UNIVERSITY OF TECHNOLOGY
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Fast and direct inverse nonequispaced Fourier transforms

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Problem formulation

Motivation – MRI problem

phantom ⇝ measurements ⇝ reconstruct

$\hat f_{\boldsymbol k}$ $\quad f(\boldsymbol x_j) = \sum_{\boldsymbol k\in\mathcal I_{\boldsymbol M}} \hat f_{\boldsymbol k}\, \mathrm e^{2\pi\mathrm i \boldsymbol k \boldsymbol x_j}$ $\quad h_{\boldsymbol k} \approx \hat f_{\boldsymbol k}$

Inversion problem (iNFFT)

Solve: $\boldsymbol A \hat{\boldsymbol f} = \boldsymbol f$ with $\boldsymbol A := \left(\mathrm e^{2\pi\mathrm i \boldsymbol k \boldsymbol x_j}\right)_{j=1,\,\boldsymbol k\in\mathcal I_{\boldsymbol M}}^{N}$

Given: $\boldsymbol f := (f(\boldsymbol x_j))_{j=1}^N$, $\boldsymbol x_j \in \mathbb T^d \cong \left[-\frac12,\frac12\right)^d$

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

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

Nonequispaced fast Fourier transform (NFFT)

Algorithm to efficiently evaluate trigonometric polynomials

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

at nonequispaced nodes $\boldsymbol x_j \in \mathbb T^d$, $j = 1,\dots,N$, $d\in\mathbb N$, 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 $M^d = |\mathcal I_{\boldsymbol M}| = N$
  ⇒ **FFT:** $\mathcal O(|\mathcal I_{\boldsymbol M}|\log(|\mathcal I_{\boldsymbol M}|))$
- **Complexity:** $\mathcal O(|\mathcal I_{\boldsymbol M}|\log(|\mathcal I_{\boldsymbol M}|) + N)$
- **Factorization:**

$$\boldsymbol A \approx \boldsymbol B \boldsymbol F \boldsymbol D \quad \text{and} \quad \boldsymbol A^* \approx \boldsymbol D^* \boldsymbol F^* \boldsymbol B^*$$

banded FFT diagonal

Unitarity?

Equispaced nodes:

$$\boldsymbol A^*\boldsymbol A = N \boldsymbol I_{|\mathcal I_{\boldsymbol M}|} \quad\text{or}\quad \boldsymbol A\boldsymbol A^* = |\mathcal I_{\boldsymbol M}|\cdot \boldsymbol I_N$$

Nonequispaced nodes:

$$\boldsymbol A^*\boldsymbol A \neq N \boldsymbol I_{|\mathcal I_{\boldsymbol M}|} \quad\text{and}\quad \boldsymbol A\boldsymbol A^* \neq |\mathcal I_{\boldsymbol M}|\cdot \boldsymbol I_N$$

Direct methods

vs. iterated methods (multiple iteration steps)

reconstruction = same number of arithmetic operations as single adjoint NFFT

⇒ highly profit in setting of fixed $\boldsymbol x_j$

precomputation: has to be done only once
reconstruction: for each measurement
⇝ adjoint NFFT very fast

Direct inversion approaches

Sampling density compensation

Basic idea

Find suitable matrix $\boldsymbol X$ with

$$\boldsymbol X \boldsymbol A \approx \boldsymbol I_{|\mathcal I_{\boldsymbol M}|},$$

since then

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

Reminder – Equispaced nodes:

$$\boldsymbol X = \boldsymbol A^*\cdot N^{-1}$$

Simplest generalization:

$$\boldsymbol X = \boldsymbol A^* \boldsymbol W,$$

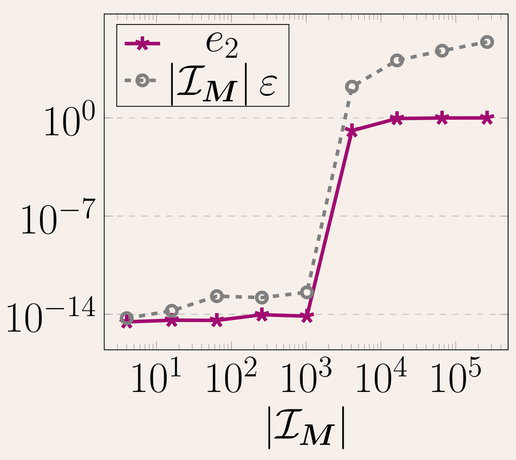
i. e., additional weighting due to nonequispaced sampling

Computation scheme

Exactness condition: An exact reconstruction $\hat{\boldsymbol f} = \boldsymbol A^*\boldsymbol W \boldsymbol f$ is given if $|\mathcal I_{2\boldsymbol M}| < N$ and

$$\sum_{j=1}^N w_j\, \mathrm e^{2\pi\mathrm i \boldsymbol k \boldsymbol x_j} = \delta_{\boldsymbol 0,\boldsymbol k}, \quad \boldsymbol k\in\mathcal I_{2\boldsymbol M}.$$

Practice: by means of normal equations



Algorithm 1 [2, 3]

1. Precompute weights $\boldsymbol W$
2. Compute scaled coeffs $\boldsymbol W \boldsymbol f$
3. Adjoint NFFT

Error bound [2]

In case of small residuals $\varepsilon_{\boldsymbol k}\in\mathbb R$ there exists an $\varepsilon \ge 0$ such that

$$\|\boldsymbol A^*\boldsymbol W \boldsymbol f - \hat{\boldsymbol f}\|_2 \le \varepsilon\, |\mathcal I_{\boldsymbol M}| \cdot \|\hat{\boldsymbol f}\|_2.$$

Optimization of banded matrix

Basic idea

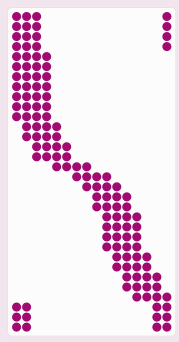
Recap:

(i) $\hat{\boldsymbol f} \approx \boldsymbol D^*\boldsymbol F^*\boldsymbol B^*\boldsymbol W \boldsymbol f =: \boldsymbol D^*\boldsymbol F^*\boldsymbol B^*\boldsymbol g$

(ii) $\hat{\boldsymbol f} \approx \boldsymbol D^*\boldsymbol F^*\boldsymbol B^*\boldsymbol W \boldsymbol f =: \boldsymbol D^*\boldsymbol F^*\tilde{\boldsymbol B}^*\boldsymbol f$

⇒ Optimization of banded $\boldsymbol B$ (only N degrees of freedom)

Now: optimize all nonzero entries
⇝ modification of $\boldsymbol B$
⇝ preserve structure and complexity



Computation scheme

Consider:

$$\|\boldsymbol D^*\boldsymbol F^*\tilde{\boldsymbol B}^*\boldsymbol f - \hat{\boldsymbol f}\|_2 \le \left\|\boldsymbol D^*\boldsymbol F^*\tilde{\boldsymbol B}^*\boldsymbol A - \boldsymbol I_{|\mathcal I_{\boldsymbol M}|}\right\|_{\mathrm F}\|\hat{\boldsymbol f}\|_2$$

⇝ $\boldsymbol A^*\tilde{\boldsymbol B}$ pseudoinverse of $\boldsymbol F\boldsymbol D$
⇝ given since $\boldsymbol F^*\boldsymbol F = |\mathcal I_{\boldsymbol M_\sigma}|\,\boldsymbol I_{|\mathcal I_{\boldsymbol M}|}$

Optimization problem:

$$\underset{\tilde{\boldsymbol B}\text{ banded}}{\text{Minimize}}\ \left\|\boldsymbol A^*\tilde{\boldsymbol B} - \tfrac{1}{|\mathcal I_{\boldsymbol M_\sigma}|}\boldsymbol D^{-1}\boldsymbol F^*\right\|_{\mathrm F}^2 = \sum_{l\in\mathcal I_{\boldsymbol M_\sigma}} \left\|\boldsymbol A_l^*\tilde{\boldsymbol b}_l - \tfrac{1}{|\mathcal I_{\boldsymbol M_\sigma}|}\boldsymbol D^{-1}\boldsymbol f_l\right\|_2^2$$

Algorithm 2 [1, 2]

1. Precompute matrix $\boldsymbol B_{\mathrm{opt}}$
2. Modified adjoint NFFT

Error bound [2]

In case of small residuals $\varepsilon_\ell \ge 0$ there exists an $\varepsilon \ge 0$ such that

$$\|\boldsymbol h_{\mathrm{opt}} - \hat{\boldsymbol f}\|_2^2 \le \varepsilon\, |\mathcal I_{\boldsymbol M}|\cdot \|\hat{\boldsymbol f}\|_2^2.$$

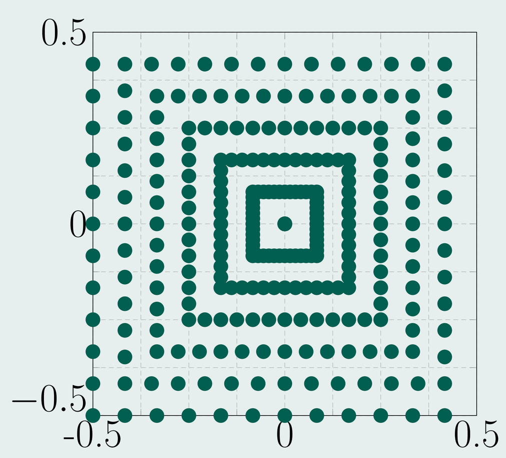
Numerics – Shepp-Logan phantom

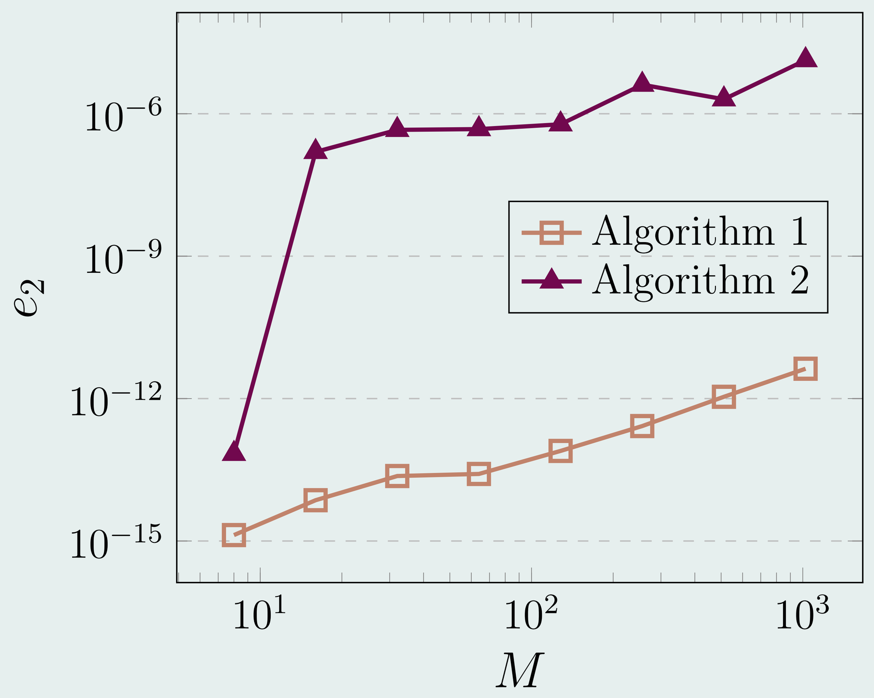
Example with $|\mathcal I_{2\boldsymbol M}| < N$

- Relative errors

$$e_2 := \frac{\|\tilde{\boldsymbol h} - \hat{\boldsymbol f}\|_2}{\|\hat{\boldsymbol f}\|_2}$$

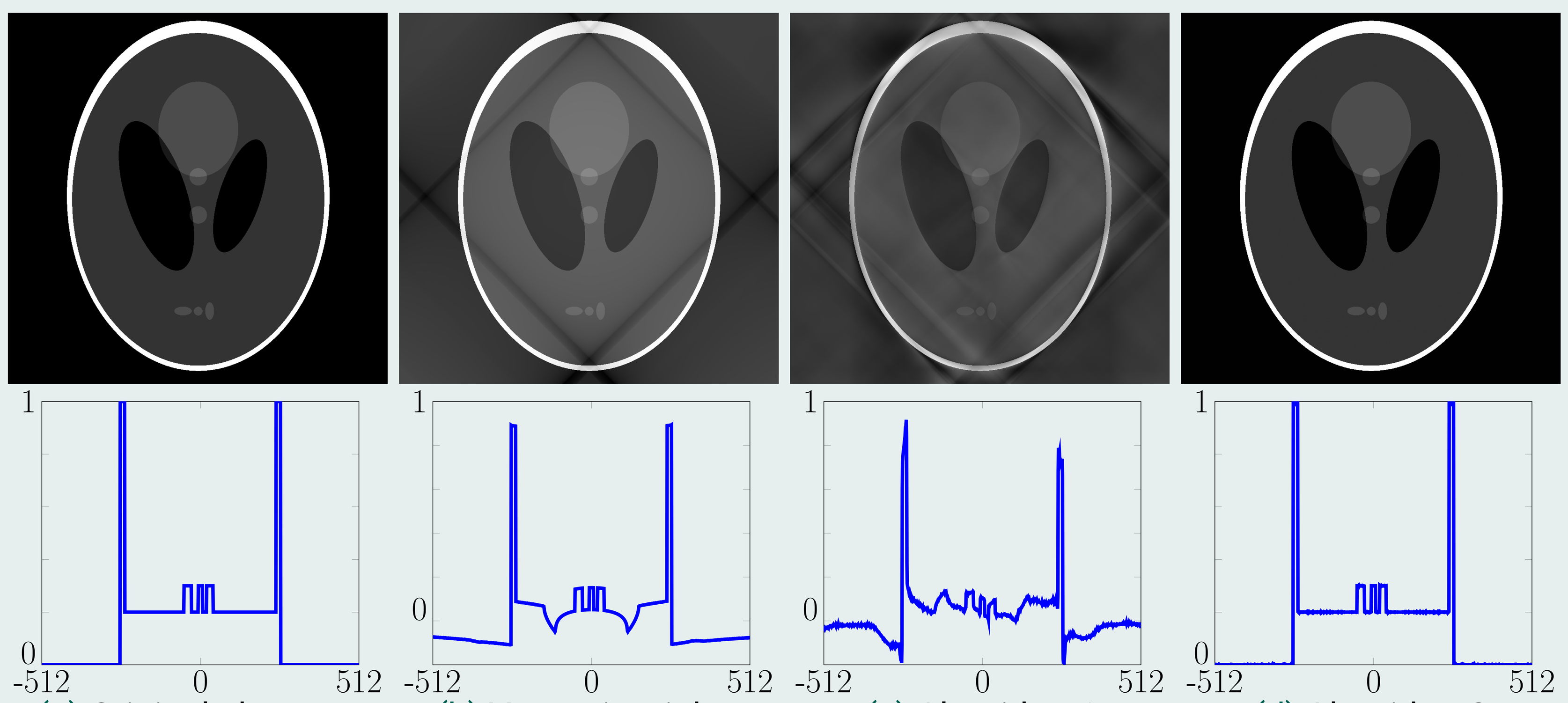
- phantom size $M\times M$
- linogram grid of size $N = 8M^2$





Example with $|\mathcal I_{2\boldsymbol M}| > N$

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



(a) Original phantom
(b) Voronoi weights $e_2 = 5.3040e-01$
(c) Algorithm 1 $e_2 = 5.0585e-01$
(d) Algorithm 2 $e_2 = 2.2737e-03$

[1] Kircheis, Potts. Efficient multivariate inversion of the nonequispaced fast Fourier transform. *PAMM, 20(1):e202000120, 2021.*
[2] Kircheis, Potts. Fast and direct inversion methods for the multivariate nonequispaced fast Fourier transform. *Front. Appl. Math. Stat. 9:1155484, 2023.*
[3] Kircheis, Potts. Optimal density compensation factors for the reconstruction of the Fourier transform of bandlimited functions. *arXiv, 2304.00094, 2023.*

Related work
NFFT – [Plonka, P., Steidl, Tasche 18]
Iteration – [Kunis, P. 07], [Scarnati, Gelb 19]
Density comp. for MRI – [Eggers, K., P. 22]
Frame-theoretical approach – [K., P. 19]

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