Object Oriented Model for Parameter Estimation of Partially Separable Functions

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Introduction. In parameter estimation the goal is to fit a model function that depends on adjustable parameters to a set of observed data. This is done by defining a merit function (e.g. mean square error) to measure the agreement between the data and the model function and by minimising this function. This article focuses on *structural* or *partially separable* model functions, where the actual model function is a sum of *component* functions, e.g. a spectrum consisting of a sum of spectral lines.

Numerous algorithms has been presented for model fitting tasks in the literature but usually from the numerical analysis viewpoint, treating the model as a plain vector of parameters plus a function. However, the natural representation of the model may be highly structural consisting of several component functions. Moreover the component functions may have common parameters or other dependencies between their parameters. The flat model representation is therefore inconvenient for the user and it is the application developers task to provide a conversion to and from the structural representation.

In this article an object oriented model is presented to serve as an intermediate link between the above two representations, providing simultaneously the interface for the optimisation algorithms and the structured view for the user.

Object oriented model. The model is a collection of classes comprising a core to represent structured model functions. These core classes implement the basic structural and flat views to the model function, as well as the mechanisms for function value and derivative calculations. The core also handles the possible relations between the parameters. The extension of the core model for a specific application is done by providing a class for each type of component function. Only member functions for calculating the values of the component functions are required in these classes. The model utilises *automatic differentiation* [1] to compute the derivatives, so explicit code for analytical derivatives is not needed. By exploiting the partial separability of the model functions, automatic differentiation can be implemented efficiently.

The core classes implement all the functionality needed for manipulating component functions and their parameters. The user interface for this task can therefore be built solely based on the core classes. Adding new classes to the model hierarchy does not cause any need for changes in the interfacing code. An example of a user interface built in this manner is given.

In the structural representation of model functions inheritance and dynamic binding is used. Therefore we loose something in computational efficiency. Efficiency of the model is discussed and it is shown, that the speed decrease compared to low level code is not very significant. The persistence, i.e. the ability store and retrieve the objects of the model is also considered.

The model was developed while working on nuclear magnetic resonance (NMR) spectra estimation. A case study of NMR-spectral fitting is therefore conveyed through the article to clarify the ideas presented.

The are scantly descriptions of object orientation together with parameter estimation in the literature. Related work can be found from [3, 4] containing descriptions of computer systems sharing some similarities with our model. See [2] for the description of the NMR analysis software built using the object oriented model presented here.

Conclusions. Traditionally object oriented programming is not very popular in numerical codes, where efficiency is of utmost importance. However, by careful design the penalty of replacing low level codes with more abstract ones is quite moderate. The main result of this paper is to show that using object oriented principles a flexible and extendible framework for expressing structural functions can be built without sacrificing efficiency in the evaluation of the function values and derivatives.

References

[1] Rall L.B.: Automatic differentiation: Techniques and Applications, Lecture Notes in Computer Science 120, Springer-Verlag, Berlin 1981

[2] Järvi J.: A PC-program for automated analysis of NMR spectrum series, Computer Methods and Programs in Biomedicine **52** (1997) 213-222

[3] Majoras R. E., Richardson W. M., Seymour R. S.: An object-oriented approach to evaluating multiple spectral models, Journal of Radioanalytical and Nuclear Chemistry **193** (1995) 207-210

[4] van Tongeren B. P. O., Boxman R. D. C., Deumens J. W., van Leeuwen J. P., Mehlkopf A. F., van Ormondt D., de Beer R., QUANSIS, An object-oriented data-analysis system for in vivo NMR signals, Journal of Magnetic Resonance Analysis, **2** (1996) 75-84.