A robust and prior knowledge independent method to interpret non-negative least squares (NNLS) T2 relaxation results

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A robust and prior knowledge independent method to interpret non-negative least squares (NNLS) T_2 relaxation results

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The fitting of an NMR signal decay in a weighted sum of exponentials is an ill-posed problem, i.e. different sets of relaxation times and amplitudes will lead to the same least-squares distance between the model and the experimental noisy data. To analyze such data, the classical pipe consists in performing a non-negative least squares (NNLS) algorithm combined with a regularization to smooth the T_2 distribution. However, a critical step of this approach deals with the choice of the operator and then of the corresponding regularization parameter which significantly affects the T_2 distribution. These parameters are usually chosen based on the operator experience as well as prior knowledge on the sample.

In this work, we propose to analyze NNLS results without regularization to circumvent these drawbacks. Our approach is based on the analysis of NNLS outputs by cumulative distribution functions (cdf) and not by probability density functions (pdf) as it is usually done. This concept is validated in different simulations for which the true T_2 distributions are built from discrete to continuous functions. Simulation results showed that the T_2 amplitude measured at a plateau of the cdf is unbiased and (almost) independent of both the decomposition basis and the signal-to-noise ratio. This observation allows to quantitatively interpret the NNLS inversions, especially when the true distribution is continuous. We suggest that NNLS by itself suffices in many situations, provided that cdf plateau can be discernable. The degrees of freedom to adjust in the method are then limited to the decomposition basis. To exemplify, this pragmatic and fruitful approach is applied on real NMR data obtained by spectroscopy and imaging.