PREDICTING WINTER WHEAT BIOMASS AND GRAIN PROTEIN CONTENT

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Abstract

This paper addresses the problem of predicting biomass and grain protein content using improved particle filtering (IPF). First, we propose to use the IPF for improving nonlinear and non-Gaussian crop model predictions. In case of standard particle filtering (PF), the latest observation is not considered for the evaluation of the weights of the particles as the importance function is taken to be equal to the prior density function. Unlike the PF which depends on the choice of sampling distribution used to estimate the posterior distribution, the IPF yields an optimum choice of the sampling distribution based on minimizing Kullback-Leibler divergence, which also accounts for the observed data. Second, we apply the state estimation techniques PF and IPF for predicting biomass and grain protein content. In a first step, we present an application of the IPF to a simple dynamic crop model with the aim to predict a single state variable, namely winter wheat biomass. In a second step, we apply the IPF for updating predictions of complex nonlinear crop models in order to predict protein grain content. The performance of the estimation techniques is evaluated on a synthetic example in terms of estimation accuracy and root mean square error.

Keywords: Crop model; Bayesian methods; Grain protein; Biomass.

1. Introduction

Dynamic crop models such as EPIC [1], WOFOST [2], DAISY[3], STICS [4], and SALUS [5] are 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,…). They are developed to predict crop yield and quality or to optimize the farming practices in order to satisfy agricultural 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.

For example, it is useful to predict the evolution of variables, such as the biomass and the grain protein content during the crop lifecycle. State estimation techniques can be of a great value to solve that problem since they have the potential to estimate simultaneously the variables and several parameters. As an example, involved parameters are the radiation use efficiency, the maximal value of the ratio of intercepted to incident radiation, the coefficient of extinction of radiation, the maximal value of LAI, ... The estimation problem that is addressed here can be viewed as an optimal filtering problem, in which the posterior distribution of the unobserved state, given the sequence of observed data and the state evolution model, is recursively updated.

Several state estimation techniques are developed and used to estimate state and parameters in environmental systems [6, 7, 8, 9]. These techniques include the extended Kalman filter (EKF) [10, 11], the unscented Kalman filter (UKF) [11, 12], the particle filter (PF) [13, 14], the variational Bayesian filter (VBF) [15, 16, 17, 18] and more recently the improved particle filter (IPF) [19].

The objectives of this paper are twofold. The first objective is to use improved Particle filtering (IPF) based on Kullback-Leibler divergence minimization for improving nonlinear and non-Gaussian crop model predictions, by assuming time-varying statistical parameters.

The second objective is to apply the state estimation techniques PF and IPF for predicting biomass and grain protein content. In a first step, we present an application of the IPF to a simple dynamic crop model with the aim to predict a single state variable, namely winter wheat biomass. In a second step, we apply the IPF for updating predictions of complex nonlinear crop models in order to predict protein grain content.

The rest of the paper is organized as follows. In Section 2, a description of an improved particle filtering for nonlinear crop model predictions is presented. Then, in Section 3, the performances of the proposed new improved particle filtering are evaluated and compared to the standard particle filtering through the application cases. Finally, some concluding remarks are presented in Section 4.

2. Description of Improved Particle Filtering

Particle filtering suffers from one major drawback. Its efficient implementation requires the ability to sample from $p\left(z_k \mid z_{k-1}\right)$, which does not take into account the current observed data, y_k, and thus many particles can be wasted in low likelihood (sparse) areas [20]. This issue is addressed by the

proposed improved particle filter (IPF), which is described in the next sub-section.

2.1. Improved Particle Filtering (IPF)

The distribution of interest for the state takes the form of a marginal posterior distribution $p(z_k|y_{0:k})$. The proposed extended Bayesian sampling algorithm (also named as improved particle filtering, IPF) is proposed for approximating intractable integrals arising in Bayesian statistics. By using a separable approximating distribution $\hat{q}(z_k) = \hat{q}(z_k|z_{0:k-1}, y_{0:k}) = \Pi_i \hat{q}(z_k^i)$ to lower bound the marginal likelihood, an analytical approximation to the posterior probability $p(z_k|y_{0:k})$ is provided by minimizing the Kullback-Leibler divergence (KLD) [18]:

$$D_{KL}(\hat{q}\|p) = \int \hat{q}(z_k|z_{0:k-1}, y_{0:k}) \log \frac{\hat{q}(z_k|z_{0:k-1}, y_{0:k})}{p(z_k|z_{0:k-1}, y_{0:k})} dz_k \quad (1)$$

Where,

$$\hat{q}(z_k|z_{0:k-1}, y_{0:k}) = \Pi_i \hat{q}(z_k^i|z_{0:k-1}, y_{0:k}) = \hat{q}(z_k)\hat{q}(\mu_k)\hat{q}(\lambda_k) \quad (2)$$

Minimizing the KLD subject to the constraint $\int \hat{q}(z_k)dz_k = \Pi_i \int \hat{q}(z_k^i)dz_k^i = 1$, the Lagrange
multiplier scheme is used to yield the following approximate distribution [21],

$$\hat{q}(z_k^i) \propto \exp\left[E\left(\log(p(y_{0:k}, z_k)\right)_{\Pi j \neq i \hat{q}(z_k^j)}\right] \quad (3)$$

where $E\left(\log(p(y_{0:k}, z_k)\right)_{\Pi j \neq i \hat{q}(z_k^j)}$ denotes the expectation operator relative to the distribution $\hat{q}(z_k^j)$. Therefore, these dependent parameters can be jointly and iteratively updated. Taking into account the separable approximate distribution $\hat{q}(z_{k-1}^j)$ at time $k-1$, the posterior distribution $p(z_k|y_{0:k})$ is sequentially approximated according to the following scheme:

$$\hat{p}(z_k|y_{0:k}) \propto p(y_k|z_k)p(z_k, \lambda_k|\mu_k)q_p(\mu_k) \quad (4)$$

where $$q_p(\mu_k) = \int p(\mu_k|\mu_{k-1})\hat{q}(\mu_{k-1})d\mu_{k-1}$$

Hence, the particles $\{z_{0:k}^{(i)}\}_{i=0}^{N}$ are sampled according to the following optimal function:

$$\hat{q}(z_k^i) = \int \mathrm{N}(z_k^i | \mu_k, \lambda_k) p(\mu_k, \lambda_k | z_k^i) p(z_k | z_k^i) \hat{q}(\mu_{k-1}) d\mu_k d\lambda_k \quad (5)$$

The recursive estimate of the importance weights can be derived as follows:

$$l_k^{(i)} = l_k^{(i-1)} \frac{p(y_{0:k} | z_{0:k}^{(i)}) p(z_k^{(i)} | z_{0:k-1}^{(i)})}{\hat{q}(z_k | z_{0:k-1}, y_{0:k})} \quad (6)$$

Equation (5) provides a mechanism to sequentially update the importance weights, given an appropriate choice of proposal distribution, $\hat{q}(z_k | z_{0:k-1}, y_{0:k})$. Then, the estimate of the augmented state $\hat{z}_k$ can be approximated by a Monte Carlo scheme as follows:

$$\hat{z}_k = \sum_{i=0}^{N} l_k^{(i)} z_k^{(i)} \quad (7)$$

3. Simulation Results Analysis

3.1. Case 1 : A simple example: a dynamic model simulating wheat biomass

3.1.1. The overall formalism

In this section, we describe a simple dynamic crop model that will be used to compare the performances of PF and IPF. The crop model has a single state variable representing above-ground winter-wheat biomass. This state variable is simulated on a daily basis in function of the daily temperature and the daily incoming radiation according to the classical method presented in ([22]). The biomass at time *k*+1 is linearly related to the biomass at time *k* as follows:

$$Biom_{k+1} = Biom_k + E_b E_{i\max} \left(1 - e^{-K LAI_k}\right) PAR_k + w_k \quad , \quad (8)$$

where k is the day number since sowing, $Biom_k$ is the true above-ground plant biomass on day k, PAR_k is the incoming photossynthetically active radiation on day k, LAI_k is the leaf-area index on day k and w_k is a random term representing the model error. The crop biomass at sowing is set equal to zero: $Biom_1 = 0$. LAI_k

is calculated in function of the cumulative degree-days (over a basis of 0°C) from sowing until day k, noted T_t , as follows ([23]):

$$LAI_k = L_{\max}\left(\frac{1}{1+e^{-A[T_k - T_{s1}]}} - e^{-B[T_k - T_{s2}]}\right), \quad (9)$$

where the parameter T_{s2} is set equal to $\frac{1}{B\log\left(1+e^{AT_{s1}}\right)}$ in order to have $LAI_1 = 0$.

The model includes two input variables $X_k = [T_k, PAR_k]'$ and seven parameters $\left(E_b, E_{i\max}, K, L_{\max}, A, B, T_{s1}\right)$. E_b is the radiation use efficiency which expresses the biomass produced per unit of intercepted radiation, $E_{i\max}$ is the maximal value of the ratio of intercepted to incident radiation, K is the coefficient of extinction of radiation, $L_{\max}$ is the maximal value of LAI, T_{s1} defines a temperature threshold, and A and B are two additional parameters. At this stage, the parameter values are assumed to be known and obtained from ([23]).

We suppose that N measurements of biomass, $y_1, y_2, y_3, \ldots, y_N$, are made at different times before harvest on the site-year of interest. In practice, values of y_k can be derived from plant samples or from remote-sensing data. We assume that each measurement y_k is related to the biomass $Biom_k$ by

$$y_k = Biom_k + v_k \quad (10)$$

where v_k is a random term representing measurement errors. In the next section we show how such measurements can be used to improve the accuracy of biomass predictions.

3.1.2. Numerical application

3.1.2.1. Estimation of the biomass

Based on the equation (10), the Biomass is estimated at each date of measurement using both PF and IPF algorithms (Fig. 1). Table 1 illustrates the Root Mean Square Error (RMSE) using the two algorithms PF and IPF. Fig. 1 and Table 1 show that IPF outperforms PF, these advantages of the IPF are due to the fact it provides an optimum choice of the sampling distribution used to approximate the posterior density function, which also accounts for the observed data.

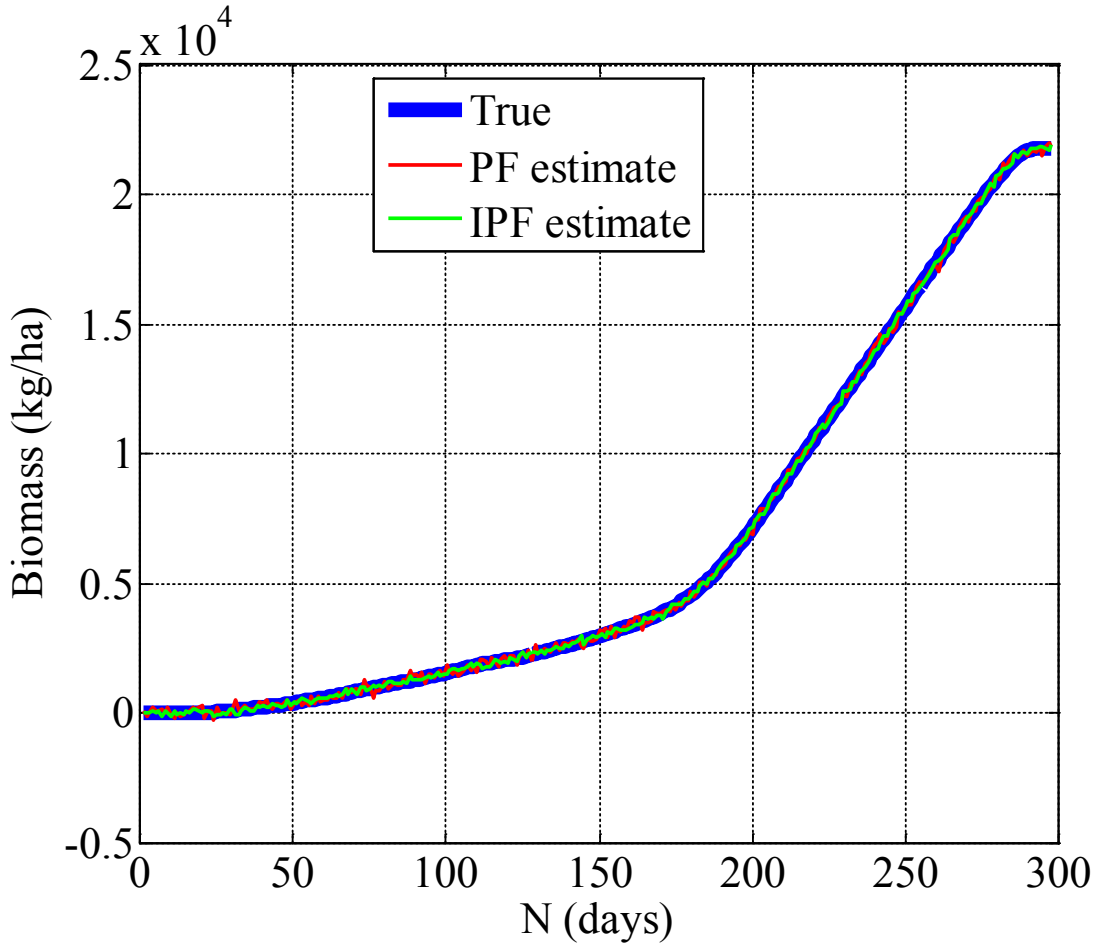

Fig. 1. Estimation of state variable Biomass versus N (days) using PF and IPF techniques.

Technique	ERROR Biomass Kg/ha
PF	6.113
IPF	4.245

Table 1. ERROR of estimated Biomass

3.2. Case 2 : IPF for complex nonlinear crop models

3.2.1. The overall formalism

A nonlinear complex crop model can be defined by:

$$x_k = f\left(x_{k-1}, u_{k-1}, \theta_{k-1}, w_{k-1}\right) \quad (11)$$

Suppose that a measurement y_k is available at time k and that y_k is related to the state variable vector by:

$$y_k = h(x_k, u_k, \theta_k, v_k) \tag{12}$$

Note that in equations (11) and (12). The process and measurement noise vectors have the following properties:

$$E[w_k] = 0, \quad E[w_k w_k^T] = Q_k, \quad E[v_k] = 0, \quad E[v_k v_k^T] = R_k.$$

The function f is used to predict the value of the state vector at some time step (k) given its value at the previous time step $(k-1)$, and the function h relates the measured vector (y_k) to the state vector (x_k) at the same time step. 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, and the matrices, Q_k and R_k represent the covariance matrices of the process and measurement noise vectors, respectively.

Since 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:

$$\theta_k = \theta_{k-1} + \gamma_{k-1} \tag{13}$$

where γ_{k-1} is white noise. In other words, the parameter vector model (13) 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:

$$z_k = \begin{bmatrix} x_k \\ \theta_k \end{bmatrix} = \begin{bmatrix} f(x_{k-1}, u_{k-1}, \theta_{k-1}, w_{k-1}) \\ \theta_{k-1} + \gamma_{k-1} \end{bmatrix} \tag{14}$$

where z_k 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,

$$\varepsilon_{k-1} = \begin{bmatrix} w_{k-1} \\ \gamma_{k-1} \end{bmatrix} \quad (15)$$

the models (11) and (12) can be written as:

$$\begin{aligned} z_k &= \Im\left(z_{k-1}, u_{k-1}, \varepsilon_{k-1}\right) \\ y_k &= \Re\left(z_k, u_k, v_k\right) \end{aligned} \quad (16)$$

where the two nonlinear differentiable functions $\Im$ and $\Re$ in equation (16) are nonlinear differentiable functions that describe the changes in the state variables over discrete time. The function $\Im$ is used to predict the value of the state vector at some time step (k) given its value at the previous time step $(k-1)$, and the function $\Re$ relates the measured vector y_k to the state vector z_k at the same time step.

3.2.2. Application to a crop model predicting grain protein content

The AZODYN crop model ([24]) is a nonlinear dynamic model simulating winter-wheat crop in function of environmental variables (characteristics of the crop at the end of winter, soil characteristics, climate) and of nitrogen fertilization (dates and rates of fertilizer applications). We consider a particular site-year (2008-2009). This model can be used to predict grain yield, soil mineral nitrogen, and grain protein content at harvest. AZODYN is a useful tool for studying the effects of nitrogen management on crop yield, grain quality and risk of pollution by nitrate ([25]). Before flowering, five state variables are simulated each day by AZODYN: nitrogen uptake (NU), dry matter (DM), nitrogen-nutrition index (NNI), leaf-area index (LAI), soil mineral nitrogen supply (SNS). We consider chlorophyll-content measurements obtained with a chlorophyll meter. These measurements are correlated to one of the model state variables, namely nitrogen uptake, and can be easily performed by farmers, collecting-firm operators, or farmers' advisors. Here, we suppose that only one chlorophyll-content measurement is performed at flowering and that this measurement is linearly related to the model state variables as follows:

$$\mathrm{y}m_k = \mu + H\mathrm{x}m_k + \mathrm{vm}_k \quad (17)$$

where $\mathrm{y}m_k$ and $\mathrm{x}m_k$ are, respectively, the chlorophyll-content measurement and the (5×1) vector of the true state-variable values at flowering, μ is an intercept parameter, and H is a one-row matrix defined by $H = (\alpha,0,0,0)$ where α is

the slope of the linear equation relating the measurement to nitrogen uptake. We assume that the error term vm_k is Normally distributed, $vm_k \sim N(0,R)$. The IPF is used to update the five states variables nitrogen uptake (NU), dry matter (DM), nitrogen-nutrition index (NNI), leaf-area index (LAI), soil mineral nitrogen supply (SNS) given a single chlorophyll-content measurement ym_k performed at flowering. Yield and grain protein content at harvest are then estimated from the updated state variables.

Figures 2, 3 and Table 2 show the estimation of the two states variables Yield and grain protein content using PF and IPF. The results show the performance of IPF over PF, the efficiency of IPF is due to the fact it uses the KLD divergence to compute the optimum sampling distribution used to approximate the posterior density function, which also accounts for the observed data.

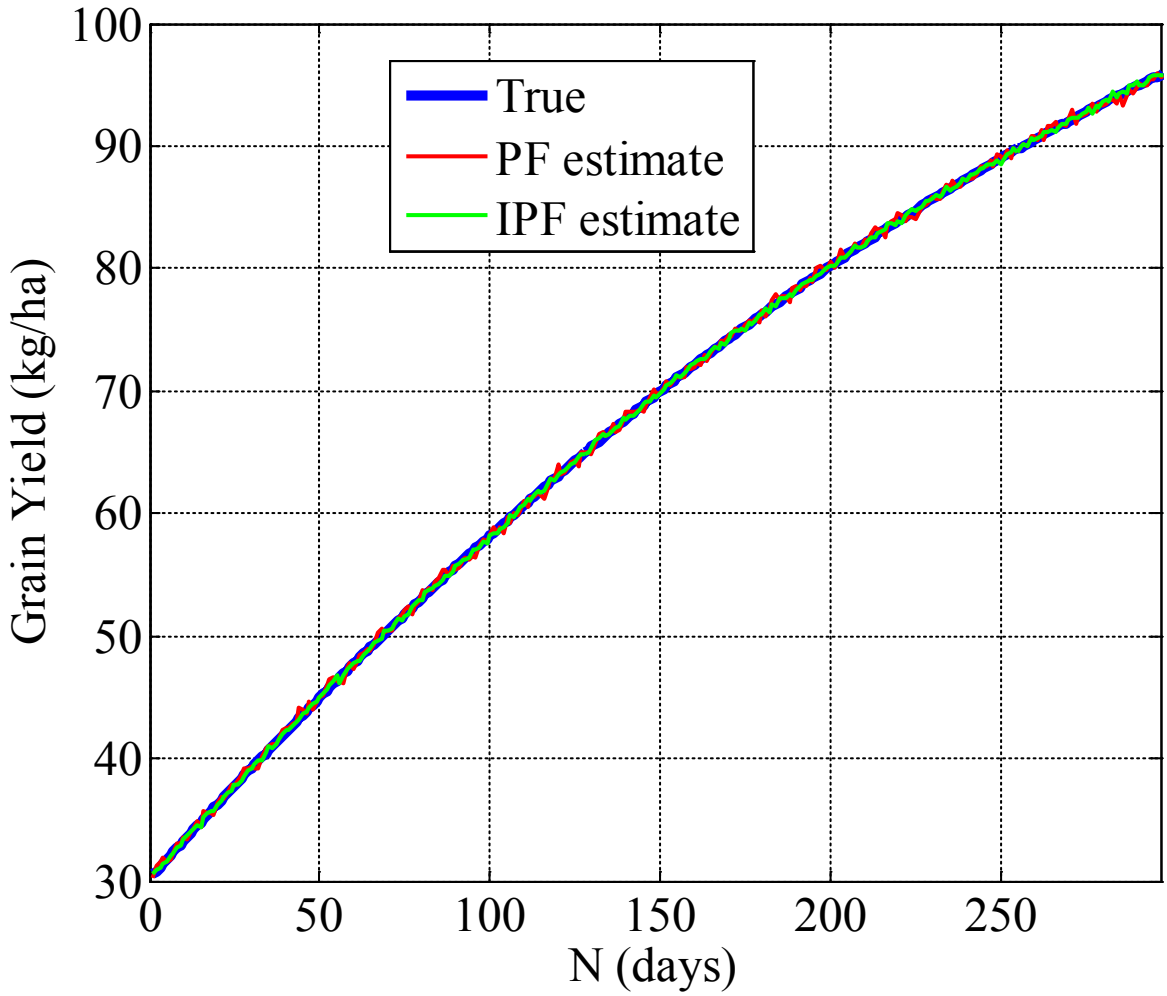

Fig. 2. Updated value of grain protein content (kg/ha) versus N (days) using PF and IPF techniques.

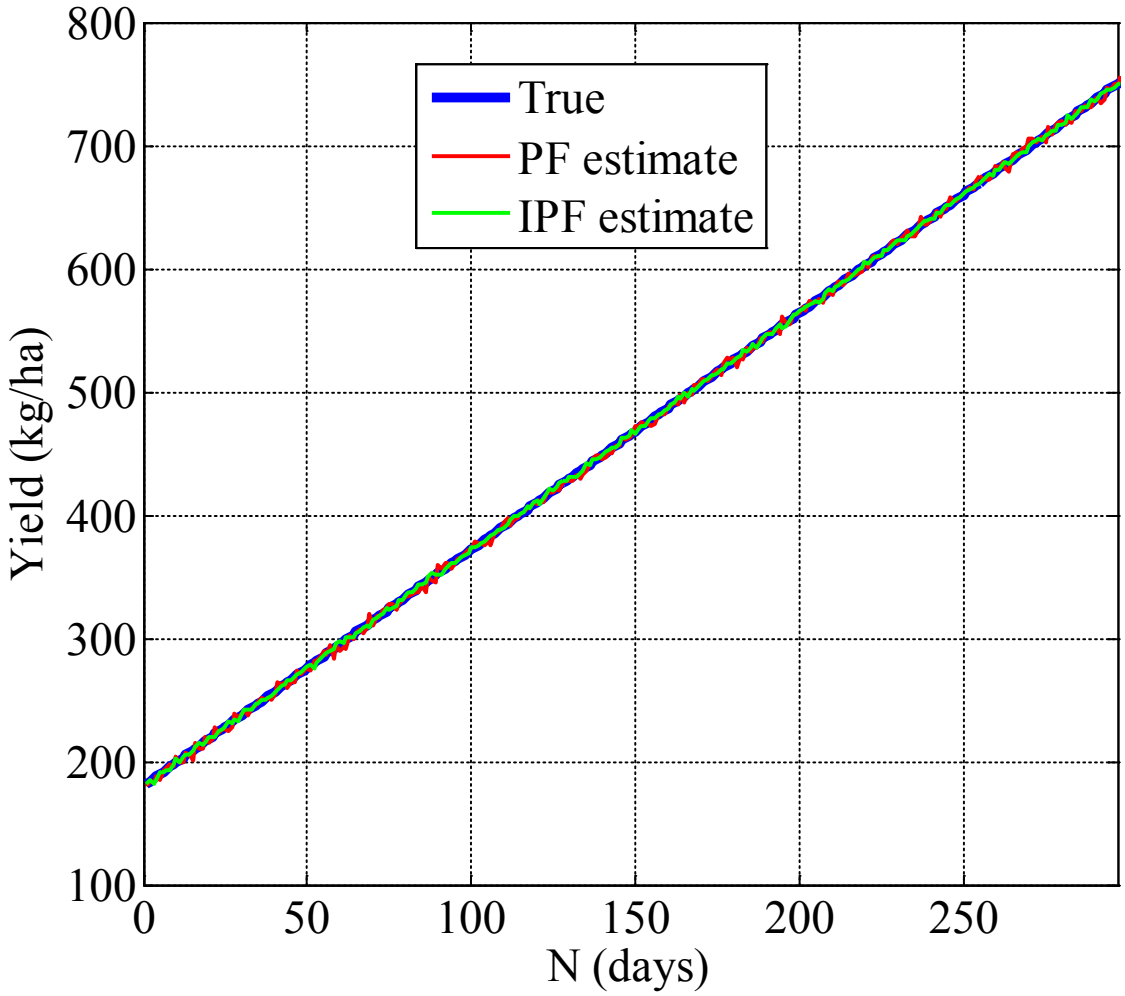

Fig. 3 Updated value of yield (kg/ha) versus N (Days) using PF and IPF techniques.

Table 6. ERROR of estimated states

	Technique	ERROR
	Yield	grain protein content
PF	0.942	0. 0603
IPF	0.736	0.0381

4. Conclusions

In this paper, we developed an improved Particle Filter (IPF) for crop model predictions. Specifically, two comparative studies are performed. In the first comparative study, we presented a simple application of the new IPF to a linear dynamic crop model predicting only one state variable, namely winter wheat

biomass. In the second comparative study, we used the proposed IPF for updating predictions of complex nonlinear crop models. In this case, the proposed IPF is applied to a nonlinear model predicting an important winter-wheat quality criterion and grain protein content. The results of both comparative studies show that the IPF 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 IPF yields an optimum choice of the sampling distribution, which also accounts for the observed data. The performance of the proposed method is evaluated on a synthetic example in terms of estimation accuracy, and root mean square error.

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