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Multipole Expansions and Pseudospectral Cardinal Functions: A New Generalization of the Fast Fourier Transform

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The polynomial or trigonometric interpolant of an arbitrary function $f(x)$ may be represented as a "cardinal function" series whose coefficients are the values of $f(x)$ at the interpolation points. We show that the cardinal series is *identical* to the sum of the forces due to a set of N point charges (with appropriate force laws). It follows that the cardinal series can be summed via the fast multipole method (FMM) in $O(N \log_2 N)$ operations, which is much cheaper than the $O(N^2)$ cost of direct summation. The FMM is slower than the fast Fourier transform (FFT), so the latter should always be used where applicable. However, the multipole expansion succeeds where the FFT fails. In particular, the FMM can be used to evaluate Fourier and Chebyshev series on an *irregular* grid as is needed when adaptively regridding in a time integration. Also, the multipole expansion can be applied to basis sets for which the FFT is inapplicable even on the canonical grid including Legendre polynomials, Hermite and Laguerre functions, spherical harmonics, and sinc functions. © 1992 Academic Press, Inc.

1. INTRODUCTION

The pseudospectral family of numerical methods approximate a function $f(x)$ by a series of the form [1–6]

$$f(x) \approx \sum_{j=1}^{N} f(x_j)\, C_j(x), \tag{1}$$

where the grid points x_j and cardinal functions $C_j(x)$ are determined by the choice of underlying basis functions. For the Whittaker cardinal or sinc basis, for example, which is appropriate for the unbounded interval $x \in [-\infty, \infty]$,

$$x_j = hj, \qquad C_j(x) = \frac{\sin(\pi[x - x_j]/h)}{\pi(x - x_j)/h}, \tag{2}$$

where h is the (uniform) grid spacing. By definition, the cardinal functions have the property that

$$C_j(x_i) = \delta_{ij}, \tag{3}$$

where δ_{ij} is the usual Kronecker delta function. That is to say, the cardinal functions are combinations of the underlying basis (trigonometric functions, Chebyshev polynomials, or whatever) which are chosen so that the jth function is equal to one at the jth grid point and vanishes at all the other grid points. (The cardinal functions are also known as the "Lagrange basis," the "fundamental polynomial of Lagrangian interpolation," and collectively as the "cardinal basis.") The monograph by Boyd [1] gives a full treatment.

When the solution to a time-dependent problem develops shock waves or other regions of rapid change, a common tactic is to dynamically adjust the grid at regular time intervals. First, the gradients and curvature of the solution are evaluated at the current time level. The computer code then makes a change of coordinates so that the standard pseudospectral grid in the new, computational coordinate has a high density of grid points in regions of large gradients. One essential step in this dynamic regridding is to interpolate the solution from the original grid onto the new grid.

Unfortunately, direct evaluation of the cardinal series (1) is rather expensive because we must sum N terms at each of N grid points for a total cost of $O(N^2)$ operations per transform. Alternatively, we can sum (1) via the fast Fourier transform (FFT) at a cost of only $O(N \log_2 N)$ operations. Unfortunately, the FFT is *not* applicable to evaluate $f(x)$ on an *irregularly* spaced set of points.

However, we can sum (1) at each of N points in only $O(N \log_2 N)$ operations by using the fast multipole method (FMM). As reviewed by Greengard [9, 10], the FMM is a highly efficient algorithm for evaluating series of the form

$$E(x) = \sum_{j=1}^{N} \frac{q_j}{(x - x_j)}. \tag{4}$$

The q_j are the strengths of the N point charges (in electrostatics) or the masses of the N bodies (in gravitational problems); $E(x)$ is the force or the potential. The inverse first power law in (4) may be replaced by an inverse square

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law, by a logarithmic potential like $\log(x - x_j)$, or by a wide variety of other functions without invalidating the algorithm. Although our illustrations are one-dimensional, the FMM is applicable to sums like (4) in an arbitrary number of dimensions.

Historically, the FMM was invented for many-body calculations. However, the forces and potentials exerted by a number of point charges, vortices, or masses combine to create a series which is *identical* in mathematical form to a cardinal function series.

To demonstrate this last assertion for the special case of a sinc expansion, we merely use a trigonometric identity to write

$$f(x) = \sum_j f(x_j) \frac{\sin(\pi[x - jh]/h)}{\pi(x - jh)/h}$$
$$= \frac{h \sin(\pi x/h)}{\pi} \sum_j \frac{(-1)^j f(x_j)}{x - x_j}. \tag{5}$$

The summation on the right in (5) is identical in form to (4) with the equivalence $(-1)^j f(x_j) \Leftrightarrow q_j$. The physical interpretation is very different: the $f(x_j)$ are the grid point values of a single, continuous function, whereas the q_j are the charges of N different and distinct bodies. Nevertheless, the series are term-by-term identical.

We can extend the analysis to polynomial cardinal functions—Chebyshev, Legendre, Hermite, and Laguerre functions—by noting that for orthogonal polynomials, the interpolation points are the roots of the Nth member of the orthogonal set, $\phi_N(x)$. The polynomial of degree $(N-1)$ which, as required by (3), vanishes at all but one of the grid points and is unity at the jth point is then [1, 4, 8]:

$$C_j(x) = \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)}. \tag{6}$$

The N-term cardinal series for $f(x)$ is

$$f(x) \approx \phi_N(x) \sum_{j=1}^{N} \frac{f(x_j)/\phi'_N(x_j)}{(x - x_j)}. \tag{7}$$

This is of the same form as (4) except for the extracted factor of $\phi_N(x)$.

The cardinal functions for trigonometric interpolation are [1, 3]

$$C_j(x) = (-1)^j \sin(Nx) \cot\left(\frac{x - x_j}{2}\right). \tag{8}$$

The trigonometric cardinal series too can be summed by the FMM; the only difference from (5) is that the "force law" is $\cot([x - x_j]/2)$ instead of $1/(x - x_j)$.

The derivative of the interpolated function $f(x)$ is given by a series of similar form which is obtained by differentiating the cardinal series (1) term-by-term. Again, the FMM is applicable; the effect of the differentiation is merely to change the "force law" of the corresponding N-body problem.

For Chebyshev and Fourier methods, the FMM is useful only for interpolation to a *nonstandard* grid. Although the FMM and FFT are both $O(N \log_2 N)$ algorithms, the proportionality constant is much greater for the FMM. Consequently, the traditional FFT-based methods for evaluating derivatives on the standard pseudospectral grid are much more efficient and should be used instead of the FMM.

However, the FFT is *not* applicable to sinc series, Legendre sums, spherical harmonics, Hermite functions, or Laguerre functions. For these basis sets, the FMM is an order of magnitude faster than the direct summations that have been used with these basis sets in the past.

Orszag [11] has also developed a fast transform, but one based on exploiting the three-term recurrence relations for these basis functions rather than the FMM. Orszag's algorithm, like the FMM, has a large proportionality constant. It would be interesting to compare the FMM with Orszag's fast transform, but detailed comparisons are beyond the scope of this note.

We omit a detailed description of the FMM and numerical examples because these are given in the review article and book by Greengard [7, 8]. What is novel in this work is the *identification* of cardinal series with point force summations, that is, the equivalence of the grid points values of $f(x)$ with the point charges of the corresponding N-body problem. Once this identification has been made, once this equivalence has been recognized, then the FMM applies to cardinal function series *without modification.*

In summary, pseudospectral cardinal function series (for a general function $f(x)$ and its derivatives) are identical in form to N-body series (with the appropriate force law). This implies that the cardinal series can be summed in $O(N \log_2 N)$ operations by the FMM.

The FMM is not restricted to the regular pseudospectral grid but can be applied to interpolate $f(x)$ to an *irregular* grid, as needed in dynamical regridding. The FMM can also provide an FFT-substitute for basis sets such as Legendre and Hermite functions for which the FFT is not applicable. Thus, the FMM significantly extends the range of fast pseudospectral algorithms.

Several open questions remain. First, is it possible to improve (or improve upon) the FMM by exploiting the quasi-alternating nature of the cardinal function series? (Note that the terms of a cardinal function series are strictly alternating in sign if $f(x)$ is one-signed and almost alternating if $f(x)$ is an arbitrary function.) Second, how does the FMM compare with Orszag's fast transform and other methods like the sum acceleration schemes in [12]? Third, if N-body interactions are described by series identical in form to the cardinal function approximation to a continuous function, can we reinterpret many-body models as a description of a continuous flow field, and not merely a cloud of discrete particles or vortices?

These issues must remain for future work. It is already clear, however, that the connection between N-body models and polynomial approximation is both intriguing and useful.

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