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BAYESIAN METHODS FOR PREDICTING LAI AND SOIL MOISTURE

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ABSTRACT

The prediction errors of crop models are often important due to uncertainties in the estimates of initial values of the states, in parameters, and in equations. The measurements needed to run the model are sometimes not numerous or known with some uncertainty.

In this paper, two Bayesian filtering methods were used to update the state variable values predicted by MiniSTICS model. The chosen state variates were the LAI (Leaf Area Index) of a wheat crop (*Triticum aestivum* L.) and the corresponding moisture content of two soil layers (0-20 cm and 30-50 cm). These state variates were estimated simultaneously with several parameters. The assessed filtering methods were the centralized Particle Filtering (PF) and the Variational Bayesian Filtering (VF). The former is known to be sensitive to the number of particles while the latter yields an optimal choice of the sampling distribution over the state variable by minimizing the Kullback-Leibler divergence. In fact, variational calculus leads to a simple Gaussian sampling distribution whose parameters (estimated iteratively) depends on the observed data. On basis of a case study, the VF method was found more efficient than the PF method. Indeed, with the VF, the Root Mean Square Error (RMSE) of the three estimated states was smaller and the convergence of the all parameters was ensured.

Keywords: Crop model, nonlinear states and parameters estimation, Variational Bayesian filter, LAI and soil moisture predicting, STICS model.

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, type of tillage, 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 remain important due to uncertainties in (i) the estimates of initial values of the states, (ii) the input data, (iii) the parameter values, and (iv) the equations and formalisms used to represent the reality (physically based or empirical). 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 lack of measurement accuracy is rather difficult to estimate.

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. In this context, state/parameter model estimation may be considered as an optimal filtering problem, which consists of recursively updating the posterior distribution of the unobserved state given the sequence of observed data and the state evolution model.

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 by Makowski et al. (2004). The method remains computationally efficient, but is limited by its strong assumption. The authors 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, 2009) 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 models. But till now, there are few studies with encouraging works considering simultaneous estimation of states and model parameters where the nonlinear 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 untractable (Kotecha and Djuric, 2003). To overcome this drawback, a nonparametric Monte Carlo sampling based method called Particle Filtering (PF) has recently gained popularity (Doucet and Tadic, 2003). The latter method presents several advantages since: (i) it can account for the constraint of small number of data samples, (ii) the online update of the filtering distribution and its compression are simultaneously performed, and (iii) it yields an optimal choice of the sampling distribution over the state variable by minimizing the Kullback-Leibler (KL) divergence.

Recently, a variational filtering (VF) has been proposed for solving the non linear parameter estimation problem (Mansouri et al., 2009), but till now, the method has been applied only for the tracking/localization in wireless sensor networks problem. The variational Bayesian 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 availability of small number of measured data samples, and the larger number of model parameters.

The objectives of the paper are to compare two methods (PF and VF) for estimating important state variates 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 (0-20 cm and 30-50 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 which has several advantages since it can reduce the computing and execution times and has the nice property to be good dynamic model, ensuring the robustness of data processing and estimation.

MATERIAL AND METHODS

Problem Statement

Let a nonlinear state space model be described as follows:

$$\dot{x} = g\left(x, u, \theta, w\right)$$
$$y = l\left(x, u, \theta, v\right) \tag{1}$$

where $x \in R^n$ is a vector of the state variables, $u \in R^p$ is a vector of the input variables, $\theta \in R^q$ is an unknown parameter vector, $y \in R^m$ is a vector of the measured variables, g and l are nonlinear differentiable functions, and $w \in R^n$ and $v \in R^m$ are respectively process and measurement noise. Discretizing the state space model (1), the discrete model can be written as follows:

$$x_k = f\left(x_{k-1}, u_{k-1}, \theta_{k-1}, w_{k-1}\right)$$
$$y_k = h\left(x_k, u_k, \theta_k, v_k\right) \tag{2}$$

which describes the state variables at some time step (k) in terms of their values at a previous time step ($k-1$). Let the process and measurement noise vectors have the following properties:

$$E[w_k]=0,\ E\left[w_k w_k^T\right]=Q_k,\ E[v_k]=0,\ E\left[v_k v_k^T\right]=R_k$$

Since in this problem, we are interested to estimate the state vector x_k, as well as the parameter vector θ_k, let's assume that the parameter vector is described by the following model:

$$\theta_k = \theta_{k-1} + \gamma_{k-1} \tag{3}$$

where γ_{k-1} is white noise. In other words, the parameter vector model (3) corresponds to a stationary process, with an identity transition matrix, driven by white noise. We can define a new state vector that augments the two vectors together as follows:

$$z_k = \begin{bmatrix} x_k \\ \theta_k \end{bmatrix} = \begin{bmatrix} f\left(x_{k-1}, u_{k-1}, \theta_{k-1}, w_{k-1}\right) \\ \theta_{k-1} + \gamma_{k-1} \end{bmatrix} \tag{4}$$

where $z_k \in R^{n+q}$ is assumed to follow a Gaussian model as $z_k \sim N(\mu_k, \lambda_k)$, and where at any time k the expectation μ_k and the covariance matrix λ_k are both constants. Also, defining the augmented vector,

$$\varepsilon_{k-1} = \begin{bmatrix} w_{k-1} \\ \gamma_{k-1} \end{bmatrix} \tag{5}$$

the model (2) can be written as:

$$\begin{aligned} z_k &= \Im\left(z_{k-1}, u_{k-1}, \varepsilon_{k-1}\right) \\ y_k &= \Re\left(z_k, u_k, v_k\right) \end{aligned} \tag{6}$$

Variational Bayesian Filter

The distribution of interest for state estimation takes the form of a marginal posterior distribution $p\left(z_k \mid y_{1:k}\right)$. The variational Bayesian method is proposed for approximating intractable integrals arising in Bayesian statistics. Using a separable approximating distribution $q(z_k) = \prod_i q(z_k^i)$ to minimize the lower bound of the marginal likelihood, an analytical approximation of the posterior probability $p\left(z_k \mid y_{1:k}\right)$ is provided by minimizing the Kullback-Leibler (KL) divergence:

$$D_{KL}(q\|p) = \int q(z_k)\log\frac{q(z_k)}{p(z_k|y_{1:k})}dz_k \qquad (7)$$

where $q(z_k) = \prod_i q(z_k^i)$.

To minimize the KL divergence subject to the constraint $\int q(z_k)dz_k = 1 = \prod_i \int q(z_k^i)dz_k^i = 1$, the Lagrange multiplier method is used, yielding the following approximate distribution (Vermaak et al., 2003),

$$q(z_k^i) \propto exp < \log p(y_{1:k}, z_k) >_{\prod_{j\neq i} q(z_k^j)}, \qquad (8)$$

where $<.>_{q(z_k^j)}$ denotes the expectation operator relative to the distribution $q(z_k^j)$. Therefore, these dependent parameters can be jointly and iteratively updated. Taking into account the separable approximate distribution $q(z_{k-1})$ at time $k-1$, the filtering distribution $p(y_{1:k}, z_k)$ is sequentially approximated according to the following scheme:

$$\hat{p}(y_{1:k}, z_k) \propto p(y_k, z_k)p(z_k) \qquad (9)$$

Therefore, through a simple integral with respect to μ_{k-1}, the filtering distribution $p(z_k|y_{1:k})$ can be sequentially updated. However, the state z_k does not have a tractable approximate distribution because of the nature of the system model. By combining equations (8) and (9), we have

$$q(z_k) \propto p(y_k, z_k)N\left(<\mu_k>,<\lambda_k>\right) \qquad (10)$$

This form immediately suggests an IS procedure, where samples are drawn from the Gaussian distribution $N(<\mu_k>,<\lambda_k>)$ and weighted according to their likelihoods:

$$z_k^{(i)} \sim N\left(<\mu_k>,<\lambda_k>\right), l_k^{(i)} \propto \prod_{j=1}^N p\left(z_k^j|y_{1:k}^{(i)}\right) \qquad (11)$$

Then, the estimate of the augmented state $\hat{z}_k$ can be approximated by a Monte Carlo scheme:

$$\hat{z}_k = \sum_{i=1}^N z_k^{(i)}l_k^{(i)} \qquad (12)$$

In the Bayesian inference framework, besides updating the filtering distribution $p(z_k|y_{1:k})$, the predictive distribution $p(z_k|y_{1:k-1})$ needs to be computed. The predictive distribution $p(z_k|y_{1:k-1})$ can be efficiently updated by variational inference. Taking into account the separable approximate

distribution $q(z_{k-1}) \propto p(z_{k-1}|y_{k-1})$, the predictive distribution can be expressed as

$$p(z_k \,|y_{1:k-1}) = \int p(z_k \,|z_{k-1})q(z_{k-1})\,dz_{k-1} \qquad (13)$$

The predictive distribution that minimizes the Kullback-Leibler divergence yields the following Gaussian distribution:

$$q_{k|k-1}(z_k) = N\left(<\mu_k>_{q_{k|k-1}}, <\lambda_k>_{q_{k|k-1}}\right) \qquad (14)$$

and the predictive expectations of the state can be evaluated by the following expressions:

$$<z_k>_{q_{k|k-1}} = <\mu_k>_{q_{k|k-1}},$$

$$<z_k z_k^T>_{q_{k|k-1}} = <\lambda_k>_{q_{k|k-1}}^{-1} + <\mu_k>_{q_{k|k-1}} <\mu_k>_{q_{k|k-1}}^T \qquad (15)$$

Compared with the PF, the computational cost and the memory requirements associated with the VF are dramatically reduced by the variational approximation in the prediction phase. In fact, the expectations involved in the computation of the predictive distribution have closed forms, avoiding the use of Monte Carlo integration.

Case study and crop model presentation

The original data were issued from experiments carried out on a silty soil in Belgium, with a wheat crop (*Triticum aestivum* L., cultivar Julius), during 3 consecutive years, the crop seasons 2008-09, 2009-10 and 2010-11. A wireless monitoring system (eKo pro series system, Crossbow) completed by a micrometeorological station was used for measuring continuously soil and climate characteristics. Especially, the measurements of soil water content were performed at 20 and 50 cm depth. The plant characteristics (LAI and biomass) were also measured using reference techniques at regular intervals along the crop seasons.

The model for which the methods were tested is Mini STICS model (Makowski et al., 2004). These are the 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 explanatory 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. The model structure can be derived from the basic conservation laws, namely material and energy balances. However, the model involves several parameters that are usually not known, which include the radiation use efficiency which expresses 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 are presented at Table 1. The parameter values were the ones determined in Makowski et al. (2004).

Problem Formulation

Based on the equations described in Makowski et al. (2004), the mathematical model LSM of the LAI and Soil Moisture is given by:

$$
\begin{aligned}
LAI(t-1) &= f_1(LAI(t-1)+\theta) \\
HUR1(t) &= f_1(HUR1(t-1)+\theta) \\
HUR2(t) &= f_1(HUR2(t-1)+\theta)
\end{aligned}
\tag{16}
$$

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 (16) using a sampling interval of Δt (one day), it can be written as,

$$
\begin{aligned}
LAI_k &= [g_1(\theta)]\Delta t &&+ LAI_{k-1} + w_{k-1}^1 \\
HUR1_k &= [g_2(\theta)]\Delta t &&+ HUR1_{k-1} + w_{k-1}^2 \\
HUR2_k &= [g_3(\theta)]\Delta t &&+ HUR2_{k-1} + w_{k-1}^3
\end{aligned}
\tag{17}
$$

where $w_{j\in\{1,\ldots,3\}}^j$ is a process Gaussian noise with zero mean and known variance $\sigma_{\gamma^j}^2$. Up to now, the model (17) assumes that the parameters θ are constant. These parameters are $ADENS, DLAIMAX$, and $PSISTURG$. $ADENS$ is the parameter of compensation between stem number and plant density, $DLAIMAX$ is the maximum rate of the setting up of LAI, and $PSISTURG$ is the absolute value of the potential of the beginning of decrease in the cellular extension. If we are interested in estimating some (or all) of these parameters, the equations describing their evolution are also needed:

$$
\begin{aligned}
ADENS_k &= ADENS_{k-1} + \gamma_{k-1}^1 \\
DLAIMAX_k &= DLAIMAX_{k-1} + \gamma_{k-1}^2 \\
PSISTURG_k &= PSISTURG_{k-1} + \gamma_{k-1}^3
\end{aligned}
\tag{18}
$$

where $\gamma_{j\in\{1,\ldots,3\}}^j$ is a process Gaussian noise with zero mean and known variance $\sigma_{\gamma^j}^2$. Combining (17) and (18), one obtains:

Table 1. LSM model parameters and physical properties

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(m2.l.s.m−2.degreedays−1)	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

$$f_1 : LAI_k = [g_1(\theta_{k-1})]\Delta t + LAI_{k-1} + w_{k-1}^1$$
$$f_2 : HUR1_k = [g_2(\theta_{k-1})]\Delta t + HUR1_{k-1} + w_{k-1}^2$$
$$f_3 : HUR2_k = [g_3(\theta_{k-1})]\Delta t + HUR2_{k-1} + w_{k-1}^3$$

$$f_4 : ADENS_k = ADENS_{k-1} + \gamma_{k-1}^1$$
$$f_5 :: DLAIMAX_k = DLAIMAX_{k-1} + \gamma_{k-1}^2$$
$$f_6 : PSISTURG_k = PSISTURG_{k-1} + \gamma_{k-1}^3$$

$$(19)$$

where $f_{k\in\{1,...,6\}}$ are some nonlinear functions and where $w = (w_1, w_2, w_3)^T$ and $\gamma = (\gamma_1, \gamma_2, \gamma_3)^T$ are respectively the measurement and process noise vector, which quantify randomness at both levels. In other words, we are forming the augmented state: $z_k = (x_k, \theta_k)^T$ which is the vector that we wish to estimate. It can be given by a 6 by 1 matrix:

$$x_k(1,:) \rightarrow LAI_k$$
$$x_k(2,:) \rightarrow HUR1_k$$
$$x_k(3,:) \rightarrow HUR2_k$$
$$x_k(4,:) \rightarrow ADENS_k$$
$$x_k(5,:) \rightarrow DLAIMAX_k$$
$$x_k(6,:) \rightarrow PSISTURG_k$$

$$(21)$$

The idea here is that, if a dynamic model structure is available and if dynamic measurements of the state variables are available, the model parameters can be estimated using one of state estimation technique. State estimation is a system-engineering approach, in which the states (and sometimes the parameters) of a state space model can be estimated given time-series dynamic measurements of some of the state variables. In this work, the PF and VF will be used as state estimation technique. Their abilities to solve this nonlinear state estimation problem will be tested through different cases, which are summarized below. In all cases, it is assumed that three states ($LAI, HUR1$ and $HUR2$) are measured.

i) Case 1: the three states ($LAI, HUR1$ and $HUR2$) along with the parameter $ADENS$ be estimated.
ii) Case 2: the three states ($LAI, HUR1$ and $HUR2$) along with the parameter $ADENS$, and $DLAIMAX$ will be estimated.
iii) Case 3: the three states ($LAI, HUR1$ and $HUR2$) along with the parameter $ADENS$, $DLAIMAX$ and $PSISTURG$ will be estimated.

Sampling data generation

To go further in the research, data to run the model are necessary. To generate these original dynamic data, the model was first used to simulate the responses LAI_k, $HUR1_k$, $HUR2_k$ as functions of time of the first recorded

climatic variable of the crop season "2008-2009". The sampling time used for discretization was 1 day.

Moreover, to characterize the ability of the different approaches to estimate both at same time, the states and the parameters, we have chosen "true" parameter values (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 so obtained simulated states, which are assumed to be noise free, are then contaminated with zero mean Gaussian errors, i.e., the measurement noise $v_{k-1} \sim N(0, \sigma_v^2)$, where $\sigma_v^2 = 0.1$.
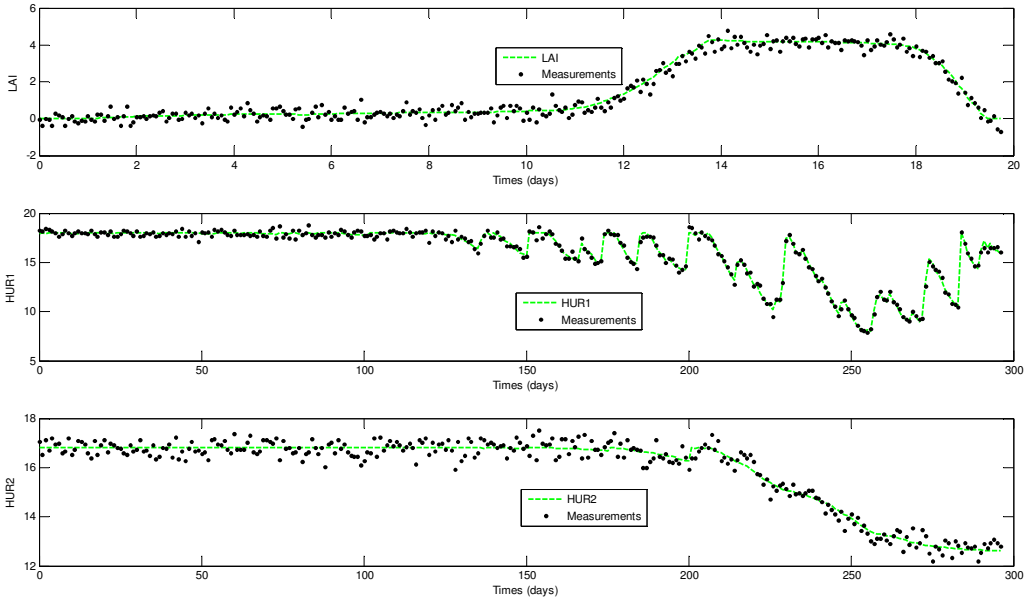

Fig. 1. Simulated LSM data used in estimation: state variables (*LAI* leaf area index, *HUR*1 volumetric water content of the layer 1; *HUR*2 volumetric water content of the layer 2).

SIMULATIONS RESULTS ANALYSIS

In this section, we are interested in examining the effect of the number of estimated parameters on the estimation performances of PF and VF and in estimating the states and parameters of the LSM process model.

State and parameter estimation results corresponding to case 1 and 3 and using PF and VF are shown in Fig. 2 to 5. Table 2 compare the estimation performances of PF and VF for case 1 in terms of RMSE for the three states *LAI*, *HUR*1 and *HUR*2 (with respect to the noise free data) and the mean of the estimated

parameter $DLAIMAX$ at steady state. Tables 3, and 4 provide similar comparisons for cases 2 and 3, respectively, (i.e., estimating the three states and the parameters $ADENS$ and $DLAIMAX$ in case 2, and estimating the three states and the parameters $ADENS$, $DLAIMAX$ and $PSISTURG$ in case 3).

Comparing the estimation performances of PF and VF, it has been observed, as expected, that the root mean square errors (RMSE) of estimated states increase for both estimation techniques as the number of estimated states and parameters increases.

Table 2. Root mean square errors (RMSE) of estimated states and mean of estimated parameters - case 1

Technique	RMSE			Mean at steady state
	LAI	$HUR1$	$HUR2$	$ADENS$
PF	0.0365	0.0376	0.0257	−0.8
VF	0.0198	0.0191	0.0126	−0.8

Table 3. Root mean square errors (RMSE) of estimated states and mean of estimated parameters – case 2

Technique	RMSE			Mean at steady state	
	LAI	$HUR1$	$HUR2$	$ADENS$	$DLAIMAX$
PF	0.0790	0.0808	0.0533	−0.8	0.0078
VF	0.0378	0.0389	0.0245	−0.8	0.0078

Table 4. Root mean square errors (RMSE) of estimated states and mean of estimated parameters - case 3

Technique	RMSE			Mean at steady state		
	LAI	$HUR1$	$HUR2$	$ADENS$	$DLAIMAX$	$PSISTURG$
PF	0.1146	0.1186	0.0774	−0.8	0.0078	did not converge
VF	0.0608	0.0586	0.0369	−0.8	0.0078	0.0078

VF shows improved estimation performance over PF in estimating the states and parameters in all cases. The RMSE of the estimated states (with respect to the noise free data) is higher using PF than VF. The parameters convergence to the true value is obtained more quickly with VF than PF. Furthermore, in case 3, where three parameters ($ADENS$, $DLAIMAX$ and $PSISTURG$) had to be estimated, the estimate of $PSISTURG$ did not converge to the true value while a convergence was quickly obtained with VF.
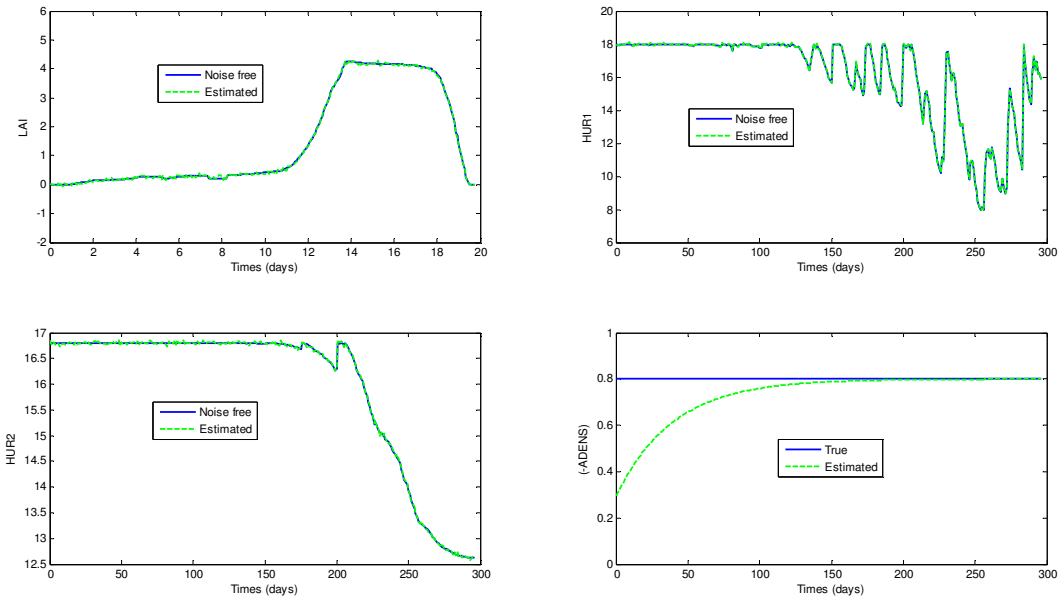
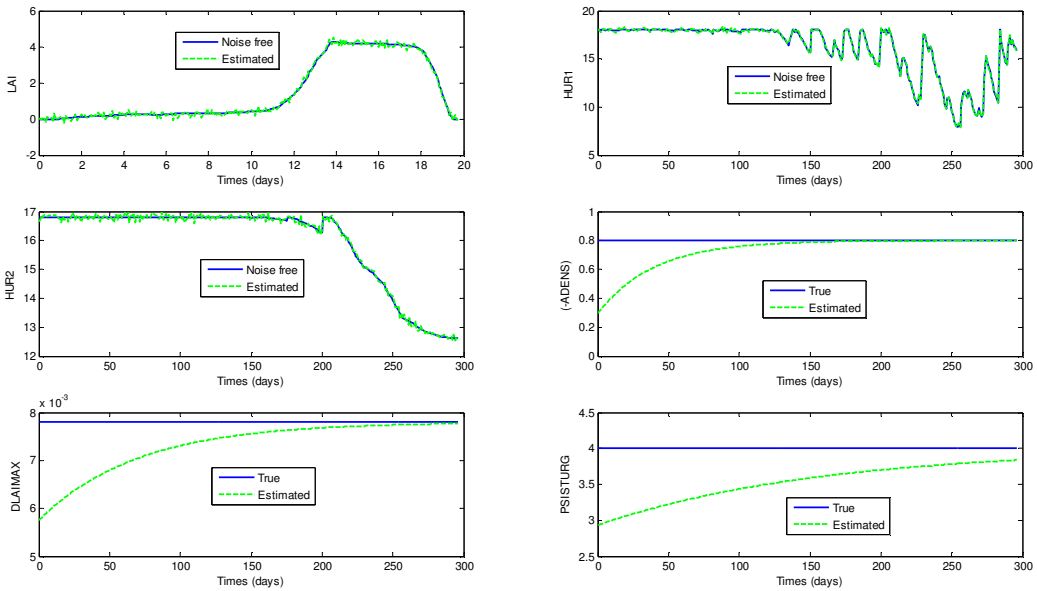**Fig. 2. Estimation using PF - Case 1: Estimation of LAI, HUR1, HUR2; ADENS.**

Fig. 3. Estimation using PF - Case 3: Estimation of LAI, HUR1, HUR2; ADENS, DLAIMAX, PSISTURG.
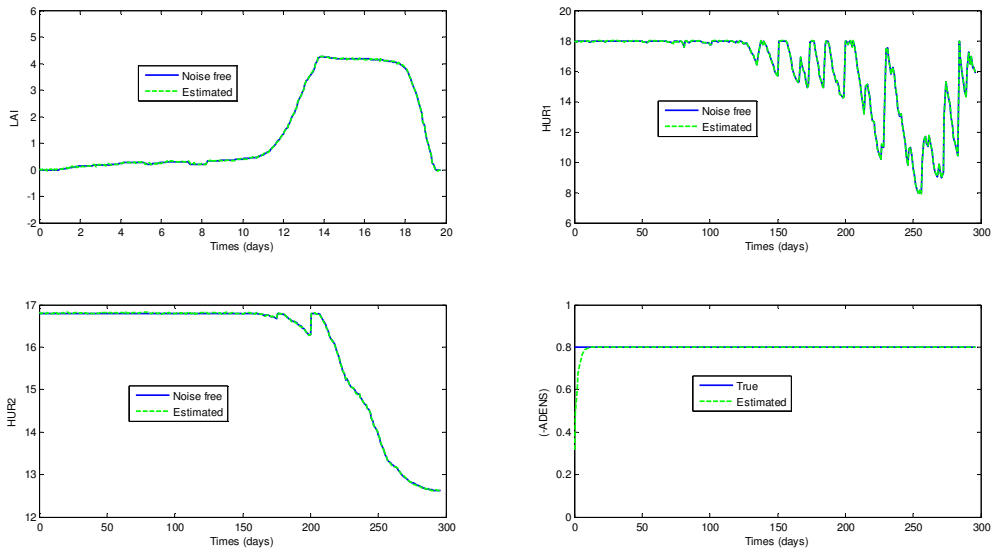
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Fig. 4. Estimation using VF - Case 1: Estimation of LAI, HUR1, HUR2; ADENS.
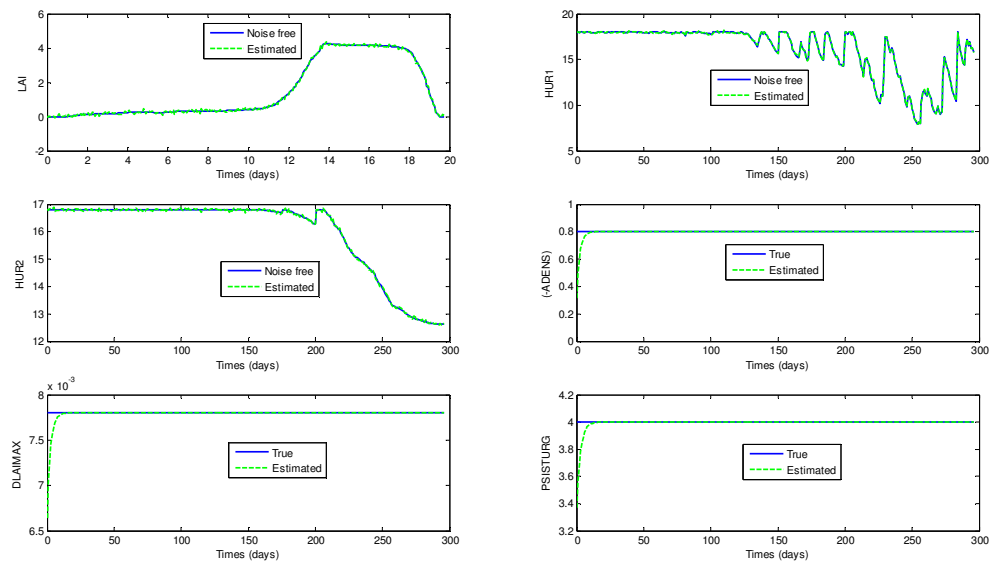

Fig. 5. Estimation using VF - Case 3: Estimation of LAI, HUR1, HUR2; ADENS, DLAIMAX, PSISTURG.

CONCLUSIONS

A Bayesian filtering was applied on a nonlinear dynamic crop model, considered as a system assumed to progress according to a probabilistic state space model. The aim was to predict simultaneously three state variates (Leaf Area Index and soil moisture of two soil horizons) and several parameters. It has been shown that the variational Bayesian filter approach guarantees observer convergence. Furthermore, the proposed algorithm has a low computation complexity since it is directly based on the Gaussian predictive distribution of the state variable. In addition, when the number of states and parameters to estimate increases, variational Bayesian filtering also offers a benefit because it does not require us to calculate Jacobian matrices. In addition, the convergence speed of states and parameters estimation can be adjusted independently.

This conclusion could be established as we compared our method with the centralized particle filtering. Detailed case studies presented in this paper demonstrate the significantly improved performance of our approach for highly nonlinear estimation problems.

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