A Graphic Tool for Fast Interactive Spectroscopic Prior Knowledge Modeling and Prior Knowledge Database Management

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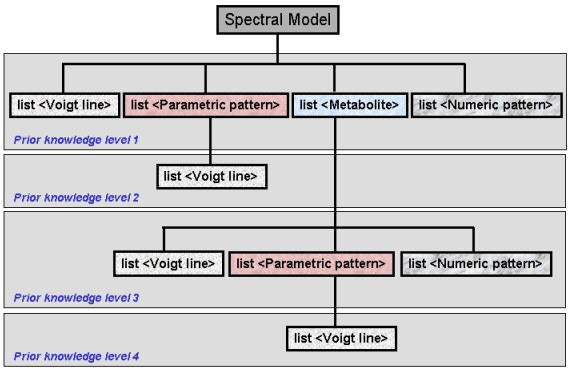
Introduction

Quantification of short echo time ^{1}H-MR spectra is not possible without imposing prior knowledge, as the complexity of the overlapping signals cannot be resolved by first principles. Several prior knowledge based fitting algorithms have been developed (LC-model *(1)*, Amares *(2),* TDFDFIT *(3),* SIT *(4)*). Prior knowledge is either obtained from *in vitro* metabolite spectra or from spectral simulation based on high resolution data. The former requires substantial work for any change in the experimental setup, while the latter has the disadvantage of neglecting experimental non-ideality (e.g. actual pulse profiles). *In vitro* metabolite spectra can either be used directly by the fitting program (e.g. *(1, 3)*) or they can be used to obtain parameterized prior knowledge *(2,3)*, which can then easily be adapted to accommodate differences between *in vitro* and *in vivo* spectra, as well as potentially different relaxation properties for different protons within a molecule. Parameterized prior knowledge also offers the possibility to link certain parameters of a group of similar entities, while leaving other parameters free to be fitted (e.g. linking T_2 's for chemically similar subgroups, while leaving chemical shift differences free to be fitted as e.g. function of pH). The parameterization of prior knowledge and the mutual linking is very tedious and error prone, if not supported by graphical tools. A special application has been developed that is based on a hierarchical spectral model to easily form and adapt parameterized prior knowledge.

Method

Every in vivo MR-spectrum can be modeled by a so called *tree* model, as displayed in the figure below. The top level node, is the mathematical model of the spectrum to be fitted, whose parameters have to be found by some non linear least square fitting method. This model spectrum node can have lists of child nodes of four different types: a. Voigt lines, b. parametric patterns, c. metabolite spectra and d. numeric patterns. Amongst these first level child nodes of different type, area, shift, phase and line width prior knowledge can be defined, denoted by prior knowledge level 1). A first level child node parametric pattern, on its turn, has one or more Voigt line typed only child nodes; between these Voigt line typed child nodes prior knowledge can exist also (prior knowledge level 2). Whereas a first level child node *numeric pattern*, which is a measured or modeled time or frequency response function, has no child nodes, a *metabolite spectrum* can have Voigt lines, parametric and numeric patterns as child nodes. Amongst child nodes of a metabolite spectrum, prior knowledge can be defined (Prior knowledge level 3). Amongst the Voigt lines of the parametric patterns defined on Prior knowledge level 3, also prior knowledge may exist, defining the fourth and deepest level of prior knowledge.



Result

An object oriented model of the above displayed tree model, has been implemented in Java 2. In order to allow easy user access to this model, a graphic user interface (Fitting Parameter Editor) has been developed. It allows the user to define graphically prior knowledge on all four levels. Prior knowledge on each prior knowledge level is separately stored in a file based database, allowing for optimal reuse. New Voigt line typed nodes can graphically be added in the spectral view, via one single mouse click. Since the TDFDFIT *(3)* application allows for parameter range constrained fitting, these constraints can also be entered via the Fitting Parameter Editor. All spectral views in application, allow for standard spectral processing like apodization, zero filling, zero and first order phase correction and eddy current correction, which can be applied to the loaded spectra via simple selections in popup menus. The application automatically generates all necessary starting value files needed by the TDFDFIT fitting program, and it can be extended to produce starting value information for other fitting programs as well. Since the fitting can be started from the application, and the results produced by the fitting program are automatically read back, the application supports fully graphical interactive refinement of the spectral model. The application also allows for direct reading of Dicom formatted spectroscopic data files (that were produced by a Siemens Sonata Scanner), without the necessity of having to export them manually (a very tedious, time consuming and error prone task), which has to be done normally in the case of off-line spectral processing. Since the application was created in an application framework that was designed originally to process and view Dicom *images*, the user can study the MR images together with the MR spectra within the same application.

Conclusion

A tool has been developed that allows for rapid interactive spectral modeling of *in vivo* spectra. Besides interactive spectral modeling, the application allows for easy build up and maintenance of metabolite prior knowledge databases. The application allows for direct loading of Dicom files that contain spectral data. Quantified spectral data can be viewed together with MRI images, allowing for a combined study (off line) of MRS data *together* with MRI data.

References

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