Fast sparse Fourier transformations for NMR spectroscopy

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Terms

- NMR- Nuclear Magnetic Resonance
- Sparse- Thinly dispersed or scattered
- IST- Iterative Soft thresholding
- FFT- Fast Fourier transformations
- IFT- Inverse Fourier transformations
Background

- NMR data is used by scientists to understand molecular structure of proteins. It is an essential step for synthesizing new protein molecules.
- For this purpose NMR spectral data is gathered from spectral equipment.
- However, taking uniform frequency data and doing calculations on it can be quite a challenge. As it would take long hours to calculate this data.
- By sparsely and randomly taking data points at certain thresholds, the calculation time can be decreased by several hours. [2]
- Goal is to reconstruct actual wavelets from sparse samples.
Background

First off for the process we sparsely sample NMR data at certain data points. After that we apply FFT to the Fourier transformed version of the wave.[2][1]
After that we apply IST (it thresholds to sections of the Fourier transformed wave) and IFT on it iteratively to build the wave [2]

At the end of our iterations we are left with the sample of the original wave. Which is used for experiments.

Using this technique the data processing time can be reduced by several hours. Which is our main goal combined with application of other faster processing techniques (if time permits).
Aims

- This project will give us an opportunity to understand Fast Fourier Transform (FFT) algorithms and their application to sparse data.

- Developed an understanding of the importance of FFT algorithms in NMR spectroscopy.

- Have implemented code to process sparsely sampled high-dimensional NMR data.

- Have profiled the code and optimized performance of execution. Maybe parallelize code if time permits.
Approach

- Sparse Sampling quality[3]
  - Under sampling can lead to loss of information in waves.

- Time
  - It can take quite a while to process this data even after applying the methods discussed.
  - Process time is platform and application build quality dependent.

- Development cycle planned on is spiral development. With milestones.

- Software used
  - Fftw
Outlook

- The project will help us understand structure of proteins as we have already discussed.
- This understanding can help us construct and synthesis proteins for medical, industrial and other purposes.
- Sparse FFT is widely used in voice processing to network signal processing, where waves are sparsely sampled at intervals. The project will focus on applying this in molecular physics.
References


2. Application of iterative soft thresholding for fast reconstruction of NMR data non-uniformly sampled with multidimensional Poisson Gap scheduling, Sven G. Hyberts, Alexander G. Milbradt, Andreas B. Wagner, Haribabu Arthanari, Gerhard Wagner