Optimal density compensation factors for the reconstruction of the Fourier transform of bandlimited functions

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joint work with Daniel Potts

Sampling Theory and Applications
Yale, July 10–14, 2023

Motivation – discrete problem

phantom

$\hat{f}_{\boldsymbol{k}}$

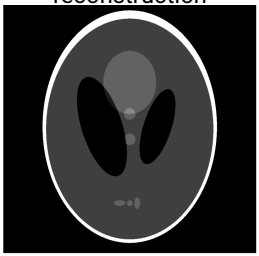
$\rightsquigarrow$

given measurements

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

$\rightsquigarrow$

reconstruction



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

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reconstruction

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$\boldsymbol{x}_j$ equispaced $\Longrightarrow$ FFT (Fast Fourier Transform)

$\boldsymbol{x}_j$ nonequispaced $\Longrightarrow$ inverse NFFT (Nonequispaced Fast Fourier Transform) **?**

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	ground truth	given measurements	aim
discrete problem	$\hat{f}_{\boldsymbol{k}}$	$f(\boldsymbol{x}_j) = \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \hat{f}_{\boldsymbol{k}} \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j}$	$\tilde{h}_{\boldsymbol{k}} \approx \hat{f}_{\boldsymbol{k}}$

$\boldsymbol{v} \in \mathbb{R}^d$, $\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}$

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continuous problem	$\hat{f}(\boldsymbol{v})$	$f(\boldsymbol{x}_j) = \int_{\left[-\frac{M}{2}, \frac{M}{2}\right)^d} \hat{f}(\boldsymbol{v}) \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_j} \, \mathrm{d}\boldsymbol{v}$	$\tilde{h}(\boldsymbol{k}) \approx \hat{f}(\boldsymbol{k})$

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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 $\boldsymbol{x}_j$, $j = 1, \ldots, N$, fixed $\quad\Longrightarrow\quad$ highly profit from direct method

1. precomputation: only once for fixed $\boldsymbol{x}_j$
2. reconstruction: for each measurement $\rightsquigarrow$ very efficient

Overview

1. Introduction
2. Discrete problem
3. Continuous problem
4. Numerical Examples

NFFT (Nonequispaced Fast Fourier Transform)

Fast algorithm to evaluate a trigonometric polynomial $\mathcal{O}(|\mathcal{I}_{\boldsymbol{M}}| \log(|\mathcal{I}_{\boldsymbol{M}}|) + N)$

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

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

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Inversion problem (iNFFT):

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

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

Basic idea

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

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

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$\Rightarrow$ Find suitable matrix $\boldsymbol{X}$ with

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

since then

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

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Reminder – Equispaced nodes:

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

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

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

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Algorithm

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

Exact reconstruction for trigonometric polynomials

Theorem (K., Potts 23)

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

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

$$\sum_{j=1}^{N} w_j \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j} = \delta_{\boldsymbol{0},\boldsymbol{k}}, \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{2M}}, \qquad \boldsymbol{A}_{|\mathcal{I}_{\boldsymbol{2M}}|}^{T} \boldsymbol{w} = \boldsymbol{e_0}$$

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

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

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

Proof

- $\{\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{\ell}\boldsymbol{x}} : \boldsymbol{\ell} \in \mathbb{Z}^d\}$ forms an orthonormal basis of $L_2(\mathbb{T}^d)$ [Plonka, Potts, Steidl, Tasche 18]
- $\boldsymbol{\ell} \in \mathcal{I}_M$ sufficient for trigonometric polynomials $f(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathcal{I}_M} \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$

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- For fixed $\boldsymbol{\ell} \in \mathcal{I}_M$ we have

$$h_{\boldsymbol{k}}^{\mathrm{w}} = \sum_{j=1}^{N} w_j\, \mathrm{e}^{2\pi\mathrm{i}(\boldsymbol{\ell}-\boldsymbol{k})\boldsymbol{x}_j}, \quad \boldsymbol{k} \in \mathcal{I}_M,$$

and

$$\hat{f}_{\boldsymbol{k}} = c_{\boldsymbol{k}}(f) = \int_{\mathbb{T}^d} \mathrm{e}^{2\pi\mathrm{i}(\boldsymbol{\ell}-\boldsymbol{k})\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x} = \delta_{\boldsymbol{\ell},\boldsymbol{k}}, \quad \boldsymbol{k} \in \mathcal{I}_M.$$

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$\rightsquigarrow$ necessary for exact solution: underdetermined system with $|\mathcal{I}_{\boldsymbol{2M}}| \leq N$ [Huybrechs 09]

Computation schemes

Aim: exact solution to

$$\boldsymbol{A}^{T}_{|\mathcal{I}_{\boldsymbol{2M}}|}\,\boldsymbol{w} = \boldsymbol{e_0} \coloneqq (\delta_{\boldsymbol{0},\boldsymbol{k}})_{\boldsymbol{k}\in\mathcal{I}_{\boldsymbol{2M}}} \qquad (*)$$

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Friendly setting ($|\mathcal{I}_{\boldsymbol{2M}}| \leq N$): unique solution given by normal eqs. of 2nd kind [K., Potts 23]

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

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- note that $(*)$ implies $\boldsymbol{A}^{*}\boldsymbol{W}\boldsymbol{A} = \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|} \implies$ minimization of $\left\|\boldsymbol{A}^{*}\boldsymbol{W}\boldsymbol{A} - \boldsymbol{I}_{|\mathcal{I}_{\boldsymbol{M}}|}\right\|_{\mathrm{F}}^{2}$
  $\rightsquigarrow$ minimizer obtained by solving $\boldsymbol{S}\boldsymbol{w} = \boldsymbol{b}$ with [Rosenfeld 98]

$$\boldsymbol{S} \coloneqq \left(\left|\left[\boldsymbol{A}\boldsymbol{A}^{*}\right]_{j,s}\right|^{2}\right)_{j,s=1}^{N} \quad \text{and} \quad \boldsymbol{b} = |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{1}_N \qquad \mathcal{O}(N^3)$$

Analogous problem for bandlimited functions

Application: MRI (Magnetic Resonance Imaging) [Rosenfeld 98], [Greengard, Lee, Inati 06], [Eggers, K., Potts 22]

no longer discrete (trigonometric polynomials) but continuous (bandlimited functions)

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(Continuous) Fourier transform:

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

$\rightsquigarrow$ bandlimited functions with maximum bandwidth M $\iff$ $\operatorname{supp}(\hat{f}\,) = \left[-\frac{M}{2}, \frac{M}{2}\right)^d$

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

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

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Now: extend previous method

Reconsideration as trigonometric polynomials

Consider 1-periodization

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$\Rightarrow$ uniquely representable by absolute convergent Fourier series [Plonka, Potts, Steidl, Tasche 18]

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with Fourier coefficients

$$c_{\boldsymbol{k}}(\tilde{f}) = \int_{\mathbb{T}^d} \tilde{f}(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{k}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x} = \int_{\mathbb{R}^d} f(\boldsymbol{x})\, \mathrm{e}^{-2\pi \mathrm{i}\boldsymbol{k}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{x} = \hat{f}(\boldsymbol{k}), \quad \boldsymbol{k}\in\mathbb{Z}^d$$

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$\rightsquigarrow$ f bandlimited with bandwidth $\boldsymbol{M}$ $\iff$ $\operatorname{supp}(\hat{f}) = \left[-\frac{M}{2}, \frac{M}{2}\right)^d$ $\implies$ $\hat{f}(\boldsymbol{k}) = 0, \boldsymbol{k}\in\mathbb{Z}^d \setminus \mathcal{I}_{\boldsymbol{M}}$

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$\Rightarrow$ exact reconstruction

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

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 $\boldsymbol{x} \in \left[-\frac{1}{2}, \frac{1}{2}\right)^d$

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$\rightsquigarrow$ have to deal with the approximation

$$\hat{f}(\boldsymbol{k}) \approx \sum_{j=1}^{N} w_j \, f(\boldsymbol{x}_j) \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j}, \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}$$

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Main cause of error: f is not known on whole $\mathbb{R}^d$

Connection to previous work

[Greengard, Lee, Inati 06]: extend approximation to whole interval

$$\hat{f}(\boldsymbol{v}) \approx \tilde{h}(\boldsymbol{v}) \coloneqq \sum_{j=1}^{N} w_j \, \tilde{f}(\boldsymbol{x}_j) \, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_j}, \quad \boldsymbol{v} \in \left[-\tfrac{M}{2}, \tfrac{M}{2}\right)^d$$

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$\Rightarrow$ inverse Fourier transform

$$f(\boldsymbol{x}_s) = \int_{\left[-\frac{M}{2}, \frac{M}{2}\right)^d} \hat{f}(\boldsymbol{v}) \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_s} \, \mathrm{d}\boldsymbol{v} \approx \int_{\left[-\frac{M}{2}, \frac{M}{2}\right)^d} \tilde{h}(\boldsymbol{v}) \, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_s} \, \mathrm{d}\boldsymbol{v} = \sum_{j=1}^{N} w_j \, \tilde{f}(\boldsymbol{x}_j) \cdot |\mathcal{I}_{\boldsymbol{M}}| \, \mathrm{sinc}\big(M\pi(\boldsymbol{x}_j - \boldsymbol{x}_s)\big)$$

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Question: Choose w_j based on this equation

$$\boldsymbol{f} \approx |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W} \tilde{\boldsymbol{f}} \approx |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W} \boldsymbol{f},$$

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$$\boldsymbol{C}_{\mathrm{n}} \coloneqq \Big(\operatorname{sinc}\big(M\pi(\boldsymbol{x}_j - \boldsymbol{x}_s)\big)\Big)_{j,s=1}^{N} \in \mathbb{R}^{N \times N}$$

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$\rightsquigarrow$ ideally aim for $\boldsymbol{I}_N = |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W}$

Exact solution? main diagonal of $|\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W} = \boldsymbol{I}_N$ reads as

$$\tfrac{1}{|\mathcal{I}_{\boldsymbol{M}}|} = w_j \operatorname{sinc}(0) = w_j, \quad j = 1, \ldots, N,$$

i. e., need $\operatorname{sinc}(M\pi(\boldsymbol{x}_j - \boldsymbol{x}_s)) = 0,\ j \neq s$ ↯ $\boldsymbol{x}_j$ nonequispaced ⇝ only approximate solution

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Least squares problem:

$$\underset{\boldsymbol{W} = \operatorname{diag}(w_j)_{j=1}^N}{\text{Minimize}} \ \| |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W} - \boldsymbol{I}_N \|_{\mathrm{F}}^2$$

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⇝ consider only nonzeros

$$\| |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{W} - \boldsymbol{I}_N \|_{\mathrm{F}}^2 = \sum_{j=1}^{N} \| |\mathcal{I}_{\boldsymbol{M}}| \cdot \boldsymbol{C}_{\mathrm{n}} \boldsymbol{w}_j - \boldsymbol{e}_j \|_2^2 = \sum_{j=1}^{N} \| |\mathcal{I}_{\boldsymbol{M}}| \cdot [\boldsymbol{C}_{\mathrm{n}}]_j \, w_j - \boldsymbol{e}_j \|_2^2$$

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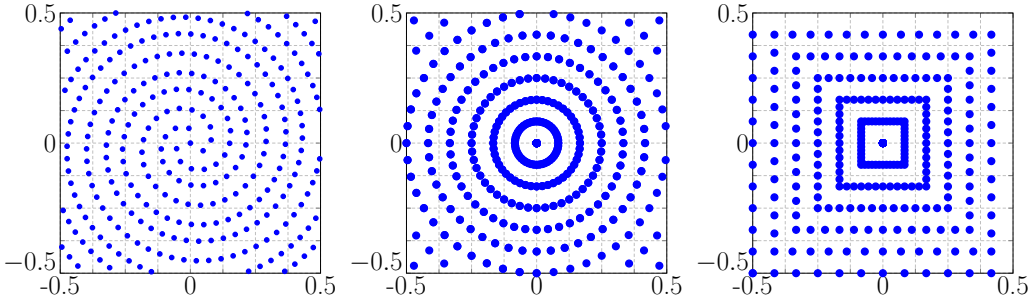
⇒ least squares solution given by

$$w_j = \frac{1}{|\mathcal{I}_{\boldsymbol{M}}|} [\boldsymbol{C}_{\mathrm{n}}]_j^{\dagger} \boldsymbol{e}_j = \; \dots \; = \frac{1}{|\mathcal{I}_{\boldsymbol{M}}|} \left(\sum_{s=1}^{N} \operatorname{sinc}^2(M\pi(\boldsymbol{x}_j - \boldsymbol{x}_s)) \right)^{-1}$$

Numerical Examples – Testing Grids



(a) Spiral grid (b) Polar (blue) and modified polar (red) grid (c) Linogram grid

Figure: Exemplary grids of size $R = 12$ and $T = 2R$.

Discrete problem – Shepp-Logan phantom

1. phantom data = Fourier coefficients $\hat{\boldsymbol{f}} := (\hat{f}_{\boldsymbol{k}})_{\boldsymbol{k}\in\mathcal{I}_M}$ of a trigonometric polynomial
2. compute the evaluations $f(\boldsymbol{x}_j) = \sum_{\boldsymbol{k}\in\mathcal{I}_M} \hat{f}_{\boldsymbol{k}}\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{x}_j}$ by means of NFFT
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Friendly setting ($|\mathcal{I}_{\boldsymbol{2M}}| \leq N$):

- linogram grid of size $R = 2M$, $T = 2R$
- phantom size $M \times M$
- relative errors

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

⇝ show exact reconstruction

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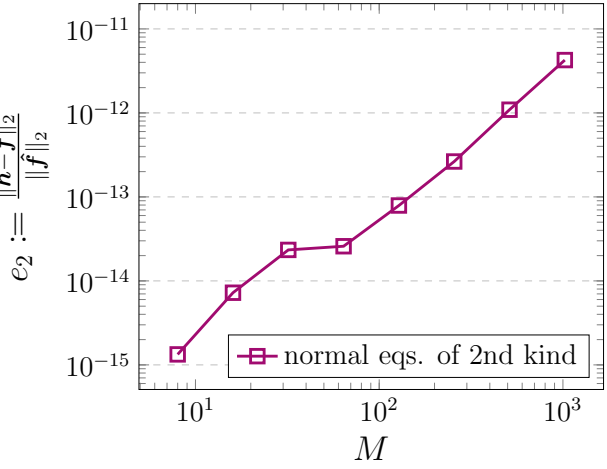
Unfriendly setting ($|\mathcal{I}_{\boldsymbol{2M}}| > N$):

- spiral grid of size $R = M, T = 2R$
- phantom of size $M = 64$

⇝ compare presented computation schemes

- normal eqs. of 2nd kind
- normal eqs. of 1st kind
- Frobenius norm minimization
  (small M necessary for being affordable)

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



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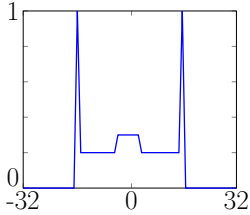
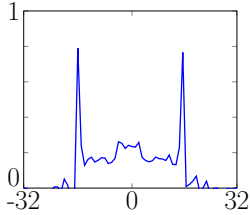
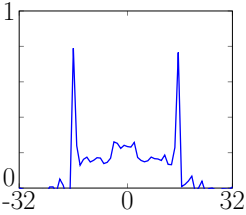


(a) Phantom



(b) Normal eqs. of 2nd kind

$e_2 = 0.2482$



(c) Normal eqs. of 1st kind

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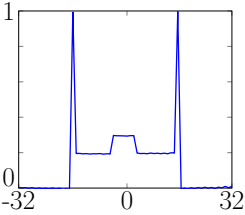

(d) Frobenius norm minimization

$e_2 = 0.1187$

Continuous problem – tensorized triangular pulse function

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

$$f(\boldsymbol{x}) = \int_{\mathbb{R}^2} \hat{f}(\boldsymbol{v})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v}\boldsymbol{x}}\, \mathrm{d}\boldsymbol{v} = b^2 \operatorname{sinc}^2(b\pi\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^2$$

$\rightsquigarrow$ bandlimited with bandwidth M for all $b \in \mathbb{N}$ with $b \leq \frac{M}{2}$

3. sample $f(\boldsymbol{x}_j)$ for given $\boldsymbol{x}_j \in \left[-\frac{1}{2}, \frac{1}{2}\right)^2, j = 1, \ldots, N$
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Setup:

- consider $|\mathcal{I}_{\boldsymbol{2M}}| \leq N$
- $M = 32$ and $b = 12$
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Sampling data:

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

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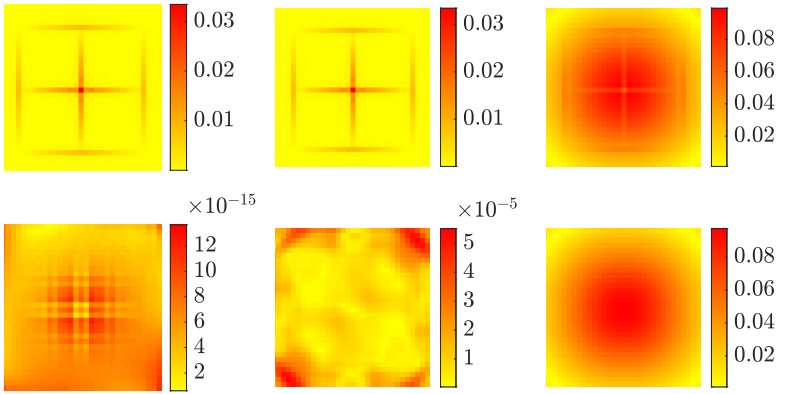
Results – real-world sampling (top) & artificial sampling (bottom)



(b) normal eqs. of 2nd kind

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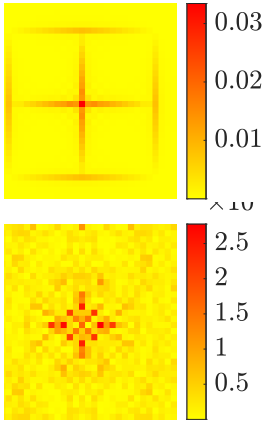
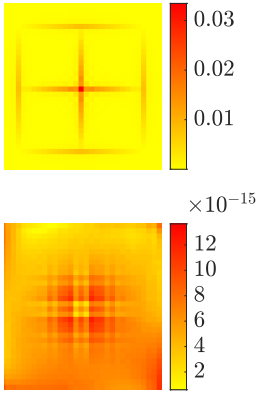
(d) [Greengard, Lee, Inati 06]

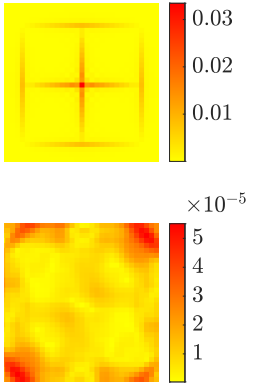
Results – real-world sampling (top) & artificial sampling (bottom)



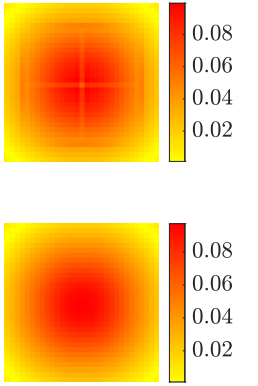
(a) equispaced setting



(b) normal eqs. of 2nd kind



(c) Frobenius norm minimization



(d) [Greengard, Lee, Inati 06]

Summary

- new direct inversion method based on sampling density compensation
- introduced for discrete problem (trigonometric polynomials)
- exact reconstruction in case $|\mathcal{I}_{\boldsymbol{2M}}| \leq N$
- extendable continuous problem (bandlimited functions)
- error solely occurs since f cannot be sampled on whole $\mathbb{R}^d$

- **K., Potts: Fast and direct inversion methods for the multivariate nonequispaced fast Fourier transform**.
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Thank you for your attention!