Sigmapoint Approach for Robust Optimization of Nonlinear Dynamic Systems

Sebastian Recker[1], Peter Kühl[2], Moritz Diehl[3] and Hans Georg Bock[4]
[1]*Aachener Verfahrenstechnik, RWTH Aachen University, Aachen, Germany*
[2]*BASF SE, Ludwigshafen, Germany*
[3]*Optimization in Engineering Center, KU Leuven, Leuven, Belgium*
[4]*Interdisciplinary Center for Scientific Computing, University of Heidelberg, Heidelberg, Germany*

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Abstract: Mathematical models describing dynamic processes contain parametric uncertainties. Robust model-based optimization thus becomes a challenging task in process engineering. Current approaches either require high computational effort or they make use of oversimplified approximations that do not capture changes in the solution structure due to nonlinear effects of the uncertain parameters on the states of the process. In this paper we propose an improved optimization approach that uses sigmapoints to characterize the space of uncertain parameters. Propagating sigmapoints through the process model and directly using them in the optimization problem allows to capture relevant nonlinearities for the uncertain parameters. Main advantages of this simple yet elegant approach are the relatively low computational burden and the independence from the optimizer, as no further derivatives are needed. The approach is applied to two examples from process engineering, a batch distillation and a semibatch reactor.

1 INTRODUCTION

In this paper we consider constrained optimization problems of the form

$$\min_{u\in\mathbb{R}^{n_u}} \Phi(x,z,u) \tag{1}$$

with

$$\Phi := \int_0^T L(x(t),z(t),u(t),p)\,dt + M(x(T),z(T)) \tag{2}$$

subject to the DAE system

$$\dot{x}(t) = f(x(t),z(t),u(t),p), \quad t\in[0,T], \tag{3}$$
$$0 = g(x(t),z(t),u(t),p), \quad t\in[0,T], \tag{4}$$

the initial value constraint

$$x(0) - x_0 = 0, \tag{5}$$

as well as control and path constraints

$$h(x(t),z(t),u(t),p) \le 0, \quad t\in[0,T]. \tag{6}$$

In this formulation $x(t)\in\mathbb{R}^{n_x}$ denotes the differential states, $z(t)\in\mathbb{R}^{n_z}$ the algebraic states, $u(t)\in\mathbb{R}^{n_u}$ the available controls, and $p\in\mathbb{R}^{n_p}$ the parameters. Such problems often arise from the model-based optimization of technical processes, e.g. in the chemical process industry.

The above formulation is based on a process model with exact parameters p. This is an idealization, which is referred to as the *nominal problem* in this paper. In most real-world problems, at least some of the parameters will not be known exactly. Rather, a set $\mathcal{P}\subset\mathbb{R}^{n_p}$ that is likely to contain p will be known or can at least be assumed. For a robust solution of the optimization problem the constraints shall be fulfilled for all parameters within this set and thus

$$h(x(t),z(t),u(t),p) \le 0 \quad \forall\, p\in\mathcal{P} \tag{7}$$

has to hold. Due to its then infinite number of constraints, this formulation is called a semi-infinite program (Blankenship and Falk, 1976). In order to solve this problem, the number of constraints has to be reduced. For this purpose we focus on the general concept of local reduction methods (Hettich and Kortanek, 1993) in this paper. Note that we do not consider the case when the model structure is not entirely known. In some cases, however, such a problem can be reformulated into one with parametric uncertainty.

A common idea to solve robust optimization prob-

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lems is to see the uncertain parameters as adverse players (Ben-Tal and Nemirovski, 1999) that try to disturb any constraint enforcement effort as strongly as possible. The task is to still meet the constraints for the worst parameter realization. This leads to minimizing the maximum negative effect of possible uncertainty realizations with respect to the constraints and results in the worst-case problem

$$\min_{u\in\mathcal{U}} \Phi(x,z,u,p) \qquad (8)$$
$$s.t. \quad \max_{p\in\mathcal{P}} h(x,z,u,p) \leq 0.$$

Due to its bi-level structure, this optimization problem is still difficult to solve numerically for general nonlinear functions.

1.1 Min-max Approximative Worst-case Reformulation

(Diehl et al., 2006) suggest an approximation for this kind of optimization problem. If the constraint functions are monotone within the parameter set and can be approximated by a Taylor expansion, the max-term of the optimization problem (8) for normally distributed parameters

$$\mathcal{P} := \left\{ p \in \mathbb{R}^{n_p} \mid \left\| \frac{1}{\gamma} \Sigma^{-\frac{1}{2}} (p - \tilde{p}) \right\|_2 \leq 1 \right\} \qquad (9)$$

with the covariance matrix Σ and the confidence level γ can be restated as:

$$\max_{p\in\mathcal{P}} h(x,z,u,p)$$
$$\approx h(x,z,u,\tilde{p}) + \gamma \left\| \Sigma^{\frac{1}{2}} \nabla_p h(x,z,u,\tilde{p}) \right\|_2 \leq 0 \qquad (10)$$

This robust optimization problem can efficiently be solved by dynamic optimization algorithms. For nonlinear DAE systems this linear approximation may lead to approximation errors and the robust enforcement of constraints will fail. A remedy is to use higher order approximations. In (Heine et al., 2006) a second order approximation of the mean and variance is suggested that can efficiently be computed by an unscented transformation.

In this article we assume all uncertain parameters to be normally distributed. Other parameter distributions can be treated within the same framework. For a derivation of robust reformulations of the optimization problem for different distributions see (Diehl et al., 2006).

While we focus on robust enforcement of constraints, note that the approach also allows to robustly treat the cost functional $\Phi(x,z,u,p)$.

1.2 Min-max Reformulation with Sufficient Condition

(Moennigmann and Marquardt, 2002) and (Diehl et al., 2008) present another approach to handle the bi-level structure of the optimization problem (8). The inner maximization problem is replaced by its sufficient condition. Due to the additional equations this extended optimization problem can be difficult to solve and results in a higher computational effort, but overcomes the problems associated with the linearization approach.

1.3 Chance-constrainted Programming

Another approach to solve optimization problems robustly, which avoids the bi-level structure caused by the worst case min-max formulation of the constraint, is the chance constrained optimization (Arellano-Garcia et al., 2003). The general constraint (7) is replaced by a probability constraint

$$P\{h(x,z,u,p) \leq 0\} \geq 1-\alpha. \qquad (11)$$

This approach requires efficient algorithms for realizing the mapping from the uncertain parameters to the uncertain constraints. As this mapping only holds for the actual set of inputs u, it has to be recalculated in each iteration of the optimization. Even if derivatives are used to avoid the computation of the mapping in each iteration (Li et al., 2008), this approach results in high computational effort.

2 A MODIFIED SIGMAPOINT APPROACH

The presented approaches either only hold for mildly nonlinear problems that can be approximated by linearization, or they result in high computational time. To combine the low computational effort of the worst-case approximation with the higher accuracy of the other two methods, we modify the usage of the unscented transformation suggested in (Heine et al., 2006). Before optimizing, modified constraints $\tilde{h}(x,z,u,p)$ shall be identified such that satisfying the new constraints results in satisfying the original constraints for all parameters inside the critical subspace with a desired probability:

$$\tilde{h}(x,z,u,p) \leq 0 \Rightarrow P\{h(x,z,u,p) \leq 0\} \geq 1-\alpha \qquad (12)$$

A possible choice of the modified constraints could be the principal axis endpoints of the constraint dis-

tribution, which correspond to the $1-\alpha$ interval[1], if the constraints are monotone within the parameter set. For constraints with moderate curvatures, this choice of the modified constraints results in an approximation that might allow to meet the original constraints for all parameters inside the uncertainty ellipsoid with nearly the desired probability. In order to identify these endpoints, the mapping of the parameter distribution onto the constraints has to be described.

An appealing method for propagating distributions through nonlinear models is the Unscented Transformation ((Julier and Uhlmann, 1996)). By choosing so called sigmapoints and weights and propagating these sigmapoints through the model, one can approximate the distribution of the constraints $\tilde{h}(x,z,u,p)$, if the weighted sigmapoints approximate the distribution of the parameters. The first two moments of the constraint distribution (the mean and the covariance) are matched exactly and the method can be extended to match additional moments (Julier and Uhlmann, 1997).

Using these moments, a possible choice of the modified constraints for normally distributed parameters is

$$\tilde{h} := h(x,z,u,\tilde{p}) + \gamma \left\| h(x,z,u,\tilde{p}) - h(x,z,u,p_i^{\mathrm{UT}}) \right\|_2, \quad i = 0,\ldots,2n_p \tag{13}$$

with the sigmapoints of the Unscented Transformation

$$\begin{aligned} p_0^{\mathrm{UT}} &= \tilde{p} \\ p_i^{\mathrm{UT}} &= \tilde{p} + \sqrt{\Sigma_i} \qquad ,i = 1,\ldots,n_p \\ p_{i+n_p}^{\mathrm{UT}} &= \tilde{p} - \sqrt{\Sigma_i} \qquad ,i = 1,\ldots,n_p, \end{aligned} \tag{14}$$

where $\sqrt{\Sigma_i}$ is the ith row or column of the matrix square root of the covariance matrix Σ. $\tilde{p}$ denotes the set of nominal parameters. As the first two moments of the distribution are matched exactly, the endpoints are matched exactly, if the constraints are normally distributed. For not normally distributed constraints the endpoints can be mismatched dramatically, as the first two moments but not the $1-\alpha$ intervals are propagated.

Applying the Unscented Transformation to industrial relevant examples has shown, that modified sigmapoints are a good approximation for the corresponding $1-\alpha$ intervals, even for not normally distributed constraints. Thus, choosing the modified constraints as

$$\tilde{h} := h(x,z,u,p_i) \le 0, \quad i = 0,\ldots,2n_p \tag{15}$$

results in satisfying the constraints for all parameters inside the critical subspace with nearly the desired probability $(1-\alpha)$, if the modified sigmapoints are chosen by

$$\begin{aligned} p_0 &= \tilde{p} \\ p_i &= \tilde{p} + \gamma\sqrt{\Sigma_i} \qquad ,i = 1,\ldots,n_p \\ p_{i+n_p} &= \tilde{p} - \gamma\sqrt{\Sigma_i} \qquad ,i = 1,\ldots,n_p. \end{aligned} \tag{16}$$

Hence, the robust optimization problem results in

$$\begin{aligned} &\min_{u\in\mathcal{U}} \Phi(x,z,u,\tilde{p}) \\ &s.t. \quad h(x,z,u,p_i) \le 0, \quad i = 0,\ldots,2n_p \end{aligned} \tag{17}$$

and can easily be solved by a standard dynamic optimizer. For normally distributed and monotone constraints the $1-\alpha$ intervals are mapped exactly. Applying this approach to industrially relevant examples has shown that also for non-normally distributed constraints the desired probability is nearly achieved.

3 APPLICATION EXAMPLE: BATCH DISTILLATION

In the following section we will revisit an example that has already been studied in previous publications of (Diehl et al., 2006; Diehl et al., 2008). We will briefly review the optimization method with the linearization of the max-term and compare their results to our new approach.

The aim of the process sketched in Figure 1 is the separation of a binary mixture and to obtain distillate with a purity of at least 99%. In the following we briefly summarize the process model.

3.1 Process Model

The content of the reboiler M_0, with x_0 the molar percentage of the lighter component, is heated, so that vapor with and equilibrium composition $y(x)$ and a constant molar flux $V = 100$ kmol/h is produced over all trays. The vapor equilibrium is expressed by the simple function $y(x) := \frac{x(1+\alpha)}{x+\alpha}$. Input to the process is the controlled reflux ratio R and a liquid molar flux $L = \frac{R}{1+R}V$, which is also assumed to be constant throughout the column, is fed back into the column. The remainder of the condensed liquid flux $V-L$, with composition x_C is collected within the distillate tank with molar holdup M_D and composition x_D. For

[1] $1-\alpha$ denotes the probability of values to lie inside the symmetric confidence interval with less then $\gamma\cdot\sigma$ from the mean, with σ representing the standard deviation (e.g. for normal distributions $\gamma = 1 \Rightarrow 1-\alpha \approx 68.3\%$, $\gamma = 3 \Rightarrow 1-\alpha \approx 99.7\%$).

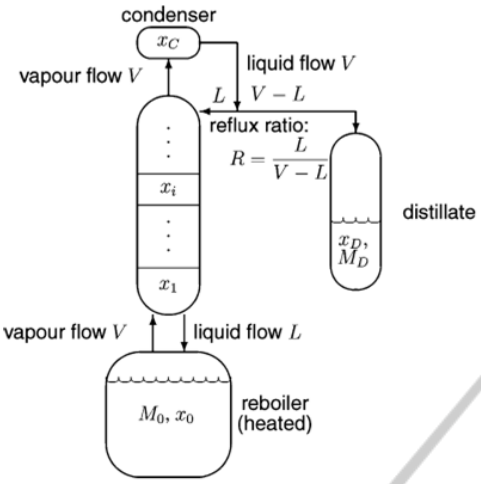

Figure 1: Sketch of the batch distillation column ((Diehl et al., 2006)).

the reboiler, we get the following ordinary differential equations:

$$\dot{M}_0 = -V + L \tag{18}$$

$$\dot{x}_0 = \frac{1}{M_0}(Lx_1 - Vy(x_0) + (V-L)x_0) \tag{19}$$

and

$$\dot{x}_i = \frac{1}{m}(Lx_{x_i+1} - Vy(x_i) + Vy(x_{i-1}) - Lx_i) \quad i = 1,\ldots,N \tag{20}$$

for the tray concentrations, where $m = 0.1$ kmol (the molar holdup of each tray) is assumed to be constant, and the number of trays is $N = 5$. For the condenser concentration x_{N+1} we obtain

$$\dot{x}_{N+1} = \frac{V}{m_c}(y(x_N) - x_{N+1}) \tag{21}$$

where $m_C = 0.1$kmol is the constant molar holdup of the condenser, and for the distillate container we obtain

$$\dot{M}_D = V - L \tag{22}$$

$$\dot{x}_D = \frac{V-L}{M_D}(x_{N+1} - x_D). \tag{23}$$

3.2 Nominal Optimization Problem

We summarize the states in $x = (M_0, x_0, x_1, \ldots, x_{N+1}, M_D, x_D)^T$ and set the control variable $u = R$. The objective is given by $\Phi := T - M_D(T)$ and reflects the two objectives of minimizing the batch time and maximizing the produced distillate. The only inequality constraint is $h := 0.99 - x_D(T) \leq 0$, i.e. the purity at the end of the batch shall exceed or equal 99%. Nominal initial values are $M_0 = 100, x_0 = 0.5, x_1 = \ldots = x_{N+1} = x_D = 1, M_D = 0.1$, and the nominal value of the equilibrium parameter is $\alpha = 0.2$. In addition there are bounds on the controlled reflux ratio, $0 \leq R \leq 15$. Figure 2 shows the solution for the nominal optimization problem, which has been solved with the software package *MUSCOD-II* ((Leineweber et al., 2003a; Leineweber et al., 2003b)) based on the direct multiple shooting approach introduced in (Bock and Plitt, 1984).

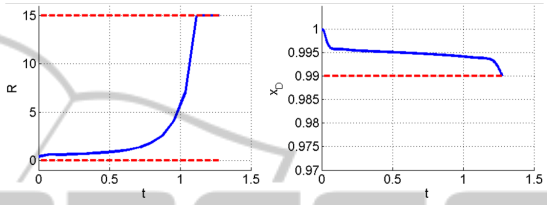

Figure 2: Nominal solution of the batch distillation problem.

3.3 Uncertain Optimization Problem

For practical problems, the aim of a robust optimization is to still meet the constraints despite the uncertainties. For this model uncertainty is certainly present in the parameter $p_1 = \alpha$ as well as in the initial feed composition $p_2 = x_0(0)$. We assume the set of the uncertain parameters to be characterized by the covariance matrix

$$\Sigma = \begin{pmatrix} 0.0278 & 0 \\ 0 & 2.5e^{-5} \end{pmatrix}. \tag{24}$$

3.4 Robust Optimization by Linearization of the Max-term

In order to robustify the optimization with respect to the critical quality specification, we reformulate the respective constraint as

$$\max_{p \in \mathcal{P}} \; 0.99 - x_D(T,p) \leq 0 \tag{25}$$

and approximate the solution of the inner maximization problem by

$$0.99 - x_D(T,\tilde{p}) - \gamma\sqrt{\Sigma_{1,1}\frac{\partial x_D(T,\tilde{p})}{\partial \alpha}^2 + \Sigma_{2,2}\frac{\partial x_D(T,\tilde{p})}{\partial x_0(0)}^2} \leq 0. \tag{26}$$

Here, $\tilde{p}$ denotes the nominal parameters and γ is set to 3, to meet the constraint with aa approximate probability of $\approx 99.7\%$. The results for this optimization are shown in Figure 3.

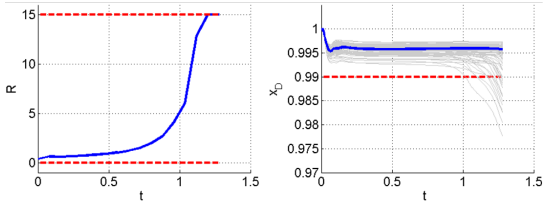

Figure 3: Robust solution of the batch distillation problem for the linearization of the max-term. Light gray lines show MonteCarlo simulations with random parameter realizations $p \in \mathcal{P}$.

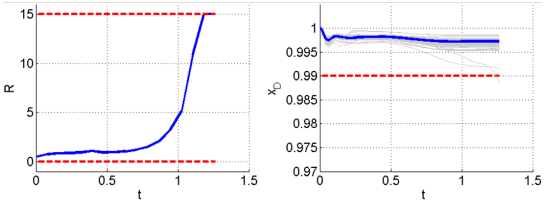

Figure 4: Robust solution of the batch distillation problem for the sigmapoint approach. Light gray lines show MonteCarlo simulations with random parameter realizations $p \in \mathcal{P}$.

Although the robust constraint (26) is active, a MonteCarlo simulation[2] of the robust profile (gray lines) shows that the desired purity at the end of the batch is not achieved with the desired probability. Obviously the linearization of the constraint function is not a sufficient approximation, as shown by (Diehl et al., 2008). Due to the special properties of this constraint function (structural changes of the constraint function for small changes in the uncertain parameter $x_0(0)$), increasing the order of the Taylor expansion would not improve the approximation with respect to the aim of staying above the desired final composition.

3.5 Robust Optimization by Sigmapoint Approach

For the sigmapoint approach, the critical constraint for the nominal parameters $\tilde{p}$ is amended by additional constraints with the sigmapoints p_i as arguments. Thus, the robust optimization problem formulation results in

$$\begin{aligned} \min_{u} \quad & T - M_D(T,\tilde{p}) \qquad (27)\\ s.t. \quad & 0.99 - x_d(T,p_0) \le 0\\ & 0.99 - x_d(T,p_1) \le 0\\ & 0.99 - x_d(T,p_2) \le 0\\ & 0.99 - x_d(T,p_3) \le 0\\ & 0.99 - x_d(T,p_4) \le 0 \end{aligned}$$

with the sigmapoints (cf. eq. 16)

$$p_0 = \tilde{p} = (6,0.5)^T, \quad p_1 = (6.5,0.5)^T,$$
$$p_2 = (6,0.516)^T, \quad p_3 = (5.5,0.5)^T, \quad p_4 = (6,0.484)^T.$$

The results of the optimization are shown in Figure 4.

[2]For the MonteCarlo simulation the trajectories for 100 normally distributed parameter realizations with mean $\tilde{p}$ and covariance matrix Σ have been computed.

A MonteCarlo simulation of this profile (gray lines) shows, that the compliance with the constraint is achieved with the desired probability.

4 APPLICATION EXAMPLE: SEMIBATCH PROCESS

The second application example is an exothermic semibatch process that been considered for optimization purposes in a previous publication of (Kuehl et al., 2005). A sketch of the process is shown in Figure 5. It describes the esterification of 2-butanol (B) with propionic anhydride (A) to 2-butyl propionate (D) and propionic acid (C). This homogeneous reaction is moderately exothermic and is catalyzed by sulphuric acid (K).

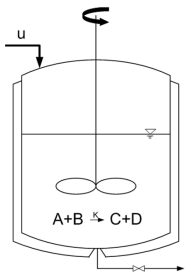

Figure 5: Sketch of the semibatch process.

The reaction is assumed to take place in a semi-batch reactor under isoperibolic conditions (e.g. constant jacket temperature). The reactor is initially charged with B and K. During the process, A is dosed to the reactor until the dosed amount of substance A is equal to the initial amount of substance B. The batch is finished once almost all B has been consumed. A model of the process can be found in the Appendix. It was originally developed by (Milewska, 2006).

4.1 Nominal Optimization Problem

Following the case study in (Kuehl et al., 2005) the objective is chosen as $\Phi := \int_0^{t_f} n_B(\tau)^2 \, d\tau$. The inequality constraints are $h_1(t) := T_R(t) - 340.5 \leq 0$ and $h_2(t) := T_{ad}(t) - 363.65 \leq 0$.

The complete optimization problem is summarized as

$$\begin{aligned} \min_u \quad & \int_0^{t_f} n_B(\tau)^2 \, d\tau \qquad (28) \\ \text{s.t.} \quad & 0 \text{ mol/s} \leq u(t) \leq 0.005 \text{ mol/s}, \\ & \int_{t_0=0}^{t_f} u(\tau) \, d\tau \leq 6.89396 \text{ mol}, \\ & T_R(t) - 340.5 \text{ K} \leq 0, \\ & T_{\text{ad}}(t) - 363.65 \text{ K} \leq 0. \end{aligned}$$

The second constraint ensures, that the maximum amount of A is not exceeded. Figure 6 shows the solution of the nominal optimization problem.

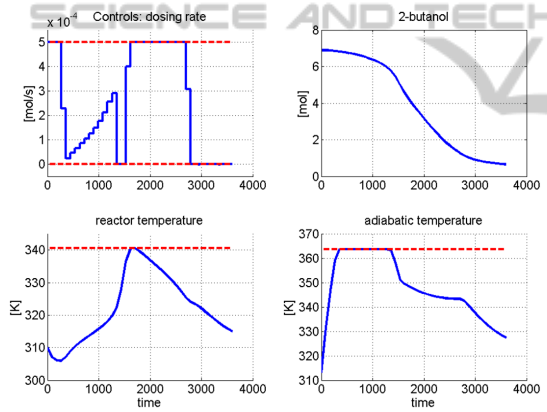

Figure 6: Nominal solution of the exothermic semibatch problem with safety constraints on reactor temperature and worst-case adiabatic temperature in case of a runaway reaction.

4.2 Uncertain Optimization Problem

Uncertainty is assumed to be present in the jacket temperature $p_1 = T_j$, due to imperfect control action and in the initial amount of catalyst $p_2 = n_K$. The covariance of the uncertain parameter space is

$$\Sigma = \begin{pmatrix} 1.2469 & 0 \\ 0 & 2.8747e^{-4} \end{pmatrix}. \qquad (29)$$

4.3 Robust Optimization by Linearization of the Max-term

To meet the constraints for all $p \in \mathcal{P}$ the approximation of the inner worst-case problem reads as

$$T_R - \gamma \sqrt{\Sigma_{1,1} \left(\frac{dT_R}{dT_j}\right)^2 + \Sigma_{2,2} \left(\frac{dT_R}{dn_K}\right)^2} - 340.5 \leq 0 \qquad (30)$$

$$T_{ad} - \gamma \sqrt{\Sigma_{1,1} \left(\frac{dT_{ad}}{dT_j}\right)^2 + \Sigma_{2,2} \left(\frac{dT_{ad}}{dn_K}\right)^2} - 363.65 \leq 0. \qquad (31)$$

Figure 7 displays the results for the robust optimization for $\gamma = 3$. Although this profile results in a safety margin to the maximal reactor temperature, a MonteCarlo simulation (gray lines) reveals, that the constraints are violated more often than allowed.

As the linearization of the uncertain constraints is computed for each iteration of the optimization, this approach is suitable for the approximation of uncertainties if the structure of the state trajectories does not change. This example shows, that even for small uncertainties (here 1% of the jacket temperatur) the structure of the trajectories can change dramatically. This strucutral change caused by the intrinsic dynamics of the system (e.g. accumulation of propionic acid) is not well approximated by the linearization. As a consequence, the solution fails to meet the constraints for the desired range of uncertain parameter.

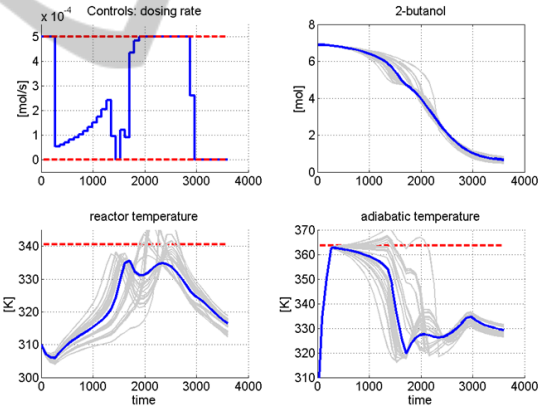

Figure 7: Robust solution of the exothermic semibatch problem for the linearization of the max-term. Light gray lines show MonteCarlo simulations with random parameter realizations $p \in \mathcal{P}$.

4.4 Robust Optimization by Sigmapoint Approach

As the sigmapoint approach tracks critical points instead of locally approximating the transformed distribution, the differing trajectories are captured in a broader range. The robust optimization problem for a desired probability level of $\gamma = 3$ results in

$$\min_u \int_0^{t_f} n_B(\tau)^2 \, d\tau \tag{32}$$
$$\text{s.t.} \quad 0 \text{ mol/s} \le u(t) \le 0.005 \text{ mol/s},$$
$$\int_{t_0=0}^{t_f} u(\tau) \, d\tau \le 6.89396 \text{ mol},$$
$$T_R(t, p_i) - 340.5 \text{ K} \le 0, \qquad i = 0, \ldots, 4$$
$$T_{\text{ad}}(t, p_i) - 363.65 \text{ K} \le 0, \qquad i = 0, \ldots, 4$$

with the sigmapoints (16)

$$p_0 = \tilde{p} = (313.15, 0.0511)^T, \quad p_1 = (314.65, 0.0511)^T$$
$$p_2 = (311.65, 0.0511)^T, \quad p_3 = (313.15, 0.0562)^T$$
$$p_4 = (313.15, 0.046)^T.$$

The optimization results are shown in Figure 8. In contrast to the robust solution presented above, even for the trajectories of the MonteCarlo simulation[3] (grey lines) compliance with the constraints is achieved with higher probability.

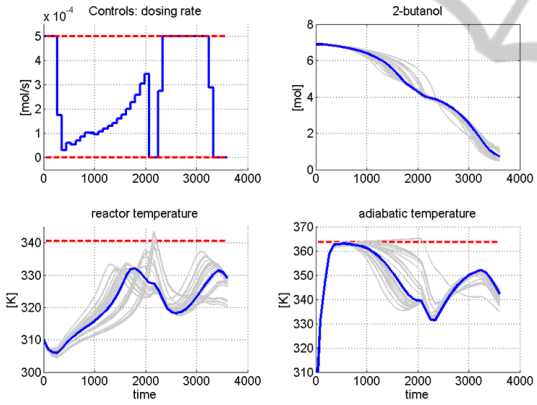

Figure 8: Robust solution of exothermic semibatch problem for the sigmapoint approach. Light gray lines show MonteCarlo simulations with random parameter realizations $p \in \mathcal{P}$.

5 CONCLUSIONS AND OUTLOOK

An improved approach for the approximative solution of robust optimization problems with parametric uncertainties has been introduced in this paper. The simple but effective idea relies on propagating sigmapoints through the nonlinear process and ensuring that these sigmapoint trajectories also meet the required constraints as part of the optimization problem. This approach does not change the original optimization problem apart from adding additional path constraints. In particular, no higher-order derivatives are required. The approach takes advantage of the beneficial properties of the unscented transformation, which allows to better track the nonlinear effect that uncertain parameters have on the constraints. This proves particularly important in cases where the structure of the optimal control problem solution changes. Examples from process engineering illustrate that even for small uncertainties these structural changes may occur and that approaches based on local linearization of the nominal trajectories may not be well suited.

In practical applications, robustly meeting critical constraints may not be the only concern. As the objective function increases with increasing robustness requirements, one typically wishes to find a compromise between robustness and the costs associated with it. Within the discussed framework, we see two approaches to adequately balance robustness and costs. One solution is to simply price constraint violations and include these costs in the objective function. The sigmapoint approach nicely supports this solution as the requested degree of robustness γ corresponds to a probability of constraint violation α. We have not yet investigated whether it is possible to directly include γ (or α respectively) as a free variable into the optimization problem.

A second solution for a balanced trade-off between robustness and performance is a robust reformulation of the objective function itself. For normally distributed parameters the reformulation of the objective functions is equivalent to that of 13 seems suitable. This has not yet been thoroughly investigated either.

Even though the sigmapoint approach has performed well on the examples shown, no performance guarantees have been established so far. There certainly exist optimization problems where the modified sigmapoints do not approximate the $1 - \alpha$ interval for the constraints well enough. In this case a possible remedy could be the propagation of additional sigmapoints at the expense of higher computational cost.

ACKNOWLEDGEMENTS

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[3]To guarantee the comparability for both MonteCarlo simulations even for the small number (25) of realizations used in this example, both simulations use the same set of normally distributed parameters for the trajectories.

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APPENDIX

The model of the semibatch process (as used in (Kuehl et al., 2005)) reads as follows:

$$\frac{dn_A}{dt} = \frac{u}{M_A} - r \cdot V \tag{33}$$

$$\frac{dn_B}{dt} = -r \cdot V \tag{34}$$

$$\frac{dn_C}{dt} = r \cdot V \tag{35}$$

$$(C_{p,I} + C_p) \cdot \frac{dT_R}{dt} = r \cdot (-\Delta H_r) \cdot V - q_{\text{dil}} - U \cdot \Omega (T_R - T_J) - \alpha \cdot (T_R - T_a) - \frac{u}{M_A} \cdot c_{p,A} \cdot (T_R - T_d) \tag{36}$$

where n_i denotes the molar amount of components $i = A,B,C,D$ and V the volume. T_R, T_J, T_a and T_d stand for the reactor, jacket, ambient and dosing temperatures. The reaction rate is denoted by r, $(-\Delta H_r)$ is the reaction enthalpy and Q_{dil} the dilution's heat. U is an overall heat transfer coefficient and Ω the heat exchanger area. The approximated heat capacity of solid inserts (stirrer, baffles) is $C_{p,I}$. C_p denotes the approximated heat capacity of the entire reaction mixture and $c_{p,i}$ is the specific molar heat capacity of component i. As the number of moles of D always equals the number of moles of C, the equation for D has been omitted. The molar concentrations c_i are calculated as $c_i = n_i/V$. The molar dosing rate u of A to the batch reactor serves as control input. The defining algebraic equations are:

$$\rho_i = M_i \left(P_i \cdot Q_i^{\left(1 - \left(\frac{T_R}{T_{c,i}}\right)\right)^{0.2857}} \right)^{-1}, \quad i = A,B,C,D \tag{37}$$

$$c_i = \frac{n_i}{V}, \quad i = A,B,C,D,K \tag{38}$$

$$c_{p,i} = a_i + b_i \cdot T_R + c_i \cdot T_R^2 + d_i \cdot T_R^3, \quad i = A,B,C,D \tag{39}$$

$$c_p = \sum_{i=A,B,C,D} c_{p,i} \cdot n_i \tag{40}$$

Table 1: List of process parameters and initial conditions.

name	value	name	value
$\Omega_{\min}$	0.0113	n_1	1.58
$V_{\min}$	0.124	n_2	0.76
d	0.155	E_a	$9.17 \cdot 10^4$
V_1	0.8	A_1	$9.35 \cdot 10^{10}$
V_2	1.6	A_2	$9.22 \cdot 10^{10}$
$C_{p,I1}$	117.3	A_3	$9.78 \cdot 10^{10}$
$C_{p,I2}$	198.4	A_4	$1.40 \cdot 10^8$
U_1	195	R	8.314
U_2	155	$(-\Delta H_r)$	59458
α	0.1	$T_R(0)$	310
T_J	313.15	$n_A(0)$	0.0
T_d	298.15	$n_B(0)$	6.894
T_a	298.85	$n_C(0)$	0.0
$m_{A,\text{total}}$	890.00	n_K	0.0511
q_0	$1.6 \cdot 10^4$		

i	A	B	C	D
M_i	0.13014	0.07412	0.07408	0.13011
a_i	683.73	242.57	94.84	206.16
b_i	-3.701	-2.313	-0.243	0.199
c_i	$9.6 \cdot 10^{-3}$	$1.07 \cdot 10^{-2}$	$2.2 \cdot 10^{-3}$	$-3.56 \cdot 10^{-4}$
d_i	$-7.46 \cdot 10^{-6}$	$-1.16 \cdot 10^{-5}$	$-2.51 \cdot 10^{-6}$	$1.04 \cdot 10^{-6}$
P_i	0.462	0.320	0.285	0.508
Q_i	0.2166	0.2088	0.1993	0.2265
$T_{c,i}$	630	536	611	578

$$C_{p,I} = C_{p,I1} + \frac{C_{p,I2} - C_{p,I1}}{V_2 - V_1}(V - V_1) \tag{41}$$

$$V = \frac{n_A M_A}{\rho_A} + \frac{n_B \cdot M_B}{\rho_B} + \frac{n_C M_C}{\rho_C} + \frac{n_C \cdot M_D}{\rho_D} \tag{42}$$

$$\Omega = \Omega_{\min} + 4 \cdot \frac{V - V_{\min}}{d} \frac{1\,\text{m}^3}{1000 \cdot 1} \tag{43}$$

$$U = U_1 + \frac{U_2 - U_1}{V_2 - V_1}(V - V_1) \tag{44}$$

$$x_A = \frac{n_A(t)}{n_A(t) + n_B(t) + 2n_C(t) + n_{\text{K}}(0)} \tag{45}$$

$$q_{\text{dil}} = q_0 \cdot e^{\frac{-x_A}{0.14}} \frac{dn_A}{dt} \tag{46}$$

$$r = \left(A_1 + A_2 \cdot c_C^{n_1}(t) + A_3 \cdot c_K^{n_2}\right) e^{\frac{-E_a}{R \cdot T_R(t)}} \cdot c_A \cdot c_B \tag{47}$$

$$T_{\text{ad}} = T_R + \frac{n_A \cdot \Delta H}{900 \cdot c_p \frac{V}{1000}} \tag{48}$$

In these equations, M_i, ρ_i, c_i denote the molar weight, density and molar concentration of component i. V_1, V_2, U_1, U_2 are geometry-dependent parameters and d is the scaled reactor diameter. The rate of heat loss to the environment is modeled by a constant α of appropriate dimension derived from a constant heat transfer coefficient and an average heat transfer surface area. The reaction rate is calculated following an Arrhenius approach; the parameters A_i and n_i are estimated from experimental data and give very good results for the semi-batch operation mode.