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Economic Stochastic Model Predictive Control Using the Unscented Kalman Filter ⋆

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Abstract: Economic model predictive control is a popular method to maximize the efficiency of a dynamic system. Often, however, uncertainties are present, which can lead to lower performance and constraint violations. In this paper, an approach is proposed that incorporates the square root Unscented Kalman filter directly into the optimal control problem to estimate the states and to propagate the mean and covariance of the states to consider noise from disturbances, parametric uncertainties and state estimation errors. The covariance is propagated up to a predefined "robust horizon" to limit open-loop covariances, and chance constraints are introduced to maintain feasibility. Often variables in chemical engineering are non-negative, which however can be violated by the Unscented Kalman filter leading to erroneous predictions. This problem is solved by log-transforming these variables to ensure consistency. The approach was verified and compared to a nominal nonlinear model predictive control algorithm on a semi-batch reactor case study with an economic objective via Monte Carlo simulations.

Keywords: Robust control, Uncertain dynamic systems, Model-based control, Co-ordinate transformations, Nonlinear filters

1. INTRODUCTION

Batch reactors are common in the chemical industry due to their flexibility. The control of batch processes is challenging, since these are operated at unsteady state and are frequently highly nonlinear. This motivates the use of nonlinear model predictive control (NMPC) (Nagy and Braatz, 2003). The objective of the NMPC is usually to track a set point, but the true objective is to maximize profit. Therefore, in economic MPC (EMPC) the cost function is given by the quantity to be maximized (Lucia et al., 2014), which has attracted significant attention in recent years (Rawlings and Amrit, 2009). For batch reactors the objective is usually a property of the final product and hence the control problem leads to a shrinking horizon implementation.

The performance of the NMPC algorithm depends on the accuracy of the model used. Models of real processes often involve substantial uncertainties, including parametric uncertainties, unaccounted disturbances and state estimation errors. In particular, economic MPC often drives the system to its constraints (Lucia et al., 2014). Most work to consider uncertainties has been in robust NMPC (RNMPC), which assumes that uncertainties are deterministic and bounded. Important methods for RNMPC are min-max NMPC (Chen et al., 1997) and tube-based NMPC (Mayne et al., 2011). An alternative to RNMPC is given by stochastic NMPC (SNMPC), which assumes that the uncertainties are given by known probability distributions. In SNMPC constraints are probabilistic and given by either chance or expectation constraints. The regulation of the probability of constraint violations allows the adjustment of the conservativeness of the solution Mesbah (2016).

In Cannon et al. (2009) a procedure for SNMPC is introduced based on successive linearization and application of a probabilistic tube method. Bradford and Imsland (2017a) proposed to use a sampling average approach with variance reduction. A popular tool in SNMPC is given by the so-called polynomial chaos expansion (PCE), which is an efficient alternative to Monte Carlo simulations to propagate probabilistic uncertainties. A major disadvantage of this approach is that the complexity with respect to the number of uncertainty parameters scales exponentially (Fagiano and Khammash, 2012). In Bradford and Imsland (2018) a similar method is proposed using Gaussian processes instead. This has the advantage that it also considers the uncertainty of the approximation itself, but otherwise suffers from the same drawbacks. Maciejowski et al. (2007) proposed a method based on the Markov chain Monte Carlo approach, which is generally more efficient than common Monte Carlo sampling based techniques, but does not take gradient information into account. Lastly, multi-stage MPC has been used to solve SNMPC problems for discrete uncertainties, which however quickly becomes intractable due to the computational complexity scaling exponentially with the size of the time horizon, number of uncertainty parameters and uncertainty levels (Goodwin et al., 2009; Lucia, 2014).

In Bradford and Imsland (2017b) the Unscented Kalman filter (UKF) is used to estimate the state for output feedback model predictive control and propagate the state estimation error and additive noise from disturbances forward in time. The predicted Gaussian distributions of the states were used to impose probabilistic constraints. A similar approach is given in Farrokhsiar and Najjaran (2012) to propagate state estimation error and additive noise for the control of nonholonomic mobile robots.

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In addition, Liu et al. (2014) and Völz and Graichen (2016) show that the unscented transformation (UT) can be used to efficiently propagate additive disturbance errors. Lastly, in Heine et al. (2006) the UT is used to propagate parametric uncertainties. A general advantage of the UT is the linear scaling with respect to the number of uncertain parameters.

In this paper the previous work is unified to take into account state estimation error from the square root UKF, noise from additive disturbances and lastly parametric uncertainties. Log-transformations are used to enforce positiveness of several variables and the square root UKF is used to guarantee positive semi-definiteness of the state covariances (Van Der Merwe and Wan, 2001). The approach was tested on a semi-batch reactor case study with an economic objective. The robustness of the approach was verified with 4 uncertain parameters and compared to a nominal NMPC approach via Monte Carlo simulations. The paper is divided into the following sections. In the next Section the general SNMPC problem is formulated. In the third Section the square root UKF is introduced and utilised to solve the SNMPC problem. Further, the concepts "robust horizon", log-transformation and linear joint state constraints are outlined. The case study to test the procedure is formulated in Section 4. Section 5 gives the results of the Monte Carlo simulations for the case study. In the last Section conclusions were drawn from the simulation results.

2. NONLINEAR MODEL PREDICTIVE CONTROL WITH LINEAR CHANCE CONSTRAINTS

The dynamic system we consider is given by a discrete time stochastic nonlinear system with parametric uncertainties and additive noise. The states and the parameters enter the nonlinear equation system in a non-additive fashion, such that it is practical to write them jointly as x_a.

$$x(k+1) = f(x_a(k), u(k)) + w(k) \tag{1}$$
$$y(k) = h(x_a(k), u(k)) + \nu(k) \tag{2}$$

where k is the discrete time, $x_a = [x^T, \theta^T]^T \in \mathbb{R}^{n_x \times n_\theta = L}$ denotes the augmented state vector with a joint dimension of L, $x \in \mathbb{R}^{n_x}$ are the states, $u \in \mathbb{R}^{n_u}$ represents the inputs, $y \in \mathbb{R}^{n_y}$ are the measurements and $\theta \in \mathbb{R}^{n_\theta}$ denotes the parametric uncertainties; the additive disturbance term w lies in $\mathbb{R}^{n_x}$ and the additive measurement noise ν lies in $\mathbb{R}^{n_y}$. The equations $f : \mathbb{R}^L \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$ and $h : \mathbb{R}^L \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ represent the dynamics of the states and the measurements respectively.

The parametric uncertainties are assumed to be Gaussian distributed with mean vector $m_\theta(k)$ and covariance matrix $\Sigma_\theta(k)$ at stage k. The additive disturbances $w(k)$ and $\nu(k)$ are assumed to be zero mean independent normal random variables with variances $\Sigma_w(k)$ and $\Sigma_\nu(k)$ at stage k respectively. The probability density of the initial state $x(0)$ is assumed to be normal with mean $\hat{x}(0)$ and covariance $\Sigma_x(0)$. Assuming that we are at stage n, let $\mathcal{Y}_n$ stand for the measurements collected thus far. Subsequently, $\mathbb{E}_{\mathcal{Y}_n}(\cdot)$ and $\mathbb{P}_{\mathcal{Y}_n}(\cdot)$ denote the expectation and probability conditioned on $\mathcal{Y}_n$ respectively (Yan and Bitmead, 2005). The goal of the SNMPC algorithm at stage n is to determine a control sequence over a finite time horizon to adjust the probability distributions of the states to optimize an objective, while adhering to predefined probabilistic constraints, given imperfect information through $\mathcal{Y}_n$. A general SNMPC problem formulation at stage n can be given as follows, with deterministic constraints on the inputs and joint, linear chance constraints on the states:

Finite-horizon SNMPC problem with chance constraints

$$\begin{aligned}
&\underset{\mathbf{u}_N}{\text{minimize}} \quad \mathbb{E}_{\mathcal{Y}_n}\left(J(N, x(n), \mathbf{u}_N)\right) \\
&\text{subject to} \\
&x(n+k+1) = f(x_a(k), u(k)) + w(n+k) \\
&y(n+k) = h(x_a(k), u(k)) + \nu(n+k) \\
&\mathbb{P}_{\mathcal{Y}_n}(l_k^{iT} x(n+k) \le g_k^i) \ge 1 - p_k^i \\
&\qquad\qquad \forall (k,i) \in \{1,\dots,N\} \times \{1,\dots,n_g\} \\
&u(n+k) \in \mathbb{U}_k \quad \forall k \in \{0,...,N-1\}
\end{aligned} \tag{3}$$

where the time horizon is given by N, n_g is the number of linear state constraints, $l_k^i \in \mathbb{R}^{n_x}$ and $g_k^i \in \mathbb{R}$ define each linear state constraint, the input constraints are represented by $\mathbb{U}_k \subset \mathbb{R}^{n_u}$, $\mathbf{u}_N := \{u(n), \dots, u(n+N-1)\}$ is a collection of inputs over the finite horizon N from an initial stage n and $J(N, x(n), \mathbf{u}_N))$ is objective function. The chance constraints are set to be violated by a probability of $p_k^i \in (0,1) \subset \mathbb{R}$.

3. INCORPORATION OF THE SQUARE ROOT UNSCENTED KALMAN FILTER

3.1 Transformation of variables with lower bound

First principle equations for batch processes are commonly given as continuous differential equations, which can be discretized using numerical integration techniques to obtain equations in the form of Eq. (1). In this work orthogonal collocation was used for numerical integration Chachuat (2007). The log-transformation is, however, directly applied to the continuous differential equation system. Many variables in chemical engineering are non-negative due to physical constraints, such as temperatures, concentrations, volumes, etc.. The methods available in literature to incorporate state constraints in the UKF are not suitable for our specific problem, since these are discontinuous (Simon, 2010). Instead, we suggest to log-transform the variables to ensure a lower bound on the variables. Let x' be the variable that cannot be lower than a. Then define x as:

$$x = \log(x' - a) \tag{4}$$

If we now work with x in the problem rather than x', then x' is guaranteed to remain larger than a, i.e. we have implicitly introduced the following constraint:

$$x' > a \tag{5}$$

The differential equation of x' can then be transformed in the following way to obtain the required differential equation of x:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\mathrm{d}x'}{\mathrm{d}t} \frac{1}{x' - a} \tag{6}$$

Lastly, given that we know x is normally distributed with mean $\hat{x}$ and covariance Σ_x, i.e. $x \sim \mathcal{N}(\hat{x}, \Sigma_x)$, x' then follows a log-normal distribution, with mean and covariance given by (Halliwell, 2015):

$$\hat{x'}_i = \exp\left(\hat{x}_i + \frac{\Sigma_{xi,i}}{2}\right) \tag{7}$$

$$\Sigma_{x'i,j} = \exp\left(\hat{x}_i + \hat{x}_j + \frac{\Sigma_{xi,i} + \Sigma_{xj,j}}{2}\right)\left(\exp(\Sigma_{xi,j}) - 1\right) \tag{8}$$

where $\hat{x'}$ and $\Sigma_{x'}$ are the mean and covariance of x' respectively

Eq. (7) can be used to obtain the state estimate for the true variable x' from x with the corresponding covariance matrix from Eq. (8).

3.2 Propagation of state probability distributions using the square root Unscented Kalman filter

The problem in Eq. (3) is intractable, since it requires the propagation of conditional probability densities of the states through nonlinear transformations. Instead we use the UT to approximate the mean and covariance of this probability density. In our case the uncertain input is given by the states and uncertain parameters. The UT creates a set of sampling points, which depend on the mean and covariance of the Gaussian distributed input. The mean and covariance of the UT are accurately estimated up to third order (Simon, 2006), which is an advantage of the UT over more conventional linearization approaches.

To obtain the state estimate the Kalman filter equations are used at stage n. For the propagation of the mean and covariance of the states the UT is repeatedly applied to Eq. (1), assuming at each stage that the output follows a Gaussian distribution. This approach is summarised in the Algorithm 1 box and illustrated in Fig. 1. The equation system is given such that $\hat{x}(n|n)$, the state estimate, is also calculated given the current measurement $y(n)$, the previous state estimate $\hat{x}(n-1|n-1)$, the previous state covariance $\Sigma_x(n-1|n-1)$ and the previous control input $u(n-1)$. Guidelines on how to set the scaling parameters ($\omega_i^{\mu}, \omega_i^{c}, \lambda$) and definitions of qr$(\cdot)$, $\cdot/\cdot$ and cholupdate$(\cdot,\cdot,\cdot)$ can be found in Van Der Merwe and Wan (2001).

The considered OCP in Eq. (3) is open-loop, which does not account for the NMPC to have reduced covariances through feedback by the state and bias update. This leads to the predicted conditional covariances to increase with k and therefore the OCP becoming increasingly conservative with larger time horizons. Eventually the OCP becomes infeasible (Yan and Bitmead, 2005). The "robust horizon" is utilised as in Bradford and Imsland (2017b), up to which the covariances are propagated to address the problem of growing covariances. Hence, for the square root UKF in the Algorithm 1 box, equations were added, such that the covariance matrix is constant after a defined "robust horizon" t_R. This is similar to Yan and Bitmead (2005) who propagates the covariance at the first stage from a Kalman filter in linear MPC. Farrokhsiar and Najjaran (2012) introduces "fake measurements". This is an interesting approach to take into account information gained to learn parameters, but is expensive since it requires additional equations.

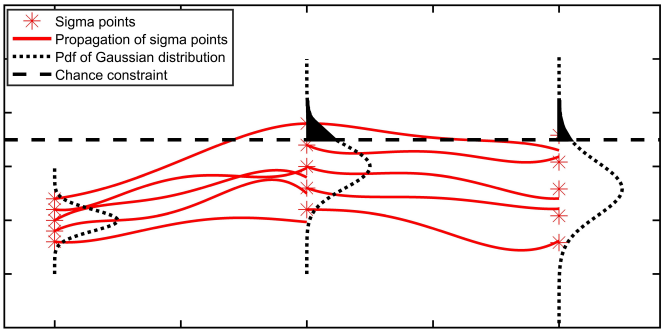

Fig. 1. Illustration of UKF SNMPC algorithm: Each Sigma point resembles a different input, which are then propagated through the nonlinear transformation to the next stage as indicated by the red lines. These are then used to estimate the mean and covariance of the Gaussian distribution of the states at the next stage. The probability of violating the chance constraint shown is given by the area under the pdf.

Algorithm 1: Square root Unscented Kalman filter with additive noise and parametric uncertainty

Initialization

Input: $\hat{x}(n-1|s),\ \Sigma_x(n-1|s),$
$u(n-1),\ y(n),\ \lambda,\ \omega^{\mu},\ \omega^{c},\ t_R,\ n,\ N$
$m_\theta(n+k),\ \forall k \in \{1,\dots,N\},$
$\Sigma_\theta(n+k),\ \forall k \in \{1,\dots,N\}$
$\Sigma_w(n+k),\ \Sigma_v(n+k)\ \forall k \in \{1,\dots,N\}$
$f(\cdot),\ h(\cdot)$

For $s = n-1, k = 0$ and $s = n,\ k \in \{1,\dots,N\}$

Definition of Sigma points

$$\hat{x}_a(n+k-1|s) = [\hat{x}(n+k-1|s)^T\ m_\theta(n+k-1)^T]^T \tag{9a}$$

$$\Sigma_a^{1/2}(n+k-1|s) = \operatorname{diag}(\Sigma_x^{1/2}(n+k-1|s), \Sigma_\theta^{1/2}(n+k-1)) \tag{9b}$$

$$\mathcal{X}(n+k-1|s) = [\hat{x}_a(n+k-1|s) \quad \hat{x}_a(n+k-1|s) + \sqrt{L+\lambda}\,\Sigma_a^{1/2}(n+k-1|s) \quad \hat{x}_a(n+k-1|s) - \sqrt{L+\lambda}\,\Sigma_a^{1/2}(n+k-1|s)] \tag{9c}$$

Covariance and mean approximation of predictions

$$\mathcal{X}_i(n+k|s) = f(\mathcal{X}_i(n+k-1|s), u(n+k-1)) \tag{10a}$$

$$\hat{x}(n+k|s) = \sum_{i=0}^{2L} \omega_i^{\mu} \mathcal{X}_i(n+k|s) \tag{10b}$$

$$\forall k \le t_R \quad \Sigma_x^{1/2}(n+k|s) = \text{qr}([\sqrt{\omega_1^c}(\mathcal{X}_{1:2L}(n+k|s) - \hat{x}(n+k|s)) \quad \Sigma_w^{1/2}(n+k)]) \tag{10c}$$

$$\forall k \le t_R \quad \Sigma_x^{1/2}(n+k|s) = \text{cholupdate}(\Sigma_x^{1/2}(n+k|s), \mathcal{X}_0(n+k|s) - \hat{x}(n+k|s), \omega_0^c) \tag{10d}$$

$$\forall k > t_R \quad \Sigma_x^{1/2}(n+k|n) = \Sigma_x^{1/2}(n+k-1|n) \tag{10e}$$

Covariance and mean approximation of observations

$$\phi_i(n|n-1) = h(\mathcal{X}_i(n|n-1), u(n-1)) \tag{11a}$$

$$\hat{y}(n|n-1) = \sum_{i=0}^{2L} \omega_i^{\mu} \phi_i(n|n-1) \tag{11b}$$

$$\Sigma_{yy}^{1/2}(n|n-1) = \text{qr}([\sqrt{\omega_1^c}(\phi_{1:2L}(n|n-1) - \hat{y}(n|n-1)) \quad \Sigma_v^{1/2}]) \tag{11c}$$

$$\Sigma_{yy}^{1/2}(n|n-1) = \text{cholupdate}(\Sigma_{yy}(n|n-1), \phi_0(n|n-1) - \hat{y}(n|n-1), \omega_0^c) \tag{11d}$$

$$\Sigma_{xy}(n|n-1) = \sum_{i=0}^{2L} \omega_i^c (\mathcal{X}^{(i)}(n|n-1) - \hat{x}(n|n-1))(\phi^{(i)}(n|n-1) - \hat{y}(n|n-1))^T \tag{11e}$$

Update of states from available measurements

$$K(n) = (\Sigma_{xy}(n|n-1)/\Sigma_{yy}^{1/2\,T}(n|n-1))/\Sigma_{yy}^{1/2}(n|n-1) \tag{12a}$$

$$\hat{x}(n|n) = \hat{x}(n|n-1) + K(n)(y(n) - \hat{y}(n|n-1)) \tag{12b}$$

$$U = K(n)\Sigma_{yy}^{1/2}(n|n-1) \tag{12c}$$

$$\Sigma_x(n|n) = \text{cholupdate}(\Sigma_x(n-1|n-1), U, -1) \tag{12d}$$

3.3 Probability constraints

The probability constraints on the states of interest are in the form of linear constraints as defined in Eq. (3):

$$\mathbb{P}(l^T x \leq g) \geq 1 - \epsilon \tag{13}$$

Using Chebychev's inequality the probability constraints in (13) can be robustly transformed to the following equation (Liu et al., 2014):

$$l^T \hat{x} + \sqrt{\beta l^T \Sigma_x l} \leq g \tag{14}$$

where $\hat{x}$ and Σ_x are the mean and covariance of x respectively and $\beta = \frac{1-\epsilon}{\epsilon}$

For the untransformed variables Eq. (13) can be directly used with the mean and covariance predicted by the square root UKF. For the transformed variables we instead use the mean and covariance given by Eq. (7) and Eq. (8) respectively. This is also done so that we can define the robust horizon.

$$\forall k > t_R \quad \Sigma_{x'}(n+k|n) = \Sigma_{x'}(n+k-1|n) \tag{15}$$

3.4 Square root UKF SNMPC formulation

Given linear chance constraints of the form in Eq. (13), a simplified SNMPC formulation can be stated as follows:

Finite horizon SNMPC problem with incorporated square root UKF and chance constraints

$$\begin{aligned}
&\underset{\mathbf{u}_N}{\text{minimize}} \quad \mathbb{E}_{\mathcal{Y}_n}(J(N, x(n), \mathbf{u}_N)) \\
&\text{subject to} \\
&\mathbb{P}_{\mathcal{Y}_n}(l_k^{iT} x(n+k) \leq g_k^i) \geq 1 - p_k^i \\
&\qquad\qquad \forall (k,i) \in \{1,\dots,N\} \times \{1,\dots,n_g\} \\
&u(n+k) \in \mathbb{U}_k \quad \forall k \in \{0,...,N-1\} \\
&(9) - (12) \text{ square root UKF based on transformed variable } x \\
&(7),(8),(15) \text{ Variance and mean of untransformed variable } x'
\end{aligned} \tag{16}$$

where the probability constraints can be reformulated as shown in Section 3.3. The open-loop problem can then be used in a receding horizon fashion to obtain a SNMPC algorithm as shown in the box for Algorithm 2.

Algorithm 2: Square root UKF SNMPC with receding horizon

Initialize: Supply $\hat{x}(0|0)$, $\Sigma_x(0|0)$, $u(0)$ and define (16)
At each sampling time $n = 1, 2, 3, \dots$

- Take measurements $y(n)$
- Solve (16) with $\hat{x}(n-1|n-1)$, $\Sigma_x(n-1|n-1)$, $u(n-1)$, $y(n)$ and obtain $u(n)$, $\hat{x}(n|n)$, $\Sigma_x(n|n)$
- Apply $u(n)$ to the real system

4. SEMI-BATCH REACTOR CASE STUDY

4.1 Semi-batch reactor model

To test the procedure the same case study as in Bradford and Imsland (2017b) based on a DAE system in Fogler (1999) is used, however parametric uncertainties were added and all the states were log-transformed. The following series reaction takes place in the reactor with H_2SO_4 as catalyst:

$$2A \xrightarrow[(1)]{k_{1A}} B \xrightarrow[(2)]{k_{2B}} 3C$$

The reactions are first order. The first reaction step is exothermic, while the second reaction step is endothermic. A heat exchanger is utilised to control the temperature. The following DAE system describes the dynamic behaviour of the semi-batch reactor:

$$\dot{C}_A = (-k_{1A} C'_A + (\theta_1 - C'_A)\frac{F}{V'})/C'_A, \tag{17a}$$

$$\dot{C}_B = (0.5 k_{1A} C'_A - k_{2B} C'_B - C'_B \frac{F}{V'})/C'_B, \tag{17b}$$

$$\dot{C}_C = (3 k_{2B} C'_B - C'_C \frac{F}{V'})/C'_C, \tag{17c}$$

$$\dot{T} = \left(\frac{(\theta_2 (T_a - T') - F\theta_1 C_{P_A}(T' - T_0)}{(C'_A C_{P_A} + C'_B C_{P_B} + C'_C C_{P_C})V' + \theta_4 C_{P_{H_2SO_4}}} + \frac{(-\Delta H_{Rx1A} k_{1A} C'_A - \Delta H_{Rx2B} k_{2B} C'_B)V'}{(C'_A C_{P_A} + C'_B C_{P_B} + C'_C C_{P_C})V' + \theta_4 C_{P_{H_2SO_4}}} \right)/T', \tag{17d}$$

$$\dot{V} = F/V', \tag{17e}$$

$$k_{1A} = \theta_3 \exp\left(-E_{1A}\left(\frac{1}{420} - \frac{1}{T'}\right)\right), \tag{17f}$$

$$k_{2B} = A_2 \exp\left(-E_{2B}\left(\frac{1}{400} - \frac{1}{T'}\right)\right), \tag{17g}$$

$$C'_A = \exp(C_A),\ C'_B = \exp(C_B),\ C'_C = \exp(C_C) \tag{17h}$$

$$T' = \exp(T),\ V' = \exp(V) \tag{17i}$$

where C'_A, C'_B, C'_C are the concentrations in moldm^{-3} of species A, B and C respectively, T' is the temperature in K of the reactor and V' is the liquid volume in dm^3. C_A, C_B, C_C, T and V are the log-transformed states of C'_A, C'_B, C'_C, T' and V' respectively. The deterministic parameters were kept at their nominal values, which can be found in Fogler (1999). The uncertain parameters are jointly given by the vector θ, which are assumed to be normally distributed, with constant mean $m_\theta = [4, 45000, 0.08, 100]^T$ and constant covariance $\Sigma_\theta = \text{diag}([0.1, 2e7, 1.6\text{e}{-4}, 5])$. The inputs of the problem are given by the flow rate of pure A entering the reactor F in dm^{3}h^{-1} and the temperature of the heat exchanger T_a in K.

In compact form we can write $x' = [C'_A, C'_B, C'_C, T', V']^T$, $x = [C_A, C_B, C_C, T, V]^T$ and $u = [F, T_a]^T$. Using orthogonal collocation the continuous time equations can be given as a discrete time equation system in the form:

$$x(k+1) = f(x(k), u(k)) + w(k) \tag{18}$$

where $f(x(k), u(k))$ describes the DAE system in Eq. (17) and $w(k)$ is additive Gaussian noise with a constant covariance matrix $\Sigma_w = \text{diag}([1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-6}, 1\text{e}{-6}])$.

Lastly, the measurement dynamics need to be defined, which are given by the following equation:

$$y(k) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} x'(k) + \nu(k) \tag{19}$$

where $\nu(k)$ is additive Gaussian noise with a constant covariance matrix $\Sigma_\nu = \text{diag}([1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-3}])$.

4.2 SNMPC problem

The OCP to be solved is formulated below. The economic objective is to maximize the amount of C at a fixed final batch time with a penalty for excessive control actions. The feed

rate can be varied between $0\text{dm}^3\text{h}^{-1}$ and $250\text{dm}^3\text{h}^{-1}$ and the heat exchanger temperature can be adjusted between $270K$ and $500K$. The liquid volume inside the semi-batch reactor is constrained to lie below 800dm^3, while the temperature is constrained to lie below 440K. The OCP problem is given by:

$$\begin{aligned}
&\underset{\mathbf{u}_N}{\text{minimize}} \quad -(\hat{x}_2(n+N|n)+\hat{x}_4(n+N|n))+\Delta U^T S \Delta U \\
&\text{subject to} \\
&\hat{x'}_3(n+k|n)+\sqrt{\beta\Sigma_{x'3,3}(n+k|n)} \leq 440 \quad \forall k \in \{1,...,N\} \\
&\hat{x'}_4(n+k|n)+\sqrt{\beta\Sigma_{x'4,4}(n+k|n)} \leq 800 \quad \forall k \in \{1,...,N\} \\
&u(n+k) \in [0,250]\times[270,500] \quad \forall k \in \{0,...,N-1\} \\
&(9)-(12) \text{ square root UKF based on transformed variable } x \\
&(7)-(8),(15) \text{ variance and mean of true variable } x'
\end{aligned} \tag{20}$$

where $\beta = \frac{\epsilon}{1-\epsilon}$, $\Delta U = [u(n+k)-u(n+k-1)]_{k\in\{1,...,N-1\}}$ and $S = \text{diag}([8\text{e}{-6}, 2\text{e}{-6}])$. For Eqs. $(9)-(12),(15)$ the robust horizon t_R was set to 2, the required scaling parameters can be determined from Van Der Merwe and Wan (2001) with $\alpha = 0.9$, $\beta = 2$ and $\kappa = 1$, $f(\cdot)$ is defined in Eq. (17) and Eq. (18) and $h(\cdot)$ in Eq. (19).

The problem objective is given at a fixed final time, such that a shrinking horizon implementation was used.

5. SIMULATION STUDIES

The final batch time was set to $4h$ with the total number of sampling points set to $N_t = 20$. The OCP in Eq. (20) was solved repeatedly using Casadi (Andersson, 2013) by employing direct collocation in Python. The degree of the polynomials was set to 4. The nonlinear programming problem was solved utilising Ipopt (Wächter and Biegler, 2006). IDAS (Hindmarsh et al., 2005) simulated the "real" plant. At time $n = 1$, Algorithm 3 needs to be initialized by with the "previous" covariance matrix, mean and control action. These were set to $\hat{x}(0|0) = [\log(1\text{e}{-3}), \log(1\text{e}{-3}), \log(1\text{e}{-3}), \log(290), \log(100)]^T$, $\Sigma_x(0|0) = \text{diag}([1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-3}, 1\text{e}{-3}])$ and $u(0) = [0, 290]^T$ respectively.

To test the robustness of the method 200 Monte Carlo simulations were performed, i.e. by sampling different realizations of parameters, additive disturbances and initial conditions for the real system, again with $\epsilon = 0.05$. The various trajectories can be seen in Fig. 4. For comparison purposes a nominal NMPC was run on 200 Monte Carlo simulations, for which the results are shown in Fig. 3. The UKF SNMPC overall performs well and leads to a relatively small number of constraint violations, while the nominal NMPC can be seen to violate both constraints substantially.

Lastly, the method was run for 3 different values of ϵ and for the nominal NMPC algorithm, with 100 Monte Carlo samples. The obtained objective values are illustrated in Fig. 2 as a box plot to highlight the trade-off between conservativeness and performance. The red line in the box plot indicates the median of the objective values, while the blue lines represent the upper and lower quartiles. The black lines give the smallest and largest value attained from the simulations, excluding outliers, shown as red crosses. We can clearly see that the median amount of C at the final batch time consistently increases with ϵ as expected, since an increase in ϵ leads to less conservativeness. The nominal NMPC algorithm leads to the largest amount of C on average.

6. CONCLUSION

Overall a new algorithm is proposed for SNMPC with efficient formulation of the probability constraints, which has been shown to be an efficient means to account for uncertainties from state estimates, disturbances and parameters for an economic model predictive control problem of a semi-batch reactor. The algorithm was able to keep nearly all 200 Monte Carlo simulations within the constraints, while it was shown that a nominal NMPC algorithm leads to significant constraint violations. In addition, important issues such as the prevention of negative concentrations were addressed by log-transformations.

7. ACKNOWLEDGEMENTS

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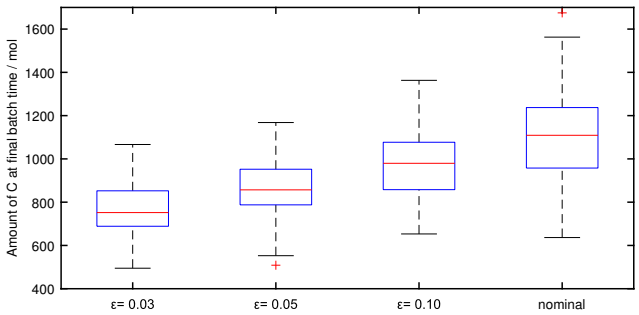

Fig. 2. Box plot of 100 Monte Carlo simulations for different values of ϵ for the UKF SNMPC algorithm based on the OCP in Eq. (20) and for the nominal NMPC algorithm

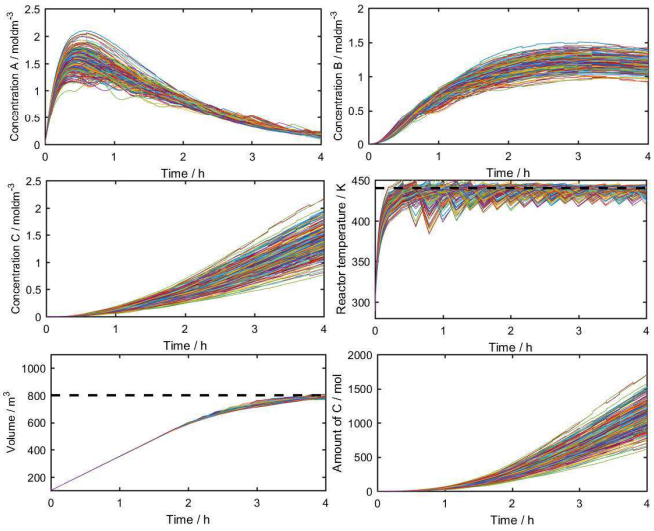

Fig. 3. 200 Monte Carlo trajectories of the "real" system from a nominal NMPC algorithm

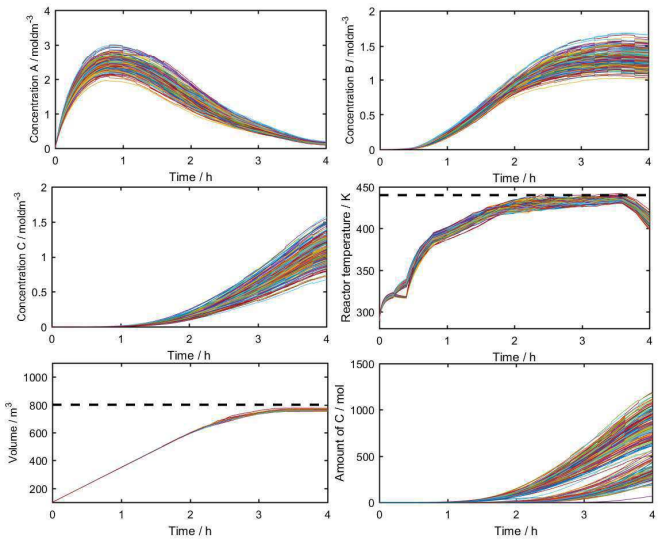

Fig. 4. 200 Monte Carlo trajectories of the "real" system from the SNMPC algorithm based on the OCP in Eq. (20) with $\epsilon = 0.05$

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