Matrix Pencil Method for High Resolution Data Processing in Low-Field NMR

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Introduction: Recent advances have made portable nuclear magnetic resonance (NMR) spectroscopy economically and practically feasible. The ease with which it can be customized makes portable NMR an extremely desirable analytical technique. However, portable NMR obtains a weaker signal with decreased resolution compared to traditional NMR. As such, one typically measures exponential decay constants at low field rather than frequencies.[1] Here, the matrix pencil method (MPM)[2,3] is explored for stable, reproducible data processing in low field NMR. Currently, the inverse Laplace transform (ILT) is the conventional method for processing data in low field NMR. However, the ILT is hindered by sensitivity to noise, poor resolution, and high computational requirements that make it difficult to apply in non-laboratory environments. Improving the efficiency of data processing could expand the applications of portable NMR and enhance the quality of information gained from correlation experiments. The MPM fits in a broad category of filter diagonalization methods for digital signal analysis, and was developed for use in radar, antenna, and acoustics technologies. The success of the MPM in other areas of signal processing makes its application to low field NMR promising.

Methods: The MPM is developed as an alternative to the ILT for data processing, due to its low noise sensitivity, high resolution, and minimal computational requirements. This advantage is gained primarily by exploiting the eigenstructure of a matrix pencil, which can be formulated directly from discretely sampled data, thereby avoiding integral transforms. Applications to both real and simulated data are shown, and the respective errors of the MPM and ILT are evaluated with Monte Carlo simulations as well as with a combinatorics-based bootstrap resampling approach.

Results and Discussion: In the cases presented here, the MPM performs better than the ILT from the standpoints of speed, resolution, and accuracy. Moreover, in the limit of zero noise, the MPM provides an analytically exact, closed-form solution to the problem of multi-exponential decomposition.

Conclusion: The key for widespread future implementation and automation of the MPM is to combine it with effective noise filters, such as singular value decomposition, multi-point moving averaging, integration smoothing methods, wavelet transforms, and sliding Fourier transform apodization. This will ultimately enable measurements of systems that have previously been inaccessible with portable NMR.

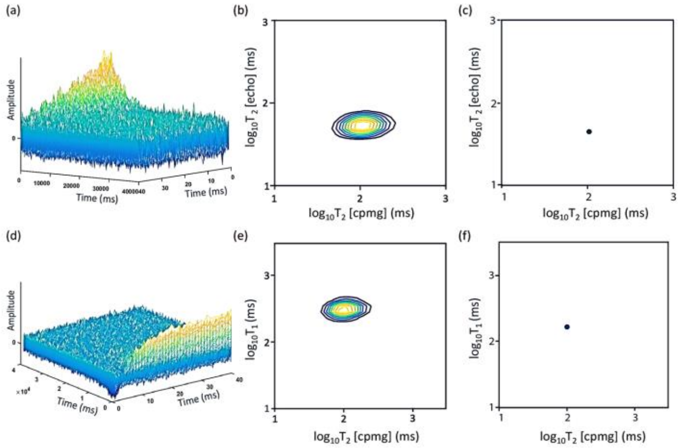

Fig. 1: Polydimethylsiloxane at 100 MPa. The raw data surface in a) is from a T_2/T_2 correlation experiment, with the corresponding spectrum processed by b) ILT and c) MPM. The raw data surface in d) is from a T_1/T_2 correlation experiment, with the corresponding spectrum processed by e) ILT and f) MPM.

References: [1] Blumich, B., Perlo, J., & Casanova, F., *Prog. Nucl. Mag. Res. Sp.*, *52*(4), 197–269. (2008). [2] Hua, Y., & Sarkar, T. K., *IEEE Trans. Sig. Proc.*, *38*(5), 814–824. (1990). [3] Lin, Y. Y., Hodgkinson, P., Ernst, M., & Pines, A., *J. Mag. Res.*, *128*(1), 30–41. (1997).