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Path-following for parametric MPCC: a flash tank case study

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Abstract

Mathematical programs with complementarity constraints (MPCC) can arise in process models that contain discrete decisions such as switches, phase changes, and flow reversal. Path-following methods are an important part of advanced-step nonlinear model predictive control (NMPC) due to the ability to deal with changes in the active-set of constraints. In this work, we introduce a path-following algorithm for parametric MPCC demonstrated on a flash tank case study. We show that this algorithm can successfully track the solution without the need for fine discretization or identifying the exact points where active-set changes occur, which are important properties for NPMC implementation.

Keywords: Mathematical programming with complementarity constraints, parametric sensitivity, path-following

1. Introduction

Nonlinear model predictive control (NMPC) is a process control method that formulates and repeatedly solves an optimization problem using a nonlinear dynamic model representation of the process as constraints. When configuring an NMPC problem, it is important to have a model that can describe the process as accurately as possible within a defined range of the process variables, and that calculations can be performed during the time between two measurements, i.e., the optimization problem needs to be rapidly solved. Systems with switches, phase changes, or flow reversal, for example, result in models with nonsmooth decisions, which make optimization problems with dynamic models challenging to solve, especially with a limited time frame. For representing such processes, complementarity constraints can be used: they specify the relationship between two variables, enforcing that at least one of them must be at its bound (Biegler, 2010). Optimization models with this type of constraint are called mathematical programs with complementarity constraints (MPCC). These models are inherently non-convex and fail to satisfy the Mangasarian–Fromovitz constraint qualification due to the complementarities, requiring reformulation strategies to handle these constraints with standard NLP solvers (Baumrucker et al., 2008).

Advanced-step NMPC (asNMPC) is a control technique that uses a prediction of the next state variables based on the current control action as the initial values (here they can be seen as parameters) to solve the optimal control problem in advance between the sampling times. When the new sample is available, the solution is updated based on the sensitivity at the optimal solution with respect to the initial state (Zavala and Biegler, 2009). Hence, computational delay between sampling and implementing the control action is reduced. A limitation of the original asNMPC is

the assumption that the active-set of constraints does not change from the optimal to the updated solutions. Path-following algorithms can be employed to handle this issue, since change in the active-set can be detected by discretizing the difference between the predicted and sampled states or by using an active-set identification method (Kungurtsev and Jaschke, 2017; Jäschke et al., 2014).

Literature on path-following of parametric MPCC (PMPCC) is scarce; to the best of the authors' knowledge, the only investigation on the topic was conducted by Kungurtsev and Jäschke (2019). They propose two algorithms: one is based on a penalty-term reformulation for MPCC (Baumrucker et al., 2008), while the other traces active-set bifurcations that stem from bi-active complementarity constraints, assuming that a reliable active-set method is available.

In general, PMPCCs pose a number of formidable challenges for numerical solution, arising from the inherent combinatorical nature of the problem and the interaction with the parameter dependence. Herein, we vastly simplify the problem by means of two key assumptions:

i due to the nature of NMPC, the exact locations of active-set changes are not required but only determination of the solution at successively given values of a scalar parameter; and,

ii that we are considering MPCC such that each complementarity constraint can only be non-simple (bi-active) at a small number of discrete points.

These two assumptions permit a much more straightforward handling of the problem yet still apply to a selection of practical problems. For example, the second assumption will be valid for most physical systems, whereby active-set changes occur only at a few discrete points (e.g. when phase transitions occur). We focus on the demonstration of this method with a flash tank case study, in which we obtain solutions for relevant points along the optimal path.

2. Background

In this section we present relevant definitions and concepts necessary for the algorithm described in the next section. We begin with the definition of complementarity constraint, roughly following the exposition in (Scheel and Scholtes, 2000). Consider a matrix-valued function $F : \mathbb{R}^n \to \mathbb{R}^{l\times q}$,

$$F(w) := \begin{bmatrix} F_{11}(w) & \dots & F_{1q}(w) \\ \vdots & \ddots & \vdots \\ F_{l1}(w) & \dots & F_{lq}(w) \end{bmatrix} \tag{1}$$

with $w \in \mathbb{R}^n$. A general complementarity constraint can be expressed as

$$F_{1k} \perp F_{2k} \perp \dots \perp F_{lk}, \quad F_{ik} \geq 0, \quad \text{for} \quad i = 1,\dots,l \quad \text{and} \quad k = 1,\dots,q \tag{2}$$

i.e., at least one entry of each column in F is zero with the remaining assuming nonnegative values. In practice, l is often equal to 2 and F_{ik} mostly represent variable bounds.

A parametric MPCC (PMPCC) is an extension of traditional parametric NLP optimization models in the sense that it contains at least one complementarity constraint and can be solved as a function of one or multiple parameters. For a parameter vector $p : \mathbb{R} \to \mathbb{R}^r$, we can define PMPCC$(p(t))$ as

$$\min_{w(p(t))} \quad \varphi(w(p(t)), p(t)) \tag{3a}$$

$$\text{s.t.} \quad h(w(p(t)), p(t)) = 0 \tag{3b}$$

$$g(w(p(t)), p(t)) \geq 0 \tag{3c}$$

$$F_{1k}(w(p(t)), p(t)) \perp \dots \perp F_{lk}(w(p(t)), p(t)) \quad \text{for} \quad k = 1,\dots,q \tag{3d}$$

$$F_{ik} \geq 0, \quad \text{for} \quad i = 1,\dots,l \quad \text{and} \quad k = 1,\dots,q \tag{3e}$$

where $\varphi : \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}$, $h : \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}^s$, $g : \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}^q$, and $F : \mathbb{R}^n \times \mathbb{R}^r \to \mathbb{R}^{l \times q}$ are smooth functions. Dropping explicit notation for dependence on t, the Lagrangian for Eqs. (3) is

$$\mathscr{L}(w(p), p, \lambda) := \varphi(w(p), p) - \mu(p)^T h(w(p), p) - \nu(p)^T g(w(p), p) - \Gamma(p) F(w(p), p) \quad (4)$$

where $\lambda = (\mu, \nu, \Gamma)$ is arranged in the natural manner by reshaping the matrix Γ columnwise into a vector. $\Gamma(p)^T F(w(p), p)$ is the inner product of the corresponding Γ with the F matrix.

The reason we define parametric optimization models is that we wish to map some interval $I_t = [t_a, t_b]$ to the solution curve $(w^*(p(t)), \lambda^*(p(t))), t \in I_t$ of PMPCC$(p(t))$ by calculating a piecewise homotopy along t. Locally, this requires calculating the sensitivity of w^* along t.

For the inequality and complementarity constraints, we define the corresponding g and F active-sets at some point $w(p)$ as $A_g(w(p)) := \{i : g_i(w(p)) = 0\}$ and $A_F(w(p)) := \{(i, j) : F_{ij} = 0\}$.

Mirroring terminology used in eigenvalue analysis, a complementarity constraint $F_{\cdot j}$ is considered *simple* at point w if only one constraint in that column $F_{\cdot j}$ is active. It is *nonsimple* if more than one constraint in $F_{\cdot j}$ is active. This latter situation is often termed 'bi-active' in the case of two active constraints.

A point $w(p)$ feasible to PMPCC$(p(t))$ is termed *weakly stationary* if there exists multipliers λ such that, where $\circ$ is the Hadamard (elementwise) product,

$$\nabla_w \mathscr{L}(w(p), p, \lambda) = 0 \quad (5a)$$
$$\nu(p) \geq 0 \quad (5b)$$
$$\nu(p)^T g(w(p), p) = 0 \quad (5c)$$
$$\Gamma(p) \circ F(w(p), p) = 0. \quad (5d)$$

A point $w(p)$ which satisfies Eqs. (5) and further satisfies that $\Gamma_{ik} \geq 0$ if there exists some $j \neq i$ such that $F_{ik}(w(p), p) = F_{jk}(w(p), p) = 0$ is termed *strongly stationary*. In plain language, this condition is stipulating that if $F_{\cdot k}$ is simple then there is no restriction on the associated Lagrange multiplier whereas if it is nonsimple then the associated Lagrange multipliers must be nonnegative. Thus, we see that for strongly stationary points, a simple complementarity constraint behaves akin to an equality constraint. The strongly active-set for g is defined as $A_g^+(w(p)) := \{i \in A_g(w(p)) : \exists\ \nu_i > 0$ satisfying Eqs. (5)$\}$.

We now describe how we obtain the sensitivity of PMPCC$(p(t))$ with respect to t by reduction locally to a parametric nonlinear program (PNLP). For $t \in I_t$, we assume that the F constraints are nonsimple or strong complementarity of the inequality constraints fails only at a (small) finite number of discrete points so that $I_t = \{t_a\} \cup I_1 \cup I_2 \cup \cdots \cup \{t_b\}$, say, where each $I_i \subset I_t$ is an open interval. Within each I_i, the complementarity constraints can then be considered as equality constraints and strong complementarity of g holds, so the PMPCC reduces to a PNLP, which is more amenable to known solution methods. Therefore, within each I_i, $A_F^+(w(p)) = A_F(w(p))$ and $A_g^+(w(p(t)))$ is invariant. For PNLP$(p(t))$, $t \in I_i$, assume that $\varphi(\cdot,\cdot)$, $h(\cdot,\cdot)$, $g(\cdot,\cdot)$, and $F(\cdot,\cdot)$ are twice continuously differentiable in a neighborhood of $w^*(p(t))$ satisfying the first-order optimality conditions, and that the linear independence constraint qualification (LICQ) and strong second order sufficient condition (SSOSC) hold. For PNLP$(t)|_{t=t_0}$, LICQ implies that the dual space is a singleton (Kyparisis, 1985), i.e., the multipliers are unique. By taking the total derivative with respect to t of the stationarity conditions and active constraints of PNLP, we obtain the following linear system

$$\underbrace{\begin{bmatrix} \nabla^2_{ww}\mathscr{L} & \nabla_w h & \nabla_w g_A & \nabla_w F_A \\ (\nabla_w h)^T & 0 & 0 & 0 \\ (\nabla_w g_A)^T & 0 & 0 & 0 \\ (\nabla_w F_A)^T & 0 & 0 & 0 \end{bmatrix}}_{M(w(p(t)),p(t))} \underbrace{\begin{bmatrix} \dot{w} \\ \dot{\lambda} \end{bmatrix}}_{\dot{v}(p(t))} = - \underbrace{\begin{bmatrix} (\nabla^2_{wp}\mathscr{L})\dot{p} \\ (\nabla_p h)\dot{p} \\ (\nabla_p g_A)\dot{p} \\ (\nabla_p F_A)\dot{p} \end{bmatrix}}_{b(w(p(t)),p(t))} \quad (6)$$

where $\dot{p} = \frac{\mathrm{d}p}{\mathrm{d}t}$, $\dot{w} = (\nabla_p w)\dot{p}$, $\dot{\lambda} = (\nabla_p \lambda)\dot{p}$, g_A includes only strongly active inequalities, F_a includes only (simple) active F constraints, and parameter dependence has been omitted for brevity.

3. Methodology

For the algorithm, we require access to a robust active-set identification method; we used an adaptation of a method in (Oberlin and Wright, 2006) along with some custom heuristics. The essential feature of the algorithm is to calculate a piecewise approximant $v(p(t)) = [\ w(p(t))\ \lambda(p(t))\ ]^T$ to the solution $v^*(p(t))$ by numerically integrating along the solution curve between active-set changes. In the canonical formulation of a first-order initial value problem, this can be expressed as $\dot{v}(p(t)) = f(t, v(p(t)))$ for $v(p(t_0)) = v_0$ where v_0 is a known initial point. From Eq. (6) and $M(p(t))$ invertible, $f(t, v(p(t)) = \dot{v}(p(t)) = M(w(p(t)), p(t))^{-1}\, b(w(p(t)), p(t))$; in practice, a linear solve is used to calculate $f(t,\cdot)$. In our implementation, we used an adaptive stepsize Runge–Kutta integrator, which maintains the truncation error within a predetermined bound by adjusting the stepsize. Event detection is used periodically to check whether an active-set change has occurred within the last integration step; this should not happen too often since the active-set identification is a comparatively expensive calculation. If an active-set change has occurred then, for the current $t_{(k)}$ held fixed, equality-constrained Newton iterations are performed with the new active-set until the error in the approximant $v(p(t))$ is sufficiently small; the number of elements in λ, and hence v, may also change if the cardinality of the active-set changes. The integration step can loosely be considered a 'predictor' step whereas the Newton iterations are a 'corrector' step. However, the error is nominally controlled by the adaptive stepsize numerical integration. Note that if the active-set identification encounters a nonsimple complementarity constraint, by assumption we can perturb $t_{(k)}$ by some small $\varepsilon > 0$ to again obtain simple complementarity constraints. This ensures the algorithm can always calculate the sensitivity.

Algorithm 1 `Path-following for PMPCC(`t`) for` $t \in I_t = [t_a, t_b]$

τ is set to maximum active-set recalculation interval
$t_{(0)} \leftarrow t_a$, $\quad \tilde{v}_{(0)} = [\ \tilde{w}_{(0)}\ \tilde{\lambda}_{(0)}\ ]^T \leftarrow v_a$ where v_a is in a neighbourhood of the initial solution
Calculate $A^+_{g,(0)} = A^+_g(\tilde{w}_{(0)})$ and $A^+_{F,(0)} = A^+_F(\tilde{w}_{(0)})$
$v_{(0)} \leftarrow$ `Newton`$(\tilde{v}_{(0)}, A^+_{g,(0)}, A^+_{F,(0)})$
$k \leftarrow 0$, $\quad t_{\mathrm{AS}} \leftarrow t_{(0)}$
repeat
  $k \leftarrow k+1$
  Perform predictor integration step to obtain approximate $(t_{(k)}, \tilde{v}_{(k)})$
  if $t_{(k)} > (t_{\mathrm{AS}} + \tau)$ **then**
    repeat
      Calculate $A^+_{g,(k)}$ and $A^+_{F,(k)}$
      if $A^+_{F,(k)}$ nonsimple **then**
        $t_{(k)} \leftarrow t_{(k)} + \varepsilon_t$
      end if
    until $A^+_{F,(k)}$ is simple
    $v_{(k)} \leftarrow$ `Newton`$(\tilde{v}_{(k)}, A^+_{g,(k)}, A^+_{F,(k)})$, $\quad t_{\mathrm{AS}} \leftarrow t_{(k)}$
  else
    $v_{(k)} \leftarrow \tilde{v}_{(k)}$
  end if
until $t \geq t_b$

It is immediately apparent that the relationship between integration stepsize $t_{(k)} - t_{(k-1)}$ and the active-set identification interval τ is important because it determines whether there will be any

transient 'overshoot' of an incorrect solution.

4. Case Study

We use the same case study presented in Kungurtsev and Jäschke (2019), in which a flash tank with a 3-component feed flow $Q \in \mathbb{R}$ and composition $z \in \mathbb{R}^3$ is simulated. We seek to analyze how the split between vapor $V \in \mathbb{R}$ and liquid $L \in \mathbb{R}$ products with composition $y \in \mathbb{R}^3$ and $x \in \mathbb{R}^3$ respectively vary with temperature $T \in \mathbb{R}$ for a fixed pressure $P \in \mathbb{R}$. For that, we set up the following optimization model

$$\min \quad \frac{1}{2}(aQ - V)^2 dt \tag{7a}$$

$$\text{s.t.} \quad \sum_{i \in \mathscr{C}} \frac{z_i(K_i - 1)}{1 + a_t(K_i - 1)} = 0 \tag{7b}$$

$$K_i = \frac{P_i^{\text{sat}}}{P} = \frac{y_i}{x_i} \quad \text{for } i \in \mathscr{C} \tag{7c}$$

$$\log_{10}(p_i^{\text{sat}}) = A_i - \frac{B_i}{T + C_i} \quad \text{for } i \in \mathscr{C} \tag{7d}$$

$$L + V = Q \tag{7e}$$

$$Lx_i + Vy_i = Qz_i \quad \text{for } i \in \mathscr{C} \tag{7f}$$

$$a - s_V + s_L - a_t = 0 \tag{7g}$$

$$0 \leq s_V \perp V \geq 0 \tag{7h}$$

$$0 \leq s_L \perp L \geq 0 \tag{7i}$$

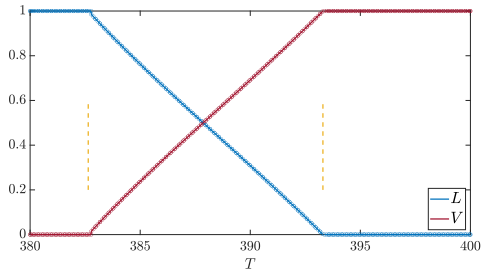
$$0 \leq a, x, y \leq 1 \tag{7j}$$

$$K, p^{\text{sat}} \geq 0. \tag{7k}$$

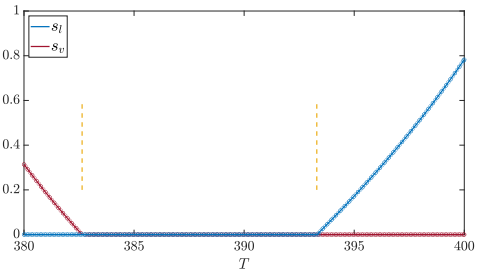
Constraint (7b) is the Rachford–Rice equation, which calculates the fraction of the feed that goes to the vapor phase, V/Q, represented by $a_t \in \mathbb{R}$. $K \in \mathbb{R}^3$ is determined by Raoult's law, given by constraint (7c). $P_i^{\text{sat}}(T) \in \mathbb{R}$ is the vapor pressure of the pure component $i \in \mathscr{C} = \{1, 2, 3\}$ at temperature T calculated using Antoine's equation (7d), where $A_i \in \mathbb{R}$, $B_i \in \mathbb{R}$ and $C_i \in \mathbb{R}$ are constants for each compound i. Constraints (7e) and (7f) correspond to the total and component-wise mass balances respectively. Constraints (7g)-(7j) are necessary to ensure that $V/Q \in [0, 1]$. The Rachford–Rice equation results in negative values and values greater than one for a_t if T is lower than the mixture's bubble point or larger than its dew point respectively, which would be physically impossible. Therefore, complementarity constraints (7h) and (7i) are considered; in the form of Eq. (2), $F_{11} = sV$, $F_{21} = V$, $F_{12} = sL$ and $F_{22} = L$. $s_L \in \mathbb{R}$ and $s_V \in \mathbb{R}$ are slack variables that represent how much a_t is lower than 0 and larger than 1 respectively. Variable $a \in \mathbb{R}$ represents the actual ratio V/Q, which is enforced by constraints (7g) and (7j). Note that $a = V/Q$ is not enforced as a hard constraint and, instead, is used as the objective function to be minimized. In this problem, temperature is the only parameter; we use $T(t_a) = 380$ and $T(t_b) = 400$.

5. Results

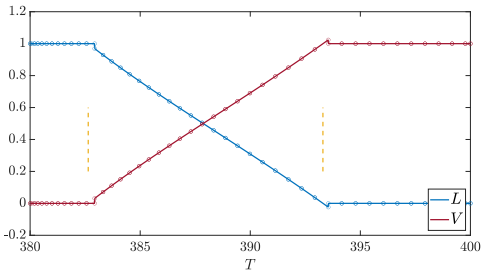
For the results presented here, the following values were used: $Q = 1$ kmol/s, $z = [0.5, 0.3, 0.2]^T$, $P = 5$ bar, $A = [3.98; 4.00; 3.93]^T$, $B = [1065; 1171; 1183]^T$, and $C = [-41.14; -48.83; -52.53]^T$. In Fig. 1a, the solution paths of primal variables L and V are shown. The maximum integration stepsize and τ in this run was set small, at 0.1, so the active-set changes are detected almost immediately after they happen. The corresponding complementarity slack variables s_l and s_v are shown in Fig. 1b. For a larger maximum stepsize of 5.0, there is less certainty where the actual active-set change happened and a jump is clearly visible, see Fig. 1d.



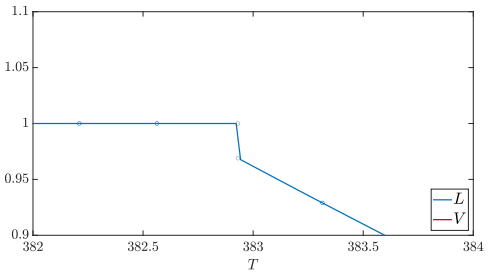
(a) Solution paths of V and L (small path-following steps).



(b) Solution paths of s_l and s_v (small path-following steps).



(c) Solution paths of V and L (large path-following steps).



(d) A local region of (c) to show jump after active-set change (large path-following steps).

Figure 1: Top row, stepsize of 0.1: (left) L (blue) and V (red) solution paths; (right) s_l and s_v paths. Bottom, stepsize of 5.0: (left) as above; (right) zoomed-in to region showing jump. Active-set changes indicated in vertical dashed lines (yellow).

6. Conclusion

We have demonstrated on the flash tank case study that the presented algorithm is a suitable method for path-following PMPCC. Since it does not require the identification of the exact location of active-set changes and that relatively coarse discretization can be used, this algorithm is a promising candidate for use in advanced-step NMPC of models with complementarities.

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