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Fast convolution with free-space Green's functions

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ABSTRACT

We introduce a fast algorithm for computing volume potentials – that is, the convolution of a translation invariant, free-space Green's function with a compactly supported source distribution defined on a uniform grid. The algorithm relies on regularizing the Fourier transform of the Green's function by cutting off the interaction in physical space beyond the domain of interest. This permits the straightforward application of trapezoidal quadrature and the standard FFT, with superalgebraic convergence for smooth data. Moreover, the method can be interpreted as employing a Nystrom discretization of the corresponding integral operator, with matrix entries which can be obtained explicitly and rapidly. This is of use in the design of preconditioners or fast direct solvers for a variety of volume integral equations. The method proposed permits the computation of any derivative of the potential, at the cost of an additional FFT.

1. Introduction

Many problems in scientific computing require the solution of a constant coefficient elliptic partial differential equation subject to suitable boundary or radiation conditions. In many cases, the free-space Green's function for the corresponding equation is known but involves nonlocal (long-range) interactions. A typical example is the Helmholtz equation in $\mathbf{R}^d$

$$\Delta\phi + k^2\phi = f,$$

where ϕ can be thought of as an acoustic potential and f a known distribution of acoustic sources, which we assume to be supported in the bounded domain $D = [-\frac{1}{2}, \frac{1}{2}]^d$. This can be done without loss of generality by rescaling the Helmholtz parameter k. The solution which satisfies the Sommerfeld radiation condition is well-known to be

$$\phi(\boldsymbol{x}) = \int_D g_k(\boldsymbol{x}-\boldsymbol{y})\, f(\boldsymbol{y})\, d\boldsymbol{y}, \tag{1}$$

where $g_k(\boldsymbol{r}) = \frac{1}{4i} H_0(kr)$ for $d = 2$ and $g_k(\boldsymbol{r}) = \frac{1}{4\pi}\frac{e^{ikr}}{r}$ for $d = 3$. Here, $r = \|\boldsymbol{r}\|_2$ and H_0 denotes the zeroth order Hankel function of the first kind.

Note that the interaction kernel is long-range, requiring fast algorithms to be practical, and singular at $r = 0$, requiring accurate quadrature techniques. In some applications, a third difficulty is that the source density f is highly inhomogeneous,

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requiring adaptive discretization. In such settings, intrinsically adaptive, hierarchical methods are required [1–4]. When the density is smooth, however, and well-resolved by a uniform mesh, it is more convenient (and generally more efficient) to use Fourier methods. We restrict our attention to the latter case in the present paper.

There are two distinct ways in which Fourier methods can be applied to the computation of (1). The first is the direct discretization of the equation with a *locally-corrected* trapezoidal rule. In the two-dimensional setting, for example, one can discretize D with a uniform mesh of N^2 points and use the approximation

$$\phi(nh, mh) \approx \sum_{\substack{n',m' \in [-\frac{N}{2}, \frac{N}{2}] \\ |n-n'|, |m-m'| > k}} g_k((n-n')h, (m-m')h)\, f(n'h, m'h)\, h^2 \quad + \\ \sum_{\substack{n',m' \in [-\frac{N}{2}, \frac{N}{2}] \\ |n-n'|, |m-m'| \leq k}} w_{n-n', m-m'} f(n'h, m'h)\,,$$

where $h = \frac{1}{N}$. Several groups have shown that kth order accuracy can be achieved in this manner by a suitable choice of weights $w_{i,j}$ (see, for example, [5–10]). The net sum takes the form of a discrete (aperiodic) convolution and, hence, can be computed using the FFT with zero-padding in $O(N^2 \log N)$ operations.

Alternatively, using the convolution theorem, one can write

$$\phi(\boldsymbol{x}) = \mathscr{F}^{-1}\left(\frac{F(s)}{|\boldsymbol{s}|^2 - k^2}\right) = \left(\frac{1}{2\pi}\right)^d \int_{\mathbf{R}^d} e^{i\boldsymbol{s}\cdot\boldsymbol{x}} \frac{F(\boldsymbol{s})}{|\boldsymbol{s}|^2 - k^2}\, d\boldsymbol{s}\,, \tag{2}$$

where

$$F(\boldsymbol{s}) = \mathscr{F}(f)(\boldsymbol{s}) = \int_D e^{-i\boldsymbol{s}\cdot\boldsymbol{x}} f(\boldsymbol{x})\, d\boldsymbol{x}\,. \tag{3}$$

$\mathscr{F}$ here denotes the Fourier transform. The fact that $f(\boldsymbol{x})$ is smooth permits us to compute the Fourier integral in (3) with "spectral" accuracy. It also ensures that the error in truncating the Fourier integral in the inverse transform (2) is rapidly decaying with $|\boldsymbol{s}|$. The principal difficulty in employing Fourier methods is the singularity $\frac{1}{|\boldsymbol{s}|^2 - k^2}$ in the integrand. In the case of the Poisson equation, this is simply $\frac{1}{|\boldsymbol{s}|^2}$.

It is possible to design high order rules for the inverse Fourier transform. In the case of the Poisson equation in three dimensions, for example, switching to spherical coordinates cancels the singularity entirely. Combining this with the nonuniform FFT yields more or less optimal schemes in terms of CPU time (see [11] and the references therein). This approach becomes technically more complicated for the Helmholtz equation, where the singularity lives on the sphere $|\boldsymbol{s}| = k$.

It turns out that there is a simple method that works for all long-range Green's functions, independent of dimension, requires only the trapezoidal rule, achieves spectral accuracy, and is accelerated by the standard FFT. Moreover, the matrix entries corresponding to this high order method are easily computed – a useful feature for either preconditioning strategies or direct solvers when using volume integral methods to solve variable coefficient partial differential equations.

Let us suppose, for the sake of simplicity, that we seek the restriction of the solution $\phi(\boldsymbol{x})$ to the unit box $D \subset \mathbf{R}^d$. Then, the maximum distance between any source and target point in D is $\sqrt{d}$. We define

$$g_k^L(\boldsymbol{r}) = \begin{cases} \dfrac{1}{4i} H_0(kr)\, \mathrm{rect}\left(\dfrac{r}{2L}\right) & \text{if } d = 2 \\ \dfrac{1}{4\pi} \dfrac{e^{ikr}}{r}\, \mathrm{rect}\left(\dfrac{r}{2L}\right) & \text{if } d = 3 \end{cases} \tag{4}$$

with $\mathrm{rect}(x)$ defined to be the characteristic function for the unit interval:

$$\mathrm{rect}(x) = \begin{cases} 1 & \text{for } |x| < 1/2 \\ 0 & \text{for } |x| > 1/2. \end{cases}$$

If we set $L > \sqrt{d}$ in d dimensions, then the solution (1) is clearly indistinguishable from

$$\phi(\boldsymbol{x}) = \int_D g_k^L(\boldsymbol{x} - \boldsymbol{y})\, f(\boldsymbol{y})\, d\boldsymbol{y}. \tag{5}$$

Since g_k^L is compactly supported, the Paley–Wiener theorem implies that its Fourier transform G_k^L is entire (and C^∞). Moreover, as we shall see below, it is straightforward to compute. In the case of the Laplace operator in three dimensions, for example, $G_0^L = 2(\frac{\sin(Ls/2)}{s})^2$. Thus, the Poisson equation in three dimensions has the solution