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Numerical stability of nonequispaced fast Fourier transforms

Daniel Potts[a,*], Manfred Tasche[b]

[a] *Chemnitz University of Technology, Department of Mathematics, D-09107 Chemnitz, Germany*
[b] *University of Rostock, Institute for Mathematics, D-18051 Rostock, Germany*

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Dedicated to Franz Locher in honor of his 65th birthday

Abstract

This paper presents some new results on numerical stability for multivariate fast Fourier transform of nonequispaced data (NFFT). In contrast to fast Fourier transform (of equispaced data), the NFFT is an approximate algorithm. In a worst case study, we show that both approximation error and roundoff error have a strong influence on the numerical stability of NFFT. Numerical tests confirm the theoretical estimates of numerical stability.

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1. Introduction

An algorithm for the discrete Fourier transform of equispaced data with low arithmetical cost is called a *fast Fourier transform* (FFT). It is very important that a fast algorithm works stably in a floating point arithmetic. It is known (see e.g. [12,22]) that univariate FFTs are very sensitive with respect to the accuracy of precomputation and that under certain conditions these algorithms can be remarkably stable. This result can be generalized to d-variate FFTs (see Lemma 5.2).

In this paper, we consider the fast computation of a d-variate discrete Fourier transform for nonequispaced data which is shortly called *nonequispaced fast Fourier transform* (NFFT). In recent years, the NFFT has attracted much attention [3,5,20,10] as a method for the fast approximate evaluation of a d-variate trigonometric polynomial at arbitrary nodes. Let M and N be even positive integers. By I_N^d we denote the index set $\{-\frac{N}{2}, \ldots, \frac{N}{2} - 1\}^d$. For given nonequispaced nodes $\boldsymbol{x}_j \in [-\frac{1}{2}, \frac{1}{2})^d$ $(j \in I_M^1)$ and given $\hat{f}_{\boldsymbol{k}} \in \mathbb{C}$ $(\boldsymbol{k} \in I_N^d)$ we are interested in a fast and

* Corresponding author.
E-mail addresses: potts@mathematik.tu-chemnitz.de (D. Potts), manfred.tasche@uni-rostock.de (M. Tasche).

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numerically stable computation of all values $f(\boldsymbol{x}_j)$ of the d-variate trigonometric polynomial

$$f(\boldsymbol{x}) := \sum_{\boldsymbol{k}\in I_N^d} \hat{f}_{\boldsymbol{k}} \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}.$$

A direct evaluation of all values $f(\boldsymbol{x}_j)$ $(j \in I_M^1)$ requires $\mathcal{O}(N^d\, M)$ arithmetical operations, too much for practical purposes. The most efficient NFFTs were proposed in [5,3]. Later, Steidl [20,6] has presented a unified approach to NFFT and has improved the estimates of the approximation error. Nowadays, software of d-variate NFFT is freely available from the homepage [14].

In contrast to FFT, the NFFT is an approximate algorithm. By NFFT, we can compute only approximate values for $f(\boldsymbol{x}_j)$. Using oversampling, we approximate the d-variate trigonometric polynomial f by g a linear combination of translates of suitable window function φ having a good localization in the time/spatial and frequency domain. Here we choose a Gaussian or Kaiser–Bessel window function. Then the Fourier coefficients of g can be easily computed by d-variate FFT. By truncation of φ by means of a cut-off parameter, we can calculate approximate values of $f(\boldsymbol{x}_j)$ in a simple and fast way. Thus the d-variate NFFT with N^d input data and M output data requires $\mathcal{O}(N^d \,\log N + M)$ arithmetical operations.

We measure the nonuniformity of this sampling grid $\{\boldsymbol{x}_j \in [-\frac{1}{2}, \frac{1}{2})^d : j \in I_M^1\}$ by a mesh norm and a separation distance. Roughly speaking, the mesh norm and the separation distance is the largest and the smallest gap between neighboring nodes, respectively. We reformulate results in [11] concerning weighted sampling of d-variate trigonometric polynomials.

In order to introduce the normwise backward stability of NFFT, we have to consider the inverse NFFT. Therefore we discuss the solvability of the linear system

$$\boldsymbol{A}_{M,N^d}^{(d)} \hat{\boldsymbol{f}} = \boldsymbol{f},$$

where

$$\boldsymbol{A}_{M,N^d}^{(d)} := \left(\mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}_j}\right)_{j\in I_M^1, \boldsymbol{k}\in I_N^d} \in \mathbb{C}^{M\times N^d} \tag{1.1}$$

is the nonequispaced Fourier matrix, $\hat{\boldsymbol{f}} := (\hat{f}_{\boldsymbol{k}})_{\boldsymbol{k}\in I_N^d} \in \mathbb{C}^{N^d}$ is an unknown vector, and $\boldsymbol{f} := (f_j)_{j\in I_M^1}$ is a given vector. In the case $N^d < M$, this linear system is overdetermined and nonsolvable in general. But we can find a convenient vector $\hat{\boldsymbol{f}}$ by weighted reconstruction, where we follow an idea in [11] and compensate the "clusters" in the sampling set by special weights. If the mesh norm of the sampling grid is smaller than $\mathcal{O}(N^{-1})$, then a weighted nonequispaced Fourier matrix is left-invertible. In the case $N^d > M$, we focus on the underdetermined and consistent linear system. We expect to interpolate the given data $f_j \in \mathbb{C}$ $(j = 0, \ldots, M-1)$ exactly by optimal interpolation via damping factors. If the separation distance of the sampling grid is greater than $\mathcal{O}(N^{-1})$, then a weighted nonequispaced Fourier matrix is right-invertible.

Now we are able to investigate a worst case roundoff error analysis for the d-variate NFFT. We propose a definition of normwise backward stability of the approximate NFFT. With other words, we consider the influences of approximation error and roundoff error together. We show that under weak assumptions, the NFFT possesses a remarkable good numerical stability. The stability depends on the norm of the left inverse or right inverse of the underlying weighted nonequispaced Fourier matrix. As usual in a worst case analysis, the errors are overestimated, especially for dimensions $d > 1$. Nevertheless the theoretical results describe the right behavior of the error which is first influenced by the approximation error and later dominated by the roundoff error. This effect is demonstrated by various numerical tests for dimensions $d = 2$ and $d = 3$.

The paper is organised as follows: After introducing the necessary notations for the NFFT in the Section 2, we collect results for sampling of trigonometric polynomials in Section 3. Then in Section 4, we introduce the inverse NFFT by means of weighted reconstruction and optimal interpolation, respectively. Further we estimate the norms of a left inverse (see Theorem 4.2) and right inverse (see Theorem 4.3) of a weighted nonequispaced Fourier matrix. Finally in Section 5, we use these results in order to prove the numerical stability of the NFFT. Various numerical examples concerning the accuracy of the forward NFFT, and the reconstruction error of the inverse NFFT are presented in Section 6.