Title: Baseline Modeling for Magnetic Resonance Spectroscopy (MRS) Using a Modified Temporal Convolution Network (mTCN)

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Introduction: Proton magnetic resonance spectroscopy (MRS) is a non-invasive technique for measuring metabolites in-vivo and can be used to measure the underlying chemical composition of a region of interest. Specifically, short echo time MRS in the brain, can be used to detect neurometabolites, such as myoinositol (mIns), suggested to reflect inflammatory processes due to gliosis, and choline (Cho), reflecting cell membrane turnover. However, quantification of these metabolites necessitates accurate modeling of the baseline and metabolites, as baseline distortions, potentially due to residual water, residual macromolecules, and lipids, can lead to incorrect estimation of metabolite peaks[1]. Accurate baseline modeling is essential for removing contaminating signals from the spectrum, such that spectral quantification reveals true metabolite values. To this end, we developed a modified temporal convolution network to predict the underlying baseline from ^{1}H MRS spectra.

Methods: Data Generation: Simulated free induction decay (FID) using synMARSS[2] was used to generate 10000 FIDs, with their respective baseline functions. FIDs were simulated with pulse shapes from 17 metabolites and 10 macromolecules using the point resolved spectroscopy (PRESS) protocol with an echo time (TE) of 30 ms, a sampling frequency of 4000 Hz, with 2048 points, and a Larmor frequency of 127.7324 MHz to mimic in vivo single voxel spectra (SVS) acquired from a General Electric (GE) Signa MR scanner. Metabolite concentrations ranged between 0 to twice the reference concentration. Macromolecules were modeled as overlapping Gaussians. Each spectrum contained macromolecules, uncorrelated Gaussian noise, and a cubic B-spline baseline, where the position of the knots followed a uniform distribution. The cubic B-spline was generated in the frequency domain, and then an inverse Fourier transform was applied and then added to the metabolite FID. All data were min-max normalized before input into the model. The dataset was then partitioned into an 80/10/10 train-validation test split. The study pipeline can be seen in Figure 1. **Model Architecture:** We developed a fully automated baseline modeling algorithm using a modified temporal convolutional network (mTCN) for optimal fitting of spectral data. The full mTCN architecture can be seen in Figure 2. The model was trained using the Adam optimizer **Statistical Analysis:** To test whether the model could accurately produce a baseline spectrum from the metabolite spectrum, the root mean square error (RMSE), the coefficient of determination (R^2), and the peak signal-to-noise ratio (PSNR) were calculated. All statistics were performed using Python 3.10.12.

Results and Discussion: The mTCN model demonstrated effective baseline modeling in proton MRS data, showing the potential to enhance the reliability of MRS in metabolite quantification (RMSE: 0.001±0.001, PSNR: 33.649±2.119, R^2:0.993±0.002). Figure 3 shows representative spectra, their ground truth baselines, and the predicted baseline. Future directions include, testing on in vivo spectral data and performing quantifications to observe potential improvements.

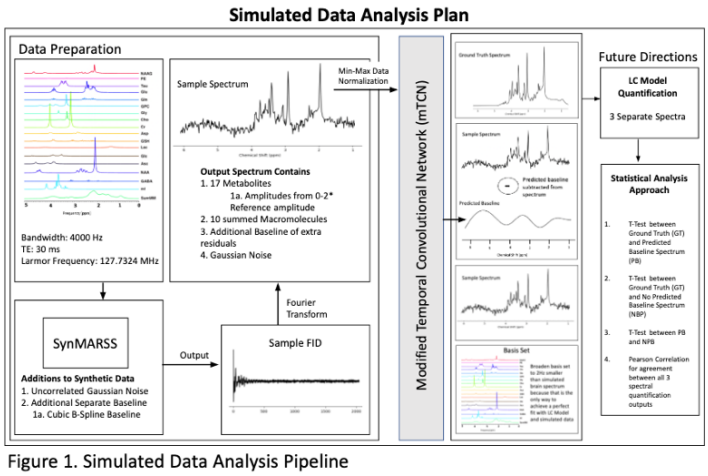

Figure 1. Simulated Data Analysis Pipeline

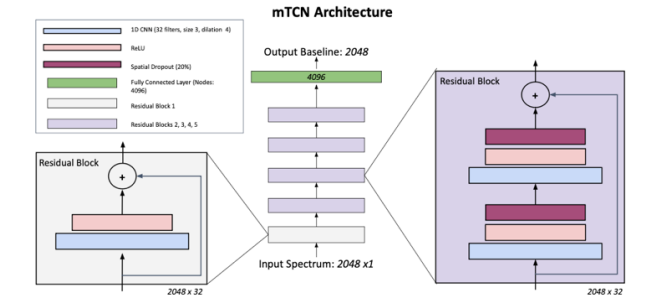

Figure 2. The Modified Temporal Convolutional Network

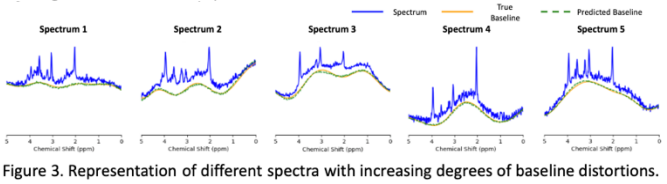

Figure 3. Representation of different spectra with increasing degrees of baseline distortions.

References

1. Wilson M. Adaptive baseline fitting for MR spectroscopy analysis. Magnetic Resonance in Med 2021;85:13–29.
2. Landheer K, Treacy M, Instrella R, et al. synMARSS-An End-To-End Platform for the Parametric Generation of Synthetic In Vivo Magnetic Resonance Spectra. *NMR Biomed*. 2025;38(3):e7001