An Accurate Algorithm for Nonuniform Fast Fourier Transforms (NUFFT's)

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***Abstract*— Based on the (m, N, q)-regular Fourier matrix, a new algorithm is proposed for fast Fourier transform (FFT) of nonuniform (unequally spaced) data. Numerical results show that the accuracy of this algorithm is much better than previously reported results with the same computation complexity of $O(N \log_2 N)$. Numerical examples are shown for the applications in computational electromagnetics.**

***Index Terms*—Discrete Fourier transforms, Fourier series, interpolation, nonuniform fast Fourier transform (NUFFT).**

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 1960's, 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 nonuniform (i.e., 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 (NUFFT) data by using a new class of matrices, the regular Fourier matrices [4]. 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 [5], 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] for $j = -N/2, \cdots, N/2 - 1$:

$$f_j = F(\alpha)_j = \sum_{k=0}^{N-1} \alpha_k e^{i\omega_k \cdot t_j} \tag{1}$$

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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 (i.e., unequally spaced).

The idea of Dutt and Rokhlin [2] for solving this problem by a regular FFT is to approximate a function $F : [-\pi, \pi] \to C$ of the form

$$F(x) = e^{-bx^2} e^{icx}, \qquad \text{for } x \in [-\pi, \pi] \tag{2}$$

where $b > 1/2$ and c is a real number, 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:

$$F(j) = s_j e^{i2\pi cj/N}, \qquad \text{for } j = -N/2, \cdots, N/2 - 1 \tag{3}$$

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:

$$s_j w^{jmc} = \sum_{k=[mc]-q/2}^{[mc]+q/2} x_{k-[mc]}(c) w^{jk} \tag{4}$$

where $[mc]$ denotes the integer nearest to mc. Defining matrices and vectors shown in (5) at the bottom of the next page, and

$$v(c) = \begin{bmatrix} s_{-N/2} w^{-\frac{N}{2}mc} \\ s_{-N/2+1} w^{(-\frac{N}{2}+1)mc} \\ \vdots \\ s_0 \\ \vdots \\ s_{N/2-1} w^{(\frac{N}{2}-1)mc} \end{bmatrix} \tag{6}$$

we obtain the equation

$$Ax(c) = v(c). \tag{7}$$

Observe that (7) is a system of N linear equations with $(q+1)$ unknowns. Since in our applications $q \ll N$, (7) cannot be expected to have an exact solution. However, we can find the *least-squares solution* of the inconsistent system (7). That is, to find $x(c)$ such that $||Ax(c) - v(c)||$ is smallest possible:

$$x(c) = F^{-1}a(c) \tag{8}$$

where

$$a(c) = A^{\dagger}(c) \cdot v(c) \tag{9}$$

and (10), shown at the bottom of the page, where $A^{\dagger}$ denotes the complex-conjugate transpose of A matrix. Observe that while A, and hence $A^{\dagger}$, depends on c, the product matrix $F(m, N, q) = A^{\dagger}A$ is independent of c and is uniquely determined by m, N and q. This remarkable property of A is of great importance because it will reduce the number of operations by our algorithms and is a crucial point of this work. The matrix $F(m, N, q)$, for $m, N, q \in \mathcal{N}$, called the (m, N, q)-*regular Fourier matrix*, is a Hermitian matrix of dimension $(q+1) \times (q+1)$. The elements of $a(c)$ are given by

$$a_k(c) = \sum_{j=-N/2}^{N/2-1} s_j e^{i\frac{2\pi}{Nm}(\{mc\}+q/2-k)j} \tag{11}$$

where $\{mc\} = mc - [mc]$, and $k = 0, \cdots, q$.

B. The NUFFT Algorithm

We may choose two different accuracy factors, namely 1) the Gaussian $s_j = e^{-b(\frac{2\pi j}{Nm})^2}$ and 2) 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 (11):

$$a_k(c) = i \sum_{\gamma=-1,1} \frac{\sin\left[\frac{\pi}{2m}(2k - \gamma - q - 2\{mc\})\right]}{1 - e^{i\frac{\pi}{Nm}(2\{mc\}+q-2k+\gamma)}}. \tag{12}$$

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 NUFFT's are required for the same ω_k points, since then one can precompute (8) for all the subsequent NUFFT's.

In summary, our NUFFT algorithm consists of following steps.

1) Compute $x_j(\omega_k)$ by (8) for all j and k.
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 Fig. 1(a) is the transverse electric field due to a transient plane wave normally incident to a thin conductive dielectric slab of 15 cm thick. The slab has $\epsilon_r = 4$ and $\sigma = 1$ S/m, and the background is vacuum. The center frequency of the transient incident wave is 166.7 MHz (a Blackman–Harris window time function). In terms of the center frequency, the slab is only $1/12$ of the wavelength in vacuum. The fast spatial variation of the field [obtained by the finite-difference time-domain (FDTD) method with a very fine grid] is depicted in Fig. 1(a) near the slab. As shown in the figure, in order to effectively describe the field variation, a fine sampling is used near the slab, while a much coarser sampling is used away from the slab where the field has a slow variation. Fig. 1(b) and (c) shows the excellent agreement of the real and imaginary parts of the (spatial) spectrum obtained by the

$$A = \begin{bmatrix} w^{-\frac{N}{2}([mc]-q/2)} & w^{-\frac{N}{2}([mc]-q/2+1)} & \cdots & w^{-\frac{N}{2}([mc]+q/2)} \\ w^{(-\frac{N}{2}+1)([mc]-q/2)} & w^{(-\frac{N}{2}+1)([mc]-q/2+1)} & \cdots & w^{(-\frac{N}{2}+1)([mc]+q/2)} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ w^{(\frac{N}{2}-1)([mc]-q/2)} & w^{(\frac{N}{2}-1)([mc]-q/2+1)} & \cdots & w^{(\frac{N}{2}-1)([mc]+q/2)} \end{bmatrix} \tag{5}$$

$$F(m, N, q) = \begin{bmatrix} N & \frac{w^{-N/2} - w^{N/2}}{1-w} & \cdots & \frac{w^{-qN/2} - w^{qN/2}}{1-w^q} \\ \frac{w^{N/2} - w^{-N/2}}{1-w^{-1}} & N & \cdots & \frac{w^{-(q-1)N/2} - w^{(q-1)N/2}}{1-w^{q-1}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{w^{qN/2} - w^{-qN/2}}{1-w^{-q}} & \frac{w^{(q-1)N/2} - w^{-(q-1)N/2}}{1-w^{-(q-1)}} & \cdots & N \end{bmatrix} \tag{10}$$

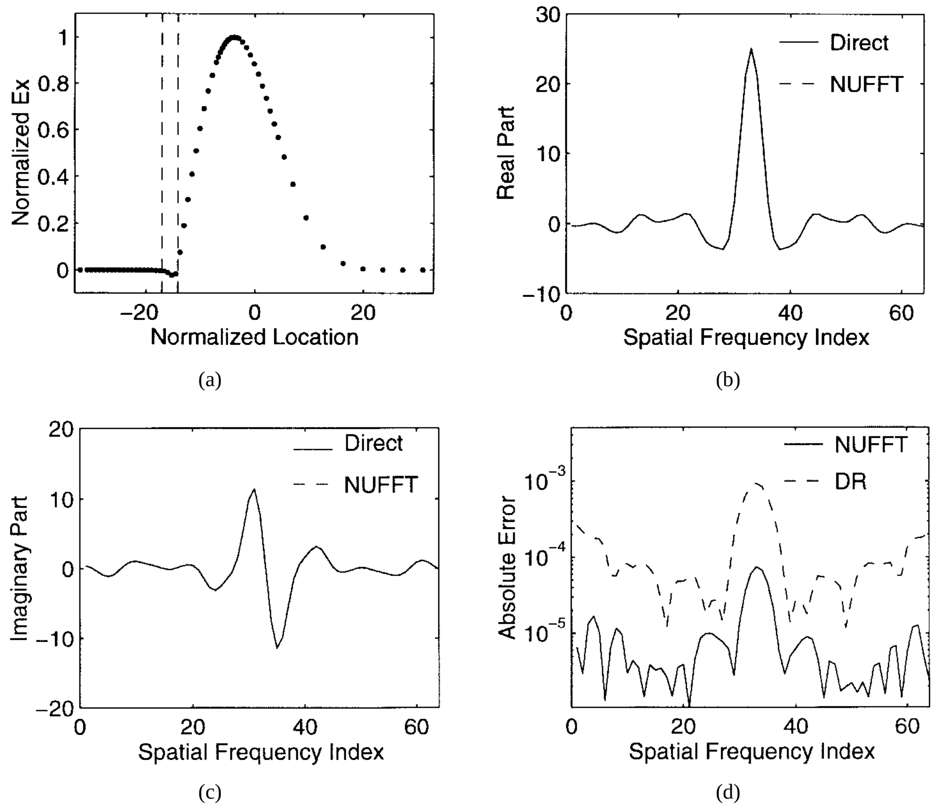

Fig. 1. (a) Spatial distribution of transient electromagnetic field near a conductive dielectric slab. Dashed lines show interfaces of the slab. Nonuniform sampling is used to increase the resolution close to the slab. (b) Real and (c) imaginary parts of the (spatial) spectrum of the field obtained by direct evaluation and by the NUFFT algorithm. (d) Absolute errors from this algorithm and that by Dutt–Rokhlin [2].

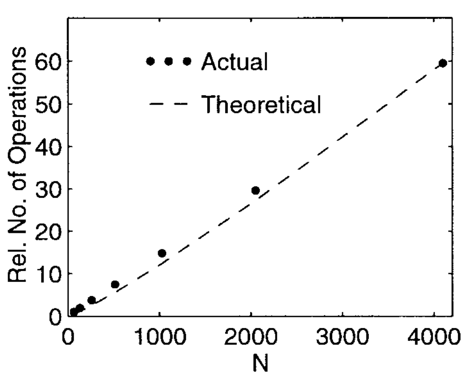

Fig. 2. Relative number of operations as a function of N. Both input data and the locations of the sampling points are random. The dashed curve is the theoretically predicted curve passing through the last point.

NUFFT (with cosine accuracy factors and $q = 8, m = 2$) and direct evaluation. Fig. 1(d) 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. This algorithm will benefit the development of a nonuniform pseudospectral time-domain (PSTD) method for Maxwell's equations [5].

Fig. 2 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 pseudorandom number generator with large variations. It clearly verifies that the algorithm is of complexity $O(N \log_2 N)$.

IV. Conclusion

Based on a class of regular Fourier matrices, a new 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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