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Modeling and prediction of nonlinear environmental system using Bayesian methods

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ABSTRACT

An environmental dynamic system is usually modeled as a nonlinear system described by a set of nonlinear ODEs. A central challenge in computational modeling of environmental systems is the determination of the model parameters. In these cases, estimating these variables or parameters from other easily obtained measurements can be extremely useful. This work addresses the problem of monitoring and modeling a leaf area index and soil moisture model (LSM) using state estimation. The performances of various conventional and state-of-the-art state estimation techniques are compared when they are utilized to achieve this objective. These techniques include the extended Kalman filter (EKF), particle filter (PF), and the more recently developed technique variational filter (VF). Specifically, two comparative studies are performed. In the first comparative study, the state variables (the leaf-area index LAI , the volumetric water content of the soil layer 1, HUR1 and the volumetric water content of the soil layer 2, HUR2) are estimated from noisy measurements of these variables, and the various estimation techniques are compared by computing the estimation root mean square error (RMSE) with respect to the noise-free data. In the second comparative study, the state variables as well as the model parameters are simultaneously estimated. In this case, in addition to comparing the performances of the various state estimation techniques, the effect of number of estimated model parameters on the accuracy and convergence of these techniques are also assessed. The results of both comparative studies show that the PF provides a higher accuracy than the EKF, which is due to the limited ability of the EKF to handle highly nonlinear processes. The results also show that the VF provides a significant improvement over the PF because, unlike the PF which depends on the choice of sampling distribution used to estimate the posterior distribution, the VF yields an optimum choice of the sampling distribution, which also accounts for the observed data. The results of the second comparative study show that, for all techniques, estimating more model parameters affects the estimation accuracy as well as the convergence of the estimated states and parameters. However, the VF can still provide both convergence as well as accuracy related advantages over other estimation methods.

1. Introduction

Crop models such as EPIC (Williams et al., 1989), WOFOST (Diepen et al., 1989), DAISY (Hansen et al., 1990), STICS (Brisson et al., 1998), and SALUS (Basso and Ritchie, 2005) are dynamic nonlinear models that describe the growth and development of a crop interacting with environmental factors (soil and climate) and agricultural practices (crop species, tillage type, fertilizer amount). They are developed to predict crop yield and quality or to optimize the farming practices in order to satisfy environmental objectives, as the reduction of nitrogen lixiviation. More recently, crop models are used to simulate the effects of climate changes on the agricultural production. Nevertheless, the prediction errors of these models may be important due to uncertainties in the estimates of initial values of the states, in input data, in the parameters, and in the equations. The measurements needed to run the model are sometimes not numerous, whereas the field spatial variability and the climatic temporal fluctuations over the field may be high. The degree of accuracy is therefore difficult to estimate, apart from numerous repetitions of measurements. For these reasons, the problem of state/parameter estimation represents a key issue in such nonlinear and non-Gaussian crop models including a large number of parameters, while measurement noise exists in the data.

Several state estimation techniques are developed and used in practice. These techniques include the extended Kalman filter, particle filter, and more recently the variational filter. The classical Kalman Filter (KF) was developed in the 1960s (Kalman, 1960), and is widely used in various engineering and science applications,

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including communications, control, machine learning, neuroscience, and many others. In the case, where the model describing the system is assumed to be linear and Gaussian, the KF provides an optimal solution (Simon, 2006; Grewal and Andrews, 2008; Aidala, 1977; Matthies et al., 1989). The KF has also been formulated in the context of Takagi–Sugeno fuzzy systems to handle nonlinear models, which can be described as a convex set of multiple linear models (Chen et al., 1998; Simon, 2003; Nounou and Nounou, 2006). It is known that the KF is computationally efficient; however, it is limited by the non-universal linear and Gaussian modeling assumptions. To relax these assumptions, the extended Kalman filter (Simon, 2006; Grewal and Andrews, 2008; Julier and Uhlmann, 1997; Ljung, 1979; Kim et al., 1994) and the unscented Kalman filter (Simon, 2006; Grewal and Andrews, 2008; Wan and Merwe, 2000; Merwe and Wan, 2001; Sarkka, 2007) are developed. In extended Kalman filtering, the model describing the system is linearized at every time sample (in order to estimate the mean and covariance matrix of the state vector), and thus the model is assumed to be differentiable. Unfortunately, for highly nonlinear or complex models, the EKF does not usually provide a satisfactory performance. On the other hand, instead of linearizing the model to approximate the mean and covariance matrix of the state vector, the UKF uses the unscented transformation to improve the approximation of these moments. In the unscented transformation, a set of samples (called sigma points) are selected and propagated through the nonlinear model, which provides more accurate approximations of the mean and covariance matrix of the state vector, and thus more accurate state estimation.

Other state estimation techniques use a Bayesian framework to estimate the state and/or parameter vector (Beal, 2003). The Bayesian framework relies on computing the probability distribution of the unobserved state given a sequence of the observed data in addition to a state evolution model. Consider an observed data set y, which is generated from a model defined by a set of unknown state variables and/or parameters z (Beal, 2003). The beliefs about the data are completely expressed via the parametric probabilistic observation model, $P(y|z)$. The learning of uncertainty or randomness of a process is solved by constructing a distribution $P(z|y)$, called the posterior distribution, which quantifies our belief about the system after obtaining the measurements. According to Bayes rule, the posterior can be expressed as:

$$P(z|y) \propto P(y|z)P(z),$$

where $P(y|z)$ is the conditional distribution of the data given the vector, z, which is called the likelihood function, and $P(z)$ is the prior distribution, which quantifies our belief about z before obtaining the measurements. Thus, Bayes rule specifies how our prior belief, quantified by the priori distribution, is updated according to the measured data y. Unfortunately, for most nonlinear systems and non-Gaussian noise observations, closed-form analytic expressions of the posterior distribution of the state vector are untractable (Kotecha and Djuric, 2003). To overcome this drawback, a non-parametric Monte Carlo sampling based method called particle filtering (Storvik, 2002; Doucet and Tadić, 2003; Poyiadjis et al., 2005) has recently gained popularity.

The Particle Filter approximates the posterior probability distribution by a set of weighted samples, called particles (Arulampalam et al., 2002). Since real-world problems usually involve high-dimensional random variables with complex uncertainty, the non-parametric and sample-based estimation of uncertainty (provided by the PF) has thus become quite popular to capture and represent the complex distribution $P(z|y)$ for nonlinear and non-Gaussian process models (Arulampalam et al., 2002). The PF has the ability to accommodate nonlinear and multi-modal dynamics, but at the cost of more computational complexity and storage requirements. Also, taking into account the stringent calculus and storage constraints, the propagation of a huge amount of particles has impeded the implementation of the PF in very challenging parameter estimation problems. As a consequence, the variational filter is proposed recently to enhance state estimation (Mansouri et al., 2009; Balaji and Friston, 2011) because VF yields an optimal choice of the sampling distribution by minimizing a Kullback–Leibler (KL) divergence criterion. In fact, variational calculus leads to a simple Gaussian sampling distribution whose parameters (which are estimated iteratively) also utilize the observed data, which provides more accurate and computationally efficient computation of the posterior distribution.

Each of the above state estimation techniques has its advantages and disadvantages. The VF can be applied to large parameter spaces, has better convergence properties, and is easier to implement than the PF, and both of them can provide improved accuracy over the EKF. The objective of this paper is to compare the performances of the EKF, PF, and VF when used to monitor and model a LSM process through the estimation of its state variables and model parameters. This comparative study is assess the accuracy and convergence of these techniques, as well as the effect of the size of the parameter space (i.e., number of estimated parameters) on the performances of these estimation techniques. Some practical challenges, however, can affect the accuracy of estimated states and/or parameters. Such challenges include the large number of states and parameters to be estimated, the presence of measurement noise in the data, and the availability of small number of measured data samples. The objective of this paper is two-fold: (i) we study the accuracy and convergence of EKF, UKF and PF techniques and (ii) we investigate the effect of the above challenges on the performances of these techniques. Then, a comparative investigation are conducted to study their performances under the same challenge mentioned above. The above analysis are performed using an environment process model representing leaf area index and soil moisture (LSM) (i.e, the leaf-area index LAI, the volumetric water content of the layer 1, HUR1 and the volumetric water content of the layer 2, HUR2) and their abilities to estimate some of the key system parameters, which are needed to define the LSM model.

The rest of the paper is organized as follows. In Section 2, a statement of the problem addressed in this paper is presented, followed by descriptions of various commonly used state estimation techniques in Section 2.2. Then, in Section 3, the performances of the various state estimation techniques are compared through their application to estimate the state variables and model parameters of a LSM process. Finally, some concluding remarks are presented in Section 4.

2. Material and methods

In this section, the mathematical formulation of the state/parameter estimation problem is developed, according to the filtering approaches that are studied. In a second step, the dynamic model simulation is presented, and the problem is formulated.

2.1. Problem statement

Here, the estimation problem of interest is formulated for a general system model. Let a nonlinear state space model be described as follows:

$$\begin{aligned} \dot{x} &= g(x, u, \theta, w), \\ y &= l(x, u, \theta, v), \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^n$ is a vector of the state variables, $u \in \mathbb{R}^p$ is a vector of the input variables, $\theta \in \mathbb{R}^q$ is an unknown parameter vector, $y \in \mathbb{R}^m$ is a vector of the measured variables, $w \in \mathbb{R}^n$ and $v \in \mathbb{R}^m$ are process