Parallelization of the Direct, Interpolative Non-Uniform Fast Fourier (NFFT) Transform for Imputation of Missing Values for Periodic Signals

Next Generation FFT Algorithms in Theory and Practice: Parallel Implementations and Applications

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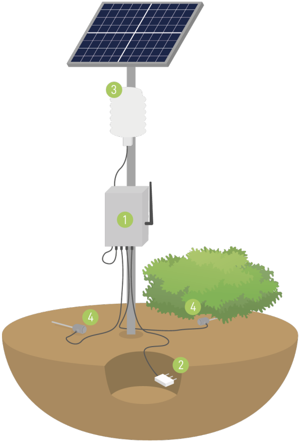

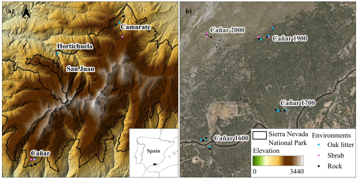

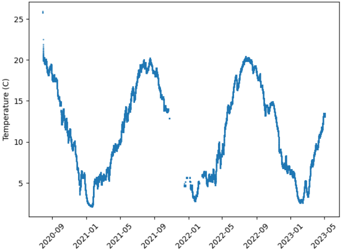

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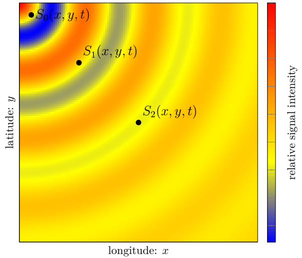
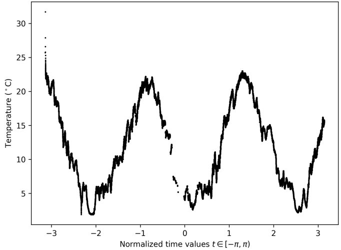


Linear model (coded effects)

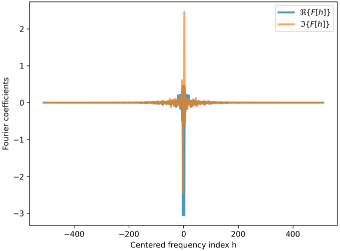
$$\mathbf{X} \in \mathbb{C}^{M \times N} \qquad \mathbf{C} \in \mathbb{R}^{M \times P}$$

$$\mathbf{X} = \mathbf{C}\Theta^H + \mathbf{E}$$

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix} \dots$$



$\longleftrightarrow$



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What is an inverse transform?

Type-I NFFTs

Let $f(x_j) \in \mathbb{R}^M$ be an irregularly sampled function on $(-\pi, \pi]$.
Let $\hat{h}_k \in \mathbb{C}^N$ be predicted Fourier coefficients in $(-N/2, N/2]$.
Define an irregular transformation matrix $\mathbf{A} \in \mathbb{C}^{N \times M}$:

$$\mathbf{A} = \left(e^{\pm \mathbf{i}\, k\, x_j}\right)_{k,j \in N,M} \quad \mathbf{A}^H\mathbf{A} \neq \alpha \mathbf{I}_M \quad \mathbf{A}\mathbf{A}^H \neq \beta \mathbf{I}_N$$

Standard	**Inverse**	**Equivalence**
Forward NFFT $\hat{\eta}_k = \mathbf{A} f(x_j)$	Inverse NFFT $\mathbf{A}^H \hat{h}_k = f(x_j)$	$\hat{\eta}_k = \hat{h}_k \Leftrightarrow \mathbf{A}^H \hat{\eta}_k = f(x_j)$
Adjoint NFFT $\hat{\phi}(x_j) = \mathbf{A}^H h_k$	Inverse adjoint NFFT $\mathbf{A}\hat{f}(x_j) = h_k$	$\hat{\phi}(x_j) = \hat{f}(x_j) \Leftrightarrow \mathbf{A}\hat{\phi}(x_j) = h_k$

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Prior work

$$\|\hat{h}_k\|^2_{\hat{\mathbf{W}}_k^{-1}} = \sum_{k\in I_N} \frac{|\hat{h}_k|^2}{\hat{w}_k} \rightarrow \min \quad \text{subject to } \mathbf{A}^H\hat{h}_k = f(x_j)^1$$
$$\mathbf{A} = \mathbf{DFB}, \quad M\mathbf{I}_N \approx \mathbf{AB}^H\mathbf{F}^H\mathbf{D}^{*2}$$

[1] Stefan Kunis and Daniel Potts. "Stability results for scattered data interpolation by trigonometric polynomials". In: *SIAM Journal on Scientific Computing* 29.4 (2007), pp. 1403–1419.

[2] Melanie Kircheis and Daniel Potts. "Direct inversion of the nonequispaced fast Fourier transform". In: *Linear Algebra and its Applications* 575 (2019), pp. 106–140.

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Weighted transforms

$$\arg\min_{\hat{h}_k} \left(\|\hat{h}_k\|^2_{\hat{\mathbf{W}}_k^{-1}} + \|\hat{h}_k - \mathbf{F}f_j\|_2^2\right)$$

Equi-spaced transformation matrix

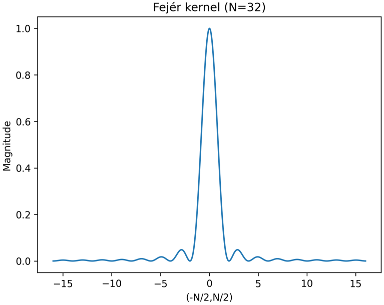
$$\mathbf{F} = \left(e^{\pm \mathbf{i}kj}\right)_{j,k\in N,M}$$
$$f_j \in (-\pi, \pi]$$
$$\hat{h}_k \in \left(-\frac{N}{2}, \frac{N-1}{2}\right)$$

Solve for $\hat{h}_k$

$$\hat{h}_k = \mathbf{F}f_j(M(\tfrac{1}{M}\hat{\mathbf{W}}_k^{-1} + \mathbf{I}))^{-1} **$$
$$\hat{h}_k = \mathbf{F}f_j\hat{\mathbf{W}}_k(M\hat{\mathbf{W}}_k + \mathbf{I}_N)^{-1}$$

Searle Identity**

$$(\mathbf{I} + \mathbf{X}^{-1})^{-1} = \mathbf{X}(\mathbf{X} + \mathbf{I})^{-1}$$



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Optimization Problem

$$\|\hat{h}_k\|^2_{\hat{\mathbf{W}}_k^{-1}} = \sum_{k \in I_N} \frac{|\hat{h}_k|^2}{\hat{w}_k} \rightarrow \min \quad \text{subject to } \mathbf{A}^H \hat{h}_k = f(x_j).$$

$$\hat{h}_k = \arg\min_{\hat{h}_k} \left(\|\hat{h}_k\|^2_{\mathbf{W}_k^{-1}} + \|\mathbf{A}^H \hat{h}_k - f(x_j)\|_2^2 \right)$$

$$\hat{h}_k = \mathbf{A} f(x_j)(\mathbf{W}_k^{-1} + \mathbf{A}\mathbf{A}^H)^{-1}$$

Woodbury Identity ($\mathbf{A}\mathbf{A}^H = \mathbf{L}\mathbf{U}$) $\mathcal{O}(N^2)$[3]

$$\left(\mathbf{W}_k^{-1} + \mathbf{L}\mathbf{U}\right)^{-1} = \mathbf{W}_k - \mathbf{W}_k \mathbf{L} \left(\mathbf{I} + \mathbf{U}\mathbf{W}_k \mathbf{L}\right)^{-1} \mathbf{U}\mathbf{W}_k$$

$$\hat{h}_k = \mathbf{A} f(x_j) \left(\mathbf{W}_k - \mathbf{W}_k \mathbf{L} \left(\mathbf{I} + \mathbf{U}\mathbf{W}_k \mathbf{L}\right)^{-1} \mathbf{U}\mathbf{W}_k \right) \quad \mathcal{O}(N^3)$$

[3] Adam W Bojanczyk et al. "On the stability of the Bareiss and related Toeplitz factorization algorithms". In: *SIAM journal on Matrix Analysis and Applications* 16.1 (1995), pp. 40–57.

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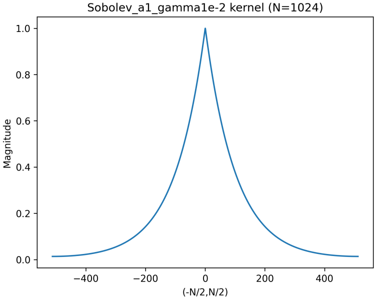
Some Results

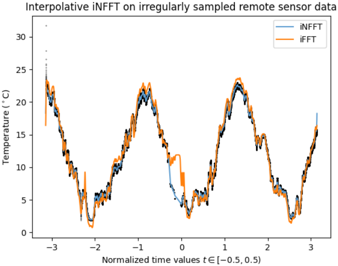
Frequency weights

$$w_k = \frac{\left(\frac{1}{4} - (k/N)^2\right)^{\beta}}{1 + \gamma\,(2\pi|k|)^{2\alpha}}$$



Reconstruction quality

$$\hat{f}_j \approx \mathbf{A}^H \hat{h}_k$$



Method	MAPE
iNFFT	0.0189
iFFT	0.0700

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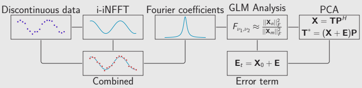
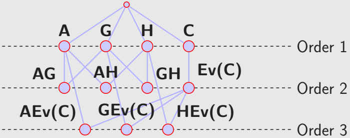
Workflow

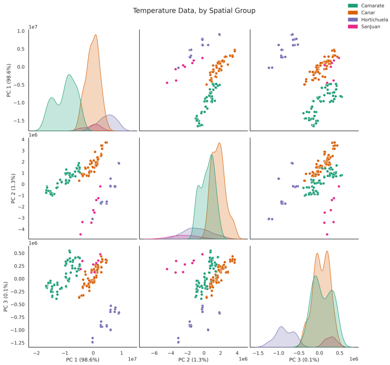


Experimental Design

$$\mathbf{X} = \mathbf{A}+\mathbf{G}+\mathbf{H}+\mathbf{C}+\mathbf{Ev(C)}+\mathbf{E}$$



SCA



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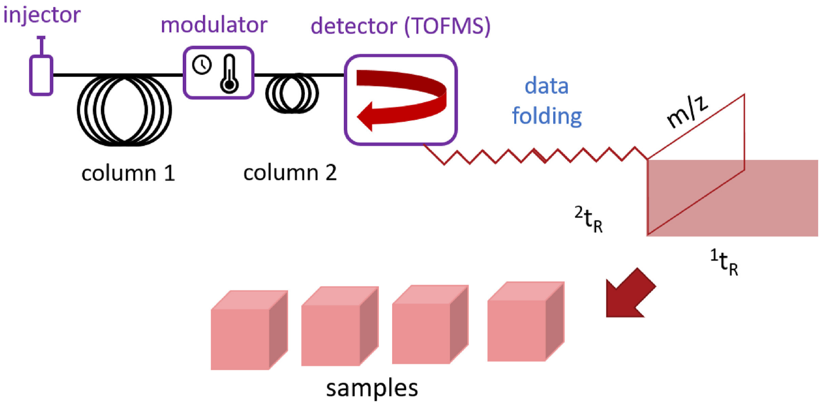
An example of multi-modal time series data



Michael D Sorochan Armstrong et al. "PARAFAC2× N: Coupled decomposition of multi-modal data with drift in N modes". In: *Analytica Chimica Acta* 1249 (2023), p. 340909

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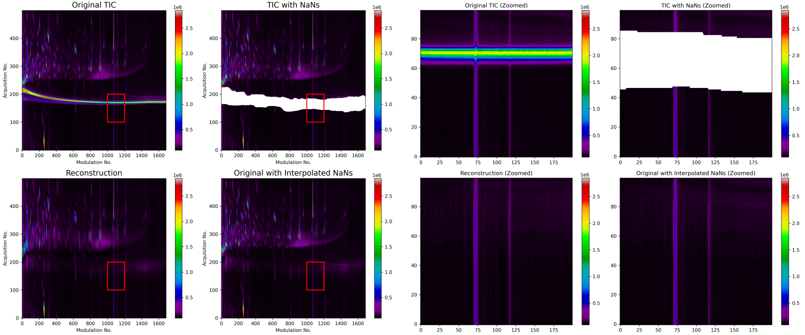
2D Transforms

$N = 32$ $\quad$ $w_k = g_{\alpha=0.5,\beta=3,\gamma=0.1}$



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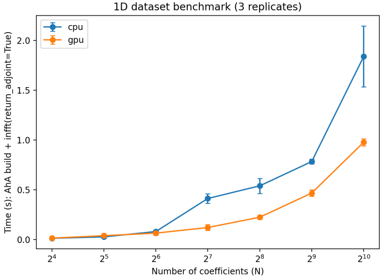
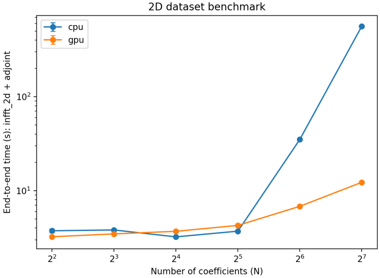
GPU Parallelization

NFFT → FINUFFT/CUFINUFFT



Algebra → NumPy / PyTorch



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PyTorch

https://github.com/mdarmstr/iinfft

Yu-hsuan Shih et al. “cuFINUFFT: a load-balanced GPU library for general-purpose nonuniform FFTs”. In: *2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE. 2021, pp. 688–697

Michael Sorochan Armstrong and José Camacho. “An Alignment-Agnostic Methodology for the Analysis of Designed Separations Data”. In: *Journal of Chemometrics* 39.2 (2025), pp. 1–12

Michael Sorochan Armstrong. “Frequency-Domain Alignment of Heterogeneous, Multidimensional Separations Data Through Complex Orthogonal Procrustes Analysis”. In: *Journal of Chemometrics* 39.7 (2025), e70042

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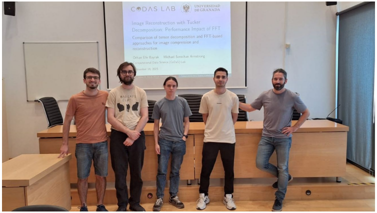
Further acknowledgements



SMART ECOMOUNTAINS

mustard
multi-scale spatio-temporal analysis of research data

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