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Design of constrained nonlinear model predictive control based on global optimisation

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Abstract

In this paper a constrained nonlinear model predictive control (CNMPC) based on deterministic global optimisation is designed. The approach adopted consists in the transformation of the dynamic optimisation problem into a nonlinear programming (NLP) problem using the method of orthogonal collocation on finite elements. Rigorous convex underestimators of the nonconvex NLP problem are then derived within a spatial branch-and-bound method and solved to global optimality. The resulting control is compared to the CNMPC based on local optimisation in the control of a single-input single-output (SISO) continuous stirred tank reactor where a set of consecutive and parallel reactions take place.

Keywords: orthogonal collocation, finite elements, dynamic optimisation, global optimisation, CNMPC

1.Introduction

The interest of global dynamic optimisation is constantly growing mainly in security analysis of processes, state observation, parameter estimation and model based predictive control. Despite the increasing interest, deterministic global methods have not been extensively investigated. Very few academic research contributions including experimental studies and numerical simulations have been recently published in the open literature. This is mainly due to the lack of methods that allow the construction of rigorous convex underestimators for nonlinear differential constraints. One class of approaches that can be applied to solve dynamic optimisation problems to global optimality consists in the discretisation of variables in order to transform the problem into a nonlinear programming (NLP) problem. This means that in the process dynamic models, described by systems of ordinary differential-algebraic equations (DAEs), both the state and control variables are discretised (known as complete discretisation). The well-established global static optimisation algorithms, mainly deterministic methods, can then be used.

The approach proposed in this paper belongs to this class and uses the orthogonal collocation method on finite elements [1, 2, 3] to convert the DAEs

into a set of algebraic constraints. The objective here is the design of constrained nonlinear model predictive control (CNMPC) based on global optimisation. The case study is a single-input single-output (SISO) continuous stirred tank reactor involving a set of consecutive and parallel reactions.

1.1.Open-loop optimal control problem

Consider a deterministic optimal control problem in Bolza form on a fixed horizon $t \in [t_0, t_f]$ with

$$\begin{aligned} \min_{\mathbf{u}(t)} \quad & J = G(\mathbf{x}(t_f)) + \int_{t_0}^{t_f} F(\mathbf{x}(t), \mathbf{u}(t))\mathrm{d}\,t \\ \text{s.t.} \quad & \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \quad \mathbf{x}(0) = \mathbf{x}_0 \\ & \mathbf{h}(\mathbf{x}(t), \mathbf{u}(t)) = \mathbf{0}, \quad \mathbf{g}(\mathbf{x}(t), \mathbf{u}(t)) \le \mathbf{0}, \\ & \mathbf{x}^L \le \mathbf{x}(t) \le \mathbf{x}^U, \quad \mathbf{u}^L \le \mathbf{u}(t) \le \mathbf{u}^U \end{aligned} \tag{1}$$

where J represents the objective function (this comprises G, the component of the objective function evaluated at final conditions, and F, the component of the objective function evaluated over a period of time. In the case of tracking problems the functional F under the integral may be given by an appropriate norm of the difference between the reference trajectory and the output trajectory, such as a weighted Euclidean norm with the particular weighting $\mathbf{Q}: \|\mathbf{x}\|_{\mathbf{Q}}^2$), $\mathbf{f}$ is a vector valued function, $\mathbf{x}(t) \in R^{n_x}$ the state variables with constant initial conditions $\mathbf{x_0}$, $\mathbf{u}(t) \in R^{n_u}$ the sequence of control variables, $\mathbf{h}$ and $\mathbf{g}$ represent some equality and inequality constraints imposed to the process.

1.2.NLP Formulation-Collocation Based Approach

One class of approaches that can be applied to solve dynamic optimisation problems such as problem (1) is total discretisation (TD) or total parametrisation (TP) method [2, 3]. It transforms the original optimisation problem (1) into a NLP by parameterising both input and state variables over finite elements using polynomials (e.g., Lagrange polynomials) or any suitable basis functions. The coefficients of these polynomials and the length of the finite elements then become the decision variables in the resulting NLP problem. Following the procedure in [4] for a given approach the complete formulation can be written as

$$\begin{aligned} \min_{z} \quad & J(\mathbf{z}) \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{z}) = \mathbf{0}, \quad \mathbf{g}(\mathbf{z}) \le \mathbf{0}, \\ & \mathbf{z}^L \le \mathbf{z} \le \mathbf{z}^U \end{aligned} \tag{2}$$

where $\mathbf{z}$ is a vector of decision variables, $\mathbf{h}$ and $\mathbf{g}$ represent the equality and inequality constraints (both linear and nonlinear) resulting from the discretisation approach. Problem (2) can be solved using any standard nonlinear programming solver.

It is important to notice that the NLP problem (2) exhibits multiple local optima mainly due to the nonlinearity of equations $\mathbf{h}$ and $\mathbf{g}$. Methods for determination of the global optimum are therefore needed.

1.3.Global Solution

Here only deterministic methods for global optimisation are considered. They are based on the generation of convex relaxations of the original non-convex problem (2). Numerous methods have been proposed for constructing such relaxations [5–9]. In this work, the branch-and-bound method [5, 6, 10, 11] is exploited to guarantee the global optimality within ε-tolerance to the solution of the non-convex NLP problem (2).

The branch-and-bound algorithm begins by constructing a relaxation of the original non-convex problem (2). This relaxation is then solved to generate a lower bound on the performance index. An upper bound is generated by the value of the non-convex objective function at any feasible point (e.g., a local minimum found by standard NLP algorithm, or a problem (2) evaluation at the solution of the relaxed problem). If these bounds are not within some ε-tolerance a branching heuristic is used to partition the current interval into two new sub-problems (e.g., bisect on one of the variables). Relaxations can be constructed on these two smaller sets, and lower and upper bound can be computed for these partitions. If the lower bound on a partition is greater than the current best upper bound, a global solution cannot exist in that partition and it is excluded from further consideration (fathoming). This process of branching, bounding and fathoming continues until the lower bound on all active partitions is within ε-tolerance of the current best upper bound.

2.Case Study

2.1.Problem Formulation

In this work we consider a benchmark control problem of the isothermal operation of a continuous stirred tank reactor (CSTR) where the Van de Vusse reactions take place [12, 13] (i.e. $\mathrm{A} \rightarrow \mathrm{B} \rightarrow \mathrm{C}$ and $2\mathrm{A} \rightarrow \mathrm{D}$). The performance index is defined as the weighted sum of squares of errors between the setpoint $c_{\mathrm{B}}^{\mathrm{set}}$ and the estimated model output $\hat{c}_{\mathrm{B}}$ predicted for the k^{th} time step in the future with $w(t_k) = 0.01$ for all $k \neq H_{\mathrm{p}}$ and $w(t_k) = 10{,}000$ for $k = H_p$. The control problem is then formulated as

$$
\begin{aligned}
&\min_{c_{\mathrm{A}}, c_{\mathrm{B}}, F/V} J = \sum_{k=1}^{H_p=30} w(t_k)\left(c_{\mathrm{B}}^{\mathrm{set}}(t_k) - \hat{c}_{\mathrm{B}}(t_k)\right)^2 \\
&\text{s.t.} \quad \frac{\mathrm{d}c_{\mathrm{A}}}{\mathrm{d}t} = (F/V)(c_{\mathrm{A0}} - c_{\mathrm{A}}) - k_1 c_{\mathrm{A}} - k_3 c_{\mathrm{A}}^2 \\
&\qquad \frac{\mathrm{d}c_{\mathrm{B}}}{\mathrm{d}t} = k_1 c_{\mathrm{A}} - k_2 c_{\mathrm{B}} - (F/V) c_{\mathrm{B}}
\end{aligned}
\tag{3}
$$

where F is the feed flow rate of A into the reactor, V is the constant reactor volume, c_{A} and c_{B} are the reactant concentrations in the reactor, and k_i are the reaction rate constants for the three reactions. In this work, $k_1 = 50\ \mathrm{h}^{-1}$,

$k_2 = 100\,\mathrm{h}^{-1}$, $k_3 = 10\,\mathrm{l\,mol}^{-1}\,\mathrm{h}^{-1}$. We assume that the volume of the reactor is constant, that the feed consists of pure component A, and that the nominal concentration of A in the feed is $c_{\mathrm{A0}} = 10\,\mathrm{mol\,l}^{-1}$. An upper bound on the input *(F/V)* is assumed to be set at $200\,\mathrm{h}^{-1}$. The objective of NMPC is to regulate the concentration of the product B in the isothermal operation of the CSTR by manipulating the control variable *(F/V)* in the presence of disturbance d which will be simulated through changes in c_{A0}. The objective function is minimised over the future time horizon H_p (equal to 30 sampling times) with a sampling time of $0.002\,\mathrm{h}$ (7.2s). At each sampling time t_k, measurements $c_{\mathrm{B}}^{\mathrm{mes}}$ are taken from the perturbed plant and output disturbance is estimated as

$$d(t_k) = c_{\mathrm{B}}^{\mathrm{mes}}(t_k) - c_{\mathrm{B}}(t_k) \tag{4}$$

where $c_{\mathrm{B}}(t_k)$ is the model output at time t_k. The updated disturbance is then assumed to be constant in dynamic optimisation over the whole prediction horizon. Therefore, the estimation of $c_{\mathrm{B}}(t)$ in the performance index is calculated as

$$\hat{c}_{\mathrm{B}}(t) = c_{\mathrm{B}}(t) + d(t_k), \quad t \geq t_k \tag{5}$$

Once the solution of the dynamic optimisation problem is found (with 8 collocation points for state variables, and considering the control variable as piecewise constant within 1 element with a length of $0.06\,\mathrm{h}$ which is the prediction horizon), the computed optimal input within the first sampling period is applied both to the actual plant and to the model. The whole procedure is repeated with the moving horizon strategy in each sampling instant.

2.2.Closed- loop results

The results obtained in the closed-loop control are summarised in Fig. 1 where five time varying curves are presented. The first one is the controlled variable (c_{B}), the second is the input or control variable (F/V), the third is the feed concentration change (c_{A0}), the fourth is the performance index (or objective function) and the last one is the computational time required to get the solution.
It should be noted that it happens to the system under consideration to exhibit a steady-state input multiplicity and thus several solutions. This point is well discussed in [12].

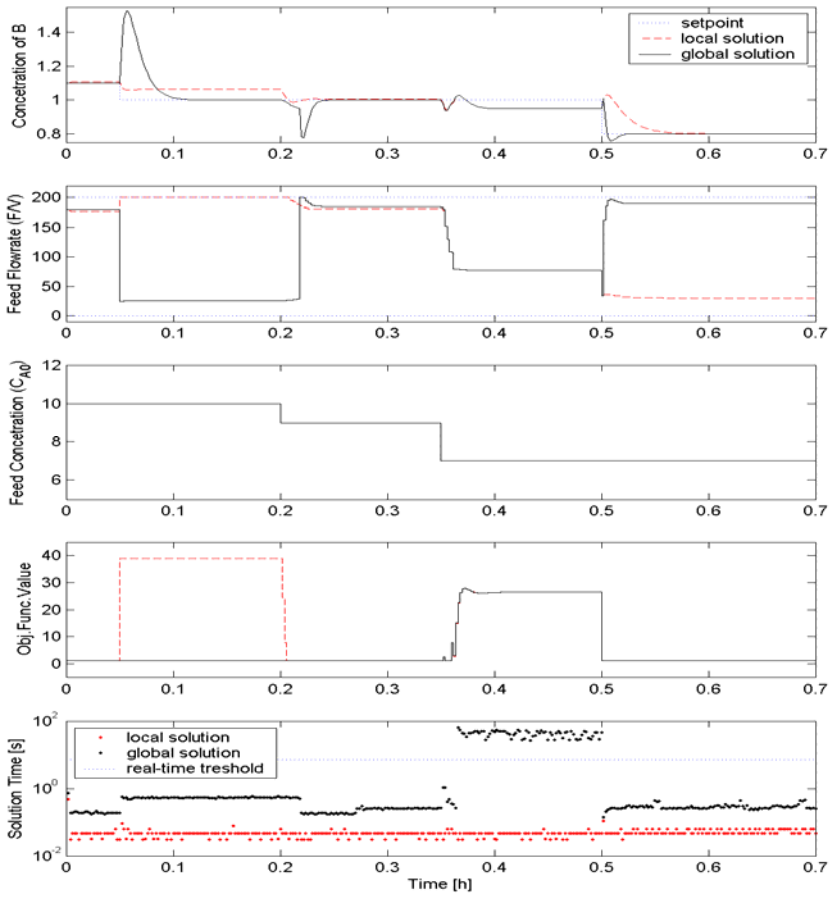

Figure 1: Closed-loop results obtained with local and global optimisation

In order to demonstrate the benefits of the global optimisation method over the local optimisation, setpoint transitions to track and disturbance loads to reject are generated as follows. The setpoint transitions are obtained by stepping the concentration c_B^{set} from 1.1 to $1\,\text{mol}\,\text{l}^{-1}$ at time $0.05\,\text{h}$ and then to $0.8\,\text{mol}\,\text{l}^{-1}$ at time $0.5\,\text{h}$ (first curve in Fig. 1). In the same way the disturbance loads are simulated by changing the feed concentration c_{A0} from 10 to $9\,\text{mol}\,\text{l}^{-1}$ at time $0.2\,\text{h}$ and to $7\,\text{mol}\,\text{l}^{-1}$ at time $0.35\,\text{h}$ (third curve in Fig. 1).

The global optimisation method leads to two significant improvements in setpoint tracking visible at setpoint changing times $0.05\,\text{h}$ and $0.5\,\text{h}$. In the first change, at time $0.05\,\text{h}$, the global algorithm chooses to use an offset free position corresponding to an input value of $F/V = 25\,\text{h}^{-1}$ (second curve in Fig. 1). The local technique is helpless as it finds the problem to be locally infeasible, forcing the relaxation to the hard terminal constraint and chooses to move in an improving direction and ends on the constraint $F/V = 200\,\text{h}^{-1}$. In this case the global method leads to significantly lower performance index than the local one (fourth curve in Fig. 1).

In the second change, at time $0.5\,\text{h}$, the locally tuned controller is able to track the setpoint offset free without issue using an input value of $F/V = 29.9\,\text{h}^{-1}$.

On other hand, the globally tuned controller finds a better solution choosing the opposite steady state input value of $F/V = 185\,\mathrm{h}^{-1}$ (second curve in Fig. 1). This gives a better setpoint tracking behaviour.
Concerning the time required to compute a solution (fifth curve in Fig. 1), in most cases the global solver is able to guarantee the global optimality within the sampling period of $7.2\,\mathrm{s}$. However, it should be mentioned, that at time of $0.35\,\mathrm{h}$ the solver can no longer achieve the desired setpoint due to a large disturbance. At this point, guaranteeing the global solution takes much more time than in previous cases and the solution is returned too late to be used for real-time purposes (within $7.2\,\mathrm{s}$). In this time instant, the best local solution is implemented and thus the guarantee on global optimality is lost. For the global optimisation method used to design the CNMPC the increase of the computation capacities or the decrease of the global optimum accuracy would probably guarantee the global optimality of the computed control.

3.Conclusions

A globally optimal NMPC algorithm has been proposed. A deterministic approach is used to find the guaranteed global optimum to the nonconvex NLP problem resulting from the simultaneous optimisation method. The algorithm has shown its capabilities to eliminate the poor performance in a simple CSTR example resulting from the suboptimal input trajectories obtained by local optimisation techniques. It has been shown, that with growing computational capabilities, the global CNMPC may be used also in real-time applications.

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