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Technical Note

Comparison of the hemodynamic filtering methods and particle filter with extended Kalman filter approximated proposal function as an efficient hemodynamic state estimation method

Serdar Aslan *

Institute of Biomedical Engineering, Boğaziçi University, Kandilli, İstanbul, Turkey

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ABSTRACT

Estimating the hidden hemodynamic states that underlie measured blood oxygen level dependent (BOLD) signals is an important model inversion challenge in functional neuroimaging. Various filtering techniques are proposed in the literature. Those are Gaussian type approximated estimation techniques like Extended Kalman filter (EKF), Unscented Kalman filter (UKF), Cubature Kalman filter (CKF) as well as stochastic inference techniques like standard particle filters (PF) and auxiliary particle filter (APF). In this technical note, we compare particle filter type algorithms and Gaussian approximated inference methods. We also implement a particular type of particle filter that approximates the optimal proposal function by the Extended Kalman filter (PF-EKF). We show that the allegation that Extended Kalman type approximated methods are poor in performance is not true. On the contrary, they are better. We tested this assertion under different parameter sets, inputs, a wide range of noise conditions and unknown initial condition. This finding is important for developing fast and accurate alternative model inversion schemes, which is the topic of our subsequent paper.

1. Introduction

The hemodynamic model describes a nonlinear relationship between the neuronal activity and observed blood oxygen level dependent (BOLD) signal. This nonlinear relationship is described by nonlinear differential equations [1–3]. Later, the hemodynamic model is extended to the stochastic differential equations by including noise terms [4–6]. With most of the imaging techniques, it is impossible to obtain a direct measurement of neuronal activity. After the fast neuronal activity, we observe a response in the hemodynamic variables like blood flow, blood venus volume and blood deoxyhemoglobin content [7]. But even then we do not directly observe the hemodynamic variables. In the fMRI technique, we observe the BOLD signal, which is a nonlinear combination of the blood venus volume and blood deoxyhemoglobin content [5]. Hence it is important to understand the nature of the hidden hemodynamic states from the observed BOLD signal.

In this technical note, we examine the implementation and performance of state estimation techniques for the fMRI signals. From the BOLD signal, by using the functional representation of the hemodynamic model, we perform state estimation.

We work with the continuous time state space and observation formulation. Subsequently we convert the model to the discrete time equivalent form. Hence, we describe the system in the most general setting as:

$$\dot{x}(t) = g(x(t), \theta, u(t)) \quad (1)$$

$$y(t) = h(x(t), \theta, u(t)) \quad (2)$$

Here, g is the nonlinear state transition function, h is the nonlinear measurement function. Both the functions have arguments as the hemodynamic state x_t at time t, parameter set θ and neuronal input $u(t)$. Hemodynamic state x_t at time t is a four-dimensional vector $x_t \in \mathbb{R}^4$. The BOLD signal y_t at time t is described as $y_t \in \mathbb{R}$.

Similar to Johnston et al. [5] we perturb the system with Wiener noise and discretize the system by the Euler–Maruyama Method and arrive the discrete time form of the above nonlinear differential equation. We define the discrete time instants as $t = t_k \triangleq k\Delta t, k = 1, 2, \ldots$. The state variables, input and measured BOLD signals are discretized by defining $x_{k+1} = x(t_k + \Delta t)$, $x_k = x(t_k)$, $u_k = u(t_k)$, $y_k = y(t_k)$. By using these definitions we arrive the following nonlinear discrete time state-space model.

$$x_{k+1} = f(x_k, \theta, u_k) + w_k \quad (3)$$

* Tel.: +90 554 569 4249.
E-mail address: serdar.aslan@gmail.com

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$$y_k = h(x_k, \theta, u_k) + v_k \quad (4)$$

where f is:

$$f(x_k, \theta, u_k) = x_k + \Delta t g(x_k, \theta, u_k) \quad (5)$$

and

$$w_k = \mathcal{N}(0, Q_k) \quad (6)$$

Here, f is the nonlinear state transition function, and h is again the nonlinear measurement function. The equality in Eq. (5) is an approximate equality because, under Euler–Maruyama approximations, the discrete state transition function is the solution to Eq. (1). This time, we have the discretized version of the state x_k where the time index is k. The state is a vector $x_k \in \mathbb{R}^4$. The measured BOLD signal y_k is from the set $y_k \in \mathbb{R}$. The state noise w_k is of Gaussian type with $\mathcal{N}(0, Q_k)$. The measurement noise v_k is also Gaussian type with $\mathcal{N}(0, R_k)$. One distinctive feature in the algorithms for PF and APF is that we can work with non-Gaussian noise also. This feature is not present in most of the model inversion techniques used in the fMRI literature. We denote by $y_1, y_2, \ldots, y_N$ or $y_{1:N}$ the discrete time observation sequence of length N. Given the (neuronal) input $u_{1:N}$, plausible assumptions about the noise and N observations y_1, $y_2, \ldots, y_N$ or $y_{1:N}$, we want to estimate $x_{1:N}$.

1.1. Estimation of the states

Due to nonlinearity of the system it is difficult to make probabilistic inferences from the observed data. In this technical note, our aim is to find the state estimation of type $p(x_k|y_{1:k})$, which is called filtering. In the filtering problem, for the time step k we take into account only the observations up to the time k. From these observations we calculate $p(x_k|y_{1:k})$. When the new observation arrives, we find the new conditional pdf $p(x_{k+1}|y_{1:k+1})$. Filtering disregards the information contained in the future values of y for the state x at time step k. However, in the smoothing we take into account all observed sequences. This provides us more accurate results for the state estimation, but at the cost of additional computation. Even the smoothing techniques requires the calculation of the filtering. For that reason, we concentrate on implementing a particular filtering technique to obtain the most accurate state estimation. Since it is impossible to calculate analytic expression for the $p(x_k|y_{1:k})$, various approximation techniques are proposed.

1.2. Gaussian approximated inference

We have closed form expression for basic state-space systems that are linear and have Gaussian shaped noise. For such cases, Kalman filter [8] and smoother algorithms [9] work optimally. For linear systems, the form of the filtering pdf is expressed exactly as Gaussian pdf's.

$$p(x_k|y_{1:k}) = \mathcal{N}(\hat{x}_{k|k}; P_{k|k}) \quad (7)$$

Here $\hat{x}_{k|k}$ is the recursive state estimate of the filtering at time k respectively. Similarly, $P_{k|k}$ is the state covariance for the filtering at time k.

For Gaussian approximated methods, we can list Extended Kalman filter (EKF) [10,11], Local Linearization filter (LLF) [4], Unscented Kalman filter (UKF) [12–14] and Cubature Kalman filter (CKF) [15], which is a specific case of UKF [16]. These methods approximate conditional estimates of the states as Gaussian pdf.

$$p(x_k|y_{1:k}) \approx \mathcal{N}(\hat{x}_{k|k}; P_{k|k}) \quad (8)$$

For the Extended Kalman filter algorithm, the state transition and measurement functions are linearized with a first-order Taylor series around the state estimates [17]. Approximating the nonlinear system with a linear state space form, the standard Kalman filter is applied. The LLF filter is the same as EKF except, in the prediction update of the state, LLF uses the discretization proposed by Jimenez et al. [18]. In UKF and CKF, Gaussian pdf's are represented by deterministically chosen points called sigma points and cubature points for UKF and CKF, respectively [19]. For prediction and measurement updates of the states, the deterministic points are transferred from the nonlinear state transition and measurement functions, respectively. The positive aspect of UKF/CKF is that there is no need for the calculation of the Jacobian matrix of the state and measurement functions.

1.3. Sample based inference

In stochastic or sampling based schemes we aim to approximate the posterior or target density with sampled distributions of particles. There are two broad categories of stochastic inference algorithms: Sequential Monte Carlo (SMC) methods and Markov Chain Monte Carlo Methods (MCMC). Since we will be dealing with dynamical systems, we deal with Sequential Monte Carlo methods. In SMC, the density functions are approximated by generating samples [20]. The error in these algorithms are decreased by increasing the sample number. For that reason, these algorithms can provide more accurate results compared to Gaussian approximated approaches, despite the increased computation time. In SMC, we sample from an easy to sample proposal function. By use of a technique called Importance Sampling, we change the weight associated with the sample (particle) to compensate for the difference between the target and proposal function [20]. We note that the target function is our desired posterior density $p(x_k|y_{1:k})$. It is crucial that we choose the proposal function such that we can sequentially update the state samples by each new observation.

1.4. Hemodynamic state estimation literature

For the deterministic type inference algorithms, several attempts were presented in the fMRI model inversion literature. In the first attempts at applying the fMRI model inversion techniques, there was zero process noise in the state transition equations [1]. Friston et al. modeled first the relation between the input and output by Volterra Kernels [1]. Subsequently, Friston performed a Bayesian estimation technique to estimate the parameters [21]. Still, the assumption was zero state noise in the hemodynamic state equations. Riera et al. [4] utilized a type of Extended Kalman filter (EKF). They introduced process noise in their method for the hemodynamic state equations. They performed EKF via the discretization method of Jimenez et al. [18]. They did not, however, use the widely used Euler–Maruyama discretization method. UKF is performed by Hu et al. for the system identification and state estimation of hemodynamic variables [22]. Riera et al. and Hu et al. performed these techniques in a filtering style [4,22]. They did not perform any smoothing algorithm. Recently, Havlicek et al. [17] performed the Square-root Cubature Kalman filter (SCKF) and Smoother (SCKS) for the system identification and hemodynamic state estimation. In this technical note, we also implemented SCKF, which is the numerical stable form of Cubature Kalman filter.

In the fMRI literature, Johnston et al. [5] made direct usage of the particle filters. Murray and Storkey implemented particle smoothers in the fMRI literature by using suboptimal particle filters [23].

Another class Bayesian filtering schemes as been introduced recently, called Generalized filtering. These are Bayesian filtering schemes in generalized coordinates of motion [24,25,6]. The schemes above can be considered special cases of Generalized filtering that only consider posterior densities over hidden states and their first order motion. In Generalized filtering, high order motion is also considered. This allows one to formulate Bayesian filtering