TECHNISCHE UNIVERSITÄT CHEMNITZ

Faculty of Mathematics
Applied Functional Analysis
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Direct inversion of the NFFT

Task

Nonequispaced fast Fourier transform (NFFT)

Fast algorithm to evaluate a trigonometric polynomial

$$f(x) = \sum_{k=-\frac{M}{2}}^{\frac{M}{2}-1} \hat{f}_k \, \mathrm{e}^{2\pi i k x}$$

at nonequispaced nodes $x_j \in \left[-\frac{1}{2}, \frac{1}{2}\right), \, j = 1, \dots, N.$

- **Complexity:** $\mathcal{O}(M \log M + N)$
- Equispaced nodes x_j and $M = N \quad \Rightarrow \quad$ **FFT:** $\mathcal{O}(N \log N)$
- Adjoint problem: fast evaluation of

  $$h_k = \sum_{j=1}^{N} f_j \, \mathrm{e}^{-2\pi i k x_j}, \quad k = -\tfrac{M}{2}, \dots, \tfrac{M}{2} - 1.$$

  $\Rightarrow$ Adjoint NFFT
- Matrix vector notation: $\boldsymbol{f} = \boldsymbol{A}\hat{\boldsymbol{f}}$ and $\boldsymbol{h} = \boldsymbol{A}^*\boldsymbol{f}$, respectively, with nonequispaced Fourier matrix

  $$\boldsymbol{A} := \left(\mathrm{e}^{2\pi i k x_j}\right)_{j=1,\, k=-\frac{M}{2}}^{N,\, \frac{M}{2}-1}$$
- Factorizations: $\boldsymbol{A} \approx \boldsymbol{B}\boldsymbol{F}\boldsymbol{D}$ and $\boldsymbol{A}^* \approx \boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^*$
  (sparse, FFT, diagonal)

Inversion (iNFFT)

Given: $f(x_j), j = 1, \dots, N$

Find: $\hat{f}_k \in \mathbb{C}, \; k = -\frac{M}{2}, \dots, \frac{M}{2} - 1$

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

Issue: in general $M \neq N$

Now: new direct method for general case and connection to frame approach

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

Basic idea

For illustration consider equispaced nodes

$$x_j = \tfrac{j}{N} \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right), \; j = -\tfrac{N}{2}, \dots, \tfrac{N}{2} - 1.$$

We obtain

$$\boldsymbol{A} = \left(\mathrm{e}^{2\pi i k \frac{j}{N}}\right)_{j=-\frac{N}{2},\, k=-\frac{M}{2}}^{\frac{N}{2}-1,\, \frac{M}{2}-1} \quad \text{and} \quad \boldsymbol{A}^* = \left(\mathrm{e}^{-2\pi i k \frac{j}{N}}\right)_{k=-\frac{M}{2},\, j=-\frac{N}{2}}^{\frac{M}{2}-1,\, \frac{N}{2}-1}$$

and hence matrix products

$\boldsymbol{A}^*\boldsymbol{A} = N\boldsymbol{I}_M$ for $M \leq N$,

$\boldsymbol{A}\boldsymbol{A}^* = M\boldsymbol{I}_N$ for $M \geq N$ with $N \mid M$.

Whereas, for nonequispaced nodes

$$x_j \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right), \; j = -\tfrac{N}{2}, \dots, \tfrac{N}{2} - 1,$$

we have

$$\boldsymbol{A}^*\boldsymbol{A} \neq N\boldsymbol{I}_M \quad \text{and} \quad \boldsymbol{A}\boldsymbol{A}^* \neq M\boldsymbol{I}_N.$$

In this case, we look for a good approximation in general:

- ⇝ approximation of the form $\boldsymbol{A}\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^* \approx M\boldsymbol{I}_N$
- ⇝ modification of matrix $\boldsymbol{B}$
- ⇝ preserve band structure and arithmetic complexity

Matrix Approach

Underdetermined setting $M > N$

Assume

$$\boldsymbol{A}\boldsymbol{D}^*\boldsymbol{F}^*\boldsymbol{B}^* \approx M\boldsymbol{I}_N \iff \boldsymbol{A}\check{\boldsymbol{f}} \approx \boldsymbol{f} \quad \forall \boldsymbol{f} \in \mathbb{C}^N.$$

Since $\boldsymbol{A}\hat{\boldsymbol{f}} = \boldsymbol{f}$ that means $\check{\boldsymbol{f}} \approx \hat{\boldsymbol{f}}$. $\Rightarrow$ Reconstruction of Fourier coefficients $\hat{f}_k$.
Leads to optimization problem in terms of columns of $\boldsymbol{B}^*$ (only nonzero entries):

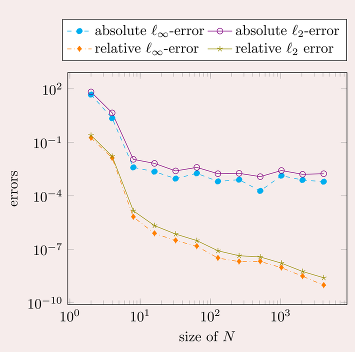
$$\underset{\boldsymbol{b}_j \in \mathbb{R}^{2m+1}}{\text{Minimize}} \; \|\boldsymbol{A}\boldsymbol{D}^*\boldsymbol{T}_j\boldsymbol{b}_j - M\boldsymbol{e}_j\|_2^2, \quad j = 1, \dots, N.$$

Can be solved via normal equations. $\Rightarrow$ precomputational algorithm: $\mathcal{O}(N^2 + M \log M)$
$\Rightarrow$ inverse NFFT: $\mathcal{O}(M \log M + N)$ (by application of modified adjoint NFFT)
$\Rightarrow$ inverse adjoint NFFT: $\mathcal{O}(M \log M + N)$ (by application of modified NFFT)

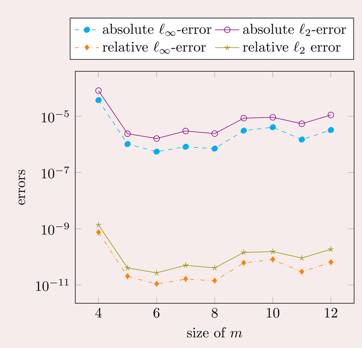
Numerical Example:

- trigonometric polynomial with $\hat{f}_k \in [1, 100]$
- jittered equispaced nodes
- absolute and relative errors per node, $r \in \{2, \infty\}$,

$$\frac{e_r^{\text{abs}}}{N} = \frac{1}{N}\|\boldsymbol{A}\check{\boldsymbol{f}} - \boldsymbol{f}\|_r \quad \text{and} \quad \frac{e_r^{\text{rel}}}{N} = \frac{\|\boldsymbol{A}\check{\boldsymbol{f}} - \boldsymbol{f}\|_r}{N\,\|\boldsymbol{f}\|_r}$$



$N = 2^c, \; c = 1, \dots, 12,$
$M = 4N$ and $m = 4.$



$N = 512, M = 2048$
and $m = 4, \dots, 12.$

Overdetermined setting $M < N$

We consider $\tilde{\boldsymbol{g}} = \boldsymbol{B}^*\boldsymbol{f}$ and $\tilde{\boldsymbol{h}} = \boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{g}}$. Set $\tilde{\boldsymbol{h}} \approx \hat{\boldsymbol{f}}$. Therefore, it holds

$$\tilde{\boldsymbol{g}} = \boldsymbol{B}^*\boldsymbol{f} = \boldsymbol{B}^*\boldsymbol{A}\hat{\boldsymbol{f}} \approx \boldsymbol{B}^*\boldsymbol{A}\tilde{\boldsymbol{h}} = \boldsymbol{B}^*\boldsymbol{A}\boldsymbol{D}^*\boldsymbol{F}^*\tilde{\boldsymbol{g}}.$$

That means $\boldsymbol{B}^*\boldsymbol{A}\boldsymbol{D}^*\boldsymbol{F}^* \approx \boldsymbol{I}_{\sigma M}$. $\Rightarrow$ Reconstruction of Fourier coefficients $\hat{f}_k$.
Leads to optimization problem in terms of the columns of $\boldsymbol{B}$ (only nonzero entries):

$$\underset{\boldsymbol{b}_j \in \mathbb{R}^{2m+1}}{\text{Minimize}} \; \|\boldsymbol{F}\boldsymbol{D}\boldsymbol{H}_l\boldsymbol{b}_l - \boldsymbol{e}_l\|_2^2, \quad l = -\tfrac{\sigma M}{2}, \dots, \tfrac{\sigma M}{2} - 1.$$

Can be solved via normal equations. $\Rightarrow$ precomputational algorithm: $\mathcal{O}(N^2M^2 + N^3M)$
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Numerical Example:

- trigonometric polynomial with $\hat{f}_k \in [1, 100]$
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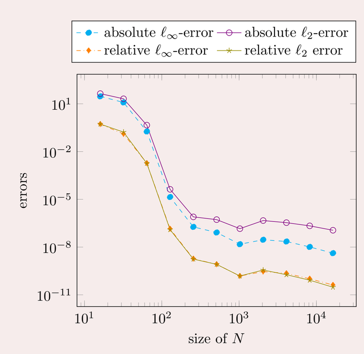

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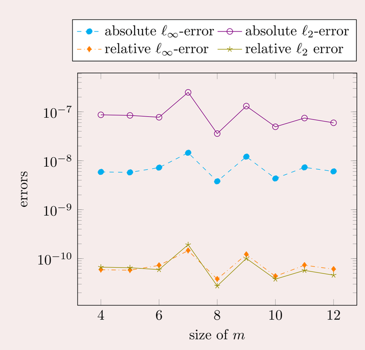

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Frame Approach

Frames

- Generalization of the concept of a basis
  ⇝ more flexible: no uniqueness, no linear independence
- **Definition:** Let $\mathcal{H}$ be a Hilbert space. A sequence $\{\varphi_j\}_{j=1}^\infty \subset \mathcal{H}$ is called a frame if there exist $A, B > 0$ such that

  $$A\|f\|^2 \leq \sum_{j=1}^{\infty} |\langle f, \varphi_j \rangle|^2 \leq B\|f\|^2 \quad \forall f \in \mathcal{H}.$$

  The operator

  $$S \colon \mathcal{H} \to \mathcal{H}, \quad Sf = \sum_{j=1}^{\infty} \langle f, \varphi_j \rangle \varphi_j,$$

  is named the frame operator.
- **Frame decomposition:** Let $\{\varphi_j\}_{j=1}^\infty$ be a frame with operator S, then

  $$f = \sum_{j=1}^{\infty} \langle f, S^{-1}\varphi_j \rangle \varphi_j = \sum_{j=1}^{\infty} \langle f, \varphi_j \rangle S^{-1}\varphi_j \quad \forall f \in \mathcal{H}.$$

  ⇝ In other words, every element in $\mathcal{H}$ can be represented as a linear combination of the elements of the frame.

$\Rightarrow$ Goal: approximate the inverse frame operator S^{-1}.

Frame-theoretical approach

We use the method of admissible frames to approximate the inverse frame operator so that we receive the approximation

$$f \approx \tilde{f} := \sum_{j=1}^{N} \sum_{l=-\frac{\sigma M}{2}}^{\frac{\sigma M}{2}-1} \langle f, \varphi_j \rangle \, p_{l,j} \, \psi_l$$

with $\boldsymbol{\Phi}^\dagger =: [p_{l,j}]_{l=-\frac{\sigma M}{2},\, j=1}^{\frac{\sigma M}{2}-1,\, N}$ is the Moore-Penrose pseudoinverse of

$$\boldsymbol{\Phi} := [\langle \varphi_j, \psi_l \rangle]_{j=1,\, l=-\frac{\sigma M}{2}}^{N,\, \frac{\sigma M}{2}-1}.$$

Workflow for iNFFT:

- Choose the frames

  $$\{\varphi_j(k) := \mathrm{e}^{-2\pi i k x_j}, \; j \in \mathbb{N}\} \text{ and } \left\{\psi_l(k) := \frac{\mathrm{e}^{-2\pi i k l/\sigma M}}{\sigma M \hat{w}(-k)}, \; l \in \mathbb{Z}\right\}.$$
- Consider the frame approximation of a function $\hat{f}$ in Fourier space.
- Evaluate it at equispaced points $k = -\frac{M}{2}, \dots, \frac{M}{2} - 1$, i.e., we have $\tilde{\hat{f}}(k) \approx \hat{f}_k$.
- Modify the adjoint NFFT such that we obtain the approximation $\tilde{h}_k \approx \tilde{\hat{f}}(k), \; k = -\frac{M}{2}, \dots, \frac{M}{2} - 1.$

Theoretical result

Define

$$\hat{\boldsymbol{h}} := (\hat{h}_k)_{k=-\frac{M}{2}}^{\frac{M}{2}-1}, \quad \text{and} \quad \tilde{\boldsymbol{h}} := (\tilde{h}_k)_{k=-\frac{M}{2}}^{\frac{M}{2}-1} = (\tilde{\hat{f}}(k))_{k=-\frac{M}{2}}^{\frac{M}{2}-1}.$$

For $\hat{\boldsymbol{w}} := \left(\frac{1}{\hat{w}(-k)}\right)_{k=-\frac{M}{2}}^{\frac{M}{2}-1}$ with $\|\hat{\boldsymbol{w}}\|_2 < \infty$ it holds:

(i) For $\sigma M < N$ we have

$$\left\|\tilde{\boldsymbol{h}} - \hat{\boldsymbol{h}}\right\|_2 \leq \frac{1}{\sqrt{\sigma M}} \|\hat{\boldsymbol{w}}\|_2 \, \|\boldsymbol{\Phi}\boldsymbol{B}^* - \boldsymbol{I}_N\|_{\mathrm{F}} \, \|\boldsymbol{\Phi}^\dagger\boldsymbol{f}\|_2.$$

(ii) For $\sigma M > N$ we have

$$\left\|\tilde{\boldsymbol{h}} - \hat{\boldsymbol{h}}\right\|_2 \leq \frac{1}{\sqrt{\sigma M}} \|\hat{\boldsymbol{w}}\|_2 \, \|\boldsymbol{B}^*\boldsymbol{\Phi} - \boldsymbol{I}_{\sigma M}\|_{\mathrm{F}} \, \|\boldsymbol{\Phi}^\dagger\boldsymbol{f}\|_2.$$

$\Rightarrow$ Minimization of Frobenius norms

Connection to iNFFT

One can show

$$\boldsymbol{\Phi}\boldsymbol{B}^* = (\boldsymbol{B}\boldsymbol{F}\boldsymbol{D}\boldsymbol{A}^*)^T \text{ as well as } \boldsymbol{B}^*\boldsymbol{\Phi} = (\boldsymbol{F}\boldsymbol{D}\boldsymbol{A}^*\boldsymbol{B})^T.$$

$\Rightarrow$ Equivalence of minimization problems
$\Rightarrow$ Equivalence of approaches

Refs

Fundamentals

Dutt, Rokhlin: **Fast Fourier transforms for nonequispaced data.** *SIAM J. Sci. Stat. Comput., 1993.*
Beylkin: **On the fast Fourier transform of functions with singularities.** *Appl. Comput. Harmon. Anal., 1995.*
Potts, Steidl, Tasche: **Fast Fourier transforms for nonequispaced data: A tutorial.** *Birkhäuser, 2001.*
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Similar approach

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Gelb, Song: **A frame theoretic approach to the nonuniform fast Fourier transform.** *SIAM J. Numer. Anal., 2014.*
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Own paper

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