Machine learning-based multi-pool Voigt fitting of Z-spectra

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INTRODUCTION:

CEST experiments involve acquiring multiple images at different saturation frequencies. As a result, a Z-spectrum is generated containing signals from molecules with protons that are coupled to water through chemical exchange or cross-relaxation.[1] The Z-spectrum contains a wealth of information, but signal components typically overlap, and separating the different components and quantifying their relative concentrations can be challenging. It is possible to separate some of the main contributions by fitting,[2-4] and traditional fitting approaches rely on least squares (LS) in combination with Lorentzian modelling of the peaks. More recently, deep learning (DL) has been successfully employed for Lorentzian fitting[5-7]. However, many Z-spectral components are broadened due to exchange and/or saturation bandwidth which renders Lorentzian modelling invalid. Recently, LS-based Voigt fitting has been proposed to improve fitting quality.[8] The present study aimed to relieve fitting time restrictions by using low complexity ML-algorithms and to compare Voigt to Lorentzian modelling.

METHODS:

Five pool Voigt (FPV) and Five pool Lorentzian (FPL) models (17 and 12 parameters, respectively, including two rNOE, DS, guanidinium proton and amide proton signals) were fitted to human 3T Z-spectral data using LS to generate training data for the corresponding ML-versions. Gradient Boosting Decision Trees (GBDT) were trained, resulting in one Voigt and one Lorentzian ML-model. Modeling accuracy was tested, and the fitting times of the ML- and corresponding LS-models were recorded. The goodness-of-fit of Voigt and Lorentzian ML-models were compared.

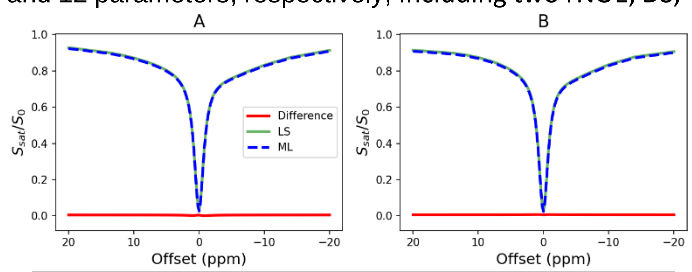

Figure 1. The modelling accuracy visualized by the fits of an in vivo sample with LS (blue) and ML (green) as well as the difference (red) for (A) FPL and (B) FPV.

RESULTS:

The modelling accuracy was excellent for both Voigt and Lorentzian ML-models as indicated by the non-significant difference between the parameters obtained by the LS-versions and the corresponding ML-versions (qualitative example in Figure 1). The average fitting time was <10 seconds/brain for ML compared to 4.6 and 15 hours/brain for LS with FPL and FPV, respectively. The goodness-of-fits of FPV-ML and FPL-ML differed significantly ($p < 0.005$), with FPV-ML showing an improvement on all tested data; an example is shown in Figure 2.

DISCUSSION:

The proposed approach provides an advantage over traditional LS in terms of fitting time. In addition, using GBDT for the fitting task reduces (time) complexity and adds interpretability compared to previous DL-based approaches[5-7]. Voigt fitting is thus valuable for broad Z-spectral components and will be even more useful for applications where higher B1 strengths are needed. However, as for all supervised ML-based methods, the proposed approach is limited by the quality of the training data. Hence, to ensure model convergence and good generalizability, high data quality must be guaranteed.

CONCLUSION:

GBDT-fitting of multi-pool Z-spectra significantly reduces fitting times compared with traditional LS-approaches, allowing fast processing of data while upholding fitting quality. This makes the method desirable in clinical settings and for large cohort research applications. The FPV-ML approach provides a statistically significant improvement of goodness-of-fit compared to FPL-ML, even for intermediate saturation powers.

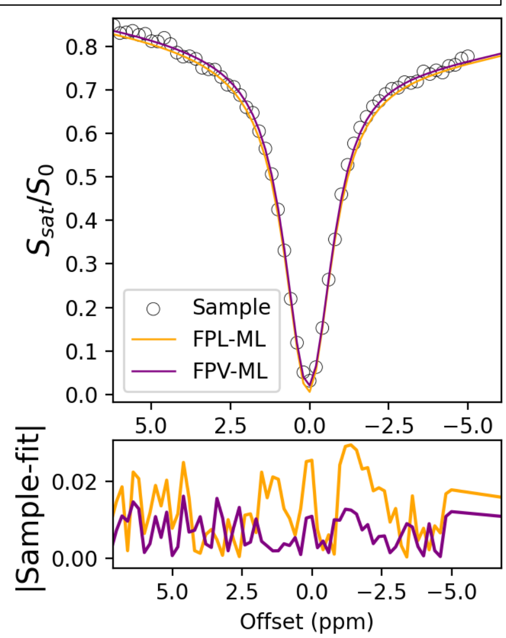

Figure 2. Top: In vivo sample (circles) fitted by the Lorentzian (orange) and Voigt (purple) ML-models. Bottom: Fitting error by FPL (orange) and FPV (purple) showing a tendency of smaller error for FPV.

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