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A Toolkit for Efficient Computation of Sensitivities in Approximate Robust Optimal Control Problems

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Abstract: Efficient solution approaches for optimal control problems where the dynamics are described by uncertain differential equations are discussed in the present paper. Problems with uncertainties can be addressed by the robust worst-case formulation. In order to numerically solve the robust counterpart for the optimal control problem several approximation techniques can be employed. In this paper we use an approach based on linearization and solution of Lyapunov differential equations. We exploit the structure of the Lyapunov equation in the optimal control context providing an efficient numerical implementation. The capabilities and computational times of the new approach are demonstrated on two (bio)chemical examples.

1. INTRODUCTION

In the present paper we consider an optimal control problem with uncertainties. Starting with an optimal control problem governed by continuous differential equations, once we apply a direct transcription method, we are dealing with a discrete counterpart of these dynamics. Therefore, in the present paper we are interested in the solution of the discrete optimal control problem specified by:

$$\underset{x\in\mathbb{R}^{(N+1)n_x},u\in\mathbb{R}^{Nn_u}}{\text{minimize}} \quad h_N(x_N) \tag{1}$$

s.t.:

$$x_{k+1} = f_{k+1}(x_k,u_k,w_{k+1}), \qquad k=0,...,N-1, \tag{2}$$

$$x_0 = \bar{x}_0 + B_0\, w_0, \tag{3}$$

$$0 \geq h_k(x_k,u_k), \tag{4}$$

where $x=(x_0^\top,...,x_N^\top)$ and $u=(u_0^\top,...,u_{N-1}^\top)$ are state and control variables, respectively. The functions f_k, $k=1,...,N$, describe the dynamic of the system, while the functions h_k, $k=0,...,N$, represent the inequality path constraints for the system. The functions f_k and h_k are assumed to be differentiable in their arguments. Note that the objective functional is in our formulation of the Mayer type and only allowed to depend on x_N. This can always be achieved by reformulating the problem using slack variables if necessary. The initial state x_0 of the dynamic system is described by the vector $\bar{x}_0 + B_0 w_0$, where the matrix $B_0 \in \mathbb{R}^{n_x\times n_w}$ is given. The vector $w_0 \in \mathbb{R}^{n_w}$ and the variables $w_k \in \mathbb{R}^{n_w}$, $k=1,...,N$, are assumed to be uncertain, i.e., they are only known to be contained in a common uncertainty set W defined by:

$$W \;:=\; \left\{ w\in\mathbb{R}^{(N+1)n_w} \;\middle|\; \|w\|_2^2 = w^\top w \leq \Gamma^2 \right\}. \tag{5}$$

Optimal control problems which consider determining an optimal time-varying trajectory for dynamic systems are encountered in many engineering applications. If the dynamic system is affected by unknown disturbances, i.e., uncertain parameters or time-varying perturbations, the situation becomes more involved and thus special solution techniques have to be applied.

The development of the robust control theory was mainly influenced by Glover and Schweppe [1971], Schweppe [1973], who analyzed linear control systems with set constrained disturbances, as well as by Zames [1981], who was significantly contributing to the development of H_∞-control. For a more general overview on the achievements in classical robust control theory, including H_∞-control, we refer to the text books Dullerud and Paganini [1999], Zhou et al. [1996] and the references therein. Lyapunov and Ricatti equations became an important field of research for analysing the stability due to the work of Kalman [1963], Bittanti et al. [1991]. Most existing stability optimization techniques are either based on the optimization of the asymptotical decay rate of the system, the optimization of the so called pseudo-spectral abscissa, or on the smoothed spectral abscissa or radius. Robust optimization approaches for nonlinear systems are commonly based on linear approximations techniques (see e.g., Diehl et al. [2006b], Houska and Diehl [2009], Nagy and Braatz [2004]).

The focus of the present paper is to develop a numerical tool for fast and efficient solution of uncertain optimal control problems. The structure of the paper is as follows. In Section 2 we start with an introduction of the basic notation for robust counterpart formulations and approximate robust optimal control. Here we particularly highlight the approach based on the solution of Lyapunov differential equation. In Section 3 we present a numerical structure exploitation technique which accelerates an existing code for approximate robust optimal control based on Lyapunov differential equations. In Section 4 it will be explained how these techniques are implemented in the framework of a new feature within the open source software `ACADO Toolkit` (Houska et al. [2011]). In Section 5 we illustrate the capabilities of the structure exploiting approach by testing it on two (bio)chemical examples. The paper concludes in Section 6 with a summary and an outlook on how the presented techniques and results might become relevant for the realization and control of more complex systems in the near future.

2. APPROXIMATE ROBUST OPTIMAL CONTROL

In order to address optimal control problems with uncertainties an approximate robust optimal control strategy based on Lyapunov differential equations is employed. In this section we formulate a robust counterpart of the optimal control problem (1) - (4) taking into account the fact that the uncertainties w are contained in the bounded uncertainty set W defined by (5). First, we collect the discrete dynamic equations into a function $g \in \mathbb{R}^{(N+1)n_x}$, specified as:

$$g(x,u,w) = \begin{pmatrix} x_0 - \bar{x}_0 - B_0\, w_0 \\ x_1 - f_1(x_0,u_0,w_1) \\ \vdots \\ x_N - f_N(x_{N-1},u_{N-1},w_N) \end{pmatrix} = 0.$$

In order to formulate a robust counterpart formulation for the discrete optimal control problem (1) - (4) we replace the discrete path constraints h_k, $k = 0,...,N-1$, by their worst case excitations ϕ_k. The functions ϕ_k, $k = 0,...,N$, are defined by:

$$\begin{aligned} \phi_k(u) \;:=\; & \underset{x\in\mathbb{R}^{(N+1)n_x},\, w\in\mathbb{R}^{(N+1)n_w}}{\text{maximize}} \quad h_k(x_k,u_k), \\ \text{s.t.} \quad & g(x,u,w) = 0, \qquad w \in W. \end{aligned} \tag{6}$$

Then, the robust counterpart of the discrete optimal control problem (1) - (4) can be formulated as:

$$\underset{u\in\mathbb{R}^{Nn_u}}{\text{minimize}} \;\; \phi_N(u) \quad \text{s.t.} \quad \phi_k(u) \le 0, \text{ for } k = 0,...,N-1. \tag{7}$$

Due to the fact that there are no suitable numerical algorithms available in order to solve min-max robust optimal control problem (7), we employ some heuristics that allow us to approximately solve this optimal control problem. There exist several possibilities for the approximation of problem (7). In the present paper linearization techniques are applied (see Nagy and Braatz [2004, 2007], Diehl et al. [2006a], Houska and Diehl [2009]).

First, the robust path constraints in (6) are linearized for the given control u around a nominal trajectory $g(x,u,0) = 0$. Then, the approximated robust path constraints $\tilde{\phi}_k(u_k)$ are defined as:

$$\tilde{\phi}_k(u) \;:=\; h_k(x_k,u_k) + \underset{\delta x\in\mathbb{R}^{(N+1)n_x},\, \delta w\in\mathbb{R}^{(N+1)n_w}}{\text{maximize}} \; \frac{\partial h_k}{\partial x}(x_k,u_k)\, \delta x, \tag{8}$$

$$\text{s.t.} \quad \frac{\partial g}{\partial x}(x,u,0)\, \delta x + \frac{\partial g}{\partial w}(x,u,0)\, \delta w \;=\; 0, \tag{9}$$

$$\delta w \in W, \tag{10}$$

where δx can be interpreted as a variation of the state variable x with respect to perturbations $\delta w \in W$, i.e., $\delta x = \frac{\partial x}{\partial w}\delta w$.

Lemma 1. The approximated robust path constraints $\tilde{\phi}_k(u_k)$ in (8) can explicitly be evaluated as

$$\tilde{\phi}_k(u) \;=\; h_k(x_k,u_k) + \Gamma \sqrt{\frac{\partial h_k}{\partial x}\, P_k \left(\frac{\partial h_k}{\partial x}\right)^{\top}},$$

where P_k is a solution of the discrete Lyapunov equation defined as:

$$P_0 = B_0\, B_0^{\top}, \tag{11}$$

$$P_k = A_k\, P_{k-1}\, A_k^{\top} + B_k\, B_k^{\top}, \qquad k = 1,...,N, \tag{12}$$

where the shorthands $A_k = \frac{\partial f_k}{\partial x_{k-1}}$ and $B_k = \frac{\partial f_k}{\partial w_k}$ are used.

Proof: First, the relation in (8) can be reformulated as follows:

$$\begin{aligned} \tilde{\phi}_k(u) \;&=\; h_k(x_k,u_k) + \max_{\delta x,\delta w} \frac{\partial h_k}{\partial x}(x_k,u_k)\, \frac{\partial x}{\partial w}\delta w \le \\ &\le h_k(x_k,u_k) + \Gamma \left\| \left(\frac{\partial x}{\partial w}\right)^{\top} \left(\frac{\partial h_k}{\partial x}(x_k,u_k)\right)^{\top} \right\|_2 = \\ &= h_k(x_k,u_k) + \Gamma \sqrt{\frac{\partial h_k}{\partial x}\, \bar{P} \left(\frac{\partial h_k}{\partial x}\right)^{\top}}, \end{aligned}$$

where the matrix $\bar{P} \in \mathbb{R}^{(N+1)n_x \times (N+1)n_x}$ is defined as:

$$\bar{P} = \left(\frac{\partial x}{\partial w}\right) \cdot \left(\frac{\partial x}{\partial w}\right)^{\top} = \begin{pmatrix} \frac{\partial x_0}{\partial w_0} & \cdots & \frac{\partial x_0}{\partial w_N} \\ \frac{\partial x_1}{\partial w_0} & \cdots & \frac{\partial x_1}{\partial w_N} \\ \vdots & & \\ \frac{\partial x_N}{\partial w_0} & \cdots & \frac{\partial x_N}{\partial w_N} \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial x_0}{\partial w_0} & \cdots & \frac{\partial x_0}{\partial w_N} \\ \frac{\partial x_1}{\partial w_0} & \cdots & \frac{\partial x_1}{\partial w_N} \\ \vdots & & \\ \frac{\partial x_N}{\partial w_0} & \cdots & \frac{\partial x_N}{\partial w_N} \end{pmatrix}^{\top}.$$

The linearized dynamics $g(x,u,w)$, specified in (9), are implicitly taken into account in $\bar{P}$ through the evaluation of sensitivities $\frac{\partial x}{\partial w}$. Due to the argument dependencies in $h_k(x_k,u_k)$, the derivative $\frac{\partial h_k}{\partial x}$ has only one non-zero $(n_h \times n_x)$ block, which correspond to the x_k - component. Thus, the product with $\bar{P}$ like

$$\left(\frac{\partial h_k}{\partial x}\right) \bar{P} \left(\frac{\partial h_k}{\partial x}\right)^{\top}$$

selects a corresponding $(n_x \times n_x)$ diagonal block $\bar{P}_k$ of the matrix $\bar{P}$ defined as:

$$\bar{P}_0 = \frac{\partial x_0}{\partial w_0}\left(\frac{\partial x_0}{\partial w_0}\right)^{\top} = B_0\, B_0^{\top}, \tag{13}$$

$$\bar{P}_k = \sum_{i=0}^{k} \frac{\partial x_k}{\partial w_i}\left(\frac{\partial x_k}{\partial w_i}\right)^{\top}, \qquad k = 1,...,N. \tag{14}$$

Closely inspecting the expressions (13) - (14), one can recognize that $\bar{P}_k$ can iteratively be evaluated as a solution of the discrete Lyapunov equation (11) - (12). This coincidence can be proved by induction.

$k = 0 : P_0 = \bar{P}_0$ by definition.

Induction step: $(k-1) \to k$. Assumption: $P_{k-1} = \bar{P}_{k-1}$.

$$\begin{aligned} \bar{P}_k &= \sum_{i=0}^{k} \frac{\partial x_k}{\partial w_i}\left(\frac{\partial x_k}{\partial w_i}\right)^{\top} = \sum_{i=0}^{k-1} \frac{\partial x_k}{\partial w_i}\left(\frac{\partial x_k}{\partial w_i}\right)^{\top} + \frac{\partial x_k}{\partial w_k}\left(\frac{\partial x_k}{\partial w_k}\right)^{\top} = \\ &= \sum_{i=0}^{k-1} \frac{\partial f_k}{\partial x_{k-1}} \frac{\partial x_{k-1}}{\partial w_i}\left(\frac{\partial x_{k-1}}{\partial w_i}\right)^{\top}\left(\frac{\partial f_k}{\partial x_{k-1}}\right)^{\top} + \frac{\partial x_k}{\partial w_k}\left(\frac{\partial x_k}{\partial w_k}\right)^{\top} = \\ &= \underbrace{\frac{\partial f_k}{\partial x_{k-1}}}_{A_k} \underbrace{\left\{\sum_{i=0}^{k-1} \frac{\partial x_{k-1}}{\partial w_i}\left(\frac{\partial x_{k-1}}{\partial w_i}\right)^{\top}\right\}}_{P_{k-1}} \left(\frac{\partial f_k}{\partial x_{k-1}}\right)^{\top} + \underbrace{\frac{\partial x_k}{\partial w_k}}_{B_k}\left(\frac{\partial x_k}{\partial w_k}\right)^{\top} = \\ &= A_k\, P_{k-1}\, A_k^{\top} + B_k\, B_k^{\top} = P_k, \end{aligned}$$

which proves the assertion of the lemma. □

Thus, the approximate robust counterpart for the discrete uncertain problem (1) - (4) can be formulated as:

$$\underset{x\in\mathbb{R}^{(N+1)n_x},u\in\mathbb{R}^{Nn_u},P\in\mathbb{R}^{Nn_x^2},\Gamma}{\text{minimize}} \quad h_N(x_N)+\Gamma\sqrt{C_N^\top P_N C_N} \tag{15}$$

$$\text{s.t.:} \quad x_{k+1} = f_{k+1}(x_k,u_k,0), \qquad k=0,\dots,N-1, \tag{16}$$

$$P_{k+1} = A_{k+1}\, P_k\, A_{k+1}^\top \;+\; B_{k+1}\, B_{k+1}^\top, \tag{17}$$

$$x_0 = \bar{x}_0, \qquad P_0 = B_0\, B_0^\top, \tag{18}$$

$$0 \geq h_k(x_k,u_k) + \Gamma\sqrt{C_k^\top\, P_k\, C_k}, \tag{19}$$

with the shorthand $C_k = \frac{\partial h_k(x_k,u_k)}{\partial x_k}$.

3. STRUCTURE EXPLOITATION FOR LYAPUNOV DIFFERENTIAL EQUATIONS

In this section we explain how the structure of differential dynamics augmented by the Lyapunov differential equation can efficiently be exploited in numerical algorithms. We consider a discrete approximate robust counterpart (15) - (19) for the uncertain optimal control problem (1) - (4), so that the Lyapunov method is employed.

Usually, derivative based approaches are applied in order to solve the discrete robust optimal control problem (15) - (19). Thus, both the differential dynamics and the corresponding discrete sensitivity equation have to be propagated simultaneously. In order to simplify notations below, the matrices $P_k \in \mathbb{R}^{n_x\times n_x}$ are transformed into vectors $p_k \in \mathbb{R}^{n_x^2}$ by applying a linear operator $l : P_k \mapsto p_k$. This operator lumps all the entries of the matrix P_k row-wise into a vector p_k, i.e.,

$$p_k = \left(P_k^{11},\dots,P_k^{1n_x},\dots,P_k^{n_x1},\dots,P_k^{n_xn_x}\right)^\top \in \mathbb{R}^{n_x^2}.$$

All the required first order sensitivities are collected into a matrix Y_{k+1}, defined as:

$$Y_{k+1} = \begin{pmatrix} \frac{\partial x_{k+1}}{\partial x_0} & \frac{\partial x_{k+1}}{\partial p_0} & \frac{\partial x_{k+1}}{\partial u_0} \\ \frac{\partial p_{k+1}}{\partial x_0} & \frac{\partial p_{k+1}}{\partial p_0} & \frac{\partial p_{k+1}}{\partial u_0} \end{pmatrix} \in \mathbb{R}^{(n_x^2+n_x)\times(n_x^2+n_x+n_u)}. \tag{20}$$

Some of the sensitivities in (20) can be obtained for free or only using a small effort if analysing and exploiting the structure of the augmented dynamics (16) - (18) (see points listed below). The rest of the required sensitivities has to be computed propagating the sensitivity equation which reads as:

$$Y_{k+1} = \begin{pmatrix} \frac{\partial f_{k+1}}{\partial x_k} & \frac{\partial f_{k+1}}{\partial p_k} \\ \frac{\partial \tilde{p}_{k+1}}{\partial x_k} & \frac{\partial \tilde{p}_{k+1}}{\partial p_k} \end{pmatrix} Y_k + \begin{pmatrix} 0 & 0 & \frac{\partial f_{k+1}}{\partial u_k} \\ 0 & 0 & \frac{\partial \tilde{p}_{k+1}}{\partial u_k} \end{pmatrix},\; Y_0 = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & 0 \end{pmatrix} \tag{21}$$

with $\mathbb{R}^{n_x^2} \ni \tilde{p}_{k+1} = l(\tilde{P}_{k+1})$ and $\tilde{P}_{k+1}$ is defined by the right hand side of the Lyapunov differential equation (17), i.e., $\tilde{P}_{k+1} = A_{k+1}\; P_k\; A_{k+1}^\top \;+\; B_{k+1}\; B_{k+1}^\top$. In order to fast and efficiently propagate the sensitivity equation (21) the structure of the augmented discrete differential dynamics can be exploited. We summarize them in the following:

- $\frac{\partial f_{k+1}}{\partial x_k} = A_k$. Thus, in (21) the upper left block in the system matrix does not need to be recalculated, since the matrix A_k is already available as an ingredient in the discrete Lyapunov differential equation.
- $\frac{\partial f_{k+1}}{\partial p_k} = 0$. The right hand side of the discrete dynamics does not depend on the discrete Lyapunov states.
- $P_k^\top = P_k$. The solution of the Lyapunov differential equation is symmetric due to its construction.
- $\frac{\partial p_{k+1}}{\partial p_0} = (A_k A_{k-1}\cdots A_0)\otimes(A_k A_{k-1}\cdots A_0)$. Because of the high dimension n_x the block $\frac{\partial p_{k+1}}{\partial p_0} \in \mathbb{R}^{n_x^2\times n_x^2}$ in the sensitivity matrix Y_{k+1} turns out to be the most computationally expensive part which has to be determined throughout the sensitivity equation. Employing the formula above this block can be obtained using only a small effort. Moreover, the product $(A_k A_{k-1}\cdots A_0)$ has anyway to be computed throughout the numerical realization since it represents an important ingredient in an optimal control algorithm.

Lemma 2. The sensitivities $\frac{\partial p_{k+1}}{\partial p_0}$ with respect to the initial value p_0 can explicitly be computed as:

$$\frac{\partial p_{k+1}}{\partial p_0} = (A_k A_{k-1}\cdots A_0)\otimes(A_k A_{k-1}\cdots A_0). \tag{22}$$

Proof: The relation (22) can be proved by induction.

$k=0$: $\frac{\partial p_1}{\partial p_0} = A_0 \otimes A_0$ by definition.

Induction step: $(k-1)\to k$.

Assumption: $\frac{\partial p_k}{\partial p_0} = (A_{k-1}A_{k-2}\cdots A_0)\otimes(A_{k-1}A_{k-2}\cdots A_0)$.

$$\frac{\partial p_{k+1}}{\partial p_0} = \frac{\partial p_{k+1}}{\partial p_k}\cdot\frac{\partial p_k}{\partial p_0} =$$
$$= (A_k\otimes A_k)\cdot(A_{k-1}A_{k-2}\cdots A_0)\otimes(A_{k-1}A_{k-2}\cdots A_0) =$$
$$= (A_k A_{k-1}\cdots A_0)\otimes(A_k A_{k-1}\cdots A_0).$$

The last equality concludes the proof.

□

An analog to the expression (22) for sensitivities of continuous Lyapunov differential equations can be found in e.g. Houska [2007].

4. PRACTICAL REALIZATION OF COMPUTING SENSITIVITIES WITHIN ACADO FRAMEWORK

The open-source software package `ACADO Toolkit` by Houska et al. [2011] enables us to solve optimal control problems by a combination of multiple shooting techniques Bock and Plitt [1984] and an SQP method. The simulation of the differential equations as well as the computation of sensitivities, which are required for the SQP iteration, are both realized within the integrators in `ACADO`. There are several integrators available.

In order to tackle the robust counterpart (15) - (19) of the optimal control problem, where the Lyapunov based approach is employed, a special type of an integrator, the so-called `LYAPINT` integrator, was developed, which represents an add-on module to the `ACADO Toolkit`. This integrator is an explicit `Runge-Kutta45` integrator with an appropriate step size control.

The `LYAPINT` integrator enables us to compute the discrete state variables x_k and the discrete Lyapunov states P_k, $k = 0,\dots,N$, specified by (16) - (18). Moreover, the required discrete sensitivities which are collected in (20) are simultaneously computed. The specific properties of the sensitivity equation, which are discussed in the previous section, are incorporated

Table 1. Class Lyapunov

Member	Description
f	right hand side of the dynamic system
A	$\frac{\partial f}{\partial x}$
B	$\frac{\partial f}{\partial w}$
P	Lyapunov matrix
x	state variable x
u	control variable u
w	disturbance function w

within the `LYAPINT` integrator, and thus enable one to fast and efficiently compute sensitivities of the discrete iteration, if the user specifies this integrator.

The class `LYAPUNOV` is implemented in the `ACADO` environment. This class contains all the information which is needed for the performance of the `LYAPINT` integrator. In Table 1 the members of this class are listed. The user allocates an object `LYAPUNOV` by calling the constructor of this class through the initialization of the Lyapunov differential equation, e.g.,

```
f << dot(P) == Lyapunov(f,A,B,P,x,u,w);
```

Moreover, the integrator `LYAPINT` has to be explicitly specified by adding the option:

```
INTEGRATOR TYPE = LYAPINT
```

Beside the standard OCP setup Houska et al. [2011] these are the only actions which are required from the user. Once the object `LYAPUNOV` exists, it will be recognized within the `ACADO` framework, and the corresponding dimensions and functions will be appropriately adopted.

Fig. 1 shows an `ACADO` implementation example. This example demonstrates how the standard toolkit syntax has to be adopted to formulate and solve an approximate robust optimal control problem, defined as:

$$\underset{x(\cdot),y(\cdot),u(\cdot),P(\cdot),\Gamma}{\text{minimize}} \int_0^{2\pi} (x(t)^2 + u(t)^2)dt \tag{23}$$

s.t. for $t \in [0, 2\pi]$:

$$\dot{x}(t) = y(t), \tag{24}$$

$$\dot{y}(t) = -x(t) - (1-u^2(t))\, y(t) + w(t), \tag{25}$$

$$\dot{P}(t) = A(t)\, P(t)\, A(t)^\top + B(t)\, B(t)^\top, \tag{26}$$

$$x(0) = 0, \qquad y(0) = 1, \qquad P(0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{27}$$

$$0 \geq x(t) - 0.6 + \Gamma\sqrt{P_{11}(t)}. \tag{28}$$

```
#include <acado_toolkit.hpp>

int main( ){

    // INTRODUCE THE VARIABLES:
    // ----------------------------
    DifferentialState     x(2);
    DifferentialState     P(2,2);
    Control               u;
    Parameter             w;
    Parameter             Gamma;

    DifferentialEquation f;
    IntermediateState rhs(2);

    rhs(0) =   x(1);
    rhs(1) =  -x(0) - (1.0-u*u)*x(1) + w;

    f << dot(x) == rhs;

    // COMPUTATION OF DERIVATIVE MATRICES
    IntermediateState A = forwardDerivative( rhs, x );
    IntermediateState B = forwardDerivative( rhs, w );

    // ALLOCATION OF THE OBJECT LYAPUNOV
    f << dot(P) == Lyapunov(f,A,B,P,x,u,w);

    // DEFINE AN OPTIMAL CONTROL PROBLEM:
    // ----------------------------------
    OCP ocp( 0.0, 2.0*M_PI, 20 );
    ocp.minimizeLagrangeTerm( x(0)*x(0) + u*u );

    ocp.subjectTo( f );

    // BOUNDARY CONDITIONS
    ocp.subjectTo( AT_START, x(0) ==  0.0 );
    ocp.subjectTo( AT_START, x(1) ==  1.0 );
    ocp.subjectTo( AT_START, w == 0.0 );
    ocp.subjectTo( AT_START, P == 0.0 );

    // ROBUSTIFIED PATH CONSTRAINT
    ocp.subjectTo( x(0) + Gamma*sqrt( P(0,0) ) <=  0.6 );

    OptimizationAlgorithm algorithm(ocp);

    // OPTION FOR THE CHOICE OF INTEGRATOR
    algorithm.set( INTEGRATOR_TYPE, LYAPINT );
    algorithm.set( INTEGRATOR_TOLERANCE, 1e-5 );
    algorithm.solve();

    return 0;
}
```

Fig. 1. Implementation example for approximated robust optimal control problem based on Lyapunov differential equation.

5. CASE STUDIES

In order to test the facilities of the `LYAPINT` integrator, two (bio)chemical test cases are studied. The description closely follows the one in Logist et al. [2011a]. For all parameter values see Logist et al. [2009a]. These problems were already discussed in the robust multi-objective context by Logist et al. [2011a,b].

5.1 Case I: Jacketed tubular chemical reactor

The first case study involves a tubular chemical reactor operating under steady-state conditions. This process can be described as follows:

$$\underset{x,u}{\text{minimize}}\ C_{\text{in}}(1 - x_1(L)) \tag{29}$$

s.t. for $z \in [0, L]$:

$$\frac{dx_1}{dz} = \frac{\alpha}{v}(1-x_1)\exp(\bar{\gamma}x_2/(1+x_2)), \tag{30}$$

$$\frac{dx_2}{dz} = \frac{\alpha\delta}{v}(1-x_1)\exp(\bar{\gamma}x_2/(1+x_2)) + \frac{\beta(z)}{v}(u - x_2), \tag{31}$$

$$x_{2,\min} \leq x_2 \leq x_{2,\max}, \qquad u_{\min} \leq u \leq u_{\max}, \qquad x(0) = (0,0)^\top. \tag{32}$$

where x_1, x_2 and u are dimensionless reactant concentration, reactor temperature and jacket temperature, respectively. The variable z is the spatial coordinate along the reactor with length L. The aim is to derive an optimal profile along the reactor for the jacket temperature $u(z)$ that minimizes the reactant concentration at the outlet L. C_{in} is the reactant concentration at the inlet. For safety reasons bounds are imposed on the reactor and the jacket temperature.

Table 2. Jacketed tubular reactor: Run-time comparison

Time for	`Runge-Kutta45`	`LYAPINT` Integrator
the whole SQP iteration	12.7 ms	10.7 ms
condensing	1.2 ms	1.1 ms
solving the QP	0.1 ms	0.1 ms
globalization	1.9 ms	1.9 ms
sensitivity generation	7.1 ms	5.3 ms

Note that the dimensionless heat transfer coefficient $w(z) = \beta(z)$ is uncertain and may vary along the reactor. This might lead to a violation of the temperature constraint in (32). Hence, in the current case a robustification of this constraint is focused on. For the given percentage γ of uncertainty on the nominal heat transfer coefficient β, i.e., $\Gamma = \gamma\,\beta$, the robustified path constraint reads as:

$$x_2(z) + \gamma\,\beta\,\sqrt{P_{2,2}(z)} \leq x_{2,\max}. \qquad (33)$$

The second term in the left hand side of the expressions in (33) is the robustness margin to the corresponding confidence level.

The approximated robust optimal control problem of the form (15) - (19) for the conversion optimization of jacketed tubular chemical reactor has been solved by using `ACADO Toolkit` and different types of integrators included therein. We have compared the performance between the `Runge-Kutta45` and the new developed `LYAPINT` integrator, where the structure of the sensitivity equation is exploited. In Table 2 the resulted run-times are listed. From this comparison one can observe the reduction in the computation time required, if we employ the `LYAPINT` integrator for the solution of the robust optimal control problem.

The exploitation of the `LYAPINT` integrator reduces the number of sensitivities to be computed in each time step from 42 to 18, which obviously impacts the computational times. Figure 2 displays the optimal state and control profiles for various γ levels.

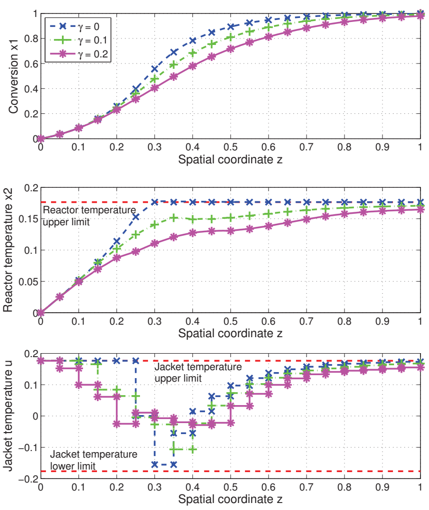

Fig. 2. Robustified jacketed tubular reactor: concentration (top), reactor temperature (middle), and jacket temperature (bottom).

5.2 *Case II: Fed-batch bioreactor*

The second problem involves a bioreactor based on the fed-batch lysine fermentation process investigated in Logist et al. [2009b]. The aim is to determine an optimal feeding profile and batch length. The process is described as follows:

$$\underset{x,u,t_f}{\text{minimize}} \quad -\frac{x_3(t_f)}{x_4(t_f)}, \qquad (34)$$

$$\text{s.t.} \quad \text{for } t \in [0, t_f]:$$

$$\frac{dx_1}{dt} = \mu\, x_1, \qquad \frac{dx_2}{dt} = -\delta\, x_1 + u\, C_{s,F}(t), \qquad (35)$$

$$\frac{dx_3}{dt} = \pi\, x_1, \qquad \frac{dx_4}{dt} = u\, C_{s,F}(t), \qquad \frac{dx_5}{dt} = u, \qquad (36)$$

$$20 \leq x_4, \qquad 5 \leq x_5 \leq 20, \qquad (37)$$

$$0 \leq u \leq 2, \qquad 20 \leq t_f \leq 40, \qquad (38)$$

$$x(0) = (0.1, 14 + \sqrt{2}w_0, 0, 0, 5)^\top. \qquad (39)$$

Here, x_1 is the biomass, x_2 the substrate, x_3 the product (lysine), x_4 the amount of substrate added and x_5 the volume. The control u is the volumetric rate of the feed stream.

For practical reasons constraints are imposed on the volume, the feed rate, the operation time and the amount of substrate added through feeding after time $t = 0$. As the process is operated in the fed-batch mode with an unspecified duration, both the feed rate $u(t)$ and the final time t_f have to be determined. The aim is to derive a feeding strategy which maximizes the yield, i.e., the ratio between the product formed and the substrate added during the process. The uncertain parameter considered in this case is the substrate concentration in the feed $w(t) = C_{s,F}(t)$, which needs a careful dosing along the batch duration. A similar uncertainty is also present in the initial amount of substrate. Consequently, the uncertainty does not only affect the possible satisfaction of constraint in (37), but also the biomass growth and lysine production. Hence, in the current case a robustification of both the constraint and the objective is concentrated on. For the given percentage γ of uncertainty on the nominal substrate concentration $C_{s,F}$, i.e., $\Gamma = \gamma\, C_{s,F}$, the robust counterpart to the constraint on the minimum amount is in this case:

$$x_4(t_f) - \gamma\, C_{s,F}\,\sqrt{t_f}\sqrt{P_{4,4}(t_f)} \geq 20. \qquad (40)$$

The batch duration t_f enters the robustness margins explicitly since the final time is a decision variable. Moreover, also a back-off in the objective is assumed to be taken into account.

The comparison between computation time needed for the approximate robust solution for yield optimization of the fed-batch bioreactor, if we employ two different integrators, the `Runge-Kutta45` and the `LYAPINT` integrator, is given in Table 3. Similar to the first case, one can observe the reduction in the computational time, if the structure exploiting `LYAPINT` integrator is used. Note, that in both examples the most computational time is spent for generation of sensitivities. Thus, in order to improve the performance of an algorithm, it is very important to reduce the run-time for computation of sensitivities, which can be achieved, e.g., by exploiting the structure as in the `LYAPINT` integrator.

Here, similar to the first case, exploiting the `LYAPINT` integrator the number of sensitivities to be computed in each time step was reduced from 420 to 120. This results in the reduction of

Table 3. Fed-batch bioreactor: Run-time comparison

Time for	Runge-Kutta45	LYAPINT Integrator
the whole SQP iteration	110 ms	51.7 ms
condensing	9.1 ms	9.1 ms
solving the QP	0.27 ms	0.58 ms
globalization	5.7 ms	4.6 ms
sensitivity generation	93.2 ms	30.1 ms

the computational times by the factor of three. Figure 3 depicts the optimal state trajectories for the first four states and the optimal controls.

Although in these small examples the computational time was not critical, one can observe a large potential for the structure exploiting method, if large dynamic systems are considered, e.g., in applications arising from chemical and mechanical engineering. This will be the subject of future investigations.

6. CONCLUSION

In this paper we have developed a structure exploitation strategy for an approximate robust optimal control approach. After reviewing an algorithm based on the solution of the Lyapunov differential equations, we explained how some structural properties of the sensitivity equation can efficiently be exploited. After that we explained how these techniques are implemented in the framework of a new feature within the open source software ACADO Toolkit. We have tested the performance of the new developed algorithm on two examples from (bio)chemical engineering and have encountered a large potential in application of the new method to dynamic systems with significant numbers of decision variables. Future research considers the application of the proposed method to advanced engineering examples and the inclusion for multi-objective optimal control [Logist et al., 2010].

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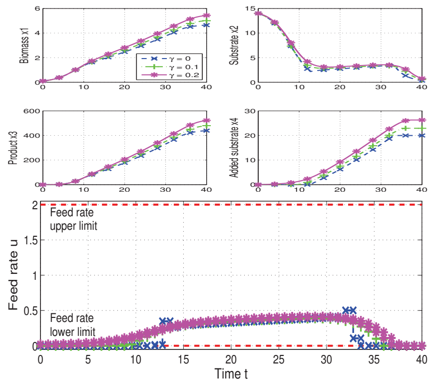

Fig. 3. Robustified fed-batch fermenter: states (top) and feed rate (bottom).

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