galerkin matrix is "*asymptotically* diagonal". Delves and Freeman's monograph [3] provides a strong theoretical foundation for this concept.

The underlying cause is that the Fourier–Galerkin discretization of $d^k u/dx^k$ is a *diagonal* matrix whose elements *grow* with row/column index j as j^k whereas the Galerkin representation of a term like $q(x)u(x)$ is a dense matrix whose elements are bounded independent of the row and column indices [1].

For an $N \times N$ two-dimensional tensor product grid, Delves' preconditioner is an $M \times M$ dense matrix plus an $(N^2 - M) \times (N^2 - M)$ diagonal matrix; all elements of both are copied from the N^2-dimensional Galerkin matrix. (The diagonal

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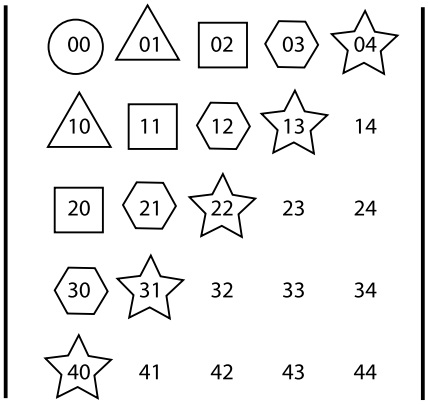

Fig. 1. Each pair of numbers gives the x and y wavenumbers of the basis function in the spectral coefficient matrix. The enclosing shapes indicate the total degree; thus, the stars enclose the five coefficients of the basis functions whose total degree is precisely four.

matrix often needs to be generalized to a banded matrix of small bandwidth, but for simplicity we restrict ourselves to a "block-and-diagonal" preconditioner here.) For ODEs, the "Delves" block is just the upper left $M \times M$ submatrix of the Galerkin matrix [1]. For PDEs, block selection is more complicated.

It is easiest to illustrate the key ideas using a Fourier cosine basis. However, for non-periodic problems, there has been an upsurge of interest in discretizations that employ "integration sparsification". A half dozen variants are compared in [6]; although the rationales seem wildly different, the ensuing discretizations are very similar. Olver and Townsend, for example, use a Petrov–Galerkin strategy with ultraspherical polynomials as the "test functions" while retaining Chebyshev polynomials as the basis functions [8,1]. The motive for this "integration sparsification" is to drastically reduce ill-conditioning, but the diagonalization or near-diagonalization of the highest derivative renders Delves' iteration much more effective as explained in our forthcoming publications [4,6,5,7].

Here, we concentrate on an issue important to both Fourier and Chebyshev discretizations. The key to minimizing both floating point operations and memory is to iterate using both a preconditioner and Fast Fourier Transform residual evaluation. It is then unnecessary to ever compute or store the $N^2 \times N^2$ Galerkin matrix [1]. (Preconditioned iterations require only direct matrix solves for the *preconditioning* matrix, here a block-and-diagonal matrix treated as two decoupled matrices of size $M \times M$ and $N \times N$ as we shall now explain.)

Multidimensional transforms are computed efficiently only as nested one-dimensional transforms, which requires writing the Fourier coefficients as an $N \times N$ matrix with "speedometer ordering"

$$a_I \equiv \text{coefficient of } \cos(mx)\cos(ny), m = 0, \ldots, (N-1);\ n = 0, \ldots, (N-1) \tag{1}$$

where $I = m + 1 + nN, I = 1, \ldots (N^2)$ as illustrated in Fig. 1. Denote the "fractional part" function by $x \equiv x - \lfloor x \rfloor$ where $\lfloor x \rfloor = \text{floor}(x)$ is the "floor" function, the largest integer $\leq x$. If $\{I/N\} > 0$, then the speedometer inverse functions are $m = N\{I/N\} - 1$ and $n = (I - m - 1)/N)$. If $\{I/N\} = 0$, then $m = N - 1$ and again $n = (I - m - 1)/N)$.

Unfortunately, asymptotic diagonal dominance depends on the growth of $m^2 + n^2$, the contribution of the second derivatives to the diagonal Galerkin matrix elements. Therefore, it is the terms of *smallest total degree* that must be included in the $M \times M$ block where the "total degree" of a basis function is

$$\text{tdeg}\big(\cos(mx)\cos(ny)\big) \equiv m + n \tag{2}$$

The number of basis functions satisfying $\text{tdeg}(\cos(mx)\cos(ny)) \leq D$ is $M = (D+2)(D+1)/2$ where D is the degree truncation and M is the size of the "Delves" block. The basis functions for the Delves block are an upper left triangular submatrix of the Fourier coefficient matrix (Fig. 1). (Delves and Freeman's theory and numerical experimentation guide the choice of D and M. Suffice it to say that for many problems, $M \ll N$ gives fast convergence [3,6,4,5,7,1].)

The bookkeeping is not onerous because the $M \times M$ block and the diagonal matrix of dimension $(N^2 - M)$ are *completely decoupled*. Solving the preconditioning matrix problem, as necessary in every iteration of whatever iteration scheme we chose, splits into two separate matrix solves.

It is easy to compute the Galerkin matrix elements of the $M \times M$ block by trapezoidal rule numerical quadrature provided that we have a mapping from the block index "jblock" to (m, n), the wavenumbers of the Fourier basis. The matrix elements of the Galerkin block are, denoting the differential operator by L and allowing the block indices to run from $jblock, kblock = 1, 2, \ldots, M$,

$$G^D_{jblock,kblock} = \frac{4}{\pi^2}\int_0^\pi dx \int_0^\pi dy \cos\big(mblock[jblock]x\big)\cos\big(nblock[jblock]y\big) \times L\cos\big(mblock[kblock]x\big)\cos\big(nblock[kblock]y\big) \tag{3}$$