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

JOHN P. BOYD

Department of Atmospheric, Oceanic, and Space Science, University of Michigan, 2455 Hayward Avenue, Ann Arbor, Michigan 48109

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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 \( O(N \log N) \) 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.

1. INTRODUCTION

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

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

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 \( x \in [-\infty, \infty] \),

\[
x_j = jh, \quad C_j(x) = \frac{\sin(p[x-x_j]/h)}{\pi(x-x_j)/h},
\]

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

\[
C_j(x_j) = \delta_{j},
\]

where \( \delta_j \) 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 \( j \)th function is equal to one at the \( j \)th 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 \( O(N \log N) \) 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 \( O(N \log N) \) 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

\[
E(x) = \sum_{j=1}^{N} \frac{q_j}{(x-x_j)},
\]

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
law, by a logarithmic potential like $\log(x - x_i)$, or by a wide
variety of other functions without invalidating the algo-

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rithm. 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

$$f(x) = \sum_j f(x_j) \frac{\sin(\pi [x - jh]/h)}{\pi [x - jh]/h}$$

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

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 inter-

pretation 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 $N$th 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 $j$th 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

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

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 differen-
tiating 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 algo-

rithm, 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 numeri-
cal 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 sum-
mations, 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 alter-
nating 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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