Direct inversion methods for the multivariate nonequispaced fast Fourier transform

Melanie Kircheis

Chemnitz University of Technology
Faculty of Mathematics

joint work with Daniel Potts

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Overview

Motivation – MRI problem

phantom

⇝ measurement ⇝

reconstruction

$$\hat{f}(\boldsymbol{v}) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{v}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x}, \quad f(\boldsymbol{x}) = \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{v})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{v}, \qquad \tilde{h}(\boldsymbol{v}) \approx \hat{f}(\boldsymbol{v})$$

special setting: evaluation points $\boldsymbol{x}_j$ are the same for every measurement

$\Rightarrow$ highly profit from direct inversion method:

① precomputation: has to be done only once for fixed $\boldsymbol{x}_j$

② reconstruction: for each measurement ⇝ should be fast algorithm

Nonequispaced fast Fourier transform

Fast algorithm to evaluate a trigonometric polynomial

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}, \quad \boldsymbol{x} \in \mathbb{T}^d \cong \left[-\tfrac{1}{2}, \tfrac{1}{2}\right)^d$$

Notation: index set $\mathcal{I}_{\boldsymbol{M}} := \left\{\boldsymbol{k} \in \mathbb{Z}^d \colon -\frac{M}{2} \leq k_t < \frac{M}{2},\, t = 1, \dots, d\right\}$ for $M \in 2\mathbb{N}$

[Dutt, Rokhlin 93], [Beylkin 95],
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(inverse) FFT: $f(\frac{\boldsymbol{j}}{M}) := \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\frac{\boldsymbol{j}}{M}}, \qquad \boldsymbol{j} \in \mathcal{I}_{\boldsymbol{M}}, M^d = |\mathcal{I}_{\boldsymbol{M}}| = N$

Complexity: $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}| \log(|\mathcal{I}_{\boldsymbol{M}}|) \qquad)$

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Complexity: $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}| \log(|\mathcal{I}_{\boldsymbol{M}}|) + N)$

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Factorizations: $\boldsymbol{A} \approx \underset{\substack{\nearrow\\ \text{banded}}}{\boldsymbol{B}}\,\underset{\substack{\uparrow\\ \text{FFT}}}{\boldsymbol{F}}\,\underset{\substack{\nwarrow\\ \text{diagonal}}}{\boldsymbol{D}}$ and $\boldsymbol{A}^* \approx \boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$

(columns of $\boldsymbol{B}$: for each $\boldsymbol{x}_j$ only $(2m+1)^d$ entries, $m \in \mathbb{N}$ given) [Nieslony, Steidl 03]

Inverse Problem

Given: $\boldsymbol{x}_j \in \mathbb{T}^d$ fixed and $f(\boldsymbol{x}_j), j = 1, \dots, N,$ for $f(\boldsymbol{x}) = \sum\limits_{\boldsymbol{k} \in \mathcal{I}_M} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$

Find: $\hat{f}_{\boldsymbol{k}} \in \mathbb{C}, \, \boldsymbol{k} \in \mathcal{I}_M$

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various applications: MRI, solution of PDEs, …

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Problems:

(1) Solve

$$\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f},$$

given: $\boldsymbol{f}$, find: $\hat{\boldsymbol{f}}$.

⇒ inverse NFFT (iNFFT)

(2) Solve

$$\boldsymbol{A}^*\boldsymbol{f} = \boldsymbol{h},$$

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⇒ inverse adjoint NFFT (iNFFT*)

Previous approaches for $d = 1$:

- iterative methods: [Feichtinger, Gröchenig 95]: CG algorithm, $N > |\mathcal{I}_M|$
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- direct methods:
  - for $N = |\mathcal{I}_{\boldsymbol{M}}|$: [Dutt, Rokhlin 93]: Lagrange interpolation & FMM
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  - general case: [K., Potts 19]: optimization of the banded matrix $\boldsymbol{B}^*$ by minimizing a certain Frobenius norm $\rightsquigarrow$ connection to frame approach

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[Averbuch et al. 08]: special approach for linogram grid, $N > |\mathcal{I}_{\boldsymbol{M}}|$
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Now: generalization of our direct method to $d > 1$

Preliminary considerations

Consider equispaced nodes

$$\boldsymbol{x_j} = \tfrac{1}{n}\boldsymbol{j} \in \mathbb{T}^d \cong \left[-\tfrac{1}{2}, \tfrac{1}{2}\right)^d, \boldsymbol{j} \in \mathcal{I}_{\boldsymbol{n}}, \boldsymbol{n} := (n, \dots, n)^T \text{ with } |\mathcal{I}_{\boldsymbol{n}}| = N$$

Obtain

$$\boldsymbol{A} = \left(\mathrm{e}^{2\pi \mathrm{i} k \frac{\boldsymbol{j}}{n}}\right)_{\boldsymbol{j}\in\mathcal{I}_{\boldsymbol{n}},\, \boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}} \quad \text{and} \quad \boldsymbol{A}^* = \left(\mathrm{e}^{-2\pi \mathrm{i} k \frac{\boldsymbol{j}}{n}}\right)_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}},\, \boldsymbol{j}\in\mathcal{I}_{\boldsymbol{n}}}$$

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$$\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \text{ for } N \geq |\mathcal{I}_{\boldsymbol{M}}|$$

$$\boldsymbol{A}\boldsymbol{A}^* = |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{I}_N \text{ for } N \leq |\mathcal{I}_{\boldsymbol{M}}| \qquad (\text{ if } |\mathcal{I}_{\boldsymbol{M}}| \text{ divisible by } N)$$

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Consider nonequispaced nodes

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$\Rightarrow$ Look for good approximation in general

Common approach - Density compensation

$$\hat{f}(\boldsymbol{v}) = \int\limits_{\mathbb{R}^d} f(\boldsymbol{x})\, \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{v}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x}$$

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Approximation computed by means of NFFT as

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Intuitive approach: Voronoi weights based on geometry

Computation of density compensation factors $\boldsymbol{W}$

$$\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$

Weighted normal equations of first kind:

[Rosenfeld 98], [Sedarat, Nishimura 00]

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[Choi, Munson 98], [Greengard, Lee, Inati 06], [Pipe, Menon 99]

$$\boldsymbol{A}\boldsymbol{A}^*\boldsymbol{W}\boldsymbol{y} = \boldsymbol{f}, \quad \boldsymbol{A}^*\boldsymbol{W}\boldsymbol{y} = \hat{\boldsymbol{f}}$$

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$$\rightsquigarrow \quad \underset{\boldsymbol{W}=\mathrm{diag}(w_j)_{j=1}^N}{\text{Minimize}} \quad \left\|\boldsymbol{A}\boldsymbol{A}^*\boldsymbol{W} - \boldsymbol{I}_N\right\|_{\mathrm{F}}^2$$

Computation of density compensation factors $\boldsymbol{W}$

$$\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$$

Weighted normal equations of first kind:

[Rosenfeld 98], [Sedarat, Nishimura 00]

$$\boldsymbol{A}^*\boldsymbol{W}\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{A}^*\boldsymbol{W}\boldsymbol{f}$$

$$\hat{\boldsymbol{f}} \approx \boldsymbol{A}^*\boldsymbol{W}\boldsymbol{f} \iff \boldsymbol{A}^*\boldsymbol{W}\boldsymbol{A} \approx \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$$

$$\rightsquigarrow \quad \underset{\boldsymbol{W}=\operatorname{diag}(w_j)_{j=1}^N}{\text{Minimize}} \quad \left\|\boldsymbol{A}^*\boldsymbol{W}\boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}\right\|_{\mathrm{F}}^2$$

Weighted normal equations of second kind:

[Choi, Munson 98], [Greengard, Lee, Inati 06], [Pipe, Menon 99]

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But: Hard to compute, huge memory requirement

Recapitulation

So far:

$$\hat{\boldsymbol{f}} \approx \boldsymbol{A}^* \boldsymbol{W} \boldsymbol{f} \approx \underset{\substack{\nearrow\\ \text{diagonal}}}{\boldsymbol{D}^*}\, \underset{\substack{\uparrow\\ \text{FFT}}}{\boldsymbol{F}^*}\, \underset{\substack{\nwarrow\\ \text{banded}}}{\boldsymbol{B}^*} \boldsymbol{W} \boldsymbol{f}$$

Interpretation perspectives:

Recapitulation

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Interpretation perspectives:

(i) Set $\boldsymbol{g} := \boldsymbol{W} \boldsymbol{f}$.

$$\Rightarrow \quad \hat{\boldsymbol{f}} \approx \boldsymbol{D}^* \boldsymbol{F}^* \boldsymbol{B}^* \boldsymbol{g}$$

$\rightsquigarrow$ ordinary NFFT, modified coefficient vector

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$$\Rightarrow \quad \hat{\boldsymbol f} \approx \boldsymbol D^* \boldsymbol F^* \tilde{\boldsymbol B}^* \boldsymbol f$$

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$\Rightarrow$ density compensation can be viewed as optimization of the banded matrix $\boldsymbol{B}$ (only N degrees of freedom)

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Now: optimize each nonzero entry of the banded matrix $\boldsymbol{B}$

Basic idea – Optimization approach

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

$$\hat{\boldsymbol{f}} \approx \boldsymbol{X}\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{X}\boldsymbol{f}.$$

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Ideas (from equispaced case) to choose appropriate $\boldsymbol{X}$:

$$\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \quad \text{and} \quad \boldsymbol{A}^* \approx \boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$$

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Aim:

⇝ approximation of the form $\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*\boldsymbol{A} \approx \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$

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- ⇝ approximation of the form $\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*\boldsymbol{A} \approx \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$
- ⇝ modification of matrix $\boldsymbol{B}$

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- ⇝ 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

Precomputational step – Optimization procedure

Define $\tilde{\boldsymbol{h}} := \boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{f}$

$$\begin{aligned}\|\tilde{\boldsymbol{h}} - \hat{\boldsymbol{f}}\|_2 &= \|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{f} - \hat{\boldsymbol{f}}\|_2 = \|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A}\hat{\boldsymbol{f}} - \hat{\boldsymbol{f}}\|_2 \\ &\leq \left\|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_M|}\right\|_{\mathrm{F}} \|\hat{\boldsymbol{f}}\|_2\end{aligned}$$

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Optimization problem:

$$\underset{\tilde{\boldsymbol{B}}\text{ banded}}{\text{Minimize}} \quad \left\|\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{B}}^*\boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_M|}\right\|_{\mathrm{F}}^2 = \left\|\boldsymbol{A}^*\tilde{\boldsymbol{B}}\boldsymbol{F}\boldsymbol{D} - \boldsymbol{I}_{|\mathcal{I}_M|}\right\|_{\mathrm{F}}^2$$

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If $\boldsymbol{A}^*\tilde{\boldsymbol{B}}$ is a pseudoinverse of $\boldsymbol{F}\boldsymbol{D}$ then $\boldsymbol{A}^*\tilde{\boldsymbol{B}}\boldsymbol{F}\boldsymbol{D} \approx \boldsymbol{I}_{|\mathcal{I}_M|}$.

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Since $\boldsymbol{F}^*\boldsymbol{F} = |\mathcal{I}_{\boldsymbol{M}_{\boldsymbol{\sigma}}}|\, \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$, a pseudoinverse is given by $\frac{1}{|\mathcal{I}_{\boldsymbol{M}_{\boldsymbol{\sigma}}}|}\boldsymbol{D}^{-1}\boldsymbol{F}^*$.

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

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$\rightsquigarrow \mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}|)$

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$\rightsquigarrow \mathcal{O}(|\mathcal{I}_M|)$

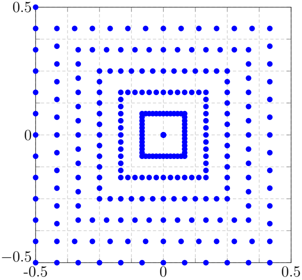
$\Rightarrow$ Inverse NFFT as well as inverse adjoint NFFT

Numerical example – Reconstruction of Shepp-Logan phantom

- phantom size 1024×1024

$\hat{\boldsymbol{f}}$

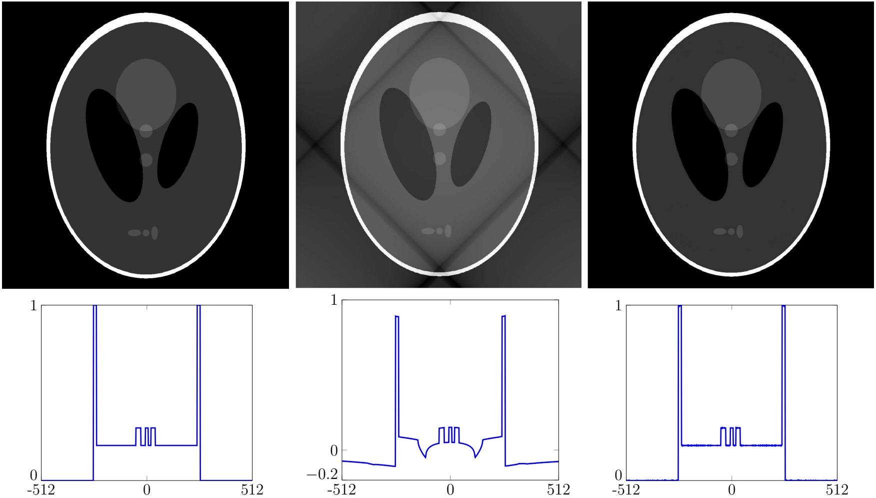
- linogram grid of size $N = 2 \cdot 1024^2$



$\boldsymbol{x}_j$

$\rightsquigarrow$ reconstruct coefficients $\tilde{\boldsymbol{h}} \approx \hat{\boldsymbol{f}}$

Reconstruction of the Shepp-Logan phantom of size 1024×1024



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

Summary

- new direct method for $d > 1$
- working in the overdetermined setting $N > |\mathcal{I}_{\boldsymbol{M}}|$
- iNFFT based on factorization $\underset{\substack{\nwarrow \\ \text{optimized}}}{\boldsymbol{B}}\boldsymbol{F}\boldsymbol{D}$ of NFFT
- fast algorithms of same complexity $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}|\log(|\mathcal{I}_{\boldsymbol{M}}|) + N)$

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Thank you for your attention!