Multi-Dimensional NMR Data Processing: From Time Domain to Frequency Domain using Wavelets and Matrix Decompositions

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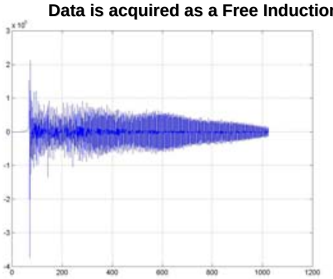
ABSTRACT:

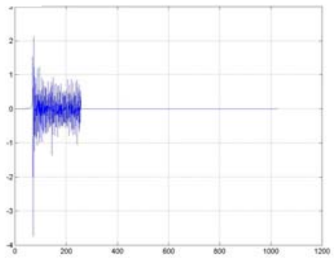
Our project focused on the problems that arise when Nuclear Magnetic Resonance (NMR) spectrums are truncated. This is a problem that crops up a lot in NMR spectrums because 2-d and 3-d spectrums are usually truncated due to major time constraints. We worked on various methods to remedy this situation, namely using Wavelet Transforms, using different methods for Peak Picking and also using Non-Negative Matrix Decomposition to decompose peaks into a more useable form.

Data is acquired as a Free Induction Decay (FID):



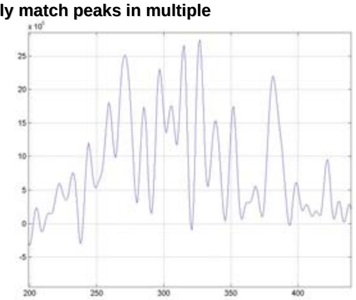
To the left is a very ideal FID in that the signal is very long and is truncated once the signal has decayed to mostly noise.

Most FIDs look more like the one to the right, where the signal is cut off very early, mostly due to time and cost constraints.



Nuclear Magnetic Resonance data is acquired as a rapidly decaying signal in the time domain. This data is very hard to interpret in the time domain because all the peaks are delocalized and overlapped, making them very hard to interpret. This makes it very useful to change to the frequency domain because it forces the peaks to become very localized and distinct and hence easier to interpret. The most common way to make this change is to apply the Fast Fourier Transform, which is very robust but also has its limitations. As part of my project I investigated the uses of the Wavelet Transform as an alternative to the Fourier Transform. The other part of my project dealt with finding an unbiased method of taking a projection of a Multi-Dimensional NMR Spectrum and representing it as a product of vectors thereby allowing one to easily match peaks in multiple projections.

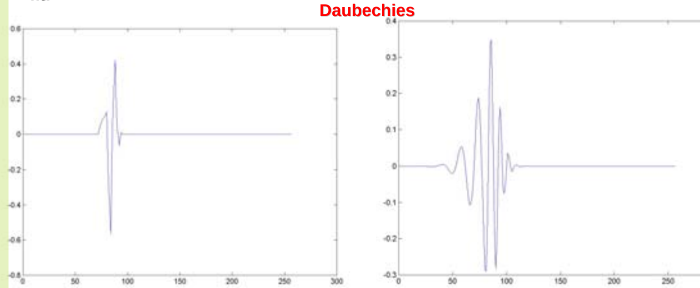
To the right is a truncated NMR Spectrum showing very broad peaks and far fewer peaks than there should be.



Wavelet Transform:

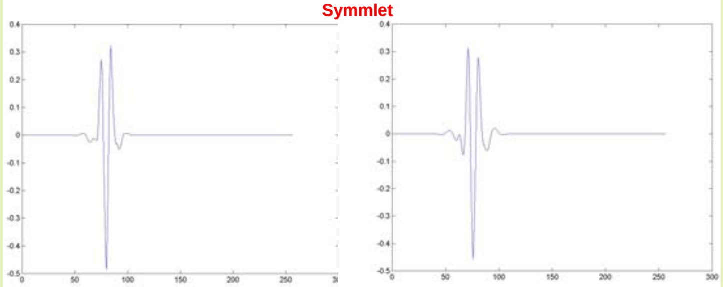
One idea that seemed very appealing to us was the idea of using the Wavelet Transform instead of using the Fourier Transform. The Fast Fourier Transform is the commonly used method to take time domain data and fit it into frequency domain data. The Wavelet Transform appealed to us because it was a very narrow and localized, which was very much like the data that we were trying to fit.

Daubechies



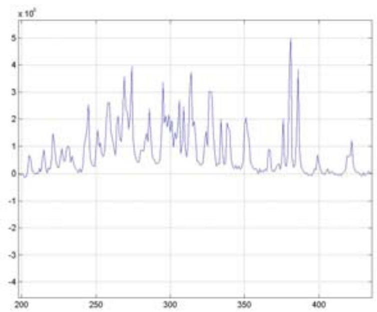
The Daubechies wavelets above have the most vanishing moments for any given support.

Symmlet



The Symmlet Wavelets above are very symmetrical and have a compact suppport.

Below is a typical 1-d NMR spectrum, which we were trying to model using the Wavelets above. The goal is to model the data using wavelets in order to better represent the narrow peaks as well as remove noise and significantly compress the data. When applied to Multi-dimensional NMR this technique would allow for faster peak matching.

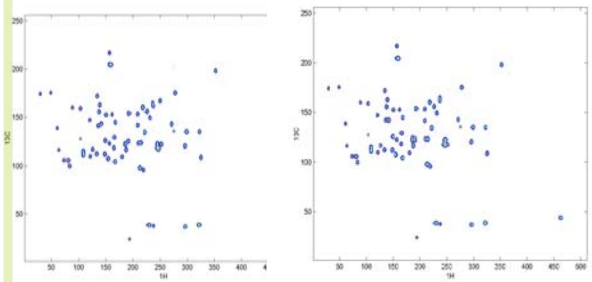


Wavelet Images were produced using WaveLab © Stanford

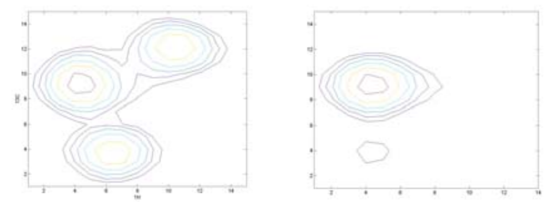
Matrix Decompositions:

The final part of my project dealt with decomposing a data matrix representing a 2-d NMR spectrum into the more useable form of a finite sum of a product of two vectors. There are many ways of achieving this using various matrix decompositions. Below are the contour plots of various 2-d NMR decompositions.

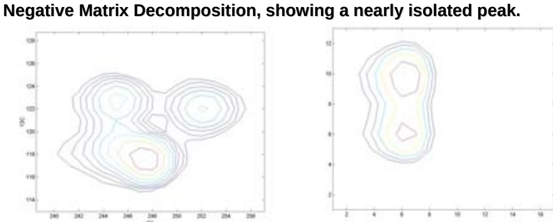
$$S(\omega_1,\omega_2,\omega_3)=\sum_i C_i S_1(\omega_1)S_2(\omega_2)S_3(\omega_3)$$



Above to the left we have the original 2-d NMR Spectrum and above to the right we have the same spectrum with each peak represented as the product of two vectors, using SVD to find the vectors. The spectrums are very similar but multiple peak overlaps are not handled well.



Above to the left we have a close-up of a 3-peak region with some overlap and to the right is the decomposition of one peak using Non-Negative Matrix Decomposition, showing a nearly isolated peak.



Above to the left we have another close-up of a 3-peak region with more overlap and to the right we have the decomposition of one peak using Non-Negative Matrix Decomposition showing major problems handling these peaks.

Conclusions: We found that using Wavelets and Non-Negative Matrix Decomposition with SVD are both very useful tools and that their applications are ubiquitous in Nuclear Magnetic Resonance.

Acknowledgements:

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