NONUNIFORM FAST FOURIER TRANSFORM (NUFFT) ALGORITHM AND ITS APPLICATIONS

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I. Introduction

Fast Fourier transform (FFT) has been enjoying widespread applications in numerical analysis and other areas of applied mathematics since Cooley and Tukey [1] established, in the 1960s, a powerful fast algorithm for calculating discrete Fourier transforms. The requirement for using FFT algorithms is that the input data must be equally spaced. In many practical situations, however, the input data is not equally spaced, and hence the regular FFT does not apply. To overcome this difficulty Dutt and Rokhlin [2] and Beylkin [3] studied the problem of FFT for nonuniform (unequally spaced) data.

We propose a new approach to achieve the fast Fourier transform for nonuniform data by using a new class of matrices, the regular Fourier matrices [4, 5]. This algorithm, also with a complexity of $O(N \log_2 N)$ where N is the number of data points, is more accurate than that proposed in [2] because our approximation error is minimized in the least-square sense.

One of the important applications of this NUFFT algorithm is to enhance the newly developed pseudospectral time-domain (PSTD) method [6], which requires only two cells per minimum wavelength, with the capability of having a nonuniform grid.

II. Formulation

Our aim is to develop a fast algorithm to find the following summation [2]:

$$f_j = F(\alpha)_j = \sum_{k=0}^{N-1} \alpha_k e^{i\omega_k \cdot t_j} \quad \text{for} \quad j = -N/2, \cdots, N/2-1, \tag{1}$$

where $\omega = \{\omega_0, \cdots, \omega_{N-1}\}$ and $t = \{t_{-N/2}, \cdots, t_{N/2-1}\}$ are finite sequences of real numbers, with $\omega_k \in [-N/2, N/2]$ for $k = 0, \cdots, N-1$ and $t_j = 2\pi j/N \in [-\pi, \pi]$ for $j = -N/2, \cdots, N/2-1$; $\alpha = \{\alpha_0, \cdots, \alpha_{N-1}\}$ and $f = \{f_{-N/2}, \cdots, f_{N/2-1}\}$ are finite sequences of complex numbers. Note that, unlike the regular FFT, ω_k's are nonuniform.

The idea of Dutt and Rokhlin [2] for solving this problem by a regular FFT is to approximate a function $F(x) = e^{-bx^2} e^{icx}$ by a small number of equally spaced points on the unit circle. We recognize that, in applications, the function F defined by (2) takes its values on a finite set only. Therefore, instead of (2), we can consider the following finite sequence

$$F(j) = s_j e^{i2\pi cj/N} \quad \text{for} \quad j = -N/2, \cdots, N/2-1, \tag{2}$$

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where $s_j > 0$ (called "accuracy factors") are chosen to minimize the approximation error. The novelty of this algorithm is that its approximation is optimal in the least-square sense, which leads to much more accurate results.

A. The regular Fourier matrices

For an integer $m \geq 2$ let $w = e^{i2\pi/mN}$, q be an even positive integer, s_j ($j = -N/2, \cdots, N/2-1$) be positive numbers, and c be a real number. Our aim is to find $x_{k-q/2}$ ($k = 0, \cdots, q$) to satisfy the following condition:

$$s_j w^{jmc} = \sum_{k=[mc]-q/2}^{[mc]+q/2} x_{k-[mc]}(c) w^{jk} \quad \text{for every} \quad j = -N/2, \cdots, N/2-1, \tag{3}$$

where $[mc]$ denotes the integer nearest to mc.

Since in our applications $q << N$, equation (3) cannot be expected to have an exact solution. However we can find the *least squares solution* of the inconsistent system (3). That is to find $x(c)$ such that $\|Ax(c) - v(c)\|$ is smallest possible. It is shown [4, 5] that

$$x(c) = F^{-1} a(c), \tag{4}$$

where

$$F_{jk}(m, N, q) = \begin{cases} N, & j = k \\ \dfrac{w^{(j-k)N/2} - w^{(k-j)N/2}}{1 - w^{(k-j)}}, & j \neq k \end{cases} \tag{5}$$

$$a_k(c) = \sum_{j=-N/2}^{N/2-1} s_j e^{i\frac{2\pi}{Nm}(\{mc\}+q/2-k)j}, \quad \text{for } k = 0, \cdots, q \tag{6}$$

and $\{mc\} = mc - [mc]$. Observe that matrix $F(m, N, q)$, called the *regular Fourier matrix*, is a Hermitian matrix of dimension $(q+1) \times (q+1)$, and is uniquely determined by m, N and q. This remarkable property of F is of great importance because it will reduce the number of operations by our algorithms and is a crucial point of this work.

B. The NUFFT Algorithm

We may choose two different accuracy factors, namely (i) the Gaussian $s_j = e^{-b(\frac{2\pi j}{Nm})^2}$ and (ii) the cosine $s_j = \cos\frac{\pi j}{Nm}$ accuracy factors. In particular, for the cosine accuracy factor, a closed-form solution can be found for (6):

$$a_k(c) = i \sum_{\gamma=-1,1} \frac{\sin[\frac{\pi}{2m}(2k - \gamma - q - 2\{mc\})]}{1 - e^{i\frac{\pi}{Nm}(2\{mc\}+q-2k+\gamma)}}. \tag{7}$$

This solution saves many arithmetic operations. Unfortunately, we are not able to find a corresponding closed-form solution for the Gaussian accuracy factors. Because of this, it is only sensible to use the Gaussian accuracy factors when many repeated NUFFTs are

required for the same ω_k points, since then one can pre-compute (4) for all the subsequent NUFFTs.

In summary, our NUFFT algorithm consists of following steps:

(1) Compute $x_j(\omega_k)$ by (4) for $j = 0, \cdots, q$ and $k = 0, \cdots, N-1$.

(2) Calculate Fourier coefficients

$$\tau_l = \sum_{j,k,[m\omega_k]+j=l} \alpha_k \cdot x_j(\omega_k).$$

(3) Use uniform FFT to evaluate

$$T_j = \sum_{k=-mN/2}^{mN/2-1} \tau_k \cdot e^{2\pi ikj/mN}.$$

(4) Scale the values to arrive at the approximated NUFFT

$$\tilde{f}_j = T_j \cdot s_j^{-1}.$$

The asymptotic number of arithmetic operations of this algorithm is $O(mN \log_2 N)$, where $m \ll N$. Usually we choose $m = 2$ and $q = 8$.

III. Numerical Results

We apply this NUFFT algorithm to perform spectral analysis of electromagnetic waves near sharp medium discontinuities. Shown in Figure 1(a) is the transverse electric field due to a transient plane wave normally incident to a thin conductive dielectric slab ($\epsilon_r = 4$ and $\sigma = 1$ S/m) of 15 cm thick. The fast spatial variation of the field (obtained by the FDTD method with a very fine grid) is depicted in Figure 1(a) near the slab, and is sampled nonuniformly. Figure 1(b) shows the excellent agreement of the (spatial) spectral amplitude obtained by the NUFFT (with cosine accuracy factors and $q = 8, m = 2$) and direct evaluation. Figure 1(c) displays the absolute error from our NUFFT algorithm and that from [2]. Quantitatively, the L_2 and L_∞ errors defined in [2] are $E_2 = 2.731 \times 10^{-6}$ and $E_\infty = 2.956 \times 10^{-6}$ for our algorithm, and $E_2 = 3.849 \times 10^{-5}$ and $E_\infty = 3.694 \times 10^{-5}$ for the algorithm in [2]. Our NUFFT algorithm is more than one order of magnitude more accurate.

Figure 1(d) shows the CPU time as a function of N in the NUFFT algorithm. Both the input data α_k and its locations ω_k ($k = 0, \cdots, N-1$) are obtained by a pseudo-random number generator with large variations. It clearly verifies that the algorithm is of complexity $O(N \log_2 N)$.

IV. Conclusions

Based on a class of regular Fourier matrices, a new nonuniform fast Fourier transform (NUFFT) algorithm is developed for unequally spaced data. With a comparable complexity of $O(N \log_2 N)$, this algorithm is much more accurate than previously reported results since it is optimal in the least squares sense. The algorithm is useful for computational electromagnetics and other fields of applied mathematics.

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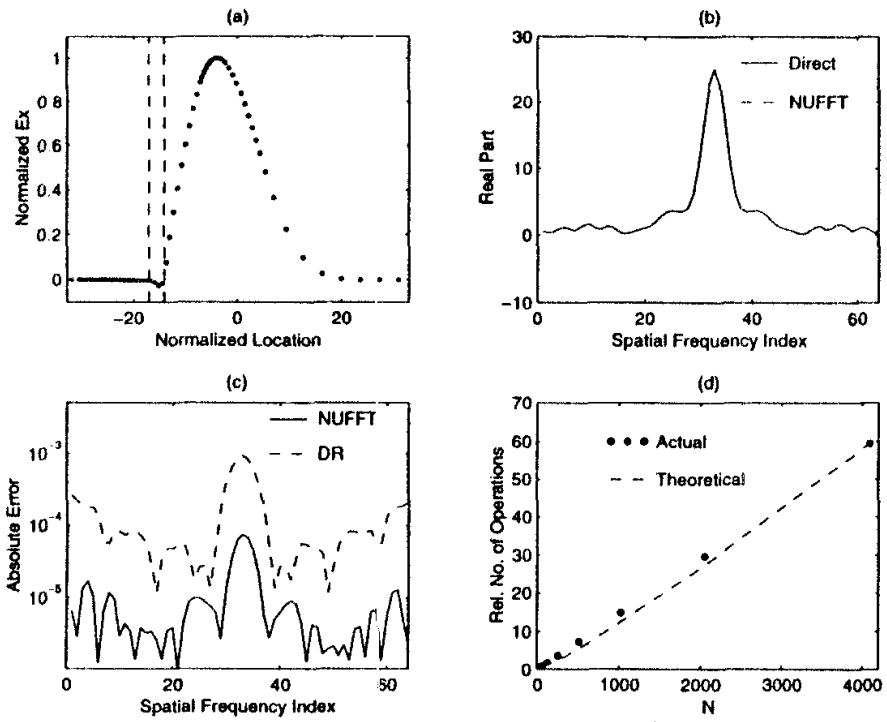

Figure 1. (a) Spatial distribution of transient electromagnetic field near a conductive dielectric slab. Dashed lines show interfaces of the slab. Nonuniform sampling is used to increase the resolution close to the slab. (b) The (spatial) spectral amplitude of the field obtained by direct evaluation and by the NUFFT algorithm. (c) Absolute errors from this algorithm and that by Dutt-Rokhlin [2]. (d) Relative number of operations as a function of N. Both input data and the locations of the sampling points are random. The dashed curve is the theoretically predicted curve $O(N \log_2 N)$ passing through the last point.