Fast acquisition of multidimensional NMR experiments by maximum entropy reconstruction of non-uniformly sampled data

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(Introduced by John Gehman)

The discrete Fourier transform (DFT) played a seminal role in the development of modern nuclear magnetic resonance (NMR) spectroscopy. Nevertheless it has a number of well-known limitations. Chief among them is the difficulty of obtaining high-resolution spectral estimates from short time records, because the ability to resolve signals with closely-spaced frequencies is largely determined by the longest evolution time sampled.

The ability to obtain accurate, high-resolution spectral estimates from short data records is critical in many applications of NMR spectroscopy because the available sampling time is limited, for example due to sample instability or simply due to constraints on available instrument time. In practice the latter is mainly encountered in multidimensional NMR experiments where the data collection time is directly proportional to the number of data samples collected in the indirect time dimensions (indirect time dimensions correspond to time delays between RF pulses; real time is referred to as the acquisition dimension). Furthermore, at very high magnetic field, the competition between the goals of short data collection time and high resolution becomes more severe as the bandwidth spanned by the nuclear resonances increases linearly with field strength, necessitating a decrease in the time between samples in order to avoid aliasing.

Non-Fourier methods of spectrum analysis provide an avenue to high-resolution spectral estimates from short data records. Over the past three decades a host of non-Fourier methods of spectrum analysis have been developed, including maximum entropy, maximum likelihood and Bayesian methods, the filter diagonalization method, G-matrix Fourier transform, back projection reconstruction, and multidimensional decomposition. These methods span a continuum of assumptions about the nature of the signal, and restrictions (or lack thereof) on the characteristics of the data sampling. MaxEnt reconstruction lies at the extreme of making few assumptions about the signal, and furthermore can be applied to data collected in essentially arbitrary fashion (non-uniform sampling, NUS).

Extensive use of synthetic and experimental, non-uniformly sampled data in 2-4 dimensions, processed using MaxEnt has enabled us to both theoretically and practically evaluate the pros and cons of this method. The results suggest the method to be resilient to false positives and robust in situations of poor signal to noise, with the consequence of producing non-linear reconstructions.