Fast and direct inverse nonequispaced Fourier transforms

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joint work with Daniel Potts

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Motivation – discrete problem

phantom

$\rightsquigarrow$ given measurements $\rightsquigarrow$

reconstruction

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

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

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

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

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

Motivation

	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)

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special setting: evaluation points $\boldsymbol{x}_j$, $j = 1, \ldots, N$, fixed $\Longrightarrow$ 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

NFFT (Nonequispaced Fast Fourier Transform)

Fast algorithm to evaluate a trigonometric polynomial

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

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

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

- 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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Matrix notation:

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

$(2m+1)^d$–sparse ↗ FFT ↑ diagonal ↖

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

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$(2m+1)^d$–sparse, FFT, diagonal

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Inversion problem (iNFFT): **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:

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

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Simplest generalization:

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

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

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Density compensation algorithm

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

Intuitive approach:
Voronoi weights based on geometry

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

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*

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

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

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

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

Proof for exactness of weights [K., Potts 23]

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

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

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

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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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$\rightsquigarrow$ efficient computation: CG algorithm combined with NFFT ✓ $\mathcal{O}(|\mathcal{I}_{\boldsymbol{2M}}| \log(|\mathcal{I}_{\boldsymbol{2M}}|) + N)$

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

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[literature study]: approaches only affordable for very small problem sizes! ✘

Recapitulation

So far:

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diagonal — FFT — $(2m+1)^d$–sparse

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Interpretation perspectives:

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

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

Recapitulation

So far:

$$\hat{f} \approx A^* W f \approx \underbrace{D^*}_{\text{diagonal}} \underbrace{F^*}_{\text{FFT}} \overbrace{B^*}^{(2m+1)^d\text{-sparse}} W f$$

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Aim: [K., Potts 21/23a]

- $\rightsquigarrow$ modification of matrix B
- $\rightsquigarrow$ preserve sparse structure and thereby arithmetic complexity

Optimization approach

0. Precompute $(2m+1)^d$–sparse matrix B ?

1. (Modified) adjoint NFFT $\mathcal{O}(|\mathcal{I}_M| \log(|\mathcal{I}_M|) + N)$

Precomputational step – Optimization procedure

[K., Potts 23]

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

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

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

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Precomputational step – Optimization procedure

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$\Rightarrow$ Compute

$$\boldsymbol{b}_\ell^{\mathrm{opt}} := \tfrac{1}{|\mathcal{I}_{M_\sigma}|} \left(\boldsymbol{A}_\ell \boldsymbol{A}_\ell^* \right)^{-1} \boldsymbol{A}_\ell \boldsymbol{D}^{-1} \boldsymbol{f}_\ell, \quad \ell \in \mathcal{I}_{M_\sigma}.$$

Compose $\boldsymbol{B}_{\mathrm{opt}}$ column-wise of the $\boldsymbol{b}_\ell^{\mathrm{opt}}$ observing the sparsity and periodicity. $\rightsquigarrow \mathcal{O}(|\mathcal{I}_M|)$

Discrete example – Shepp-Logan phantom

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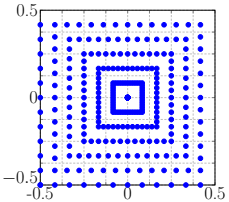
Friendly setting ($|\mathcal{I}_{2M}| \leq N$):

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

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



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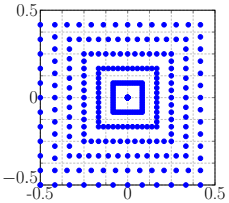
Unfriendly setting ($|\mathcal{I}_{2\boldsymbol{M}}| > N$):

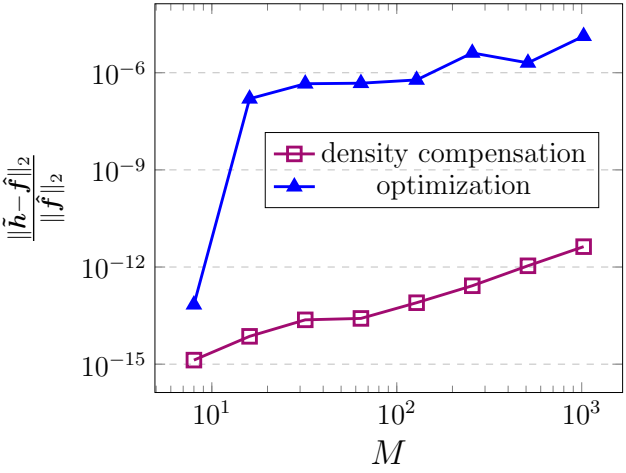
- linogram grid of size $R = M, T = 2R$
- phantom of size $M = 1024$

$\rightsquigarrow$ compare presented computation schemes

- Voronoi weights
- new density compensation factors
- optimization approach



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



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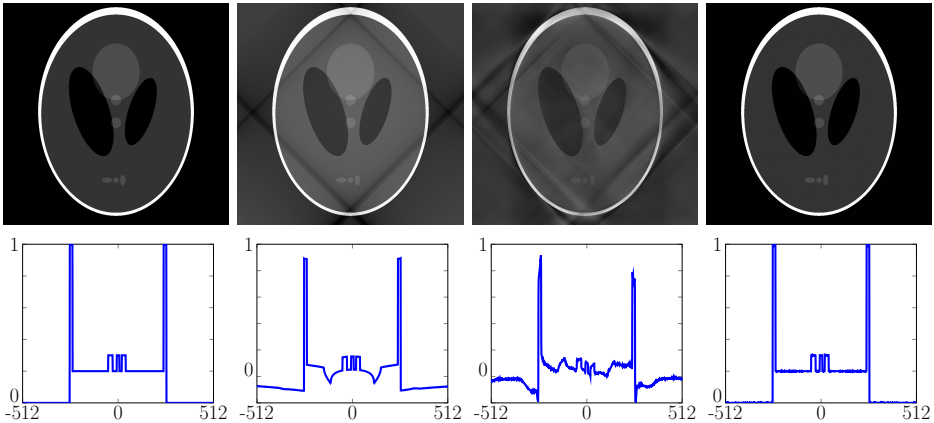

(a) Original phantom

(b) Voronoi weights
$e_2 = 5.30e-01$

(c) Density compensation
$e_2 = 5.06e-01$

(d) Optimization
$e_2 = 2.27e-03$

Summary – discrete problem

Efficient inversion methods for $\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}}$ in the form

$$\hat{\boldsymbol{f}} \approx \boldsymbol{A}^* \boldsymbol{W} \boldsymbol{f} \approx \underset{\nearrow \text{diagonal}}{\boldsymbol{D}^*} \underset{\uparrow \text{FFT}}{\boldsymbol{F}^*} \underset{\nwarrow (2m+1)^d\text{–sparse}}{\boldsymbol{B}^*} \boldsymbol{W} \boldsymbol{f}$$

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- highly overdetermined setting $|\mathcal{I}_{\boldsymbol{2M}}| < N$ (friendly setting): ✓
  $\rightsquigarrow$ exact reconstruction by density compensation – compute optimal diagonal matrix $\boldsymbol{W}$

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  ⇝ good results by optimization approach – compute optimal sparse matrix $\boldsymbol{B}$

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Open problems:

- What about the underdetermined setting $|\mathcal{I}_{\boldsymbol{M}}| > N$? ✘

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Open problems:

- What about the underdetermined setting $|\mathcal{I}_{\boldsymbol{M}}| > N$? ✘
- Stability issues (highly irregular grids) ✘
  ⇝ [Wilber, Epperly, Barnett 24]: low-rank approximation of structured matrices (Cauchy matrix)
  ⇒ "best of 2 worlds approach"?

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 $\boldsymbol{M}$ $\iff$ $\operatorname{supp}(\hat{f}) = \left[-\frac{M}{2}, \frac{M}{2}\right)^d$

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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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First step: examine forward problem (evaluation of $(*)$ instead of inversion)

Evaluation problem

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

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

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$$\implies \quad f(\boldsymbol{x}_j) = \int_{\mathbb{R}^d} \hat{f}(\boldsymbol{v})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_j}\, \mathrm{d}\boldsymbol{v} = \int_{\left[-\frac{M}{2}, \frac{M}{2}\right)^d} \hat{f}(\boldsymbol{v})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{v} \boldsymbol{x}_j}\, \mathrm{d}\boldsymbol{v} \approx \underbrace{\sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}} \hat{f}(\boldsymbol{k})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k} \boldsymbol{x}_j}}_{\text{NFFT}} \qquad (*)$$

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- designed for periodic functions
- quadrature error unclear

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Shannon Sampling Theorem ($L \geq M$)

$$f(x) = \sum_{\ell \in \mathbb{Z}} f\big(\tfrac{\ell}{L}\big)\, \mathrm{sinc}\big(L\pi\big(x - \tfrac{\ell}{L}\big)\big)$$

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with compactly supported window function, e. g. $\varphi_{\sinh}(t) \coloneqq \frac{\sinh\left(\beta \sqrt{1 - \left(\frac{Lt}{m}\right)^2}\right)}{\sinh \beta}\, \chi_{[-\frac{m}{L}, \frac{m}{L}]}(t)$ with $\beta > 0$

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$\Rightarrow$ efficient evaluation (sparse sums) + exponential error decay ($\| f - R_{\sinh,m} f \|_{C_0(\mathbb{R})} \leq C\, \mathrm{e}^{-mc}\, \| f \|_{L_2(\mathbb{R})}$)

NFFT-like procedure for bandlimited functions

Approximate f by $R_{\varphi,m} f$, where $\psi(x) = \operatorname{sinc}(x)\,\varphi(x)$, i. e.,

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$$f\big(\tfrac{\boldsymbol{\ell}}{L}\big) \approx \vartheta_{\boldsymbol{\ell}} := \frac{1}{|\mathcal{I}_{\boldsymbol{L}}|} \sum_{\boldsymbol{k} \in \mathcal{I}_{\boldsymbol{L}}} \hat{\vartheta}(\boldsymbol{k})\, \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{k}\boldsymbol{\ell}/L}, \quad \boldsymbol{\ell} \in \mathcal{I}_{\boldsymbol{L}}, \qquad \text{where} \quad \hat{\vartheta}(\boldsymbol{k}) = \begin{cases} \frac{\hat{f}(\boldsymbol{k})}{\hat{\psi}(\boldsymbol{k})} & : \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{M}}, \\ 0 & : \quad \boldsymbol{k} \in \mathcal{I}_{\boldsymbol{L}} \setminus \mathcal{I}_{\boldsymbol{M}}, \end{cases}$$

NFFT-like procedure for bandlimited functions

Approximate f by $R_{\varphi,m} f$, where $\psi(x) = \operatorname{sinc}(x)\,\varphi(x)$, i. e.,

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and thereby

$$f(\boldsymbol{x}_j) \approx (R_{\varphi,m} f)(\boldsymbol{x}_j) \approx \sum_{\boldsymbol{\ell} \in \mathcal{I}_{\boldsymbol{L}}} \vartheta_{\boldsymbol{\ell}}\, \psi\big(\boldsymbol{x}_j - \tfrac{\boldsymbol{\ell}}{L}\big)$$

$$\boldsymbol{f} \approx \boldsymbol{\Psi} \boldsymbol{F} \boldsymbol{D}_{\hat{\psi}} \hat{\boldsymbol{f}}$$

$(2m+1)^d$-sparse ↑ FFT ↖ diagonal

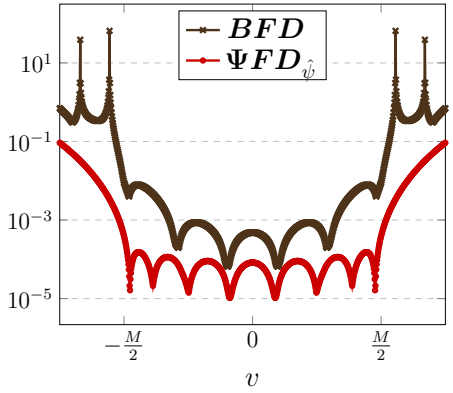
Numerical example – continuous problem

Approximation of exponential function

- $d = 1$
- $x \in \left[-\frac{1}{2} + \frac{m}{L}, \frac{1}{2} - \frac{m}{L} \right)$
- $m = 5, L = 40$
- consider pointwise error

$$e(v) := \max_{x_p, p=1,\dots,P} \left| \mathrm{e}^{2\pi \mathrm{i} v x_p} - h(x_p) \right|,$$

for $P = 10^5$ equispaced points x_p, $p = 1, \dots, P$, and $v \in \left[-\frac{M}{2}, \frac{M}{2} \right]$



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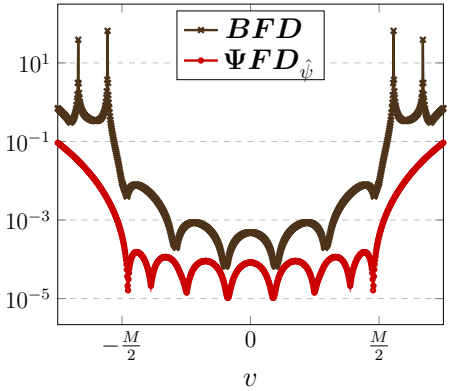

Open question: Can we use this technique also for the inversion problem?

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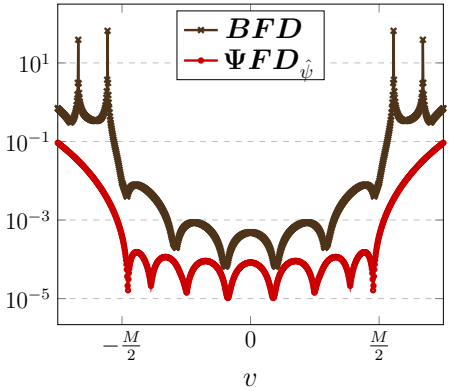

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Thank you for your attention!