Efficient multivariate inversion of the NFFT

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Overview

Nonequispaced fast Fourier transform

Fast algorithm to evaluate a trigonometric polynomial

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

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

[Dutt, Rokhlin 93], [Beylkin 95],
[Potts, Steidl, Tasche 01]

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- equispaced grid $\boldsymbol{x}_j$ and $|\mathcal{I}_{\boldsymbol{M}}| = N \quad \Rightarrow$ **FFT:** $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}| \log(|\mathcal{I}_{\boldsymbol{M}}|))$

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- Ajoint problem:

$$h_{\boldsymbol{k}} = \sum_{j=1}^{N} f_j \,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}, \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}$$

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

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- Factorizations: $\boldsymbol{A} \approx \boldsymbol{B}\boldsymbol{F}\boldsymbol{D}$ and $\boldsymbol{A}^* \approx \boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$ [Dutt, Rokhlin 93], [Beylkin 95], [Potts, Steidl, Tasche 01]

  ($\boldsymbol{B}$: sparse, $\boldsymbol{F}$: FFT, $\boldsymbol{D}$: diagonal)

iNFFT

Given: $f(\boldsymbol{x}_j), j = 1, \dots, N,$ for $f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}}$

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

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

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Problems:

(1) Solve

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

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

$\Rightarrow$ inverse NFFT

(2) Solve

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

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

$\Rightarrow$ inverse adjoint NFFT

Previous approaches for $d = 1$:

- iterative methods: [Feichtinger, Gröchenig 95]: CG algorithm, $N > |\mathcal{I}_M|$
  [Kunis, Potts 07]: CG algorithm and NFFT, $N < |\mathcal{I}_M|$

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- direct methods:
  - for $N = |\mathcal{I}_{\boldsymbol{M}}|$: [Dutt, Rokhlin 93]: Lagrange interpolation & FMM
    [Selva 18]: Lagrange interpolation & imaginary shift
  - general case: [K., Potts 19]: optimization of the sparse matrix $\boldsymbol{B}^*$ by minimizing a certain Frobenius norm $\rightsquigarrow$ connection to frame approach

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Previous approaches for $d > 1$:

[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 $d > 1$

Basic idea

Consider equispaced nodes

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

Obtain

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

Consider matrix products:

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Consider matrix products:

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

$$\boldsymbol{A}\boldsymbol{A}^* = |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{I}_N \text{ for } N \leq |\mathcal{I}_{\boldsymbol{M}}| \text{ with } N \mid |\mathcal{I}_{\boldsymbol{M}}|$$

Basic idea

Consider nonequispaced nodes

$$\boldsymbol{x}_j \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right)^d, \; j = 1, \dots, N.$$

Obtain

$$\boldsymbol{A} = \left(\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}\right)_{j=1,\dots,N,\,\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}}} \quad \text{and} \quad \boldsymbol{A}^* = \left(\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}_j}\right)_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{M}},\,j=1,\dots,N}.$$

Consider matrix products:

$$\boldsymbol{A}^*\boldsymbol{A} \neq N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$$

$$\boldsymbol{A}\boldsymbol{A}^* \neq |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{I}_N$$

Basic idea

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$\Rightarrow$ Look for good approximation in general.

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

$$\hat{\boldsymbol{f}} \approx \check{\boldsymbol{f}} := \boldsymbol{X}\boldsymbol{f}.$$

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Note: From equispaced case we know $\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}$ for $|\mathcal{I}_{\boldsymbol{M}}| \leq N$.

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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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Aim:

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

Considering

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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

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

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

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

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$$\leq \left\| \boldsymbol{D}^* \boldsymbol{F}^* \tilde{\boldsymbol{B}}^* \boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_M|} \right\|_{\mathrm{F}} \|\hat{\boldsymbol{f}}\|_2.$$

Optimization problem:

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

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

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

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

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

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

$$\|\check{\boldsymbol{f}} - \hat{\boldsymbol{f}}\|_2 = \|\boldsymbol{D}^* \boldsymbol{F}^* \tilde{\boldsymbol{B}}^* \boldsymbol{f} - \hat{\boldsymbol{f}}\|_2 = \|\boldsymbol{D}^* \boldsymbol{F}^* \tilde{\boldsymbol{B}}^* \boldsymbol{A} \hat{\boldsymbol{f}} - \hat{\boldsymbol{f}}\|_2$$
$$\leq \left\|\boldsymbol{D}^* \boldsymbol{F}^* \tilde{\boldsymbol{B}}^* \boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_M|}\right\|_{\mathrm{F}} \|\hat{\boldsymbol{f}}\|_2.$$

Optimization problem:

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

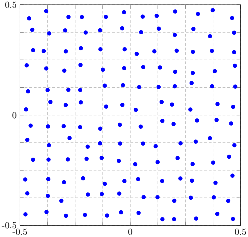
Suppose $\boldsymbol{A}^* \tilde{\boldsymbol{B}} \boldsymbol{F} \boldsymbol{D} \approx \boldsymbol{I}_{|\mathcal{I}_M|}$. $\Rightarrow$ $\boldsymbol{A}^* \tilde{\boldsymbol{B}}$ is a pseudoinverse of $\boldsymbol{F}\boldsymbol{D}$.
Since $\boldsymbol{F}^* \boldsymbol{F} = |\mathcal{I}_{\boldsymbol{M}_{\boldsymbol{\sigma}}}|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

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

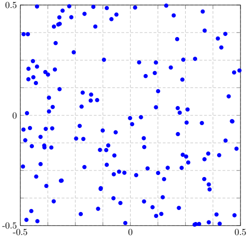
$\rightsquigarrow \mathcal{O}(|\mathcal{I}_M|)$

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

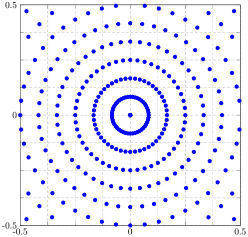
Testing Grids



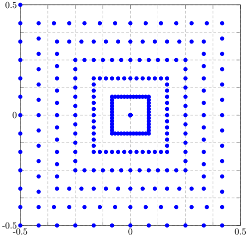
(a) Jittered



(b) Random



(c) Modified polar



(d) Linogram

Example 1 - Justification

Compare norms

$$\left\| \boldsymbol{A}^* \boldsymbol{B} \boldsymbol{F} \boldsymbol{D} - \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \right\|_{\mathrm{F}} \quad \text{and} \quad \left\| \boldsymbol{A}^* \tilde{\boldsymbol{B}} \boldsymbol{F} \boldsymbol{D} - \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \right\|_{\mathrm{F}} .$$

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Parameters:

- $\boldsymbol{M} = (12, 12)^T$
- $R \in \{4, 6, 8, 12, 16, 24, 32, 48, 64, 96, 128\}$
- $N \approx 2 \cdot R^2$

$\Rightarrow$ test in overdetermined and underdetermined setting

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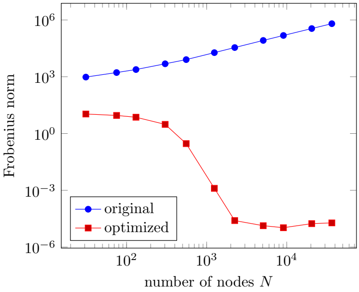

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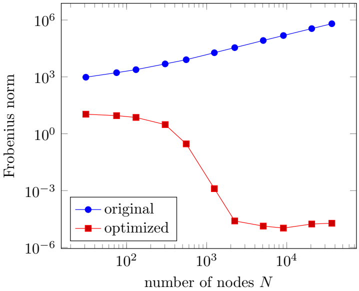

$\rightsquigarrow$ method attributed to the overdetermined setting

Example 2 - Reconstruction

Reconstruction of the Shepp-Logan phantom

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

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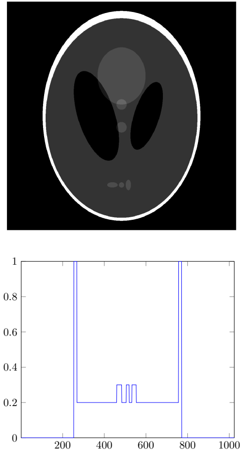
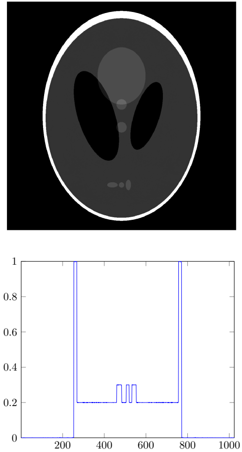
- measure relative errors $e_\infty := \frac{\|\check{\boldsymbol{f}} - \hat{\boldsymbol{f}}\|_\infty}{\|\hat{\boldsymbol{f}}\|_\infty}$

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

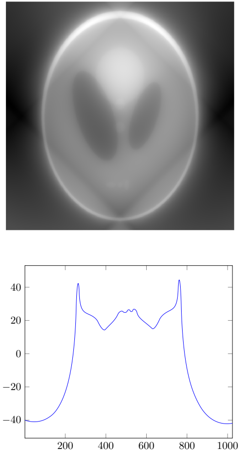


(a) Original phantom



(b) Optimization

$\rightsquigarrow e_\infty$ = 6.4462e-03



(c) NFFT

$\rightsquigarrow e_\infty$ = 1.0007e+02

Summary

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

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Thank you for your attention!