UNIVERSITY OF TECHNOLOGY
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Applied Functional Analysis
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Efficient inversion of the multivariate nonequispaced fast Fourier transform

Task

Nonequispaced fast Fourier transform (NFFT)

Fast algorithm to evaluate a trigonometric polynomial

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$$

at nonequispaced nodes $\boldsymbol{x}_j \in \mathbb{T}^d \cong \left[-\frac{1}{2},\frac{1}{2}\right)^d, j=1,\dots,N, d\in\mathbb{N}$, with index set $\mathcal{I}_{\boldsymbol{M}} := \left\{\boldsymbol{k}\in\mathbb{Z}^d\colon -\frac{M}{2}\le k_t < \frac{M}{2}, t=1,\dots,d\right\}$

- equispaced grid $\boldsymbol{x}_j$ and $M^d = |\mathcal{I}_{\boldsymbol{M}}| = N$
  $\Rightarrow$ **FFT:** $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}|\log(|\mathcal{I}_{\boldsymbol{M}}|))$
- **Complexity:** $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}|\log(|\mathcal{I}_{\boldsymbol{M}}|)+N)$
- Ajoint problem:
  $$h_{\boldsymbol{k}} = \sum_{j=1}^{N} f_j\, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}, \quad \boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}$$
- nonequispaced Fourier matrix $\boldsymbol{A} := \left(\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}\right)_{j=1,\,\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}}^{N}$
- Factorizations: $\boldsymbol{A}\approx\boldsymbol{B}\boldsymbol{F}\boldsymbol{D}$ and $\boldsymbol{A}^*\approx\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$
  sparse FFT diagonal

Inversion (iNFFT)

Given: $\boldsymbol{f} := (f(\boldsymbol{x}_j))_{j=1}^N$

Find: $\hat{\boldsymbol{f}} := (\hat{f}_{\boldsymbol{k}})_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}}, \hat{f}_{\boldsymbol{k}}\in\mathbb{C}$

Motivation: FFT is invertible
various applications: MRI, solution of PDEs, ...

Challenge: in general $N \neq |\mathcal{I}_{\boldsymbol{M}}|$

Now: new direct method for $d\ge 1$

Problems

(1) Solve
$$\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f},$$
given: $\boldsymbol{f}$, find: $\hat{\boldsymbol{f}}$. $\Rightarrow$ inverse NFFT (iNFFT)

(2) Solve
$$\boldsymbol{A}^*\boldsymbol{f} = \boldsymbol{h},$$
given.: $\boldsymbol{h}$, find.: $\boldsymbol{f}$. $\Rightarrow$ inverse adjoint NFFT (iNFFT*)

Preliminary considerations

- For illustration consider equispaced nodes
  $$\boldsymbol{x}_j = \tfrac{1}{n}\boldsymbol{j}\in\mathbb{T}^d,\ \boldsymbol{j}\in\mathcal{I}_{\boldsymbol{n}},\ \boldsymbol{n}:=(n,\dots,n)^T, \text{ with } |\mathcal{I}_{\boldsymbol{n}}| = N.$$
  Obtain
  $$\boldsymbol{A} = \left(\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\frac{\boldsymbol{j}}{n}}\right)_{\boldsymbol{j}\in\mathcal{I}_{\boldsymbol{n}},\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}} \quad\text{and}\quad \boldsymbol{A}^* = \left(\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\frac{\boldsymbol{j}}{n}}\right)_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}},\boldsymbol{j}\in\mathcal{I}_{\boldsymbol{n}}}$$
  and hence matrix products
  $$\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \text{ for } N\ge|\mathcal{I}_{\boldsymbol{M}}|,$$
  $$\boldsymbol{A}\boldsymbol{A}^* = |\mathcal{I}_{\boldsymbol{M}}|\cdot\boldsymbol{I}_N \text{ for } N\le|\mathcal{I}_{\boldsymbol{M}}| \text{ with } N \mid |\mathcal{I}_{\boldsymbol{M}}|.$$

$\Rightarrow$ In these special cases inversion given by composition of Fourier matrices.

- Whereas, for nonequispaced nodes
  $$\boldsymbol{x}_j\in\left[-\tfrac{1}{2},\tfrac{1}{2}\right)^d,\ j=1,\dots,N,$$
  we have
  $$\boldsymbol{A}^*\boldsymbol{A}\neq N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \quad\text{and}\quad \boldsymbol{A}\boldsymbol{A}^*\neq|\mathcal{I}_{\boldsymbol{M}}|\cdot\boldsymbol{I}_N.$$

$\Rightarrow$ Look for a good approximation in general.

Matrix Approach

Basic idea

Considering
$$\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$
we seek to find a matrix $\boldsymbol{X}$ such that
$$\boldsymbol{X}\boldsymbol{A}\approx\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$$
since then
$$\hat{\boldsymbol{f}}\approx\boldsymbol{X}\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{X}\boldsymbol{f}.$$

Ideas (from equispaced case) to choose appropriate $\boldsymbol{X}$:
$$\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \quad\text{and}\quad \boldsymbol{A}^*\approx\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$$

Aim:
- ⇝ approximation of the form $\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*\boldsymbol{A}\approx\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$
- ⇝ modification of matrix $\boldsymbol{B}$
- ⇝ preserve band structure and arithmetic complexity

Optimization approach

Define $\tilde{\boldsymbol{h}} := \boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{f}$. It holds
$$\|\tilde{\boldsymbol{h}}-\hat{\boldsymbol{f}}\|_2 = \|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{f}-\hat{\boldsymbol{f}}\|_2 = \|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A}\hat{\boldsymbol{f}}-\hat{\boldsymbol{f}}\|_2$$
$$\le \left\|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A}-\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}\right\|_{\mathrm{F}}\|\hat{\boldsymbol{f}}\|_2.$$

Optimization problem:
$$\underset{\tilde{\boldsymbol{B}}}{\text{Minimize}}\ \left\|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A}-\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}\right\|_{\mathrm{F}}^2 = \left\|\boldsymbol{A}^*\tilde{\boldsymbol{B}}\boldsymbol{F}\boldsymbol{D}-\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}\right\|_{\mathrm{F}}^2$$

Suppose $\boldsymbol{A}^*\tilde{\boldsymbol{B}}\boldsymbol{F}\boldsymbol{D}\approx\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$. $\Rightarrow$ $\boldsymbol{A}^*\tilde{\boldsymbol{B}}$ is a pseudoinverse of $\boldsymbol{F}\boldsymbol{D}$.
Since $\boldsymbol{F}^*\boldsymbol{F} = |\mathcal{I}_{\boldsymbol{M}_\sigma}|\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$, a pseudoinverse is given by $\frac{1}{|\mathcal{I}_{\boldsymbol{M}_\sigma}|}\boldsymbol{D}^{-1}\boldsymbol{F}^*$.

$$\rightsquigarrow\ \underset{\tilde{\boldsymbol{B}}}{\text{Minimize}}\ \left\|\boldsymbol{A}^*\tilde{\boldsymbol{B}}-\tfrac{1}{|\mathcal{I}_{\boldsymbol{M}_\sigma}|}\boldsymbol{D}^{-1}\boldsymbol{F}^*\right\|_{\mathrm{F}}^2 = \sum_{\boldsymbol{l}\in\mathcal{I}_{\boldsymbol{M}_\sigma}}\left\|\boldsymbol{A}_{\boldsymbol{l}}^*\tilde{\boldsymbol{b}}_{\boldsymbol{l}}-\tfrac{1}{|\mathcal{I}_{\boldsymbol{M}_\sigma}|}\boldsymbol{D}^{-1}\boldsymbol{f}_{\boldsymbol{l}}\right\|_2^2$$

$\Rightarrow$ inverse NFFT as well as inverse adjoint NFFT

Results

Fast optimization of the matrix $\boldsymbol{B}$

For $d,N\in\mathbb{N}$ let $\boldsymbol{x}_j\in\mathbb{T}^d, j=1,\dots,N$, as well as $\boldsymbol{\sigma}\ge\boldsymbol{1}_d$ and $\boldsymbol{M}_{\boldsymbol{\sigma}} := \boldsymbol{\sigma}\odot\boldsymbol{M}$.

1. For $\boldsymbol{l}\in\mathcal{I}_{\boldsymbol{M}_\sigma}$:
   - Determine the index set
     $$\mathcal{I}_{\boldsymbol{M}_\sigma,m}(\boldsymbol{l}) := \left\{j\in\{1,\dots,N\}\colon \exists\boldsymbol{z}\in\mathbb{Z}^d \text{ with } -m\boldsymbol{1}\le\boldsymbol{M}_{\boldsymbol{\sigma}}\odot\boldsymbol{x}_j-\boldsymbol{l}+\boldsymbol{z}\le m\boldsymbol{1}\right\}.$$
   - Compute the right side $\boldsymbol{v}_{\boldsymbol{l}} := \frac{1}{|\mathcal{I}_{\boldsymbol{M}_\sigma}|}\boldsymbol{H}_{\boldsymbol{l}}^*\boldsymbol{D}^{-1}\boldsymbol{f}_{\boldsymbol{l}}$.
   - Determine $\boldsymbol{H}_{\boldsymbol{l}}^*\boldsymbol{H}_{\boldsymbol{l}}$.
   - Solve for $\boldsymbol{H}_{\boldsymbol{l}}^*\boldsymbol{H}_{\boldsymbol{l}}$, i. e., compute
     $$\boldsymbol{b}_{\boldsymbol{l}}^{\mathrm{opt}} := \tfrac{1}{|\mathcal{I}_{\boldsymbol{M}_\sigma}|}(\boldsymbol{H}_{\boldsymbol{l}}^*\boldsymbol{H}_{\boldsymbol{l}})^{-1}\boldsymbol{H}_{\boldsymbol{l}}^*\boldsymbol{D}^{-1}\boldsymbol{f}_{\boldsymbol{l}}, \quad \boldsymbol{l}\in\mathcal{I}_{\boldsymbol{M}_\sigma}.$$
2. Compose $\boldsymbol{B}_{\mathrm{opt}}$ column-wise of the $\boldsymbol{b}_{\boldsymbol{l}}^{\mathrm{opt}}$ observing the sparsity and periodicity.

Output: optimized matrix $\boldsymbol{B}_{\mathrm{opt}}$ ⇝ $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}|)$

Workflow of iNFFT

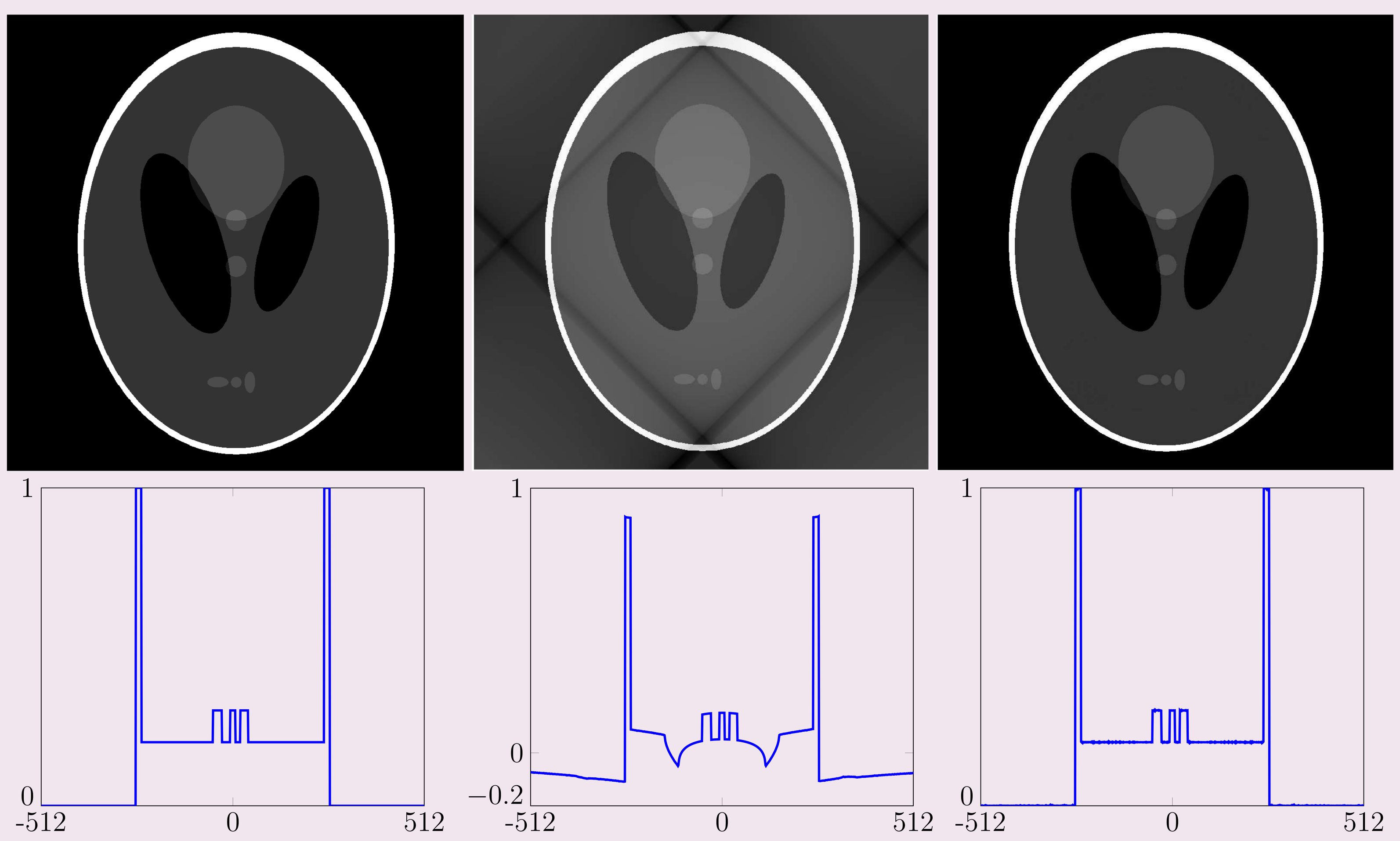
For $d,N\in\mathbb{N}$ let $\boldsymbol{x}_j\in\mathbb{T}^d, j=1,\dots,N$, as well as $\boldsymbol{f}\in\mathbb{C}^N$.

1. Compute optimized matrix $\boldsymbol{B}_{\mathrm{opt}}$.
2. Compute the approximation $\tilde{\boldsymbol{h}} = \boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}_{\mathrm{opt}}^*\boldsymbol{f}$ by means of a modified adjoint NFFT.

Output: $\tilde{\boldsymbol{h}}\approx\hat{\boldsymbol{f}}$

Example - Shepp-Logan phantom

- phantom size 1024×1024
- linogram grid of size $N = 2\cdot1024^2$



(a) Original phantom (b) Use of Voronoi weights (c) iNFFT

Refs

Fundamentals

Dutt, Rokhlin. Fast Fourier transforms for nonequispaced data. SIAM J. Sci. Stat. Comput., 1993.
Beylkin. On the fast Fourier transform of functions with singularities. Appl. Comput. Harmon. Anal., 1995.
Plonka, Potts, Steidl, Tasche. Numerical Fourier Analysis. ANHA, Birkhäuser, 2018.

Corresponding paper

M. Kircheis and D. Potts.
Efficient multivariate inversion of the nonequispaced fast Fourier transform.
PAMM, 20(1):e202000120, 2021.

NFFT Software

http://www.tu-chemnitz.de/~potts/nfft

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