

Direct inverse nonequispaced fast Fourier transforms

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joint work with Daniel Potts

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Motivation – discrete problem

phantom



$$\hat{f}_k$$



given measurements



reconstruction



$$\tilde{h}_k \approx \hat{f}_k$$

$$f(\mathbf{x}_j) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}_k e^{2\pi i \mathbf{k} \mathbf{x}_j}$$

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$$\tilde{h}_{\mathbf{k}} \approx \hat{f}_{\mathbf{k}}$$

\mathbf{x}_j equispaced \implies

FFT (Fast Fourier Transform)

\mathbf{x}_j nonequispaced \implies

inverse NFFT (Nonequispaced Fast Fourier Transform) ?

Motivation

	ground truth	given measurements	aim
discrete problem	$\hat{f}_{\mathbf{k}}$	$f(\mathbf{x}_j) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}_{\mathbf{k}} e^{2\pi i \mathbf{k} \mathbf{x}_j}$	$\tilde{h}_{\mathbf{k}} \approx \hat{f}_{\mathbf{k}}$
			$\mathbf{v} \in \mathbb{R}^d, \mathbf{k} \in \mathcal{I}_M$

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continuous problem	$\hat{f}(\mathbf{v})$	$f(\mathbf{x}_j) = \int_{[-\frac{M}{2}, \frac{M}{2}]^d} \hat{f}(\mathbf{v}) e^{2\pi i \mathbf{v} \mathbf{x}_j} d\mathbf{v}$	$\tilde{h}(\mathbf{k}) \approx \hat{f}(\mathbf{k})$ $\mathbf{v} \in \mathbb{R}^d, \mathbf{k} \in \mathcal{I}_M$

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iterated methods
 (multiple applications of the NFFT needed)

vs.

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 (realized with a single NFFT)

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special setting: evaluation points $\mathbf{x}_j, j = 1, \dots, N$, fixed

\implies highly profit from direct method

- 1 **precomputation:** only once for fixed \mathbf{x}_j
- 2 **reconstruction:** for each measurement \rightsquigarrow very efficient

Overview

- 1 Introduction
- 2 Discrete problem
- 3 Continuous problem

NFFT (Nonequispaced Fast Fourier Transform)

Fast algorithm to evaluate a trigonometric polynomial

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}_{\mathbf{k}} e^{2\pi i \mathbf{k} \mathbf{x}}$$

- index set $\mathcal{I}_M := \mathbb{Z}^d \cap \left[-\frac{M}{2}, \frac{M}{2}\right)^d$ with cardinality $|\mathcal{I}_M| = M^d$, $M \in 2\mathbb{N}$,
- Fourier coefficients $\hat{f}_{\mathbf{k}} \in \mathbb{C}$, $\mathbf{k} \in \mathcal{I}_M$,
- nonequispaced points $\mathbf{x}_j \in \mathbb{T}^d \cong \left[-\frac{1}{2}, \frac{1}{2}\right)^d$, $j = 1, \dots, N$, $N \in \mathbb{N}$

$$\mathcal{O}(|\mathcal{I}_M| \log(|\mathcal{I}_M|) + N)$$

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

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Matrix notation:

$$\mathbf{f} = \mathbf{A} \hat{\mathbf{f}} \quad \text{with} \quad \mathbf{A} = \mathbf{A}_{|\mathcal{I}_M|} := \left(e^{2\pi i \mathbf{k} \mathbf{x}_j} \right)_{j=1, \mathbf{k} \in \mathcal{I}_M}^N \in \mathbb{C}^{N \times |\mathcal{I}_M|}$$

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Factorizations: $\mathbf{A} \approx \mathbf{BFD}$ and $\mathbf{A}^* \approx \mathbf{D}^* \mathbf{F}^* \mathbf{B}^*$

$\begin{matrix} \nearrow & \uparrow & \nwarrow \\ \text{banded} & \text{FFT} & \text{diagonal} \end{matrix}$

(in each column of \mathbf{B} only $(2m + 1)^d$ entries, $m \in \mathbb{N}$ given)

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Inversion problem (iNFFT): **Given:** $\mathbf{f} := (f(\mathbf{x}_j))_{j=1}^N$ **Find:** $\hat{\mathbf{f}} := (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in \mathcal{I}_M}$ **Challenge:** in general $N \neq |\mathcal{I}_M|$

Basic idea

Equispaced nodes: $\mathbf{A}^* \mathbf{A} = N \mathbf{I}_{|\mathcal{I}_M|}$

Nonequispaced nodes: $\mathbf{A}^* \mathbf{A} \neq N \mathbf{I}_{|\mathcal{I}_M|}$

Basic idea

Equispaced nodes: $A^* A = N I_{|\mathcal{I}_M|}$

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⇒ Find suitable matrix X with

$$X A \approx I_{|\mathcal{I}_M|},$$

since then

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

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Reminder – Equispaced nodes:

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

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Simplest generalization:

$$X = A^* W \approx D^* F^* B^* W,$$

i. e., additional weighting $W := \text{diag}(w_j)_{j=1}^N$ due to nonequispaced sampling

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Nonequispaced nodes: $A^* A \neq N I_{|\mathcal{I}_M|}$

Density compensation algorithm

0. Precompute weights W ?
1. Compute scaled coefficients $W f$ $\mathcal{O}(N)$
2. Adjoint NFFT $\mathcal{O}(|\mathcal{I}_M| \log(|\mathcal{I}_M|) + N)$

Intuitive approach:

Voronoi weights based on geometry

Exact reconstruction for trigonometric polynomials

Theorem (K., Potts 23)

Let $|\mathcal{I}_{2M}| \leq N$ and $\mathbf{x}_j \in \mathbb{T}^d$, $j = 1, \dots, N$, be given.

Then the density compensation factors $w_j \in \mathbb{C}$ satisfying

$$\sum_{j=1}^N w_j e^{2\pi i \mathbf{k} \mathbf{x}_j} = \delta_{\mathbf{0}, \mathbf{k}}, \quad \mathbf{k} \in \mathcal{I}_{2M}, \quad \mathbf{A}_{|\mathcal{I}_{2M}|}^T \mathbf{w} = \mathbf{e}_0$$

are optimal,

i. e., for all trigonometric polynomials $f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}_{\mathbf{k}} e^{2\pi i \mathbf{k} \mathbf{x}}$ an exact reconstruction of the Fourier coefficients $\hat{f}_{\mathbf{k}} \in \mathbb{C}$ is given by

$$\hat{f}_{\mathbf{k}} = h_{\mathbf{k}}^w := \sum_{j=1}^N w_j f(\mathbf{x}_j) e^{-2\pi i \mathbf{k} \mathbf{x}_j}, \quad \mathbf{k} \in \mathcal{I}_M. \quad \hat{\mathbf{f}} = \mathbf{A}^* \mathbf{W} \mathbf{f}$$

$\delta_{\mathbf{0}, \mathbf{k}}$... Kronecker delta

Computation schemes

Aim: exact solution to

$$\mathbf{A}_{|\mathcal{I}_{2M}|}^T \mathbf{w} = \mathbf{e}_0 := (\delta_{0,\mathbf{k}})_{\mathbf{k} \in \mathcal{I}_{2M}} \quad (*)$$

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Friendly setting ($|\mathcal{I}_{2M}| \leq N$): unique solution given by normal eqs. of 2nd kind

[K., Potts 23]

$$\mathbf{A}_{|\mathcal{I}_{2M}|}^T \overline{\mathbf{A}_{|\mathcal{I}_{2M}|}} \mathbf{v} = \mathbf{e}_0, \quad \overline{\mathbf{A}_{|\mathcal{I}_{2M}|}} \mathbf{v} = \mathbf{w}$$

↪ efficient computation: CG algorithm combined with NFFT

$\mathcal{O}(|\mathcal{I}_{2M}| \log(|\mathcal{I}_{2M}|) + N)$

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least squares solution by normal eqs. of 1st kind

$$\overline{\mathbf{A}_{|\mathcal{I}_{2M}|}} \mathbf{A}_{|\mathcal{I}_{2M}|}^T \mathbf{w} = \overline{\mathbf{A}_{|\mathcal{I}_{2M}|}} \mathbf{e}_0$$

[K., Potts 23]: not a good approximation...

Recapitulation

So far:

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

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Interpretation perspectives:

(i) Set $g := W f$. $\Rightarrow \hat{f} \approx D^* F^* B^* g \rightsquigarrow$ ordinary NFFT, modified coefficient vector

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- (ii) Set $\tilde{B} := W B$. $\Rightarrow \hat{f} \approx D^* F^* \tilde{B}^* f \rightsquigarrow$ modified NFFT, ordinary coefficient vector

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Aim: $X = D^* F^* \tilde{B}^*$ [K., Potts 23]

\rightsquigarrow modification of matrix B

\rightsquigarrow preserve band structure and arithmetic complexity

Precomputational step – Optimization procedure

[K., Potts 23]

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

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

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Optimization problem:

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

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

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

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$$\text{Minimize}_{\tilde{B} \text{ banded}} \left\| A^* \tilde{B} - \frac{1}{|\mathcal{I}_{M_\sigma}|} D^{-1} F^* \right\|_F^2 = \sum_{\ell \in \mathcal{I}_{M_\sigma}} \left\| A_\ell^* \tilde{b}_\ell - \frac{1}{|\mathcal{I}_{M_\sigma}|} D^{-1} f_\ell \right\|_2^2$$

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[K., Potts 23]

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

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

Optimization problem:

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

If $A^* \tilde{B}$ is a pseudoinverse of FD then $A^* \tilde{B} F D \approx I_{|\mathcal{I}_M|}$.
 Since $F^* F = |\mathcal{I}_{M_\sigma}| I_{|\mathcal{I}_M|}$, a pseudoinverse is given by $\frac{1}{|\mathcal{I}_{M_\sigma}|} D^{-1} F^*$.

$$\text{Minimize}_{\tilde{B} \text{ banded}} \left\| A^* \tilde{B} - \frac{1}{|\mathcal{I}_{M_\sigma}|} D^{-1} F^* \right\|_{\mathbb{F}}^2 = \sum_{\ell \in \mathcal{I}_{M_\sigma}} \left\| A_\ell^* \tilde{b}_\ell - \frac{1}{|\mathcal{I}_{M_\sigma}|} D^{-1} f_\ell \right\|_2^2$$

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

Discrete example – Shepp-Logan phantom

- 1 phantom data = Fourier coefficients $\hat{\mathbf{f}} := (\hat{f}_{\mathbf{k}})_{\mathbf{k} \in \mathcal{I}_M}$ of a trigonometric polynomial
- 2 compute the evaluations $f(\mathbf{x}_j) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}_{\mathbf{k}} e^{2\pi i \mathbf{k} \mathbf{x}_j}$ by means of NFFT
- 3 reconstruct $\tilde{h}_{\mathbf{k}} \approx \hat{f}_{\mathbf{k}}, \mathbf{k} \in \mathcal{I}_M$



Discrete example – Shepp-Logan phantom

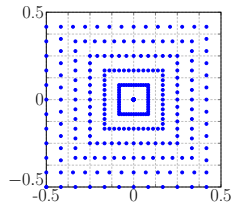
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Friendly setting ($|\mathcal{I}_{2M}| \leq N$):

- linogram grid of size $R = 2M, T = 2R$
- phantom size $M \times M$ with $M = 2^c, c = 3, \dots, 10$
- relative errors

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



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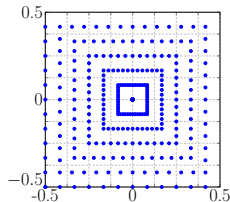
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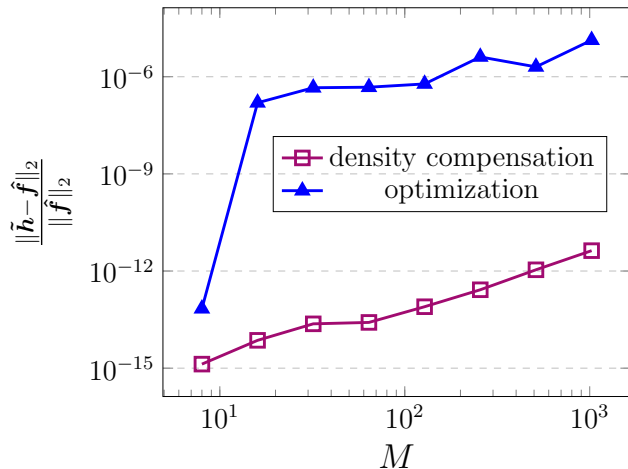
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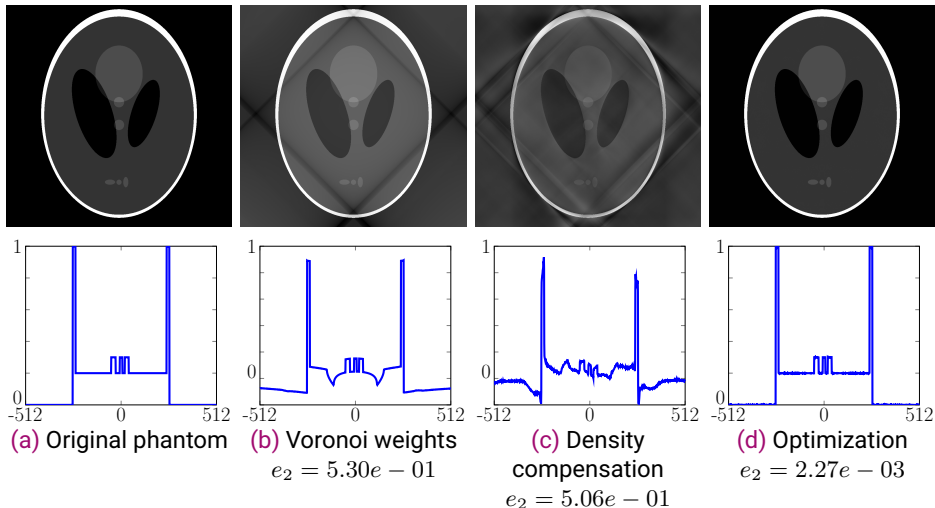
Unfriendly setting ($|\mathcal{I}_{2M}| > N$):

- linogram grid of size $R = M, T = 2R$
- phantom of size $M = 1024$
- ↪ compare presented computation schemes
 - Voronoi weights
 - new density compensation factors
 - optimization approach



Friendly setting ($|\mathcal{I}_{2M}| < N$)



Unfriendly setting ($|\mathcal{I}_{2M}| > N$)


Analogous problem for bandlimited functions

Application: MRI (Magnetic Resonance Imaging)

no longer

discrete
(trigonometric polynomials)

but

continuous
(bandlimited functions)

[Rosenfeld 98], [Greengard, Lee, Inati 06], [Eggers, K., Potts 22]

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(Continuous) Fourier transform:

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Reconstruct: evaluations $\hat{f}(\mathbf{k}) \in \mathbb{C}, \mathbf{k} \in \mathcal{I}_M$

Given: measurements $f(\mathbf{x}_j), j = 1, \dots, N$

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Now: extend previous methods

Reconsideration as trigonometric polynomials

Consider 1-periodization

$$\tilde{f}(\mathbf{x}) := \sum_{\mathbf{r} \in \mathbb{Z}^d} f(\mathbf{x} + \mathbf{r}) \in L_2(\mathbb{T}^d)$$

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⇒ density compensation method:

$$\hat{f}(\mathbf{k}) = c_{\mathbf{k}}(\tilde{f}) = \sum_{j=1}^N w_j \tilde{f}(\mathbf{x}_j) e^{-2\pi i \mathbf{k} \mathbf{x}_j}, \quad \mathbf{k} \in \mathcal{I}_M \qquad \hat{f} = \mathbf{A}^* \mathbf{W} \tilde{f}$$

Practical situation (e. g. MRI)

In practice: only hypothetical case !

periodization \tilde{f} cannot be sampled $\iff f$ cannot be sampled on whole \mathbb{R}^d

Sampling: limited coverage of space

$\rightsquigarrow f$ only known on a bounded domain, w.l.o.g. for $x \in [-\frac{1}{2}, \frac{1}{2})^d$

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\rightsquigarrow analogously also optimization method applicable

Continuous example – tensorized triangular pulse function

- 1 specify compactly supported $\hat{f}(\mathbf{v}) = g(v_1) \cdot g(v_2)$, with triangular pulse $g(v) := (1 - |v/b|) \cdot \chi_{[-b,b]}(v)$
- 2 compute inverse Fourier transform

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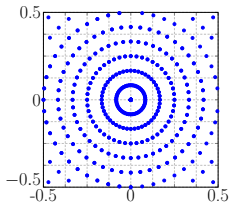
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Setup:

- consider $|\mathcal{I}_{2M}| \leq N$
- $M = 32$ and $b = 12$
- modified polar grid of size $R = 2M$, $T = 2R$
- pointwise errors $|\tilde{h} - \hat{f}|$



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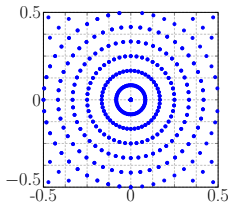
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Sampling data:

- real-world sampling $f(\mathbf{x}_j)$
- artificial sampling of the periodization

$$\tilde{f}(\mathbf{x}_j) = \sum_{\mathbf{k} \in \mathcal{I}_M} \hat{f}(\mathbf{k}) e^{2\pi i \mathbf{k} \mathbf{x}_j}$$

Results – pointwise errors $|\tilde{h} - \hat{f}|$

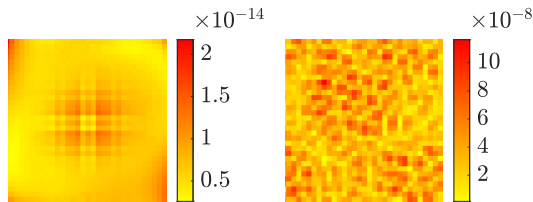
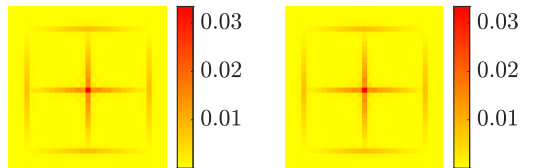
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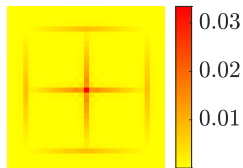
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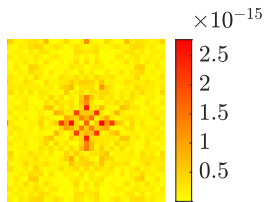
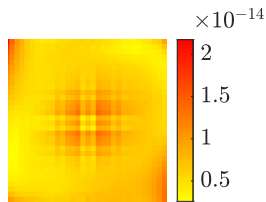
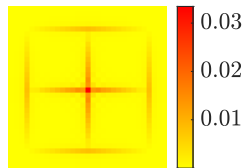
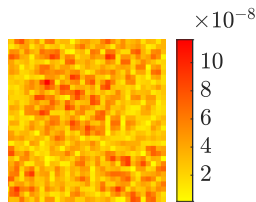
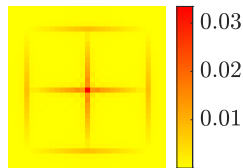


(b) Density compensation

(c) Optimization

Results – pointwise errors $|\tilde{h} - \hat{f}|$

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 (a) Equispaced points \mathbf{x}_j
 & FFT

 (b) Density
 compensation


(c) Optimization

Summary

- new direct inversion methods for $d \geq 1$, introduced for discrete problem (trigonometric polynomials)
- sampling density compensation: exact reconstruction in case $|\mathcal{I}_{2M}| \leq N$
- optimization: based on factorization $\overset{\text{optimized}}{\mathbf{BFD}}$ of NFFT, also works for $|\mathcal{I}_M| < N$
- fast algorithms of same complexity $\mathcal{O}(|\mathcal{I}_M| \log(|\mathcal{I}_M|) + N)$
- extendable to continuous problem (bandlimited functions)
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Thank you for your attention!