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Benchmark and lowfield

EUROMAR2018/271

A new approach to interpret non-negative least squares (NNLS) relaxation results

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If selected, I agree to present my work during an oral communication: Yes

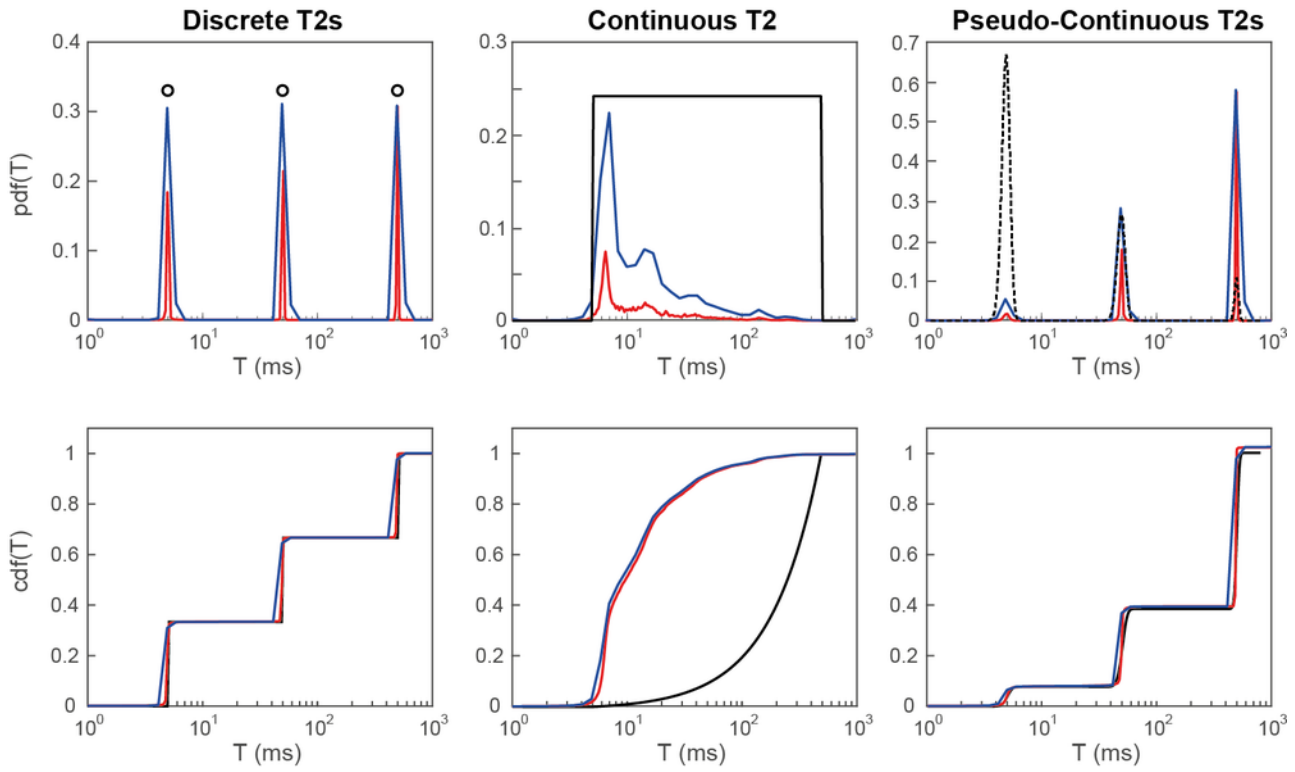
Abstract: The fitting of an NMR signal decay in a weighted sum of exponentials is an ill-posed problem, i.e. different sets of relaxation times and amplitudes will lead to the same least-squares distance between the model and the experimental noisy data. To reduce the number of solutions, an efficient strategy consists in adding a constraint of positivity on the amplitudes. Non-negative least squares (NNLS) algorithm is nowadays the most popular algorithm incorporating this constraint. By this manner, the algorithm returns a unique solution of positive amplitudes, the relaxation time values being *a priori* defined by the so-called decomposition basis. To obtain a smooth amplitude distribution, a Tikhonov regularization is most often performed. A critical step with this approach deals with the choice of the operator (i.e. norm-, slope- or curvature-smoothing) and then of the corresponding regularization parameter.¹ Because these parameters strongly affect the obtained distributions, the operator selection is based on both prior knowledge and T_2 distribution hypothesis followed by an optimization procedure.

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 (see Figure). This observation allows to quantitatively interpret the NNLS inversions, especially when the true distribution is continuous. Indeed, while the pdf are largely biased and parameter-dependent for a continuous T_2 distribution, the cdf reach a plateau for the expected amplitude. In short, 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 also applied on real NMR data obtained by spectroscopy and imaging.

Zou Y.-L. et al., Pet. Sci. (2016),13:237-246

Figure: Averaged results for 1 000 simulated T_2 NMR signal decays (SNR = 1000) analyzed with the NNLS algorithm and a decomposition basis containing either 40 (blue) or 200 (red) T_2 values logarithmically spaced between 1 and 1000 ms. The black (full or dashed) lines represent the theoretical values. Representation with the pdf (top) and the cdf (bottom) for a discrete (left), continuous (middle) or mixed (right) models.

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Disclosure of Interest: None Declared