Estimating Environmental Systems using Iterated Sigma Point Techniques: A biomass substrate hypothetical system

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A paper from the Proceedings of the
13th International Conference on Precision Agriculture
July 31 – August 4, 2016
St. Louis, Missouri, USA

Abstract. This paper addresses the problem of biomass substrate hypothetical system estimation using sigma points kalman filter (SPKF) methods. Various conventional and state-of-theart state estimation methods are compared for the estimation performance, namely the unscented Kalman filter(UKF), the central difference Kalman filter (CDKF), the square-root unscented Kalman filter (SRUKF), the square-root central difference Kalman filter (SRCDKF), the iterated unscented Kalman filter (IUKF), the iterated central difference Kalman filter (ICDKF), the iterated square root unscented Kalman filter (ISRUKF), the iterated square root central difference Kalman filter (ISRCDKF) through a biomass substrate hypothetical system with two comparative studies in terms of estimation accuracy, convergence and execution times and under constanttime and varying-time parameter constraints. In the first comparative study, the state variables are estimated from noisy measurements, 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, and the impact of the practical challenges (measurement noise and number of estimated states/parameters) on the performances of the estimation techniques are investigated. The results of both comparative studies reveal that the ISRCDKF method provides a better estimation accuracy than the IUKF, ICDKF and ISRUKF methods; while the IUKF, ICDKF, ISRUKF and ISRCDKF methods provide improved accuracy over the UKF, CDKF, SRUKF and SRCDKF methods. The benefit of the ISRCDKF method lies in its ability to provide accuracy related advantages over other estimation methods since it re-linearizes

the measurement equation by iterating an approximate maximum a posteriori estimate around the updated state, instead of relying on the predicted state. The results of the comparative studies show also that, for all the techniques, estimating more model parameters affects the estimation accuracy as well as the convergence of the estimated states and parameters. The ISRCDKF, however, still provides an improved state accuracies than the other techniques even with abrupt changes in estimated states.

I***Keywords.*** *Parameter estimation – State estimation – Particle filter – Iterated square-root central difference - Kalman.*

Introduction

The structure of a model is defined by the input, state and output variables chosen to characterize the behavior of the modeled system, the logic of the interconnections amongst all these variables, and the particular mathematical forms of the various assumed interactions. The problem in environmental systems analysis, as a structural error/uncertainty in a model becomes a source of attracting attention. Dynamic state-space models [1] are useful for describing data in many different areas, such as engineering [2], biological data [3], chemical data [4], and environmental data [5]. An important task when analyzing data by state-space models is estimation of the state and model parameters based on measurements from the observation process. Bayesian estimation filtering represents a solution of considerable importance for this type of problem definition as demonstrated by many existing algorithms based on the Bayesian filtering [6]. The Kalman filter (KF) [7], [8] has been widely used in various engineering and science applications, including communications, control, machine learning, neuroscience, and many others. When the model describing the system is assumed to be linear and Gaussian, the KF provides an optimal solution [9]. 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 (EKF) [7], [8], [10], the unscented Kalman filter (UKF) [11], the central difference Kalman filter (CDKF) ([12], [13]), the square-root unscented Kalman filter (SRUKF) [14], [15], the square-root central difference Kalman filter (SRCDKF) [16], the iterated unscented Kalman filter (IUKF) [17], [18],the iterated central difference Kalman filter (ICDKF) ([19]), the iterated squareroot unscented Kalman filter (ISRUKF) [20] and the iterated square-root central difference Kalman filter (ISRCDKF) [21] have been developed. The extended Kalman filter [7] linearizes the model describing the system to approximate the covariance matrix of the state vector. However, the EKF is not always performing especially for highly nonlinear or complex models. On behalf of linearizing the model, a class of filters called the sigma points Kalman filters (SPKF) [22] use a statical linearization technique which linearizes a nonlinear function of a random variable via a linear regression. This regression is done between n points drawn from the prior distribution of the random variable, and the nonlinear functional evaluations of those points. The sigma points family of filters has been proposed that address the issues of the EKF by making use of a deterministic sampling approach.In this approach, the state distribution is approximated and represented by a set of chosen weighted sample points which capture the true mean and covariance of the state vector. These points are propagated through the true nonlinear system and capture the posterior the mean and the covariance matrix of the state vector accurately to the 3rd order (Taylor series expansion) for any nonlinearity. As part of the sigma points Kalman filter family, the unscented Kalman filter [7], [8] is been developed and it utilizes the unscented transformation to approximate the mean and the covariance matrix of the state vector. In the unscented transformation process, a set of samples (sigma points) are selected and propagated through the nonlinear model, providing more accurate approximations of the mean and covariance matrix of the state vector. One drawback of the UKF method is that the number of sigma points is often not very large and may not adequately represent relatively complicated distributions. As an alternative to these methods, the central difference Kalman filter [12], has been developed and it uses the Sterling polynomial interpolation formula. To add some benefits of numerical stability, the square root unscented kalman filter and the square-root central difference Kalman filter [16], have been developed. The advantage of these filters is that they ensured positive semi-definiteness of the state covariances. The iterated sigma points Kalman filters methods employ an iterative procedure within a single measurement update step by resampling the sigma points till a termination criterion, based on the minimization of the maximum likelihood estimate, is satisfied. unfortunately, for most nonlinear systems and non-Gaussian noise observations, closed-form analytic expressions of the posterior distribution of the state vector are untractable [23].

The objectives of this paper is threefold: i) to estimate a nonlinear state variables and model parameters using sigma points kalman filter methods and extensions of biomass substrate hypothetical system. ii) to investigate the effects of practical challenges (such as measurement noise and number of estimated states/parameters) on the performances of the techniques. To study the effect of measurement noise on the estimation performances, several measurement noise levels will be considered. Then, the estimation performances of the techniques will be evaluated for different noise levels. Also, to study the effect of the number of estimated states/parameters on the estimation performances of all the techniques, the estimation performance will be studied for different numbers of estimated states and parameters. iii) to apply the techniques to estimate the state variables as well as the model parameters of scalar nonlinear system and 2nd order LTI system. The performances of the estimation techniques will be compared to each others by computing the execution times as well as the estimation root mean square error (RMSE) with respect to the noise-free data. The organization of the paper is as follows. In Section II, the state estimation problem is presented. Then, in Section III, the state estimation methods are described. After that, in Section IV, the performance of the various state estimation techniques are compared for their application to estimate the state variables and model parameters in biomass substrate hypothetical system. Conclusions are presented in Section V.

II. State Estimation Problem

Next, we present the formulation of the state estimation problem.

A. Problem Description and Formulation

The estimation problem of interest is formulated for a system model. Consider a nonlinear complex model described as follows:

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

where $x \in R^n$ 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, $w \in R^n$ and $v \in R^m$ are process and measurement noise vectors, respectively, and g and l are nonlinear differentiable functions. Discretizing the state space model (1), the discrete model can be written as follows:

$$\begin{aligned} x_k &= f(x_{k-1}, u_{k-1}, \theta_{k-1}, v_{k-1}), \\ y_k &= h(x_k, u_k, \theta_k, \eta_k), \end{aligned} \tag{2}$$

which describes the state variables at some time step (k) in terms of their values at a previous time step ($k-1$). Since we are interested in estimating 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:

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

which means that it corresponds to a stationary process, with an identity transition matrix, driven by white noise. In order to include the parameter vector θ_k into the state estimation problem, let's define a new state vector z_k that augments the state vector x_k and the parameter vector θ_k as follows:

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

where $z_k \in R^{n+q}$. Also, defining the augmented noise vector as:

$$\epsilon_{k-1} = \begin{bmatrix} v_{k-1} \\ \gamma_{k-1} \end{bmatrix}, \tag{5}$$

the model (2) can be written as,

$$z_k = \mathfrak{F}(z_{k-1}, u_{k-1}, \epsilon_{k-1}), \tag{6}$$

$$y_k = \mathfrak{R}(z_k, u_k, \eta_k), \tag{7}$$

where F and R are differentiable nonlinear functions. Thus, the objective here is to estimate the augmented state vector z_k, given the measurements vector y_k.

III. Description of State Estimation Methods

A. Unscented Kalman Filter (UKF) Method

The unscented Kalman filter is a sigma points kalman filter tat uses the unscented transformation. This transformation is a method for calculating the statistics of a random variable that undergoes a nonlinear mapping. It is built on the theory that "it is easier to approximate a probability distribution than an arbitrary nonlinear function".

The state distribution is represented by a Gaussian random variable (GRV) and by a set of deterministically chosen points. These points capture the true mean and covariance of the GRV and also capture the posterior mean and covariance accurately to the second order for any nonlinearity and to the third order for Gaussian inputs. Assume that a random variable $z \in R^L$ with mean $\bar{z}$ and covariance P_z is transformed by a nonlinear function, $y = f(z)$. In order to find the statistics of y, define $2L+1$ sigma vectors as follows:

$$\begin{aligned} Z_0 &= \bar{z} \\ Z_i &= \bar{z} + (\sqrt{(L+\lambda)\mathbf{P}_z})_i \quad i = 1, \ldots, L \\ Z_i &= \bar{z} - (\sqrt{(L+\lambda)\mathbf{P}_z})_i \quad i = L+1, \ldots, 2L \end{aligned} \tag{8}$$

where $\lambda = \epsilon^2(L + k) - L$ is a scaling parameter and $(\sqrt{(L+\lambda)P_z})_i$ denotes the i^{th} column of the matrix square root $(L+\lambda)P_z$. The constant $10^{-4} < \epsilon < 1$ determines the spread of the sigma points around z. The constant k is a secondary scaling parameter which is usually set to zero or $3 - L$ ([24]). Then, these sigma points are propagated through the nonlinear function, i.e.,

$$Y_i = f(Z_i) \quad i = 0, \ldots, 2L \tag{9}$$

and the mean and covariance matrix of y can be approximated as weighted sample mean and covariance of the transformed sigma points of Yi as follows:

$$\overline{\mathbf{y}} \approx \sum_{i=0}^{2L} W_i^{(m)} Y_i, \qquad (10)$$

$$\text{and} \quad \mathbf{P}_z \approx \sum_{i=0}^{2L} W_i^{(c)} (Y_i - \overline{\mathbf{y}})(Y_i - \overline{\mathbf{y}})^T,$$

where the weights are given by:

$$W_i^{(m)} = \frac{\lambda}{\lambda + r}$$

$$W_0^{(c)} = \frac{\lambda}{\lambda + r} + (1 - \alpha^2 + \xi) \qquad (11)$$

$$\text{and} \quad W_i^{(m)} = W_i^{(c)} = \frac{1}{2(\lambda + r)} \quad i = 0, \ldots, 2L.$$

The parameter ξ is utilized to incorporate prior knowledge about the distribution of z . It has been revealed that for a Gaussian and non-Gaussian variables, the unscented transformation results in approximations that are precise up to the third and second order, respectively. The algorithm includes two steps: Prediction and Update. In the prediction step, we calculate the predicted state estimate $\hat{z}_{k-1}$ and the predicted estimate covariance P_k. In the update step, we calculate the updated state estimate $\hat{z}_k$ and the updated estimate covariance P_k after calculating the innovation residual $P_{z_k y_k}$ and the optimal Kalman gain K_k

B. Central Difference Kalman Filter (CDKF) Method

The central difference Kalman filter is another filter from the family of sigma points kalman filter. This filter is based on Sterling polynomial interpolation formula instead of the unscented transformation used in UKF. The CDKF is similar to the UKF with the same or superior performance. However, it has an advantage over the UKF that it uses only one parameter instead of three parameters in the UKF. The CDKF uses a symmetric set of (2L+1) sigma points which are calculated as follow,

$$\begin{aligned} Z_0 &= \hat{z} \\ Z_i &= \hat{z} + (h\sqrt{P_z})_i \quad i = 1, \ldots, L \qquad (12) \\ Z_i &= \hat{z} - (h\sqrt{P_z})_i \quad i = L+1, \ldots, 2L, \end{aligned}$$

where L is the dimension of the state z, h is a scaling parameter (the optimal value is h = p3) and i indicates the i-th column of the matrix. These sigma point are propagated through the nonlinear function to form the set of the posterior sigma points,

$$Y_i = f(\Psi_i) \quad i = 0, \ldots, 2L \qquad (13)$$

Within the above results, the sterling approximation estimates of the mean $\hat{z}$, covariance P_y and cross covariance $P_{z,y}$ are obtained through a linear regression of weighted point,

$$\hat{y} = \sum_{i=0}^{2L} W_i^{(m)} Y_i, \qquad (14)$$

$$P_{\tilde{y}} = \sum_{i=1}^{L} W_i^{(c1)} [Y_{i,k|k-1} + Y_{i+L,K|k-1}][Y_{i,k|k-1} + Y_{i+L,k|k-1}]^T$$

$$+ \sum_{i=1}^{L} W_i^{(c2)} [Y_{i,k|k-1} + Y_{i+L,k|k-1} - 2Y_0][Y_{i,k|k-1} + Y_{i+L,k|k-1} + 2Y_0]^T, \qquad (15)$$

$$P_{z_k y_k} = \sqrt{W_i^{(c1)} P_z}\, [\Psi_i - \hat{z}]\, [Y_{1:L,k|k-1} + Y_{i+L:2L,k|k-1}]^T. \qquad (16)$$

The set of corresponding weights for the mean $W_{(m)\,i}$ which are used to compute the posterior mean is defined as

$$W_0^{(m)} = \frac{h^2 - L}{h^2}, \qquad W_i^{(m)} = \frac{1}{2h^2}, \qquad (17)$$

and the set of corresponding weights for the covariance $W_{(c)\,0}$ which is used to recover the covariance and the crosscovariance is defined as,

$$W_i^{(c1)} = \frac{l}{4h^2}, \qquad W_i^{(c2)} = \frac{h^2 - 1}{4h^4}, \qquad i = 1, \ldots, 2L \qquad (18)$$

C. Square Root Unscented Kalman Filter (SRUKF) Method

One drawback of the UKF is that it requires the calculation of the matrix square-root $S_k S_k^T = P_k$, at each time step. However, in the SRUKF, S_k will be propagated directly, avoiding the computational complexity to refactorize at each time step [25].

The SRUKF is initialized with a state mean vector and the square root of a covariance.

$$\hat{x}_0 = E[x_0], \tag{19}$$

and,

$$S_0 = chol\{E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T]\}, \tag{20}$$

$$\Psi_{k-1} = [\hat{x}_{k-1} \quad \hat{x}_{k-1} + hS_{k-1} \quad \hat{x}_{k-1} - hS_{k-1}]. \tag{21}$$

The Cholesky factorization decomposes a symmetric, positive-definite matrix into the product of a lower-triangular matrix and its transpose. This new matrix is utilized directly to obtain the sigma points: The scaling constant h is expressed as,

$$h = \sqrt{L\alpha^2}, \tag{22}$$

where α is a tunable parameter less than one. The sigma points are then went through the nonlinear process system, which predicts the current attitude based on each sigma point.

$$\Psi_{k|k-1} = f[\Psi_{k-1}]. \tag{23}$$

The estimated state mean and square root covariance are calculated from the transformed sigma points using,

$$\hat{x}_k^- = \sum_{i=0}^{2L} W_i^{(m)} \Psi_{i,k|k-1}, \tag{24}$$

$$S_k^- = qr\left\{\left[\sqrt{W_1^{(c)}}(\Psi_{1:2L,k|k-1} - \hat{x}_k^-)\sqrt{R^v}\right]\right\}, \tag{25}$$

$$S_k^- = cholupdate\left\{S_k^-, \Psi_{0,k} - \hat{x}_k^-, W_0^{(c)}\right\}, \tag{26}$$

where, $W_{(c)\,0} = 2(1 - \alpha^2 + 1^2\beta)$, $W_{(m)\,0} = 1 - \alpha^2$, $W_{(m)\,i} = W_{(c)\,i} = 1^2 2L\_2\beta)$, β is a tunable parameter used to include prior distribution. The transformed sigma points are then used to predict the measurements using the measurement model:

$$Y_{k|k-1} = h[\Psi_{k|k-1}]. \tag{27}$$

The expected measurement $\hat{y}_k$ and square root covariance of $\tilde{y}_k = y_k - \hat{y}_k^-$ (called the innovation) are given by the unscented transform expressions just as for the process model:

$$\hat{y}_k^- = \sum_{i=0}^{2L} W_i^{(m)} y_{i,k|k-1} \tag{28}$$

$$S_{\tilde{y}_k} = qr\left\{\left[\sqrt{W_1^{(c)}}(Y_{1:2L,k|k-1} - \hat{y}_k)\sqrt{R_k^v}\right]\right\}, \tag{29}$$

$$S_{\tilde{y}_k} = cholupdate\left\{S_{\tilde{y}_k}, Y_{0,k} - \hat{y}_k, W_0^{(c)}\right\}. \tag{30}$$

In an attempt to find out how much to adjust the predicted state mean and covariance based on the actual measurement, the Kalman gain matrix K_k is calculated as follows

$$P_{x_k y_k} = \sum_{i=0}^{2L} W_i^{(c)} [\Psi_{i,k|k-1} - \hat{x}_k^-][Y_{i,k|k-1} - \hat{y}_k^-]^T, \tag{31}$$

$$K_k = P_{x_k y_k} / S_{\tilde{y}_k}^T / S_{\tilde{y}_k}. \tag{32}$$

Finally, the state mean and covariance are updated using the actual measurement and the Kalman gain matrix:

$$\hat{x}_k = \hat{x}_k^- + K_k(y_k - \hat{y}_k^-), \tag{33}$$

$$U = K_k S_{\tilde{y}_k}, \tag{34}$$

$$S_k = cholupdate\{S_k^-, U, -1\}. \tag{35}$$

where, Rw is the process noise covariance, Rv is themeasurement noise covariance, chol - is Cholesky method of matrix factorization, qr is QR matrix decomposition andcholupdate is a Cholesky factor updating.

D. Square Root Central Difference Kalman Filter (SRCDKF) Method

The SRCDKF is initialized with a state mean vector and the square root of a covariance.

$$\hat{s}_0 = E[z_0], \quad (36)$$

and,

$$S_0 = chol\{E[(z_0 - \hat{s}_0)(z_0 - \hat{s}_0)']\}. \quad (37)$$

After the cholesky factorisation we obtain the sigma points:

$$\Psi_{k-1} = [\hat{s}_{k-1} \;\; \hat{s}_{k-1} + hS_{k-1} \;\; \hat{s}_{k-1} - hS_{k-1}]. \quad (38)$$

The scaling constant h is is a tunable parameter used to include prior distribution. For Gaussian random variables, the optimal value of h is expressed as,

$$h = \sqrt{3}. \quad (39)$$

The sigma points are then went through the nonlinear process system, which predicts the current attitude based on each sigma point.

$$\Psi_{k|k-1} = f[\Psi_{k-1}]. \quad (40)$$

The estimated state mean and square root covariance are calculated from the transformed sigma points using,

$$\hat{s}_k^- = \sum_{i=0}^{2L} W_i^{(m)} \Psi_{i,k|k-1}, \quad (41)$$

The next step, the sigma-point for measurement update is calculated as,

$$\Psi_{k|k-1} = [\hat{s}_{k|k-1} \;\; \hat{s}_{k|k-1} + hS_{k|k-1} \;\; \hat{s}_{k|k-1} - hS_{k|k-1}]. \quad (42)$$

The transformed sigma points are then used to predict the measurements using the measurement model:

$$Y_{k|k-1} = h[\Psi_{k|k-1}]. \quad (43)$$

The expected measurement ˆy− k and square root covariance of ˜yk = yk−ˆy− k (called the innovation) are given by expressions just as for the process model:

$$\hat{y}_k^- = \sum_{i=0}^{2L} W_i^{(m)} Y_{i,j}. \quad (44)$$

In an attempt to find out how much to adjust the predicted state mean and covariance based on the actual measurement, the Kalman gain matrix Kk is calculated as follows:

$$P_{z_k y_k} = W_1^{(c1)} S_k^- [Y_{1:L,j} - Y_{L+1:2L,j}]^T. \quad (45)$$

$$K_{k,j} = P_{z_k y_k} / S_k^T / S_{\tilde{y}_k}. \quad (46)$$

Then, the state mean and covariance are updated using the actual measurement and the Kalman gain matrix is:

$$\hat{s}_k = \hat{s}_k^- + K_k(y_k - \hat{y}_k^-). \quad (47)$$

$$U = K_k S_{y_k}. \quad (48)$$

$$S_k = cholupdate\{S_k^-, U, -1\}. \quad (49)$$

E. Iterated Sigma Point Kalman filters (ISPKF) Methods

In order to achieve superior performance of the statical linearization methods in terms of efficiency and accuracy, the iterated sigma points kalman filters have been developed.These filters include the iterated unscented Kalman filter (IUKF), the iterated central difference Kalman filter (ICDKF), the iterated square root unscented Kalman filter (ISRUKF) and the iterated square root central difference Kalman filter (ISRCDKF). The major difference between the iterated sigma points kalman filters and the sigma points kalman filters is shown in the step where the updated state estimation is calculated using the predicted state and the observation. Instead of relying on the predicted state, the observation equation is re-linearized over times by iterating an approximate maximum a posteriori estimate, so the state estimate will be more accurate. When the state prediction bzk and the covariance Pk are calculated, we set an iteration loop. In the first step, for each instant k (k _ 1), the augmented state estimate bzk and the covariance matrix Pk have been evaluated. In the second step, new sigma points have been generated. Then, we recalculate in the third step the equations of the measurements update step. Finally, we stop the iteration when the termination criterion, based on the minimization of the maximum likelihood estimate, is satisfied. The iterated sigma points methods have the ability to provide accuracy over other estimation methods since it re-linearizes the measurement equation by iterating an approximate maximum a posteriori estimate around the updated state, instead of relying on the predicted state.

In the next section, the sigma points kalman filter methods performances will be assessed and compared to iterated sigma points kalman filter methods. The performances of UKF, IUKF, CDKF, ICDKF, SRUKF, ISRUKF, SRCDKF and ISRCDKF methods will be evaluated through biomass substrate hypothetical system under time-varying and timeconstant parameter constraints with two comparative studies

TABLE I
PARAMETER VALUES IN THE MODEL OF THE HYPOTHETICAL SYSTEM

states/parameters	Initial values
$x_1(t)$	5
$x_2(t)$	2
u_{max}	0.3
Ks	3.0
Y	0.6
q_0	0.1

in terms of estimation accuracy, convergence and execution times.

IV. SIMULATION RESULTS

A. A biomass-substrate hypothetical system

The hypothetical nonlinear system of biomass-substrate interaction, taking place in a single continuously stirred tank reactor (CSTR)[26] is defined by the following set of ordinary differential equations:

$$\frac{dx_1(t)}{dt} = -q_0 x_1(t) + u x_1(t)\frac{x_2(t)}{Ks + x_2(t)} + q_0 u_1(t) \quad (50)$$

$$\frac{dx_2(t)}{dt} = -q_0 x_2(t) - \frac{1}{Y} u x_1(t)\frac{x_2(t)}{Ks + x_2(t)} + q_0 u_2(t) \quad (51)$$

where, u1(t) and x1(t) are the concentrations of biomassin the influent and the tank at time t. u2(t) and x2(t) are the concentrations of growth-limiting substrate in the store (CSTR) at time t. Ks is the saturation constant of the substrate, umax is the maximum growth rate of the biomass, Y is the yield coefficient of biomass on substrate and q0 is the dilution rate.

The concentration u1(t) is set to zero, and concentration u2(t) is defined as follows:

$$\begin{cases} u_2(t) = 30; \ if \ 0 <= t \ mod \ 40 < 20; \\ u_2(t) = 10; \ if \ 20 <= t \ mod \ 40 < 40; \end{cases} \quad (52)$$

The parameter values in the model of the hypotheticalsystem are presented in table I. For all simulations, the following parameters are used. The sampling frequency is 100Hz (T = 0. 01sec), y1(t) and y2(t) are the observed time series of x1(t) and x2(t), respectively. They are corrupted with white Gaussian measurement error i.e., a measurement noise vk s N(0, σ 2 v), with σ 2 v = 10–3.

B. Generation of Dynamic Data

In the first step we are interested to compare the estimation performances of the Sigma Point Kalman Filter methods [27] presented by : UKF, CDKF, SRUKF, SRCDKF, with their iterations IUKF, ICDKF, ISRUKF, ISRCDKF, in estimating two state variables with parameters of the environmental system under time-varying and time-constant parameter constraints, based on the model equations described in Equation 50:

$$\begin{cases} x_1(t) = f_1(x_1(t-1), \theta) \\ x_2(t) = f_2(x_2(t-1), \theta) \end{cases} \quad (53)$$

where t is the time step, f1,2 are the corresponding model function, and θ is the vector of parameters driving the simulations. Here, we therefore assume that some of the states are wrong simulated by the model, and our objective is to re-estimate them, under the hypothesis that the states are measured at some moment, along the season. Discretizing the model (53) using a sampling interval of _t, it can be written as:

$$\begin{cases} x_{1_k} = \left[g_1(\theta)\right]\Delta t + x_{1_{k-1}} + w_k^1 \\ x_{2k} = \left[g_2(\theta)\right]\Delta t + x_{2_{k-1}} + w_k^2 \end{cases} \quad (54)$$

where, wj , j 2 {1, 2} is a measurement Gaussian noise with zero mean and known variance σ 2 wj .

C. Case 1: Time invariant parameter and state estimation

1) Comparative Study 1: State estimation using SP and ISP techniques:: At this point of the research, the model

parameters are assumed to be constants. Next, we consider the state vector that we wish to estimate:

$$x_k = x_k = [x_{1k}\ x_{2k}]^T,$$

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

$$\text{RMSE} = \sqrt{E\left((\mathbf{x} - \hat{\mathbf{x}})^2\right)} \qquad (55)$$

Where x (resp. bx) is the true parameter/state (resp. the estimated parameter/state). The simulation results of estimating the two states : the biomass-substrate index x1k-x2k using the Sigma Point (UKF, CDKF, SRUKF, SRCDKF) and the Iterated Sigma Point (IUKF, ICDKF, ISRUKF, ISRCDKF) are shown in Figures 1. Also, the estimation root mean square errors (RMSE) and time executions for the estimated states are shown in Table 2. It can be observed from Figure 1 and Table II that the SP resulted in the worst performance of all estimation techniques, which is expected due to the limited ability of the SP to accurately estimate the mean and covariance matrix of the estimated states through linearization of the nonlinear process model. The results also show that the ISP provides a significant improvement over the SP, which is due to the fact that the ISP yields an optimal choice of the sampling distribution with the iterative schemes.

2) Comparative Study 2: States and parameters estimation using SP and ISP techniques: The model (54) assumes that the parameters are fixed and/or are determined previously. However, the model involves several parameters that are usually not exactly known, or that have to be estimated. Estimating these parameters, to completely define the model, usually requires several experiment setups, which can be expensive and challenging in practice. Let's thus consider that some of the parameter have to be estimated to improve the simulations, by example the umax, Ks, Y and q0 parameters. umax is the maximum growth rate, Ks is the saturation

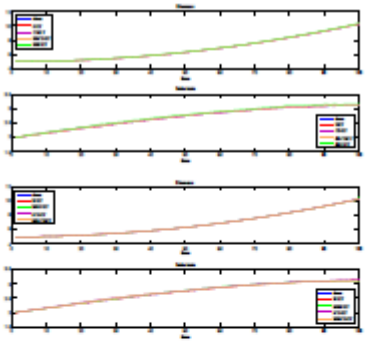


Fig. 1. Estimation of the two states (x_1 and x_2) using SP and ISP methods

TABLE II
ROOT MEAN SQUARE ERRORS (RMSE) OF ESTIMATED STATES FOR SP AND ISP METHODS

Techniques	x_1	x_2	Execution Time
UKF	0.0232	0.0223	0.058
CDKF	0.0227	0.0217	0.047
SRUKF	0.0217	0.0210	0.064
SRCDKF	0.0212	0.0207	0.065
IUKF	0.0216	0.0206	0.104
ICDKF	0.0208	0.0204	0.068
ISRUKF	0.0199	0.0200	0.076
ISRCDKF	0.0192	0.0194	0.065

constant of the substrate x2, Y is the yield coefficient ofx1 and q0 is the dilution rate. To estimate these parameters, the following equations that describe their evolution are also needed:

$$\begin{cases} u_{max_k} = u_{max_{k-1}} + \gamma_k^1 \\ K s_k = K s_{k-1} + \gamma_k^2 \\ Y_k = Y_{k-1} + \gamma_k^3 \\ q_{0_k} = q_{0_{k-1}} + \gamma_k^4 \end{cases} \qquad (56)$$

where, $\gamma_{j,\ j\in\{1,..,4\}}$ is a process Gaussian noise with zero mean and known variance σ^2_j.
The model (54) needs to incorporate the evolution of these parameters as follows:

$$\begin{cases} x_{1k} = \left[g_1(\theta_{k-1})\right]\Delta t + x_{1k-1} + w_k^1 \\ x_{2k} = \left[g_2(\theta_{k-1})\right]\Delta t + x_{2k-1} + w_k^2 \end{cases} \quad (57)$$

Where, g is nonlinear differentiable function, it can be used to compute the predicted state from the previous estimate. Hence, the discrete nonlinear system model of the Biomass substrate can be written as:

$$\begin{cases} f1 : x_{1k} = \left[g_1(\theta_{k-1})\right]\Delta t + x_{1k-1} + w_k^1 \\ f2 : x_{2k} = \left[g_2(\theta_{k-1})\right]\Delta t + x_{2k-1} + w_k^2 \\ f3 : u_{maxk} = u_{maxk-1} + \gamma_k^1 \\ f4 : Ks_k = Ks_{k-1} + \gamma_k^2 \\ f5 : Y_k = Y_{k-1} + \gamma_k^3 \\ f6 : q_{0k} = q_{0k-1} + \gamma_k^4 \end{cases} \quad (58)$$

where, f_k, $k \in \{1,\ldots,6\}$ are nonlinear functions, it is desired toestimate the parameter vector θ given dynamic measurements of the state variables x_1 and x_2. In the following, we denote $w = (w_1\ w_2)^T$, and $\gamma = (\gamma_1\ \gamma_2\ \gamma_3\ \gamma_4)^T$, respectively the measurement and process noise vectors, which quantify (i) errors in the measurements and (ii) randomness in the process. Note that we are forming the augmented state: $z_k = [x_k\ \theta_k]^T = [x_{1k}\ x_{2k}\ u_{maxk}\ Ks_k\ y_k\ q_{0k}]^T$, as a 6 by 1 matrix with the following:

$$\begin{cases} x_k(1,:) & -> & x_{1k} \\ x_k(2,:) & -> & x_{2k} \\ \theta_k(1,:) & -> & u_{maxk} \\ \theta_k(2,:) & -> & Ks_k \\ \theta_k(3,:) & -> & Y_k \\ \theta_k(4,:) & -> & q_{0k} \end{cases} \quad (59)$$

The idea here is that, if a dynamic model structure isavailable, the model parameters can be estimated using one of state estimation technique. State estimation is a systemengineering 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.

It can be seen from the results presented in Figure 2 that the ISP extensions presented by IUKF, ICDKF, ISRUKF, ISRCDKF methods outperform the SP methods UKF, CDKF, SRUKF, SRCDKF. We can show also, that the ISRCDKF shows relative improvement over all other techniques. These results confirm the results obtained in the first comparative study, where only the states variables are estimated. The advantages of the ISRCDKF over the other techniques can also be seen through their abilities to estimate the model parameters. For example, IUKF, ICDKF ISRUKF, ISRCDKF could took longer to estimate a model parameters than UKF, CDKF, SRUKF, SRCDKF, (see Figure 2). The ISRCDKF, however, could estimate all the model parameters in all cases. Next, we present the estimation performance using the state estimation techniques where the model is assumed to be time varying parameter.

D. Case 2: Time varying parameters and state estimation

For the purpose of demonstration [28], we will now linearize the model (50) in its assumptions about the kinetic interactions between biomass and substrate by substituting:

$$\theta(t) = -\frac{1}{Y}u\frac{x_1(t)}{Ks + x_2(t)}, \quad (60)$$

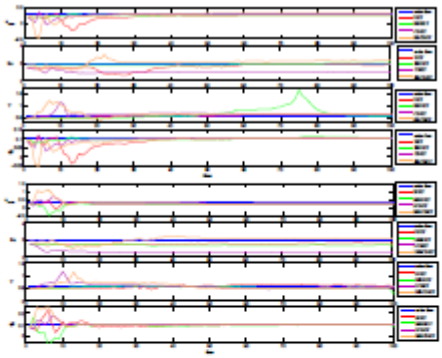


Fig. 2. Estimation of the states and all parameters(x_1, x_2, u_{max}, Ks, Y and q_0) using SP and ISP

TABLE III
INITIAL VALUES AND LEADING DIAGONAL ELEMENTS

states/parameters	Initial values
$x_1(t)$	5
$x_2(t)$	2
$\theta(t)$	0.001
Y	0.6

into Equations (61) and (62). This leads to a linear system of the form:

$$\frac{dx_1(t)}{dt} = -q_0 x_1(t) - Y\theta(t)x_2(t) + q_0 u_1(t), \qquad (61)$$

and,

$$\frac{dx_2(t)}{dt} = -q_0 x_1(t) + \theta(t)x_2(t) + q_0 u_2(t), \qquad (62)$$

in which, θ (t) is a time-varying parameter reflecting the possibility of a changing structure in the dynamics of the state variables (x1(t) and x2(t)). From a priori information, Y is known to be time-invariant, while θ (t) is idealized as a random walk (RW) parameter. The initial values of states for this example are given in Table III.

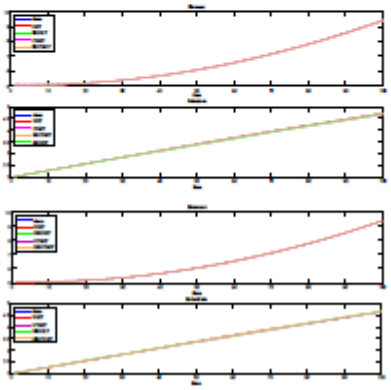
Figure 3 and Table IV present the estimation performance for estimating the two states x1 and x2 under time-varying parameter constraint using different sigma points methods in terms of RMSE and execution times.

The state and parameter estimation results for the second cases using SP and ISP methods extensions are shown in Figure 4. The estimation of the state variables and parameter(s) is performed using UKF, CDKF, SRUKF, SRCDKF, IUKF, ICDKF, ISRUKF, ISRCDKF, and the simulation results for the state variables and the model parameters are shown in Table V. For example, Table V, provides a comparisons for estimating the two states and the parameters Y and θ. It can also be shown from Table V, that the ISRCDKF method, however, still provides advantages over other methods in terms of the estimation accuracy. These advantages are dueto the fact that it uses a better proposal distribution that takes the latest observation into account.

TABLE IV
ROOT MEAN SQUARE ERRORS (RMSE) OF ESTIMATED STATES FOR SP AND ISP METHODS

Techniques	x_1	x_2	Execution Time
UKF	0.0184	0.0187	0.041
CDKF	0.0182	0.0185	0.038
SRUKF	0.0181	0.0184	0.043
SRCDKF	0.0180	0.0183	0.042
IUKF	0.0179	0.0182	0.046
ICDKF	0.0178	0.0177	0.045
ISRUKF	0.0175	0.0176	0.05
ISRCDKF	0.0172	0.0174	0.048

Fig. 3. Estimation of the two states (x_1 and x_2) using SP and ISP methods.



Conclusion or Summary

In this paper, various sigma points Kalman filter based methods are used to estimate a nonlinear state variables and model parameters. They are compared for the estimation performance through a biomass substrate hypothetical system in two comparative studies. In the first comparative study, the state variables are estimated from noisy measurements of these variables, and the various estimation

TABLE V
ROOT MEAN SQUARE ERRORS OF ESTIMATED STATES AND MEAN OF ESTIMATED PARAMETERS

Technique	RMSE		Means at steady state		Execution Time
	x_1	x_2	Y	θ	
UKF	0.0209	0.0180	0.7000	0.5032	0.043
CDKF	0.0207	0.0179	0.06933	0.5151	0.04
SRUKF	0.0201	0.0175	0.6888	0.5251	0.046
SRCDKF	0.0200	0.0174	0.6616	0.5369	0.048
IUKF	0.0199	0.0172	0.06550	0.4998	0.042
ICDKF	0.0197	0.0171	0.06364	0.5372	0.047
ISRUKF	0.0196	0.0168	0.06324	0.5531	0.05
ISRCDKF	0.0193	0.0167	0.06290	0.4984	0.049

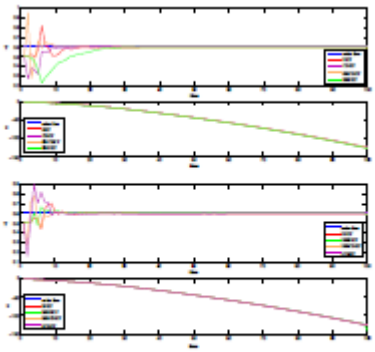


Fig. 4. Estimation of the two states and two parameters (x_1, x_2, Y and θ) using SP and ISP methods.

techniques are compared by computing the estimation root mean square error 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 the number of estimated model parameters on the accuracy and convergence of these techniques is also assessed. The results of the second comparative study show that, for all the techniques, estimating more model parameters affects the estimation accuracy as well as the convergence of the estimated states and parameters. The iterated square root central difference Kalman method, however, still provides advantages over other methods in terms of the estimation accuracy, convergence and execution times.

Acknowledgements

The authors gratefully acknowledge financial support from the Fonds de la Recherche Scientifique - FNRS..

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