A Superfast Direct Solver for Nonuniform Discrete Fourier Transform of Type 3

Jingyu Liu

School of Mathematical Sciences, Fudan University

June 2, 2025

NUDFT

Nonuniform discrete Fourier transform (NUDFT):

$$f_j = \sum_{k=0}^{N-1} \mathrm{e}^{2\pi \mathrm{i} x_j \omega_k} u_k, \quad 0 \le j \le M-1,$$

- $M \ge N$.
- Samples: $\{x_j\}_{j=0}^{M-1} \subset [0,1)$.
- Frequencies: $\{\omega_k\}_{k=0}^{N-1} \subset [-1/2, N-1/2)$.
- Coefficients: $\{u_k\}_{k=0}^{N-1} \subset \mathbb{C}$.
- Right hand side (RHS): $\{f_j\}_{j=0}^{M-1} \subset \mathbb{C}$.

NUFFT and INUDFT

Fast forward computation:

- Uniform case (FFT): $x_j = j/M$ and $\omega_k = k$.
  Complexity: $\mathscr{O}(M \log M)$ [Cooley and Tukey 1965]
- Nonuniform case (NUFFT)
  - Type 1: Equispaced samples, i.e., $x_j = j/M$;
  - Type 2: Integer frequencies, i.e., $\omega_k = k$;
  - Type 3: Nonequispaced samples and noninteger frequencies.

  Complexity: $\mathscr{O}(M + N \log N)$ [Dutt and Rokhlin 1993], [Greengard and Lee 2004], [Barnett, Magland, and Klinteberg 2019]

Problem (Inverse NUDFT Problem, INUDFT)

Given samples $\{x_j\}$ and frequencies $\{\omega_k\}$, determine the coefficients $\{u_k\}$ from the RHS $\{f_j\}$.

Displacement Structure of INUDFT-II Matrix

Method in [Wilber, Epperly, and Barnett 2024]:
Let $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{F}^{-1}$ where $\mathbf{F}$ is the standard $N \times N$ DFT matrix, then

$$\boldsymbol{\Gamma}\tilde{\mathbf{A}} - \tilde{\mathbf{A}}\mathbf{D} = \mathbf{a}\mathbf{b}^*,$$

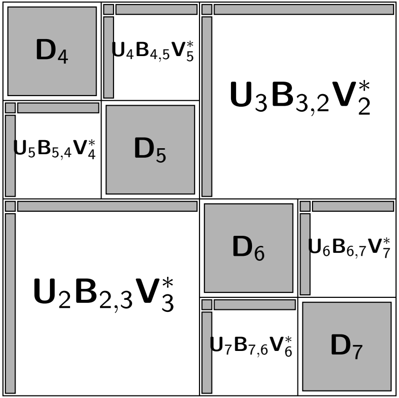
where

- $\boldsymbol{\Gamma} = \mathrm{diag}\big(\{\exp(2\pi \mathrm{i} x_j)\}_j\big)$;
- $\mathbf{D} = \mathrm{diag}\big(\{\exp(-2\pi \mathrm{i} k/N)\}_k\big)$;
- $a_j = \gamma_j^N - 1$;
- $b_k = \exp(-2\pi \mathrm{i} k/N)/N$.

The matrix $\tilde{\mathbf{A}}$ is called to have the displacement structure.

HSS Matrix Approximation

[Beckermann and Townsend 2017]: displacement structure $\Rightarrow$ low-rank.
The authors use a HSS matrix to approximate $\tilde{\mathbf{A}}$.



$$\mathbf{U}_2 = \begin{bmatrix} \mathbf{U}_4\mathbf{R}_4 \\ \mathbf{U}_5\mathbf{R}_5 \end{bmatrix}, \quad \mathbf{V}_2 = \begin{bmatrix} \mathbf{V}_4\mathbf{W}_4 \\ \mathbf{V}_5\mathbf{W}_5 \end{bmatrix},$$

$$\mathbf{U}_3 = \begin{bmatrix} \mathbf{U}_6\mathbf{R}_7 \\ \mathbf{U}_6\mathbf{R}_7 \end{bmatrix}, \quad \mathbf{V}_3 = \begin{bmatrix} \mathbf{V}_6\mathbf{W}_6 \\ \mathbf{V}_7\mathbf{W}_7 \end{bmatrix}.$$

[Wilber 2021]: fADI-based construction for HSS matrices.
[Xi et al. 2014]: URV factorization-based superfast least-squares solver for HSS matrices.

A Superfast Direct Solver of INUDFT-II

Algorithm 1: INUDFT–II

Input: Samples $\{x_j\}_{j=0}^{M-1}$ and RHS $\{f_j\}_{j=0}^{M-1}$.
Output: Coefficients $\{u_k\}_{k=0}^{N-1}$.
Approximate $\tilde{\mathbf{A}} = \mathbf{A}\mathbf{F}^{-1}$ by an HSS matrix $\tilde{\mathbf{A}}_{\mathrm{HSS}}$.
Solve $\mathbf{v} = \arg\min_{\mathbf{w}} \|\tilde{\mathbf{A}}_{\mathrm{HSS}}\mathbf{w} - \mathbf{f}\|_2$ by the URV factorization.
Compute $\mathbf{u} = \mathbf{F}\mathbf{v}$.

Fast structure in NUDFT-II:

$$\mathbf{A}_{\mathrm{fast}} = \tilde{\mathbf{A}}_{\mathrm{HSS}}\mathbf{F},$$
$$\mathbf{A}_{\mathrm{fast}}^{\dagger} = \mathbf{F}^{-1}\tilde{\mathbf{A}}_{\mathrm{HSS}}^{\dagger}.$$

Complexity:

- Construction and factorization: $\mathscr{O}(k^2M)$.
- Solution: $\mathscr{O}(kM + N\log N)$.

Motivation

Fact: $\{\mathrm{e}^{2\pi\mathrm{i}\ell x}\}_{\ell\in\mathbb{Z}}$ is an orthogonal basis of $L^2[0,1]$.
For NUDFT-III matrix:

$$\mathbf{A}(j,k) = \mathrm{e}^{2\pi\mathrm{i}x_j\omega_k} \approx \sum_{-R\le\ell\le N-1+R} \mathrm{e}^{2\pi\mathrm{i}x_j\ell} Q_{\ell,k},$$

where $Q_{\ell,k} = \mathrm{e}^{-\pi\mathrm{i}(\ell-\omega_k)} \sin\big(\pi(\ell-\omega_k)\big)/\big(\pi(\ell-\omega_k)\big)$.
Or, in matrix form,

$$\mathbf{A} = \mathbf{B}\mathbf{Q} + \mathbf{E},$$

Proposition

Suppose $\{x_j\}$ are IID uniform random variables in $[0,1)$ and $R\ge 2$, then $\mathbf{E}$ is a random matrix satisfying $\mathbb{E}\mathbf{E} = \mathbf{0}$ and

$$\mathbb{E}\|\mathbf{E}\|_{\mathrm{F}}^2 \le \|\mathbf{A}\|_{\mathrm{F}}^2 \frac{2}{\pi^2}\frac{1}{R-3/2}.$$

Practical Algorithm

Denoting $\mathbf{H} = \mathbf{B}^{\dagger}\mathbf{A}$, we have

$$\mathbf{H} = \mathbf{Q} + \mathbf{B}^{\dagger}\mathbf{E},$$
$$\mathbf{A} = \mathbf{B}\mathbf{H} + \left(\mathbf{I} - \mathbf{B}\mathbf{B}^{\dagger}\right)\mathbf{E}.$$

- $\mathbf{B}$ is a NUDFT-II matrix possessing a fast structure;
- $\mathbf{Q}$ is a kernel matrix, can be compressed into an HSS matrix;
- $\mathbf{H}$ can be empirically compressed into an HSS matrix;
- $\mathbf{I} - \mathbf{B}\mathbf{B}^{\dagger}$ is a projection matrix.

The Construction of $\mathbf{H}_{\mathrm{HSS}}$

Goal: Find an efficient way to construct $\mathbf{H} = \mathbf{B}_{\mathrm{fast}}^{\dagger}\mathbf{A}$.

- Fast forward computation on $\mathbf{A}$: NUFFT.
- Fast forward computation on $\mathbf{B}_{\mathrm{fast}}^{\dagger}$: URV factorization and FFT.

Black-box setting: Compress a matrix into its HSS form through matrix-vector multiplication.

Method in [Levitt and Martinsson 2024]: Random sampling.
Complexity: $\mathscr{O}(k^2 N + k T_{\mathrm{mult}})$.

Algorithm 2: INUDFT-III

Input: Samples $\{x_j\}_{j=0}^{M-1}$, frequencies $\{\omega_k\}_{k=0}^{N-1}$, RHS $\{f_j\}_{j=0}^{M-1}$.
Output: Coefficients $\{u_k\}_{k=0}^{N-1}$.
Construct a superfast direct solver $\mathbf{B}_{\mathrm{fast}}$.
Compress $\mathbf{H} = \mathbf{B}_{\mathrm{fast}}^{\dagger}\mathbf{A}$ into an HSS matrix $\mathbf{H}_{\mathrm{HSS}}$.
Compute the URV factorization of $\mathbf{H}_{\mathrm{HSS}}$.
Calculate $\mathbf{u} = \mathbf{H}_{\mathrm{HSS}}^{-1}\mathbf{B}_{\mathrm{fast}}^{\dagger}\mathbf{f}$.

Fast structure in NUDFT-III:

$$\mathbf{A}_{\mathrm{fast}} = \mathbf{B}_{\mathrm{fast}}\mathbf{H}_{\mathrm{HSS}},$$
$$\mathbf{A}_{\mathrm{fast}}^{\dagger} = \mathbf{H}_{\mathrm{HSS}}^{-1}\mathbf{B}_{\mathrm{fast}}^{\dagger}.$$

Complexity:

- Construction and factorization: $\mathscr{O}(k^2M + kN\log N)$.
- Solution: $\mathscr{O}(kM + N\log N)$.

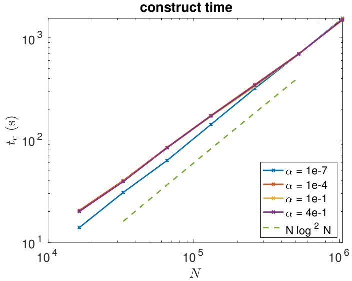
Experiment Setting

- $M = 4N$.
- Samples are IID uniform random variables in $[0, 1)$.
- Frequencies are perturbed integers given by

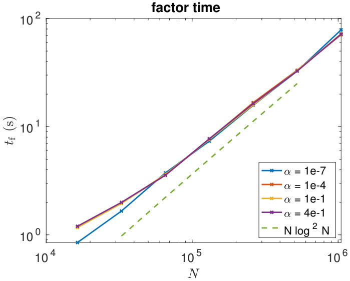
$$\omega_k = k + \alpha\psi_k, \quad 0 \leq k \leq N - 1,$$

where $\{\psi_k\}$ are IID uniform RVs on $[-1, 1]$ and $0 \leq \alpha < 1/2$ controls the non-uniformity.

INUDFT-III Construction

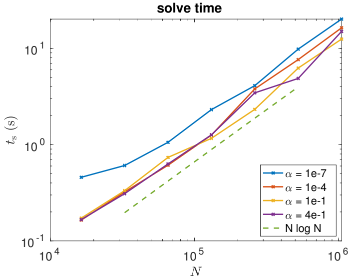


(a) Construction time.

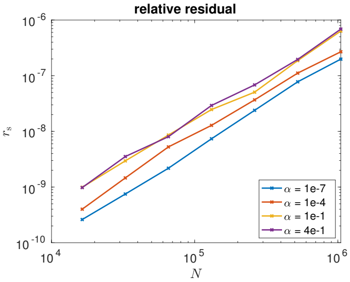


(b) Factorization time.

INUDFT-III Direct Solver



(a) Solution time.



(b) Relative residual.

Preconditioner of CG

N	method	$\alpha = 4\text{e-}1$			
		t_{pre}	t_{iter}	n_{iter}	r_{s}
131072	CG	-	x	x	x
	PCG	1.7e+02	2.4e+01	9	1.0e-14
262144	CG	-	x	x	x
	PCG	3.4e+02	4.6e+01	8	7.1e-15
524288	CG	-	x	x	x
	PCG	7.0e+02	1.0e+02	9	4.1e-14
1048576	CG	-	x	x	x
	PCG	1.5e+03	2.1e+02	8	7.7e-13

Table: Time cost, iteration number and relative residual of CG and PCG when $\alpha = 0.4$. The marker "x" means iterative method does not converge in 500 steps.

Conclusions and Future Work

Conclusions:

- A superfast direct solver for INUDFT-III;
- The direct solver could be used as an efficient preconditioner;
- Error bound of forward approximation when samples are uniform RVs.

Future work:

- Theoretical analysis on the NUDFT matrix;
- Extension to 2D and 3D problems;
- A method on regularized least-squares problem.

Thanks for listening!