Prediction of non-linear time-variant dynamic crop model using bayesian methods

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Abstract

This work addresses the problem of predicting a non-linear time-variant leaf area index and soil moisture model (LSM) using state estimation. These techniques include the extended Kalman filter (EKF), particle filter (PF) and the more recently developed technique, variational filter (VF). In the comparative study, the state variables (the leaf-area index LAI, the volumetric water content of the layer 1, HUR1 and the volumetric water content of the 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 with respect to the noise-free data. The results show that VF provides a significant improvement over EKF and PF.

Keywords: crop model, variational filter, extended Kalman filter, particle filter, LAI, soil moisture prediction

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 non-linear 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, etc.). They are developed to predict crop yield and quality or to optimize the farming practices in order to satisfy environmental objectives, such as the reduction of nitrogen leaching. More recently, crop models have been used to simulate the effects of climate changes on 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 estimation represents a key issue in such non-linear and non-Gaussian crop models including a large number of parameters, while measurement noise exists in the data. The estimation problem has been addressed with several methods, such as the Kalman Filter (KF) which provides an optimal Bayesian solution but is limited by the non-universal Gaussian modeling assumptions. An application of this technique to a linear dynamic crop model predicting a single state variable 'winter wheat biomass' is presented in Makowski *et al.* (2004). The method is computationally efficient, but its performance is limited by the non-universal Gaussian modeling assumptions. Makowski *et al.* (2004) showed how the model predictions can be sequentially updated by using several measurements, and studied the sensitivity of the results to the variance of the model errors. The Ensemble Kalman Filtering (EnKF) (Xiao *et al.*, 2009), Extended Kalman Filtering (EKF) (Calvet, 2000), and the Unscented Kalman Filtering (UKF) (Wan and Merwe, 2000) have been proposed to improve the KF flexibility. Xiao *et al.* (2009) have developed a real-time inversion technique to estimate LAI (Leaf Area Index) from MODIS data using a coupled dynamic and radiative transfer model. They used the EnKF technique to update LAI recursively by combining predictions from the

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dynamic model while MODIS reflectance data predictions from the dynamic model have been used with the EnKF method to estimate real-time LAI from time series MODIS reflectance data. Until now, there are a few studies, with encouraging results, considering estimation of states where the non-linear observed system is assumed to progress according to a probabilistic state space model. For most non-linear models and non-Gaussian noise observations, closed form analytic expression of the posterior distribution of the state is intractable (Kotecha and Djuric, 2003). Recently, a variational filtering (VF) has been proposed for solving the nonlinear parameter estimation problem encountered in crop models. Mansouri *et al.* (2013) used a Bayesian sampling method for modeling and prediction of non-linear environmental systems, where the non-linear observed system was assumed to progress according to a probabilistic state space model. In this investigation, the state vector to be estimated (at any time instant) was assumed to follow a Gaussian model, where the expectation and the covariance matrix are constants. The variational filter can be applied to large parameter spaces, has better convergence properties and is easier to implement than the particle filter. Both of them can provide improved accuracy over the extended Kalman filter. Nevertheless, some practical challenges can affect the accuracy of estimated states and/or parameters, namely the presence of measurement noise in the data, the restricted availability of the measured data samples, and the larger number of model parameters.

In the current work, we propose to extend the variational filter to better handle non-linear and non-Gaussian processes (where no *a priori* information about the states and parameters is available), by assuming time-varying statistical parameters.

The objectives of the paper are to compare three methods (EKF, PF and VF) for estimating important state variables of crop models. The LAI (Leaf Area Index) determines the photosynthetic primary production and the plant evapotranspiration and is thus a key state to characterize the plant growth. The moisture content of two soil layers (20 and 50 cm) was considered as it affects the capacity of plants to extract water and soil nutrients. The comparison will rely on the computation of the RMSE and the number of parameters that can be accurately predicted. The model used in this study is mini STICS (Makowski e*t al.*, 2006). Using mini STICS model has several advantages since: (1) it can reduce the computing and execution times of the STICS model; and (2) it has the nice property to be a good dynamic model, ensuring the robustness of data processing and estimation.

Problem formulation

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

Problem statement

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

$$\begin{aligned} z_k &= f(z_{k-1}, u_{k-1}, \theta_{k-1}, w_{k-1}) \\ y_k &= h(z_k, u_k, \theta_k, v_k) \end{aligned} \tag{1}$$

where k is an index corresponding to the time, z_k is the vector of state variables assumed to follow a Gaussian model where at any time k the expectation μ_k and the covariance matrix λ_k are both constants. Also, defining the augmented vector, u_k is the vector of input variables, θ_k is a parameter vector (assumed to be known), y_k is the vector of the measured variables, w_k and v_k are respectively model and measurement noise vectors, g and l are non-linear differentiable functions, the first one determines the new state variables as a function of the precedent situation, while the second expresses the dependence of the measurements. We assume that the error terms, w_k and v_k, have normal distributions with zero expectation, and that they are mutually independent.

Time-variant evolution systems(TVES)
Instead of the kinematic parametric model which is usually used in estimation problems, we employ a time-variant evolution systems (Vermaak *et al.*, 2003). This model is more appropriate to practical non-linear and non-Gaussian situations where no *a priori* information on the state value is available. The state variable z_k at instant k is assumed to follow a Gaussian model, where the expectation μ_k and the precision matrix λ_k are both random. Gaussian distribution for the expectation and Wishart distribution for the precision matrix form a practical choice for the filtering implementation. The hidden state z_k is extended to an augmented state $\alpha_k = (z_k, \mu_k \lambda_k)$, yielding a hierarchical model as follows:

$$\begin{cases} \mu_k \approx N\left(\mu_k \middle| \mu_{k-1}, \bar{\lambda}\right) \\ \lambda_k \approx W\left(\lambda_k \middle| \bar{S}\right) \\ z_k \approx N\left(\mu_k \middle| \lambda_k\right) \end{cases} \qquad (2)$$

where the fixed hyper-parameters $\bar{\lambda}$, $\bar{s}$ and $\bar{n}$ are respectively the random walk precision matrix, the degrees of freedom and the precision of the Wishart distribution. Note that assuming random mean and covariance for the state z_k leads to a prior probability distribution covering a wide range of tail behaviours allowing discrete jumps in the state variable. In fact, the marginal state distribution is obtained by integrating over the mean and precision matrix:

$$p(z_k \mid z_{k-1}) = \int p(z_k \mid \mu_k, \lambda_k)p(\mu_k, \lambda_k \mid x_{k-1})d\mu_k \lambda_k \qquad (3)$$

where the integration with respect to the precision matrix leads to the known class of scale mixture distributions (Vermaak *et al.*, 2003). Low values of the degrees of freedom $\bar{n}$ reflect the heavy tails of the marginal distribution $p(z_k \mid z_{k-1})$.

Simulation results analysis

Crop model description
The data used in this paper derive from an experiment designed to study wheat growth response (*Triticum aestivum* L., cultivar Julius) under different nitrogen fertilization levels during the crop season 2008-09. The experimental blocks were prepared on two soil types (loamy and sandy loam), corresponding to the agro-environmental conditions of the Hesbaye region in Belgium. The measurements were the results of four repetitions by date, nitrogen level and soil type. Each repetition was performed on a small block (2×6 m) within the original experiment as a complete randomised block distribution, spread over the field within each soil type, to ensure measurement independence. A wireless micro-sensor network was used to continuously characterize the soil (water content, suction, temperature) at two depths (20 and 50 cm) and the atmosphere (radiation, temperature, relative humidity, wind speed) within the vegetation. Pluviometry data were also acquired in the experimental field. LAI, biomass and soil nitrogen content were regularly measured manually. The model for which the methods were tested is Mini STICS model (Tremblay and Wallach, 2004). Its structure can be derived from the basic conservation laws, namely material and energy balances. It contains dynamic equations that indicate how each state variable evolves from one day to the next as a function of the current values of the state variables, of the input variables and of the parameters values. Encoding these equations over time allows one to eliminate the intermediate values of the state variables and relate the state variables at any time to the explanatory variables on each day up to that time. However, the model involves several parameters that are usually not known, which include the radiation use efficiency expressing the biomass produced per unit of intercepted radiation,

the maximal value of the ratio of intercepted to incident radiation, the coefficient of extinction of radiation, etc. The model parameters determined by Makowski *et al.* (2004) are presented in Table 1. Based on the equations described in Makowski *et al.* (2004), the mathematical model LSM of the LAI and Soil Moisture is given by:

$$\begin{aligned} LAI(t) &= f_1(LAI(t-1)+\theta) \\ HUR1(t) &= f_2(HUR1(t-1)+\theta) \\ HUR2(t) &= f_3(HUR2(t-1)+\theta) \end{aligned} \tag{4}$$

Where t is the time, $f_{1\text{-}3}$ are the corresponding model functions and θ is the vector of parameters driving the simulations (Table 1). *LAI* is the leaf area index and *HUR1* (resp. *HUR2*) is the volumetric water content of the layer 1 (resp. the layer 2). Discretizing the model (15) using a sampling interval of Δ_t (one day), one obtains:

$$\begin{aligned} LAI_k &= [f_1(\theta)]\Delta t + LAI_{k-1} + w_{k-1}^1 \\ HUR1_k &= [f_2(\theta)]\Delta t + HUR1_{k-1} + w_{k-1}^2 \\ HUR2_k &= [f_3(\theta)]\Delta t + HUR2_{k-1} + w_{k-1}^3 \end{aligned} \tag{5}$$

where $w^j_{j\in(1,\ldots,3)}$ is a process Gaussian noise with zero mean and known variance $\sigma^2_{\gamma^j}$. In other words, we are forming the augmented state which is the vector that we wish to estimate. It can be given by a 3 by 1 matrix:

$$\begin{aligned} z_k(1,:) &\rightarrow LAI_k \\ z_k(2,:) &\rightarrow HUR1_k \\ z_k(3,:) &\rightarrow HUR2_k \end{aligned} \tag{6}$$

Table 1. Model parameters (Tremblay and Wallach, 2004).

Parameter name	Meaning	True value
ADENS (-)	Parameter of compensation between stem number and plant density	-0.8
BDENS (plants/m^2)	Maximum density above which there is competition between plants	1.25
CROIRAC (cm degree – day^{-1})	Growth rate of the root front	0.25
DLAIMAX (m^2 leaves/ m^2 soil/degreedays)	Maximum rate of the setting up of LAI	0.0078
EXTIN (-)	Extinction coefficient of photosynthetic active radiation in the canopy	0.9
KMAX (-)	Maximum crop coefficient for water requirements	1.2
LVOPT (cm root/cm^3 s)	Optimum root density	0.5
PSISTO (bars)	Absolute value of the potential of stomatal closing	10
PSISTURG (bars)	Absolute value of the potential of the beginning of decrease in the cellular extension	4
RAY ON (cm)	Average radius of roots	0.02
TCMIN (°C)	Minimum temperature of growth	6
TCOPT (°C)	Optimum temperature of growth	32
ZPENTE (cm)	Depth where the root density is 1/2 of the surface root density for the reference profile	120
ZPRLIM (cm)	Maximum depth of the root profile for the reference profile	150

Sampling data generation

To obtain original dynamic data, the model was first used to simulate the temporal responses LAI_k, $HUR1_k$, $HUR2_k$ on the basis of the recorded climatic variables. The sampling time used for discretization was 1 day. Moreover, to characterize the ability of the different approaches to estimate both the states and the parameters at the same time, 'true' parameter values were chosen (Table 1). The advantage of working by simulation rather than on real data is that the true parameter values are known. It is thus possible to calculate the quality of the estimated parameters and the predictive quality of the adjusted model for each method. The drawback is that the generality of the results is hard to know. The results may depend on the details of the model, on the way the data are generated and on the specific data that are used. The simulated values, assumed to be noise free, are shown in Figure 1. The sampling time used for discretization is 1 day and the LSM model parameters as well as other physical properties were determined by Tremblay and Wallach (2004). The evolution of LAI during the wheat's lifecycle presents the three expected phases, growth, stability and senescence. Daily variations of shallow ground water show fluctuations that were damped in the subsoil layer. These simulated states were then contaminated with zero mean Gaussian errors, i.e. the measurement noise $v_{k-1} \sim N\left(0,\sigma_v^2\right)$ where $\sigma_v^2 = 0.1$.

Estimation of state variables from noisy measurements

We consider the state vector that we wish to estimate as:

$$z_k = [LAI_k, HUR1_k, HUR2_k] \tag{7}$$

Eventually, to perform comparison between the techniques, the estimation root mean square errors (RMSE) criteria will be used and calculated on the states (with respect to the noise free data):

$$RMSE = \sqrt{E((x-\hat{x})^2)} \tag{8}$$

where x (resp. $\hat{x}$) is the true state (resp. the estimated state).

The simulation results of estimating the three states: the leaf-area index LAI_k, $HUR1_k$ the volumetric water content of the layer 1 and $HUR2_k$ the volumetric water content of the layer 2 using EKF, PF and

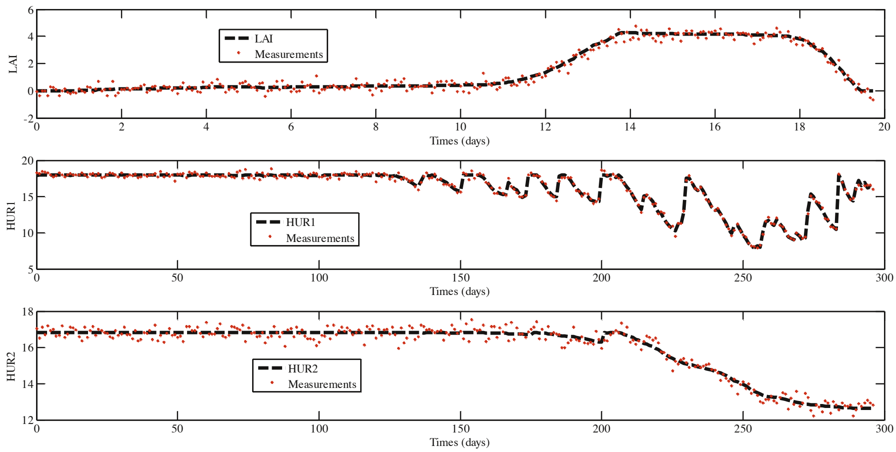

Figure 1. Simulated LSM data used in estimation: state variables (*LAI* leaf area index, *HUR1*volumetric water content of the layer 1; *HUR2* volumetric water content of the layer 2).

VF are shown in Figure 2(a,b,c), Figure 2(d,e,f) and Figure 2(g,h,i), respectively. Also, the estimation root mean square errors (RMSE) for the estimated states are shown in Table 2. It can be observed from Figure 2 and Table 2 that EKF resulted in the worst performance of all estimation techniques, which is expected due to the limited ability of EKF to accurately estimate the mean and covariance matrix of the estimated states through linearization of the non-linear process model. The results also show that the VF provides a significant improvement over the PF, which is due to the fact that the VF yields an optimal choice of the sampling distribution, $p(\alpha_k|\alpha_{k-1}, y_k)$, by minimizing a KL divergence criterion that also utilizes the observed data y_k.

Conclusions

In this paper, state estimation techniques are used to predict three state variables (Leaf area index (LAI) and soil moisture model for a winter wheat crop). Various state estimation techniques, which include the extended Kalman filter (EKF), particle filter (PF), and variational filter (VF), are compared as they are used to achieve this objective. In the comparative study, EKF, PF and VF are used to estimate the three state variables (Leaf area index (LAI) and the moisture content of the two

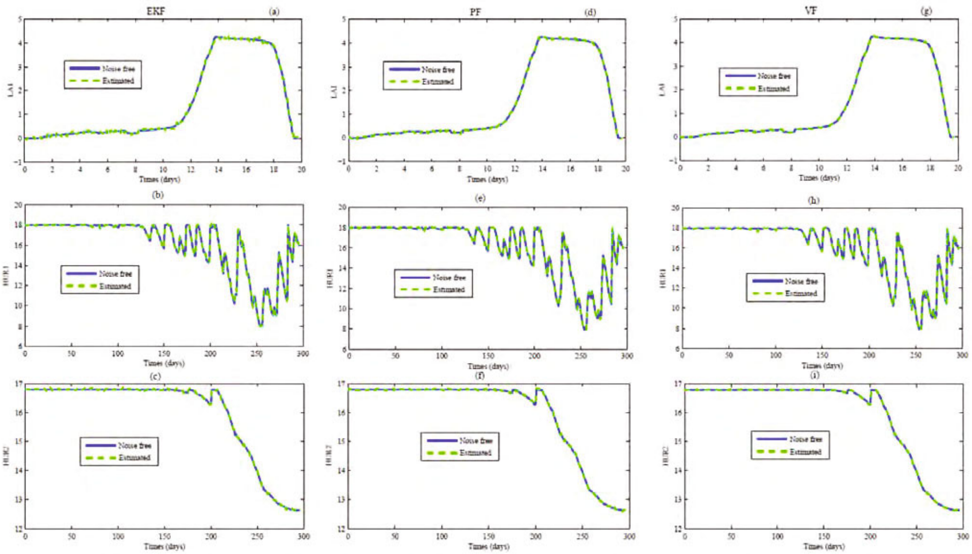

Figure 2. Estimation of state variables using various state estimation techniques.

Table 2. Root mean square errors (RMSE) of estimated states.

Technique	RMSE		
	LAI	HUR1	HUR2
EKF	0.0634	0.0598	0.0297
PF	0.0358	0.0347	0.0251
VF	0.0190	0.0187	0.0122

top soil layers) of the LSM process. The simulation results of comparative studies show that the PF provides a higher accuracy than the EKF due to the limited ability of the EKF to deal with highly non-linear process models. The results also show that the VF provides a significant improvement over the PF. This is 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 utilizes the observed data. The VF, however, still provides advantages over other methods with respect to estimation accuracy.

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