³¹P Magnetic Resonance Spectroscopy analyzed and quantified by Convolutional Neural Network (CNN)

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Synopsis

Phosphorus magnetic resonance spectroscopy imaging (³¹P-MRSI) allows the probing of biological compounds that hold fundamental cellular information. High resolution MRSI at 3T suffers from low signal-to-noise ratio (SNR) inherent to the nuclear low sensitivity. This is accentuated in the MRSI in comparison to unlocalized free induction decay (FID) where acquired volumes are smaller and consequently lower the SNR. Our Convolutional Neural Network (CNN) based algorithm perform efficient quantification of metabolite and is compared to last-square fitting algorithm. Our model was trained with a simulated dataset and tested with both simulated spectra and real spectra from 3D ³¹P-MRSI acquired in kidneys.

Introduction

Among nuclei measurable by NMR, phosphorus (³¹P) is the most noteworthy behind the proton nucleus (¹H) for its in-vivo application [1]. Phosphorus magnetic resonance spectroscopy (MRS) is a unique tool for monitoring cellular metabolism [2, 3]. Current state-of-the-art methods for identi- cation relies on non-linear tting algorithms such as AMARES [4], LCModel [5], QUEST or SVD techniques [6]. Machine learning has proven to be e cient numerical analysis for spectra analysis, with its ability to identify patterns features in data [7]. Recently, deep-learning techniques of CNN are used to perform ¹H-MRS analysis and have shown at least comparable results as the current tting model [8, 9, 10]. This work presents an optimized method based on CNN algorithm combined with realistic data simulation to train an algorithm capable of accurate metabolite concentration estimation from ³¹P-MRS data and ex-vivo 3D ³¹P-MRSI of kidneys.

Methods

Metabolites of interest were selected: phosphocreatine (PCr), inorganic phosphate (Pi), adenosine triphosphate (α -ATP, β -ATP and γ -ATP), phosphomonoester (PME) including adenosine monophosphate (AMP), nicotinamide adenine dinucleotide (NAD+ and NADH) and phosphodiester (PDE). Simulated spectra contain 2048 points for a bandwidth of 4000 Hz, covering 80 ppm centered on the PCr frequency.

First, spectra were quantified with a fitting method that is based on prior knowledge for spectral signature, peaks chemical shift and coupling constant. Once identified, the peaks are estimated with Gaussian shape curves, as illustrated in Figure 1.

As second analysis, quantification was performed with the CNN. Supervised learning approach was achieved with a simulated and labeled training data-set. Following exact density matrix computation for each metabolite resonance, 10⁶ spectra were generated with 33 independent variables, as shown on the Figure 2. The spectral parameters: concentration, zero and first order phase, frequency shift, peak width, white noise and added baseline were randomly determined for each specimen with normal distribution centered at the expected physiological values. From the 10⁶ spectra, 999000 of them were used for the training and 1000 for validation of the CNN, an other 1000 were used for testing. As a quality metric, the coefficient of determination R^2 was used. The CNN received as input the complex values of the entire ³¹P spectrum and returns a multidimensional array that include the estimation of the metabolites concentration and the values of the parameters for each voxel.

Results

Figure 3 shows the coefficients of determination R^2 for each metabolite. This evaluation is made on the testing data set, and it shows a very high ability to recover the values of the metabolite concentration as all values are above 0.96.

Figure 4 shows a slice of a 3D ³¹P-CSI-MRS and its corresponding T2 image of pig's kidneys. The concentration map shows the ATP present in the kidney graft, as estimated by the fitting algorithm.

Discussion

The CNN shows encouraging preliminary results for MRSI spectra analysis. On test data-set, CNN is able to correctly estimate metabolite concentration. We aim to compare performance of the CNN with respect to the traditional fitting on the in-vivo data-set.

The gain provided by the use of CNN is the instantaneous processing time in comparison with traditional fitting methods. Also the ability to create training set with widely distributed parameters should provide more robustness to CNN spectral analysis.

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Figures



Figure 1 : Fitting of true data FID with non-linear least-square algorithm. Pi and ATPs concentrations were estimated after phases and baseline correction.



Figure 2: MRS signal simulation is performed with the top formula with the listed independent variables. The metabolite signal $M_m(t)$ is the sum of all metabolite resonances, and the peak width is estimated with combination of a Lorentzian and a Gaussian function. An example of simulated spectrum is displayed at the bottom.



Figure 3: Values of the coeffcients of determination R² for each metabolite.



Figure 4: T2 image of kidneys MRI with its corresponding mapping of ATP level.

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