



A deconvolution scheme for the stochastic metabolic/hemodynamic model (sMHM) based on the square root cubature Kalman filter and maximum likelihood estimation

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ABSTRACT

Based on clinical data collected using different brain imaging and recording techniques, brain researchers built mathematical models of the activity in the human brain. To test these models they simulate them by performing on those models a virtual brain experiment, and compare the outputs from those with the real brain activity recordings. The models can be a basis for understanding what goes wrong in brain diseases and brain disorders and potentially help to create new drugs for these conditions. Metabolic Hemodynamic Model (MHM) is one of these models that describes the changes in metabolic and hemodynamic responses during functional brain activity, formulated in a continuous-discrete state space form. MHM calibration is a decisive step for successfully capture the changes in the latent variables that can not be directly observed and predicting the brain activity related to these changes, this requires having suitable techniques that permit us to estimate both the hidden states and parameters of the MHM. The method proposed in this paper is a combination of the Square Root Cubature Kalman Filter (SCKF) and Maximum Likelihood Estimation (MLE), it uses gradient-based optimization algorithms for optimizing the objective function. Numerical results obtained with simulated data are presented to illustrate the effectiveness of the proposed method to estimate the states, parameters and regenerating the BOLD signal even when the data are contaminated with high noise level. In the proposed method, it will be explained how the gradient can be calculated with a new developed SCKF-like recursion and the result, whenever there is a vast amount of data, so much less time can be spent analyzing it compared to the time spent when the data is analyzed using finite differences. The goal of these attempts is to construct a formal system that will produce theoretical results that are corresponding to what is found in reality.

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1. Introduction

Functional magnetic resonance imaging (fMRI) represents one of the most powerful and noninvasive tools that has ever been developed, by virtue of its capability to image human brain function. The goal of research interest in fMRI is to understand the neural mechanisms behind how we see, hear, think, feel and move. One of the most promising fields in which the fMRI was extensively used is Cognitive Neuroscience, which focuses on the study of working memory, decision making, perception, sensation, reasoning, acquisition of knowledge and behavior.

Electricity is the language of the brain. Brain activity means the tiny electrical signals (action potentials) that the neurons send to each other. Unfortunately, that's not what the fMRI scanner is measuring, the scanner measures the indirect consequences of neural activity (the hemodynamic responses). It measures the oxygen level in the activated areas in the brain and for that why the signal that is measured is called Blood Oxygen Level Dependent signal or in short BOLD signal.

The idea that changes in cerebral blood flow (CBF), cerebral metabolic rates of oxygen (CMRO₂) and glucose (CMR_{GLC}) consumption could be triggered by increasing neuronal activity, is the basis of functional neuroimaging techniques like fMRI and PET [1]. When the neurons increase their activity they give orders to the blood vessels to get more blood flow to the region concerned because it needs more oxygen and glucose. The question here is how do the neurons communicate with the blood vessels? This is called the neurovascular coupling.

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During the last two decades, several mathematical models of the neurovascular coupling had emerged. Among the first researchers who have been interested in modeling the brain activity Buxton et al. [2,3] and Friston et al. [4]. Where several assumptions concerning the modeling of the delivery of the O_2 to the brain, the nonlinear aspects of the BOLD response and others were the basis for developing the models that will be cited below.

In the Balloon model [3] the blood flow through the capillary is linked to the volume (v) and total deoxyhemoglobin content (q) by means of nonlinear ordinary differential equations (ODEs), and the measured BOLD signal is computed by a nonlinear function of v and q . The blood flow through the capillary representing the input to the Balloon model was assumed to be a trapezoidal function with a certain rise time and duration. Balloon Winkessel model [5] is a reformulation of the proposed balloon model by taking into consideration the effect of the capillary and venous compliance, more specifically the resistance of the venous compartment to changes in blood volume. Friston et al. [6] extended this model [3] to incorporate the relationship between the neuronal activity and the blood flow. Hence, the role of the neuronal activity in the generation of the BOLD signal.

The emergence of such models raised a great challenge for designing methods that can help in estimating the hidden states, neuronal activity and identifying model parameters. Probably the first work attempted to handle this problem was made by Friston et al. [6] using Volterra kernels to estimate the parameters of the hemodynamic model. Based on some studies that showed the presence of fluctuations in the metabolic responses [7,8] and vascular responses [9–12], it would be better to take into account these physiological fluctuations. In Riera et al. [13] the hemodynamic model is generalized to incorporate a Wiener process at the level of the process equation representing the physiological noise. The author's idea was to use the local linearization filter based on the truncated Ito-Taylor expansion and the composite trapezoidal rule to estimate both the hidden states and parameters of the balloon hemodynamic model.

There are so many works that have been made during the last few years to address the problem of fitting previously cited models. Additionally, to what already mentioned, there is the approach based on Kalman filtering where some of its variants were used to infer the hemodynamic model states and parameters. We mention for example the Extended Kalman Filter (EKF) [14], Unscented Kalman Filter (UKF) [15] and the Particle Filter (PF) [16], regarding particle filter Croce et al. [17,18] recently published two interesting paper where the hemodynamic model is inverted using both electrical and metabolic recordings. The Square Root Cubature Kalman Filter (SCKF) belong to the class of nonlinear Kalman filters, introduced by Arasaratnam and Haykin [19] particularly for solving high-dimensional state estimation problem. From the literature, this technique appears to outperform the conventional nonlinear filters like EKF and UKF. It has been used successfully to invert the hemodynamic model, this inversion provides estimates of both the hidden states and model parameters as well as the neuronal activity [20]. Recently Karam et al. [21] proposed a nonlinear neural network to estimate the states and the input, also a new solution methodology based on a regularized Newton method and cubature Kalman filter, has been used in [22] to calibrate the hemodynamic model.

For better understanding of the brain activity and to be able to construct plausible models describing this activity, a considerable knowledge about all physiological phenomena involved in the generation of the BOLD signal is needed. Sotero and Trujillo-Barreto [23] proposed one of the more advanced models of the neurovascular coupling, the Metabolic Hemodynamic Model (MHM) linking the excitatory/inhibitory activity to the fMRI signal taking into

account the metabolic effects such that the cerebral metabolic rate of glucose consumption CMR_{Glc} .

In this paper, we propose a new approach to estimate the states and parameters of the stochastic MHM (sMHM), based on the SCKF and MLE. To implement this approach we need to maximize the likelihood function (minimize the negative log-likelihood function). We use a gradient-based minimization algorithm for finding the minimum of the negative log-likelihood function, this requires the computation of log-likelihood function and its gradient. The log-likelihood function is approximated via the prediction error decomposition, computed using the predicted measurement and the innovation matrix from the SCKF measurement update steps. We are using MATLAB version R2015b, if we do not have gradients, solvers approximate gradients by means of finite differences. So, providing gradients can save time and increase the accuracy. The common sources of error in finite differences are round-off error and computer rounding, hence finite differences can lead to a futile point. In this case, a solver can stop and supply a gradient allows it to proceed. We show that the gradient of the negative log-likelihood function can be computed analytically based on SCKF sensitivity equations obtained by differentiating the SCKF equations. The new method replaces the standard method based on Cubature Kalman Filter (CKF) [24].

To demonstrate the effectiveness of the proposed method we fitted the sMHM to synthetic data, and present the results to show that the proposed solution methodology can obtain accurate estimates of the hidden states and model parameters.

This paper is organized as follows: in Section 2 we review the sMHM, its nonlinear continuous-discrete state space form, some numerical approximation methods to solve such a system as well as the proposed solution methodology. Section 3 is devoted to present and discuss the results of the inversion and identification of two nonlinear model with a special attention to the sMHM model.

2. Material and methods

Building models of the activity in the human brain, based on neurophysiological data has practical applications. These models are used to generate simulated neuroimaging signals, if we can understand something from these signals maybe we can better diagnosis brain diseases, brain disorders, and hence find the treatment [25–27]. Another important use of this understanding of the brain is to help design chips and computers which a brain like and can be used in future robots, intelligent information systems and Brain-Computer Interface BCI where the goal is to establish nonmuscular connections between a human brain and computer by translating the minds of a user into computer commands, an interesting research in this field with some related methods (computational algorithms) can be found in the papers recently published by Zhang et al. [28,29] and Wang et al. [30]. Many of these models are often formulated in continuous-discrete state space form. One of these models called the stochastic metabolic hemodynamic model (sMHM) [31] that will be the subject of this research paper. The question that our research answers is: given simulated data, how much of the true hidden states signals can we recover from this simulated data, and what are the most probable parameters that can generate the data?

The Kalman filter (KF) is originally developed to estimate the states knowing the parameters. In practical models, the parameters are usually unknown, this means that we have to perform a complete inversion and estimate both the hidden states and parameters. There are several approaches that can be used to estimate the states and parameters in a nonlinear discrete-time state space model. Three methods are commonly used, dual filtering approach [32] where two Kalman filters are run simultaneously in an iter-

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