PIECEWISE M-STATIONARITY OF LOCAL MINIMIZERS OF MPCCS AND CONVERGENCE OF NCP-BASED BOUNDING METHODS

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Abstract. This paper focuses on solving mathematical programs with complementarity constraints (MPCCs) by assuming neither MPCC linear independence constraint qualification (MPCC-LICQ) nor lower/upper level strict complementarity at the solution. First, necessary conditions for MPCC local optimality and sufficient conditions for convergence to B-stationarity are investigated. Under MPCC-Abadie constraint qualification (MPCC-ACQ), we show that a local minimizer of an MPCC is "piecewise M-stationary"; a weakly stationary point of an MPCC is B-stationary if the related linear program with complementarity constraints (LPCC) is bounded below; furthermore, B-stationarity can be obtained from piecewise M-stationarity. Then convergence properties of the Bounding Algorithm proposed in [29] are analyzed. C- and M- stationarity of a limit point generated by the method are developed; an inequality variant of this method offers an alternative viewpoint to understand the behavior when approaching a limit point which is not S-stationary. In addition, a few practical issues related to convergence to a non-strongly stationary solution are discussed.

Key words. complementarity constraints, B-stationarity, constraint qualification, duality, NCP

1. Introduction. We consider mathematical programs with complementarity constraints (MPCCs) of the form

min
$$f(z)$$

s.t. $g(z) \le 0$,
 $h(z) = 0$,
 $0 \le G_i(z) \perp H_i(z) \ge 0$, $i = 1 \dots m$,

where $(f, g, h, G, H) : \mathbb{R}^n \to \mathbb{R}^{1+n_g+n_h+m+m}$ are differentiable functions. At a feasible point \bar{z} of the MPCC, define the following index sets:

$$I_{g}(\bar{z}) = \{i \mid g_{i}(\bar{z}) = 0\},\$$

$$\alpha(\bar{z}) = \{i \mid G_{i}(\bar{z}) = 0, H_{i}(\bar{z}) > 0\},\$$

$$\gamma(\bar{z}) = \{i \mid G_{i}(\bar{z}) > 0, H_{i}(\bar{z}) = 0\},\$$

$$\beta(\bar{z}) = \{i \mid G_{i}(\bar{z}) = 0, H_{i}(\bar{z}) = 0\}.$$

- A feasible point \bar{z} is weakly stationary, if there exist multipliers $\bar{\lambda} = (\bar{\lambda}^g, \bar{\lambda}^h, \bar{\lambda}^G, \bar{\lambda}^H)$
- with $\bar{\lambda}^g \geq 0$, such that 25

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$$0 = \nabla f(\bar{z}) + \sum_{i \in I_g(\bar{z})} \bar{\lambda}_i^g \nabla g_i(\bar{z}) + \sum_{i=1}^{n_h} \bar{\lambda}_i^h \nabla h_i(\bar{z}) - \sum_{i \in \alpha(\bar{z}) \cup \beta(\bar{z})} \bar{\lambda}_i^G \nabla G_i(\bar{z}) - \sum_{i \in \gamma(\bar{z}) \cup \beta(\bar{z})} \bar{\lambda}_i^H \nabla H_i(\bar{z}).$$

27 Further, a weakly stationary point \bar{z} is also

- S-stationary (strongly stationary), if $\bar{\lambda}_i^G, \bar{\lambda}_i^H \geq 0$ for all $i \in \beta(\bar{z})$; M-stationary, if either $\bar{\lambda}_i^G, \bar{\lambda}_i^H \geq 0$ or $\bar{\lambda}_i^G, \bar{\lambda}_i^H = 0$ for all $i \in \beta(\bar{z})$; C-stationary, if $\bar{\lambda}_i^G, \bar{\lambda}_i^H \geq 0$ for all $i \in \beta(\bar{z})$; A-Stationary, if either $\bar{\lambda}_i^G \geq 0$ or $\bar{\lambda}_i^H \geq 0$ for all $i \in \beta(\bar{z})$.

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32 **1.1. Local optimality and geometry simplification.** A local minimizer \bar{z} of MPCC (1.1) is a B-stationary point at which the following condition holds

34 (1.4)
$$\nabla f(\bar{z})^T d \ge 0, \quad \forall d \in \mathcal{T}(\bar{z}),$$

where $\mathcal{T}(\bar{z})$ is the tangent cone of the MPCC at the point \bar{z} . If the feasible region is regular at \bar{z} in the sense of Clarke (see [24, Definition 6.4][4, Section 1]), this condition

37 is the same as

38 (1.5)
$$\nabla f(\bar{z}) \in \mathcal{T}(\bar{z})^*,$$

where $\mathcal{T}(\bar{z})^*$ is the dual cone of $\mathcal{T}(\bar{z})$. Verifying these conditions directly is generally nontrivial. In practice, it is desirable to employ linearized cones to reconstruct the first-order optimality condition (1.4) or (1.5). Constraint qualifications (CQs) play an important role in this task.

Standard linearization of $\mathcal{T}(\bar{z})$ can be carried out (see [8, Eqs. (10)-(11)]), by replacing the complementarity constraints $0 \le G(z) \perp H(z) \ge 0$ with

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$$G(z) \ge 0, \quad H(z) \ge 0, \quad G(z)^T H(z) = 0.$$

46 Then linearization of these constraints gives

$$G_{i}(\bar{z}) + \nabla G_{i}(\bar{z})^{T} d \geq 0, \quad i = 1, \dots, m,$$

$$H_{i}(\bar{z}) + \nabla H_{i}(\bar{z})^{T} d \geq 0, \quad i = 1, \dots, m,$$

$$G_{i}(\bar{z})H_{i}(\bar{z}) + H_{i}(\bar{z})\nabla G_{i}(\bar{z})^{T} d + G_{i}(\bar{z})\nabla H_{i}(\bar{z})^{T} d = 0, \quad i = 1, \dots, m.$$

48 Using the index sets defined by (1.2), we obtain the linearized tangent cone

$$\mathcal{T}^{lin}(\bar{z}) = \{d \mid \nabla g_i(\bar{z})^T d \leq 0, \qquad \forall i \in I_g(\bar{z}), \\ \nabla h_i(\bar{z})^T d = 0, \qquad \forall i = 1, \dots, n_h, \\ \nabla G_i(\bar{z})^T d = 0, \qquad \forall i \in \alpha(\bar{z}), \\ \nabla H_i(\bar{z})^T d = 0, \qquad \forall i \in \gamma(\bar{z}), \\ \nabla G_i(\bar{z})^T d \geq 0, \quad \nabla H_i(\bar{z})^T d \geq 0, \quad \forall i \in \beta(\bar{z})\}.$$

50 Its dual cone is given by

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$$\mathcal{T}^{lin}(\bar{z})^* = \{w \mid w^T d \ge 0, \ \forall d \in \mathcal{T}^{lin}(\bar{z})\}$$

$$= \{w \mid 0 = w + \sum_{i \in I_g(\bar{z})} \bar{\lambda}_i^g \nabla g_i(\bar{z}) + \sum_{i=1}^{n_h} \bar{\lambda}_i^h \nabla h_i(\bar{z}) - \sum_{i \in \alpha(\bar{z})} \bar{\lambda}_i^G \nabla G_i(\bar{z}) - \sum_{i \in \gamma(\bar{z})} \bar{\lambda}_i^H \nabla H_i(\bar{z})$$

$$- \sum_{i \in \beta(\bar{z})} \bar{\lambda}_i^G \nabla G_i(\bar{z}) - \sum_{i \in \beta(\bar{z})} \bar{\lambda}_i^H \nabla H_i(\bar{z});$$

$$\bar{\lambda}_i^g \ge 0, \ \forall i \in I_g(\bar{z}); \ \bar{\lambda}_i^G \ge 0, \bar{\lambda}_i^H \ge 0, \ \forall i \in \beta(\bar{z})\}.$$

By assuming $\mathcal{T}(\bar{z}) = \mathcal{T}^{lin}(\bar{z})$ or $\mathcal{T}(\bar{z})^* = \mathcal{T}^{lin}(\bar{z})^*$, the condition (1.4) or (1.5) can be rebuilt based on the linearized cone. This converts first-order optimality of MPCC

(1.1) into that of the relaxed NLP

RNLP: min
$$f(z)$$

s.t. $g(z) \leq 0$,
 $h(z) = 0$,
 $G_i(z) = 0$, $i \in \alpha(\bar{z})$,
 $H_i(z) = 0$, $i \in \gamma(\bar{z})$,
 $G_i(z) \geq 0$, $H_i(z) \geq 0$, $i \in \beta(\bar{z})$,

and thus justifies using the KKT conditions for RNLP, i.e., the S-stationarity conditions, as a necessary first-order condition (see also [9, Theorem 4.1]).

Since NLP-CQs are usually too strong for MPCCs, constraint qualifications customized for complementarity constraints have been proposed. MPCC-ACQ and MPCC-GCQ are MPCC variants of the standard Abadie and Guignard constraint qualifications, which are implemented by simplifying the geometry of the MPCC problem while preserving the complementarity structure. MPCC-ACQ assumes $\mathcal{T}(\bar{z}) = \mathcal{T}_{\text{MPCC}}^{lin}(\bar{z})$, where the latter is the MPCC-linearized tangent cone at \bar{z} and is defined in [8] as

$$\mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z}) = \{d \mid \nabla g_i(\bar{z})^T d \leq 0, \qquad \forall i \in I_g(\bar{z}), \\ \nabla h_i(\bar{z})^T d = 0, \qquad \forall i = 1, \dots, n_h, \\ \nabla G_i(\bar{z})^T d = 0, \qquad \forall i \in \alpha(\bar{z}), \\ \nabla H_i(\bar{z})^T d = 0, \qquad \forall i \in \gamma(\bar{z}), \\ \nabla G_i(\bar{z})^T d \geq 0, \qquad \forall i \in \beta(\bar{z}), \\ \nabla H_i(\bar{z})^T d \geq 0, \qquad \forall i \in \beta(\bar{z}), \\ (\nabla G_i(\bar{z})^T d) \cdot (\nabla H_i(\bar{z})^T d) = 0, \quad \forall i \in \beta(\bar{z}) \}.$$

Then the condition (1.4) can be expressed as:

66 (1.7)
$$\nabla f(\bar{z})^T d \ge 0, \quad \forall d \in \mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z}).$$

67 MPCC-GCQ assumes $\mathcal{T}(\bar{z})^* = \mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z})^*$ [10], where the latter is described by

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$$\mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z})^* = \{ w | w^T d \ge 0, \ \forall d \in \mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z}) \}.$$

MPCC-GCQ is implied by MPCC-ACQ, but the converse is in general not true. Their relations are analogous to the relations between NLP-GCQ and NLP-ACQ. Examples showing that NLP-GCQ and MPCC-GCQ have a better chance to be satisfied, even if NLP-ACQ and MPCC-ACQ do not hold, can be found in [27, Example 1.3] and [10, Example 2.1], respectively. Intuitively, the property that a dual cone, such as $\mathcal{T}^{lin}(\bar{z})^*$ and $\mathcal{T}^{lin}_{\text{MPCC}}(\bar{z})^*$, is always convex, even if the tangent cone, such as $\mathcal{T}^{lin}(\bar{z})$ and $\mathcal{T}^{lin}_{\text{MPCC}}(\bar{z})$, is nonconvex, offers the opportunity for NLP-GCQ and MPCC-GCQ to hold more generally. Note that despite the fact that a tangent cone is not necessarily equal to the closure of its convex hull, their dual cones are the same. It has been established that under MPCC-GCQ, M-stationarity is a necessary first-order condition [10, Theorem 3.1]. In addition, Fritz John type M-stationarity has been derived at a local minimizer of an MPCC without requiring a constraint qualification [20, Theorem 3.1].

1.2. Degeneracy. To seek a solution of MPCC (1.1), many NLP-based schemes have been proposed. The original intention is to avoid dealing with the complementarity structure explicitly. In general, these schemes are designed to solve a sequence of regularized NLPs, yielding a sequence of stationary points z^k which is hoped to approximate a solution of MPCC (1.1). An important ingredient is to characterize conditions under which, as the regularization factor vanishes or stabilizes, a limit point of $\{z^k\}$ is a stationary point of the MPCC in some sense. For some representative work see [26, 12, 23, 22, 18, 19, 28, 11, 1].

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A difficulty in establishing stationarity of a limit point arises as the point is degenerate (on the lower level), namely, a sequence $\{z^k\} \to \bar{z}$ at which $\beta(\bar{z}) \neq \emptyset$. Fukushima and Pang studied the behavior of a sequence $\{z^k\}$ which is composed of KKT points of NLPs formulated by smoothing the MPCC with perturbed Fischer-Burmeister functions. The condition of asymptotic weak nondegeneracy was proposed, meaning that for every $i \in \beta(\bar{z})$, $G_i(z^k)$ and $H_i(z^k)$ approach zero in the same order of magnitude. Under this condition and second-order necessary conditions at every z^k , together with MPCC linear independence constraint qualification (MPCC-LICQ) at \bar{z} , it has been proved that \bar{z} is a B-stationary point of the MPCC [12, Theorem 3.1]. However, the condition of asymptotic weak nondegeneracy is hard to enforce in practice. Replacing this condition with upper level strict complementarity (ULSC), namely, $\bar{\lambda}_i^G \bar{\lambda}_i^H \neq 0$ for all $i \in \beta(\bar{z})$, Scholtes recovered B-stationarity of a limit point of a regularization scheme [26, Corollary 3.4]. Kadrani et al. developed a regularization method whose limit points were shown to be M-stationary under MPCC-LICQ, and S-stationary under additional assumption of asymptotic weak nondegeneracy (see [18]). The result on M-stationarity was later proved valid under the weaker MPCC constant positive linear dependence (MPCC-CPLD) assumption (see [16]). Results under weaker assumptions also include, for example, that C-stationarity convergence of the method by Steffensen and Ulbrich under MPCC constant rank constraint qualification (MPCC-CRCQ) [28] and under MPCC-CPLD [15], and M-stationarity convergence of the method by Kanzow and Schwartz under MPCC-CPLD [19]. Theoretical and numerical comparison of some of these methods can be found in [16].

Besides diverse methods for reformulating complementarity constraints, many popular algorithmic frameworks in nonlinear programming have been exploited to deal with complementarity as well as the potential degeneracy. The sequential quadratic programming (SQP) method in its pure form applied to MPCCs was investigated in [11]. By introducing slack variables into the reformulation of general complementarity constraints, superlinear convergence to a S-stationary point was established under MPCC-LICQ and regularity conditions (Theorems 5.7 and 5.14 therein). An alternative SQP method which retained the superlinear convergence while relaxing some of the assumptions was analyzed in [2], where an adaptive elastic mode was invoked to enforce either feasibility of the QP subproblems or complementarity at the iterates (Theorems 4.5 and 4.6 therein). Interior-penalty methods for MPCCs were studied in [22]; global convergence to a S-stationary point was proved under MPCC-LICQ and a condition on the behavior of the penalty parameters (Theorem 3.4 and Corollary 3.5 therein); superlinear convergence to a S-stationary point was proved under certain regularity conditions (Theorem 4.5 therein); in particular, relations between interior-penalty and interior-relaxation methods were established, which allows to extend some convergence results derived for one approach to the other. Convergence of augmented Lagrangian methods were investigated under MPCC-LICQ [17, Theorem 3.2], where a limit point was proved to be S-stationary in the case of bounded multiplier sequence, and C-stationary in the presence of unbounded multiplier sequence.

The results were improved in [1] for a second-order method (Theorem 3.2 therein), where S-stationarity was established under a weaker MPCC-relaxed constant positive linear dependence (MPCC-RCPLD) condition, and convergence in the presence of unbounded multipliers was proved to be M-stationary under MPCC-LICQ. Comparison of more augmented Lagrangian methods for MPCCs can be found in [14].

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In Section 2, we derive a property of "piecewise M-stationarity" at a local minimizer of MPCC (1.1) at which MPCC-ACQ holds. In Section 3, we characterize conditions that guarantee a feasible point of MPCC (1.1) to be B-stationary under MPCC-ACQ. The discussions in Sections 2 and 3 are independent of particular MPCC methods/algorithms. On the other hand, in Section 4, we analyze convergence properties of the NCP-based bounding methods we proposed in [29]. In Section 5, we discuss some practical issues for MPCC methods, when approaching a solution of MPCC (1.1) which is not S-stationary. Section 6 summarizes main results of this paper.

- 2. Characterization of MPCC local minimizers. This section discusses properties pertaining to a local minimizer of an MPCC. In this section we discuss from the point of view of the NLPs constituting the MPCC problem.
- 2.1. Piecewise NLP-GCQ. Given a feasible point \bar{z} of MPCC (1.1), partitions of $\beta(\bar{z})$ comprise the set $\mathcal{P}(\beta(\bar{z})) = \{(\beta_1, \beta_2) \mid \beta_1 \cap \beta_2 = \emptyset, \beta_1 \cup \beta_2 = \beta(\bar{z})\}$. A NLP problem defined on every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$ is

$$\begin{aligned} \text{NLP}_{(\beta_1,\beta_2)}: & & \min \quad f(z) \\ & & \text{s.t.} \quad g(z) \leq 0, \\ & & h(z) = 0, \\ & & G_i(z) = 0, \qquad \qquad i \in \alpha(\bar{z}), \\ & & H_i(z) = 0, \qquad \qquad i \in \gamma(\bar{z}), \\ & & G_i(z) = 0, \ H_i(z) \geq 0, \quad i \in \beta_1, \\ & & G_i(z) \geq 0, \ H_i(z) = 0, \quad i \in \beta_2. \end{aligned}$$

LEMMA 2.1. Let \bar{z} be a local minimizer of MPCC (1.1) at which MPCC-ACQ holds. Then for every $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, NLP-GCQ holds at \bar{z} for NLP $_{(\beta_1,\beta_2)}$.

155 *Proof.* Since \bar{z} is a local minimizer of MPCC (1.1), we have from B-stationarity 156 of \bar{z} that

157 (2.2)
$$\nabla f(\bar{z})^T d \ge 0, \quad \forall d \in \mathcal{T}(\bar{z}).$$

58 MPCC-ACQ at \bar{z} and [8, Lemma 3.1] give that

159 (2.3)
$$\mathcal{T}(\bar{z}) = \left[\mathcal{T}_{\mathrm{MPCC}}^{lin}(\bar{z}) = \bigcup_{\substack{(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z})) \\ 5}} \mathcal{T}_{(\beta_1, \beta_2)}^{lin}(\bar{z}) \right],$$

where $\mathcal{T}^{lin}_{(\beta_1,\beta_2)}(\bar{z})$ is the linearized tangent cone of $NLP_{(\beta_1,\beta_2)}$ at \bar{z} and is given by

$$\mathcal{T}_{(\beta_{1},\beta_{2})}^{lin}(\bar{z}) = \{d \mid \nabla g_{i}(\bar{z})^{T}d \leq 0, \qquad \forall i \in I_{g}(\bar{z}), \\ \nabla h_{i}(\bar{z})^{T}d = 0, \qquad \forall i = 1, \dots, n_{h}, \\ \nabla G_{i}(\bar{z})^{T}d = 0, \qquad \forall i \in \alpha(\bar{z}), \\ \nabla H_{i}(\bar{z})^{T}d = 0, \qquad \forall i \in \gamma(\bar{z}), \\ \nabla G_{i}(\bar{z})^{T}d = 0, \quad \nabla H_{i}(\bar{z})^{T}d \geq 0, \quad \forall i \in \beta_{1}, \\ \nabla G_{i}(\bar{z})^{T}d \geq 0, \quad \nabla H_{i}(\bar{z})^{T}d = 0, \quad \forall i \in \beta_{2}\}.$$

Relations (2.2) and (2.3) together imply that for every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$,

$$\nabla f(\bar{z})^T d \ge 0, \quad \forall d \in \mathcal{T}_{(\beta_1, \beta_2)}^{lin}(\bar{z}),$$

164 namely, that

165 (2.4)
$$\nabla f(\bar{z}) \in \mathcal{T}_{(\beta_1,\beta_2)}^{lin}(\bar{z})^*, \quad \forall (\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z})).$$

On the other hand, \bar{z} is also a local minimizer of $NLP_{(\beta_1,\beta_2)}$ for every $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$ (see [25, Eq.(3)]). Hence, we have [13, Lemma 4.3]

168 (2.5)
$$\nabla f(\bar{z}) \in \mathcal{T}_{(\beta_1, \beta_2)}(\bar{z})^*, \quad \forall (\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z})).$$

169 Combining (2.4) and (2.5) yields

170 (2.6)
$$\mathcal{T}_{(\beta_1,\beta_2)}(\bar{z})^* = \mathcal{T}_{(\beta_1,\beta_2)}^{lin}(\bar{z})^*, \quad \forall (\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z})),$$

indicating that NLP-GCQ holds at \bar{z} for every NLP_(\beta_1,\beta_2) with $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$.

172 **2.2.** Piecewise M-stationarity.

THEOREM 2.2. Let \bar{z} be a local minimizer of MPCC (1.1) at which MPCC-ACQ holds. Then for every $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, there exist $NLP_{(\beta_1, \beta_2)}$ suitable multipliers at \bar{z} , that satisfy M-stationarity.

176 Proof. Since \bar{z} is a local minimizer of the MPCC, there exist a scalar $\lambda_0 \geq 0$ 177 and multipliers $\lambda_I^g \geq 0, \lambda^h, \lambda_\alpha^G, \lambda_\gamma^H, \zeta$, such that $(\lambda_0, \lambda_I^g, \lambda^h, \lambda_\alpha^G, \lambda_\gamma^H, \zeta) \neq 0$ and the 178 following condition holds (see [6, Theorem 6.1.1][25, Lemma 1 and proof][27, Section 179 2.2]):

$$0 \in \lambda_0 \nabla f(\bar{z}) + \nabla g_I(\bar{z}) \lambda_I^g + \nabla h(\bar{z}) \lambda^h - \nabla G_{\alpha}(\bar{z}) \lambda_{\alpha}^G - \nabla H_{\gamma}(\bar{z}) \lambda_{\gamma}^H$$

$$- \sum_{i \in \beta(\bar{z})} \zeta_i \operatorname{conv} \{ \nabla G_i(\bar{z}), \nabla H_i(\bar{z}) \},$$

where g_I denotes the constraints $\{g_i | \forall i \in I_g(\bar{z})\}$, and, similarly, $G_{\alpha}, H_{\gamma}, G_{\beta}$, and H_{β} denote the constraints related to the index sets $\alpha(\bar{z}), \gamma(\bar{z})$, and $\beta(\bar{z})$; the term conv $\{\nabla G_i(\bar{z}), \nabla H_i(\bar{z})\}$ represents the convex hull consisting of all convex combinations of $\nabla G_i(\bar{z})$ and $\nabla H_i(\bar{z})$. Note that for every $i \in \beta(\bar{z}), \nabla G_i(\bar{z})$ and $\nabla H_i(\bar{z})$ do not act on the condition independently; instead, they are associated with a common multiplier ζ_i .

Let $\theta_i \nabla G_i(\bar{z}) + (1 - \theta_i) \nabla H_i(\bar{z})$ with some $\theta_i \in [0, 1]$ be an element of the convex hull, then we have

$$0 = \lambda_0 \nabla f(\bar{z}) + \nabla g_I(\bar{z}) \lambda_I^g + \nabla h(\bar{z}) \lambda^h - \nabla G_{\alpha}(\bar{z}) \lambda_{\alpha}^G - \nabla H_{\gamma}(\bar{z}) \lambda_{\gamma}^H$$

$$- \sum_{i \in \beta_1} \underbrace{\zeta_i \theta_i}_{\lambda_i^G} \nabla G_i(\bar{z}) - \sum_{i \in \beta_1} \underbrace{\zeta_i (1 - \theta_i)}_{\lambda_i^H} \nabla H_i(\bar{z})$$

$$- \sum_{i \in \beta_2} \underbrace{\zeta_i \theta_i}_{\lambda_i^G} \nabla G_i(\bar{z}) - \sum_{i \in \beta_2} \underbrace{\zeta_i (1 - \theta_i)}_{\lambda_i^H} \nabla H_i(\bar{z}).$$

- For every $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, this system has a solution with $\lambda_0 = 1$ and $\lambda_I^g, \lambda_{\beta_1}^H, \lambda_{\beta_2}^G \ge 1$ 0, because \bar{z} is a local minimizer of every $\text{NLP}_{(\beta_1,\beta_2)}$ at which NLP-GCQ holds (see
- 192 Lemma 2.1). It follows from $\lambda_{\beta_1}^H, \lambda_{\beta_2}^G \geq 0$ that

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$$i \in \beta_1 \begin{cases} \zeta_i \geq 0 \implies \exists \theta_i \in [0, 1], & \lambda_i^G \geq 0, \lambda_i^H \geq 0; \\ \zeta_i < 0 \implies \theta_i = 1, & \lambda_i^G = \zeta_i < 0, \lambda_i^H = 0. \end{cases}$$

$$i \in \beta_2 \begin{cases} \zeta_i \geq 0 \implies \exists \theta_i \in [0, 1], & \lambda_i^G \geq 0, \lambda_i^H \geq 0; \\ \zeta_i < 0 \implies \theta_i = 0, & \lambda_i^G = 0, \lambda_i^H = \zeta_i < 0. \end{cases}$$

- Hence, for every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, there exist KKT multipliers for $\text{NLP}_{(\beta_1, \beta_2)}$ such that $\lambda_i^G, \lambda_i^H \geq 0$ or $\lambda_i^G \lambda_i^H = 0$ for all $i \in \beta(\bar{z})$. This completes the proof.
- According to Theorem 2.2, M-stationarity pertaining to a local minimizer \bar{z} of MPCC (1.1) is a piecewise property under MPCC-ACQ. Unless \bar{z} is S-stationary, there does not exist a set of MPCC multipliers which satisfies M-stationarity and is suitable for every $NLP_{(\beta_1,\beta_2)}$.
 - 3. Sufficient conditions for B-stationarity. Suppose that MPCC-ACQ holds at a feasible point \bar{z} of MPCC (1.1). According to the condition (1.7), \bar{z} is a B-stationary point of the MPCC if and only if d=0 solves the following linear program with complementarity constraints (LPCC):

min
$$\nabla f(\bar{z})^T d$$

s.t. $\nabla g_I(\bar{z})^T d \leq 0$,
 $\nabla h(\bar{z})^T d = 0$,
 $\nabla G_{\alpha}(\bar{z})^T d = 0$,
 $\nabla H_{\gamma}(\bar{z})^T d = 0$,
 $0 \leq \nabla G_{\beta}(\bar{z})^T d \perp \nabla H_{\beta}(\bar{z})^T d \geq 0$.

The LPCC is a combination of classical linear programs each defined on a partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$ as follows:

$$LP_{(\beta_{1},\beta_{2})}: \quad \min \quad obj(d) = \nabla f(\bar{z})^{T}d$$
s.t.
$$\nabla g_{I}(\bar{z})^{T}d \leq 0,$$

$$\nabla h(\bar{z})^{T}d = 0,$$

$$\nabla G_{\alpha}(\bar{z})^{T}d = 0,$$

$$\nabla H_{\gamma}(\bar{z})^{T}d = 0,$$

$$\nabla G_{\beta_{1}}(\bar{z})^{T}d = 0,$$

$$\nabla G_{\beta_{2}}(\bar{z})^{T}d \geq 0,$$

$$\nabla H_{\beta_{2}}(\bar{z})^{T}d \geq 0,$$

$$\nabla H_{\beta_{2}}(\bar{z})^{T}d \geq 0,$$

The dual problem of (3.2) is given by

$$\begin{aligned} \operatorname{LP}^{dual}_{(\beta_1,\beta_2)}: & \max obj^{dual}(\eta) = \eta^T \cdot 0 \\ & \text{s.t. } \eta_I^g \geq 0, \\ & \eta^h \text{ free,} \\ & \eta_\alpha^G \text{ free,} \\ & 209 \quad (3.3) \end{aligned} \qquad \begin{aligned} \eta_I^H & \text{free,} \\ & \eta_{\beta_1}^G \text{ free,} & \eta_{\beta_1}^H \geq 0, \\ & \eta_{\beta_2}^G \geq 0, \quad \eta_{\beta_2}^H \text{ free,} \\ & 0 = \nabla f(\bar{z}) + \nabla g_I(\bar{z}) \eta_I^g + \nabla h(\bar{z}) \eta^h - \nabla G_\alpha(\bar{z}) \eta_\alpha^G - \nabla H_\gamma(\bar{z}) \eta_\gamma^H \\ & - \nabla G_{\beta_1}(\bar{z}) \eta_{\beta_1}^G - \nabla H_{\beta_1}(\bar{z}) \eta_{\beta_1}^H - \nabla G_{\beta_2}(\bar{z}) \eta_{\beta_2}^G - \nabla H_{\beta_2}(\bar{z}) \eta_{\beta_2}^H. \end{aligned}$$

Duality theory characterizes the relations between the primal and the dual problems as follows.

- (D1) If d is a feasible point of the primal problem (3.2) and η is a feasible point of the dual problem (3.3), then $obj^{dual}(\eta) \leq obj(d)$. [5, Theorem 4.3]
- (D2) If the dual problem is infeasible, then either the primal problem is infeasible, or the optimal cost of the primal problem is $-\infty$. If the primal problem is infeasible, then either the dual problem is infeasible, or the optimal cost of the dual problem is ∞ . [5, Corollary 4.1 and Table 4.2]
- (D3) Let d and η be feasible points of the primal (3.2) and the dual (3.3), respectively, and suppose that $obj^{dual}(\eta) = obj(d)$. Then d and η are optimal solutions to the primal and the dual, respectively. [5, Corollary 4.2]

THEOREM 3.1. Suppose that MPCC (1.1) is solvable (feasible and bounded below). If \bar{z} is a weakly stationary point at which MPCC-ACQ holds, then, either there exists a partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$ such that $LP_{(\beta_1, \beta_2)}$ is unbounded below, or \bar{z} is B-stationary.

Proof. Recall that under MPCC-ACQ, \bar{z} is B-stationary if and only if d=0 solves LPCC (3.1). Consider the linear programs (3.2) that comprise the LPCC. For every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, the primal problem $LP_{(\beta_1, \beta_2)}$ has a feasible solution d=0. Whether d=0 is also optimal to each of the problems, depends on situations of the dual problems. In the case where there exists a partition $(\hat{\beta}_1, \hat{\beta}_2) \in \mathcal{P}(\beta(\bar{z}))$ such that the dual problem $LP_{(\hat{\beta}_1, \hat{\beta}_2)}^{dual}$ is infeasible, it follows from the result (D2) of duality theory that the primal problem $LP_{(\hat{\beta}_1, \hat{\beta}_2)}^{dual}$ is either infeasible or unbounded below.

Since d=0 is feasible to the primal problem, it follows that the primal problem is unbounded below. In this case, no feasible point of $LP_{(\hat{\beta}_1,\hat{\beta}_2)}$ can be optimal; \bar{z} cannot be optimal to $LP_{(\hat{\beta}_1,\hat{\beta}_2)}$ either and therefore cannot be B-stationary.

In the other case, every dual problem $LP^{dual}_{(\beta_1,\beta_2)}$ has a feasible solution. Since the feasible solution d=0 to the primal and any feasible solution η to the dual yield $obj(d)=obj^{dual}(\eta)=0$, we have from the result (D3) of duality theory that d=0 is an optimal solution to the primal problem $LP_{(\beta_1,\beta_2)}$. Because this is the case for every partition $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$, then d=0 solves LPCC (3.1) and \bar{z} is B-stationary.

It is worth noting that whenever a dual problem $LP^{dual}_{(\beta_1,\beta_2)}$ is feasible, its solution provides KKT multipliers for $NLP_{(\beta_1,\beta_2)}$. This provides a bridge between optimality of d=0 for $LP_{(\beta_1,\beta_2)}$ and that \bar{z} is a KKT point of $NLP_{(\beta_1,\beta_2)}$. Based on this observation, we arrive at the following condition for B-stationarity.

Theorem 3.2. Let \bar{z} be a feasible point of MPCC (1.1) at which MPCC-ACQ holds. Then \bar{z} is B-stationary if \bar{z} is piecewise M-stationary.

Proof. If \bar{z} is piecewise M-stationary, then \bar{z} is a KKT point of every $NLP_{(\beta_1,\beta_2)}$ with $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$. On each of the partitions, the KKT multipliers form a feasible point of $LP_{(\beta_1,\beta_2)}^{dual}$, and therefore d=0 is optimal to $LP_{(\beta_1,\beta_2)}$. As a result, d=0 is optimal to LPCC (3.1) and \bar{z} is a B-stationary point of the MPCC.

3.1. Example: *scholtes4*. This example illustrates that a weakly stationary point is also B-stationary under appropriate conditions, as stated by Theorems 3.1 and 3.2.

Problem scholtes4 from the MacMPEC collection [21] is given by

$$\begin{aligned} & \text{min} & z_1 + z_2 - z_3 & \text{multipliers} \\ & \text{s.t.} & -4z_1 + z_3 \leq 0, & \lambda_1 \\ & -4z_2 + z_3 \leq 0, & \lambda_2 \\ & 0 \leq z_1 \perp z_2 \geq 0. & \sigma_1, \sigma_2 \end{aligned}$$

Since the functions in the constraints are linear, MPCC-ACQ holds at every feasible point of the problem. Consider a weakly stationary point $\bar{z} = (\bar{z}_1, \bar{z}_2, \bar{z}_3)$ at which $\beta(\bar{z}) \neq \emptyset$, which is the case of interest. This gives that $\bar{z} = (0, 0, 0)$ and $\beta(\bar{z}) = \{1\}$.

To verify B-stationarity of \bar{z} , we check whether \bar{z} is a KKT point of $NLP_{(\beta_1,\beta_2)}$ for every $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$. Since \bar{z} is weakly stationary, we have

$$0 = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} + \lambda_1 \begin{bmatrix} -4 \\ 0 \\ 1 \end{bmatrix} + \lambda_2 \begin{bmatrix} 0 \\ -4 \\ 1 \end{bmatrix} - \sigma_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} - \sigma_2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

261 which implies

$$\lambda_1 + \lambda_2 = 1,$$

$$\sigma_1 + \sigma_2 = -2.$$

For the partitions $(\beta_1, \beta_2) = (\{1\}, \emptyset)$ and $(\beta_1, \beta_2) = (\emptyset, \{1\})$, since $(\sigma_1, \sigma_2) = (-2, 0)$ and $(\sigma_1, \sigma_2) = (0, -2)$, respectively, lead to suitable KKT multipliers for the corresponding NLPs, the point \bar{z} is piecewise M-stationary and therefore B-stationary (Theorem 3.2). Also, existence of the KKT multipliers ensures feasibility of the dual problems, which implies that no primal problem is unbounded below at \bar{z} , and again \bar{z} is B-stationary (Theorem 3.1).

3.2. Example: Unboundedness. Even if an MPCC is bounded below, a component LP of the LPCC at a feasible point of the MPCC may be unbounded below. Consider the problem given by

min
$$f(z) = (z_1 - 1)^2 + z_2^2$$
 multipliers
s.t. $0 \le z_1 \perp z_2 \ge 0$. σ_1, σ_2

The unique minimizer is $z^* = (1,0)$ (so that $\beta(z^*) = \emptyset$), which is also a minimizer of the RNLP and therefore is S-stationary. Now consider the point $\bar{z} = (0,0)$ and $\beta(\bar{z}) = \{1\}$. MPCC-LICQ holds at \bar{z} ; the weak stationarity conditions give the multipliers $(\sigma_1, \sigma_2) = (-2, 0)$ and therefore \bar{z} is M-stationary. However, \bar{z} is not B-stationary, because for $(\beta_1, \beta_2) = (\emptyset, \{1\})$, LP_{(β_1, β_2)} is unbounded below (the optimal cost is $-\infty$), and every feasible direction $d = (d_1 > 0, d_2 = 0)$ leads to $\nabla f(\bar{z})^T d = -2d_1 < 0$.

3.3. Unboundedness detection. When MPCC-LICQ holds at a feasible point \bar{z} of an MPCC, B-stationarity is equivalent to S-stationarity, and it is evident whether or not \bar{z} is B-stationary. Otherwise, in the absence of MPCC-LICQ, if there exist n linearly independent active constraints at \bar{z} , the following gives a method to decide whether \bar{z} is B-stationary.

As discussed in Theorem 3.1 under MPCC-ACQ, \bar{z} is not B-stationary when there exists a primal problem $LP_{(\beta_1,\beta_2)}$ which is unbounded below. To detect whether unbounded primal problems exist, we design an LP problem based on each $LP_{(\beta_1,\beta_2)}$, such that the designed problem has an optimal solution which indicates whether the original $LP_{(\beta_1,\beta_2)}$ is unbounded below. To design such a problem, we introduce an additional constraint into $LP_{(\beta_1,\beta_2)}$ as follows:

$$\widetilde{LP}_{(\beta_{1},\beta_{2})}: \quad \min \quad \widetilde{obj}(d) = \nabla f(\bar{z})^{T} d$$
s.t.
$$\nabla g_{I}(\bar{z})^{T} d \leq 0,$$

$$\nabla h(\bar{z})^{T} d = 0,$$

$$\nabla G_{\alpha}(\bar{z})^{T} d = 0,$$

$$\nabla H_{\gamma}(\bar{z})^{T} d = 0,$$

$$\nabla G_{\beta_{1}}(\bar{z})^{T} d = 0,$$

$$\nabla G_{\beta_{1}}(\bar{z})^{T} d = 0, \quad \nabla H_{\beta_{1}}(\bar{z})^{T} d \geq 0,$$

$$\nabla G_{\beta_{2}}(\bar{z})^{T} d \geq 0, \quad \nabla H_{\beta_{2}}(\bar{z})^{T} d = 0,$$

$$\left[-\sum_{i \in I_{g}} \nabla g_{i}(\bar{z}) + \sum_{i=1}^{n_{h}} \nabla h_{i}(\bar{z}) + \sum_{i \in \alpha \cup \beta} \nabla G_{i}(\bar{z}) + \sum_{i \in \gamma \cup \beta} \nabla H_{i}(\bar{z}) \right]^{T} d \leq r,$$

where r > 0 is an arbitrary positive scalar. Note that the constraints of $LP_{(\beta_1,\beta_2)}$ can be restated in the form of $A^Td \geq 0$, while the additional constraint is in the form of $\sum A_i^Td \leq r$ with A_i being the *i*th column of the coefficient matrix A. When n out of the columns of A are linearly independent, they span the space \mathbb{R}^n and the set of all these constraints $(A^Td \geq 0 \text{ and } \sum A_i^Td \leq r)$ defines the lower and upper bounds of $d \in \mathbb{R}^n$. As a consequence, the problem $\widetilde{LP}_{(\beta_1,\beta_2)}$ is confined in a nonempty and bounded feasible region and thus has an optimal solution which is an extreme point.

298 The corresponding dual problem is

$$\widetilde{\operatorname{LP}}_{(\beta_{1},\beta_{2})}^{dual}: \quad \max \quad \widetilde{obj}^{dual}(\eta,\mu) = [\eta^{T},\mu] \cdot \begin{bmatrix} 0 \\ -r \end{bmatrix}$$
s.t. $\eta_{I}^{g} \geq 0$,
$$\eta^{h} \text{ free},$$

$$\eta_{\gamma}^{G} \text{ free},$$

$$\eta_{\gamma}^{H} \text{ free},$$

$$\eta_{\beta_{1}}^{G} \text{ free},$$

$$\eta_{\beta_{1}}^{G} \text{ free},$$

$$\eta_{\beta_{2}}^{G} \geq 0, \quad \eta_{\beta_{2}}^{H} \text{ free},$$

$$\mu \geq 0,$$

$$0 = \nabla f(\bar{z}) + \nabla g_{I}(\bar{z})(\eta_{I}^{g} - \mu) + \nabla h(\bar{z})(\eta^{h} + \mu)$$

$$- \nabla G_{\alpha}(\bar{z})(\eta_{\alpha}^{G} - \mu) - \nabla H_{\gamma}(\bar{z})(\eta_{\beta_{1}}^{H} - \mu)$$

$$- \nabla G_{\beta_{1}}(\bar{z})(\eta_{\beta_{1}}^{G} - \mu) - \nabla H_{\beta_{1}}(\bar{z})(\eta_{\beta_{1}}^{H} - \mu)$$

$$- \nabla G_{\beta_{2}}(\bar{z})(\eta_{\beta_{2}}^{G} - \mu) - \nabla H_{\beta_{2}}(\bar{z})(\eta_{\beta_{2}}^{H} - \mu).$$

Since the modified primal problem has a finite optimal solution, so does the modified dual problem (according to duality theory).

To detect whether the original primal problem $LP_{(\beta_1,\beta_2)}$ is unbounded below, we 302 solve the modified problem $\widetilde{LP}_{(\beta_1,\beta_2)}$ with a scalar r>0. If the solution gives that 303 the multiplier of the additional constraint is $\mu = 0$, then d = 0 is optimal to $\widetilde{LP}_{(\beta_1,\beta_2)}$, 304 because $\widetilde{obj}(d) = \widetilde{obj}^{dual}(\eta, \mu) = 0$. Obviously, in this case d = 0 is also optimal to 305 the original problem $LP_{(\beta_1,\beta_2)}$. On the other hand, if the solution of the modified 306 primal problem gives the multiplier $\mu > 0$, then the additional constraint is active 307 and $\widetilde{\mathrm{LP}}_{(\beta_1,\beta_2)}$ is solved by some $d \neq 0$, with the optimal costs $\widetilde{obj}(d) = \widetilde{obj}^{dual}(\eta,\mu) =$ 308 $-\mu r < 0$. Since this nonzero d locates in $\mathcal{T}^{lin}_{(\beta_1,\beta_2)}(\bar{z})$ and $obj(d) = \widetilde{obj}(d) = -\mu r$, $LP_{(\beta_1,\beta_2)}$ cannot be optimal at d=0, and is in fact unbounded below. To summarize, 309 310 if every $LP_{(\beta_1,\beta_2)}$ has a solution with the multiplier $\mu=0$, then none of the original 311 primal problem $LP_{(\beta_1,\beta_2)}$ is unbounded below, and as a result, d=0 solves LPCC 312 (3.1) and \bar{z} is B-stationary. 313

- 4. Convergence of NCP-based bounding methods. The results of Sections 2 and 3 are independent of methods/algorithms designed for solving MPCCs. In the sequel, we investigate convergence properties of the NCP-based bounding methods we proposed in [29].
- 4.1. Brief review of a bounding scheme. In [29] we proposed an algorithm to seek a solution of MPCC (1.1) by solving a sequence of NLP problems of the form

BA(
$$\epsilon$$
): min $f(z)$ multipliers s.t. $g(z) \leq 0,$ u^g
$$h(z) = 0, \qquad u^h$$

$$\Phi_i^{\epsilon}(z) + p_i = 0, \ i = 1 \dots m, \qquad u_i^{\Phi}$$

321 where

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315

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$$\Phi_i^{\epsilon}(z) = \frac{1}{2} \left(G_i(z) + H_i(z) - \sqrt{(G_i(z) - H_i(z))^2 + \epsilon^2} \right)$$

is a NCP function with a smoothing factor $\epsilon > 0$, and the parameter p_i is adjusted adaptively (to take a value of zero or $\epsilon/2$). Define the Lagrangian for the program BA(ϵ) as

$$\mathcal{L}(z, u) = f(z) + \sum_{i \in I_q(z)} u_i^g g_i(z) + \sum_{i=1}^{n_h} u_i^h h_i(z) - \sum_{i=1}^m u_i^{\Phi} (\Phi_i^{\epsilon}(z) + p_i).$$

 $346 \\ 347$

As $\epsilon \to 0$, a sequence of KKT points of BA(ϵ) tends to a limit point. Main results of this method are summarized below, and more details can be found in [29].

• Feasibility: The perturbed NCP function (4.2) is used to approximate the complementarity constraints in MPCC (1.1), and the largest difference between them is $\epsilon/2$ (see [29, Proposition 1.7]). When $\epsilon>0$, every feasible point z of $\mathrm{BA}(\epsilon)$ satisfies

(4.3)
$$\Phi_i^{\epsilon}(z) + p_i = 0 \quad \Leftrightarrow \\
G_i(z) + p_i > 0, \ H_i(z) + p_i > 0, \ (G_i(z) + p_i)(H_i(z) + p_i) = \epsilon^2/4,$$

whose limit at $\epsilon = 0$ (thus $p_i = 0$) recovers the complementarity $0 \le G_i(z) \perp H_i(z) \ge 0$. Therefore, $\Phi_i^0(z)$ is a so-called NCP function, which represents a complementarity constraint with a suitable nonlinear and usually nondifferentiable equation.

- Sensitivity and Bounding: At a KKT point z(p) of $\mathrm{BA}(\epsilon)$, the sensitivities $\frac{\mathrm{d}f(z(p))}{\mathrm{d}p_i}$ are given by $-u_i^{\Phi}$ for $i=1\ldots m$, provided that NLP-LICQ, second-order sufficient conditions, and strict complementarity hold at z(p). This observation throws some light on the design of the Bounding Algorithm. We take advantage of the sensitivities at z(p) to adjust the parameters p_i , with the aim of improving the objective at the subsequent solution of $\mathrm{BA}(\epsilon)$, and thus yielding an efficient isolation of a solution to the MPCC. When $\epsilon > 0$ is sufficiently small, z(p) is an ϵ -approximate solution to the MPCC, which includes an $O(\epsilon^2)$ correction arising from the adjustment of the parameters p_i .
- Convergence: The following convergence results have been established under MPCC-LICQ, for the Bounding Algorithm applied to equality constrained $BA(\epsilon)$.
 - (i) Suppose that MPCC-LICQ holds at a feasible point of the MPCC, then in a neighborhood of this point, NLP-LICQ holds at every feasible point of $BA(\epsilon)$, whenever $\epsilon > 0$ is sufficiently small.
 - (ii) Suppose that a sequence of KKT points of programs $BA(\epsilon)$ tends to a limit point as $\epsilon \to 0$, at which MPCC-LICQ holds, then the limit point is C-stationary.
 - (iii) In addition, suppose that the reduced Hessian of the Lagrangian at each of the KKT points of programs $BA(\epsilon)$ is bounded below when $\epsilon > 0$ is sufficiently small, then the limit point is M-stationary.

A natural question is how does the Bounding Algorithm behave in the absence of MPCC-LICQ. In this section, we investigate stationarity of a limit point of this method without assuming MPCC-LICQ. Further, we explore more convergence features by taking advantage of an inequality variant of $BA(\epsilon)$. We note that this variant is a modification of the Lin-Fukushima algorithm [23], which we call MLF.

4.2. Bounding Algorithm. Based on the formulation $BA(\epsilon)$, a Bounding Algorithm was proposed in [29] by noting that the sensitivities $\frac{df(z(p))}{dp_i}$ are given by $-u_i^{\Phi}$

for $i = 1 \dots m$. The sensitivities can be exploited to adjust the parameters p_i so as 367 368 to improve the objective f(z(p)). The main idea of the Bounding Algorithm is given below to facilitate the later analysis. 369

For any parameters $p_i, p_i' \in [0, \epsilon/2]$ with $\epsilon > 0$ for $i = 1, \ldots, m$, and the corre-370 sponding solutions z(p) and z(p') to $BA(\epsilon)$, it is straightforward to show that

372
$$f(z(p')) = f(z(p)) + \left\lceil \frac{\mathrm{d}f(z(p))}{\mathrm{d}p} \right\rceil^T (p'-p) + O(\|p'-p\|^2).$$

Noting that the sensitivities $\frac{\mathrm{d}f(z(p))}{\mathrm{d}p}$ are given by $-u^{\Phi}$, we have that

374
$$f(z(p)) - \frac{\epsilon}{2} \sum_{i=1}^{m} |u_i^{\Phi}(p)| - |O(\epsilon^2)| \le f(z(p')) \le f(z(p)) + \frac{\epsilon}{2} \sum_{i=1}^{m} |u_i^{\Phi}(p)| + |O(\epsilon^2)|.$$

- This relation explains the approximation to a solution of the MPCC by the following 375 Bounding Algorithm.
 - Initialization: Specify initial smoothing factor $\epsilon^0 > 0$, reducing factor $\kappa \in$ (0,1), initial point z^0 , solution tolerance $\epsilon_{\rm tol} > 0$. Set initial parameters $p^0 \leftarrow 0$, counter $k \leftarrow 0$.
- Main loop: While $\epsilon^k \geq \epsilon_{\text{tol}}$, do the following. 380 Step 1. Solve the program $BA(\epsilon^k)$ with parameters p^k , to obtain a stationary point z^k and multipliers $u^k = (u^{g,k}, u^{h,\bar{k}}, u^{\Phi,k})$. Step 2. Approximate the upper bound of the MPCC with 383

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$$f^{up} = f(z^k) + \epsilon^k \sum_{i=1}^m |u_i^{\Phi,k}|.$$

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Step 3. Approximate the lower bound of the MPCC as follows. Define the 385 index sets 386

$$P_0 = \{i \mid p_i^k = 0 \text{ and } u_i^{\Phi,k} > 0\},\$$
 $P_{\epsilon} = \{i \mid p_i^k = \epsilon^k/2 \text{ and } u_i^{\Phi,k} < 0\}.$

Then the following settings would reduce $f(z^k)$: 388

$$p_i^k \leftarrow \epsilon^k/2, \quad \forall i \in P_0, \ p_i^k \leftarrow 0, \quad \forall i \in P_\epsilon.$$

The objective with the adjustment of p^k would approximately be 390

$$f^{low} = f(z^k) - \epsilon^k \sum_{i \in P_0 \cup P_\epsilon} |u_i^{\Phi,k}|.$$

Step 4. Update the parameters ϵ and p. Set $\epsilon^{k+1} \leftarrow \kappa \epsilon^k$, and 392

$$p_i^{k+1} = \begin{cases} \epsilon^{k+1}/2, & i \in P_0, \\ 0, & i \in P_{\epsilon}, \\ \kappa p_i^k, & \text{otherwise.} \end{cases}$$

Step 5. Set $k \leftarrow k+1$ and go to Step 1. 394

4.3. Derivatives of smoothed NCP function. With $\epsilon > 0$, the first and 396 second derivatives of the function $\Phi_i^{\epsilon}(z)$ in (4.2) are given by

$$\nabla_{G}\Phi_{i}^{\epsilon}(z) = \frac{1}{2} - \frac{G_{i}(z) - H_{i}(z)}{2\sqrt{(G_{i}(z) - H_{i}(z))^{2} + \epsilon^{2}}},$$

$$\nabla_{H}\Phi_{i}^{\epsilon}(z) = \frac{1}{2} + \frac{G_{i}(z) - H_{i}(z)}{2\sqrt{(G_{i}(z) - H_{i}(z))^{2} + \epsilon^{2}}},$$

$$\nabla_{GG}\Phi_{i}^{\epsilon}(z) = \nabla_{HH}\Phi_{i}^{\epsilon}(z) = \frac{-\epsilon^{2}}{2[(G_{i}(z) - H_{i}(z))^{2} + \epsilon^{2}]^{3/2}},$$

$$\nabla_{GH}\Phi_{i}^{\epsilon}(z) = \nabla_{HG}\Phi_{i}^{\epsilon}(z) = \frac{\epsilon^{2}}{2[(G_{i}(z) - H_{i}(z))^{2} + \epsilon^{2}]^{3/2}}.$$

398 Let z satisfy $\Phi_i^{\epsilon}(z) + p_i = 0$ with $\epsilon > 0$. It follows from (4.3) that

399
$$\sqrt{(G_i(z) - H_i(z))^2 + \epsilon^2} = \sqrt{((G_i(z) + p_i) - (H_i(z) + p_i))^2 + \epsilon^2}$$

$$= \sqrt{(G_i(z) + p_i)^2 + (H_i(z) + p_i)^2 + 2(G_i(z) + p_i)(H_i(z) + p_i)}$$

$$= |G_i(z) + H_i(z) + 2p_i| = G_i(z) + H_i(z) + 2p_i.$$

Using this and $(G_i(z) + p_i)(H_i(z) + p_i) = \epsilon^2/4$, we can rephrase the above derivatives as

$$\nabla_{G}\Phi_{i}^{\epsilon}(z) = \frac{H_{i}(z) + p_{i}}{G_{i}(z) + H_{i}(z) + 2p_{i}},$$

$$\nabla_{H}\Phi_{i}^{\epsilon}(z) = \frac{G_{i}(z) + p_{i}}{G_{i}(z) + H_{i}(z) + 2p_{i}},$$

$$\nabla_{GG}\Phi_{i}^{\epsilon}(z) = \nabla_{HH}\Phi_{i}^{\epsilon}(z) = \frac{-2(G_{i}(z) + p_{i})(H_{i}(z) + p_{i})}{(G_{i}(z) + H_{i}(z) + 2p_{i})^{3}},$$

$$\nabla_{GH}\Phi_{i}^{\epsilon}(z) = \nabla_{HG}\Phi_{i}^{\epsilon}(z) = \frac{2(G_{i}(z) + p_{i})(H_{i}(z) + p_{i})}{(G_{i}(z) + H_{i}(z) + 2p_{i})^{3}}.$$

4.4. C-stationarity. Let a sequence $\{z^k\} \to \bar{z}$ as $\epsilon^k \to 0$, where every z^k is a KKT point of BA(ϵ^k). Assuming a particular MPCC-CQ at \bar{z} usually amounts to assuming a certain NLP-CQ at \bar{z} or in its neighborhood. For example, MPCC-LICQ at \bar{z} usually implies the presence of NLP-LICQ in a neighborhood of \bar{z} for every feasible point of a regularized NLP problem (e.g., [12, Theorem 3.1][26, Lemma 2.1][29, Theorems 3.1 and 3.2]), and MPCC-MFCQ at \bar{z} implies the presence of NLP-MFCQ at \bar{z} for every NLP_(\beta_1,\beta_2) with $(\beta_1,\beta_2) \in \mathcal{P}(\beta(\bar{z}))$ [8, Lemma 3.5].

Instead of requiring a particular constraint qualification at \bar{z} , the following establishes C-stationarity of \bar{z} based on stationarity of z^k for BA(ϵ^k) and boundedness of the Lagrange multipliers associated with z^k . From a practical point of view, an advantage of the analysis under such settings is that in the course of $\{z^k\} \to \bar{z}$, whether or not the NLP solutions are successful, and whether or not the NLP multipliers at the solutions are bounded, are usually easy to detect in numerical experiments, then it follows whether or not the results developed under such circumstance are applicable. Note that such settings are weaker than requiring NLP-MFCQ at z^k , because the whole set of Lagrange multipliers at z^k need not be bounded.

THEOREM 4.1. For a sequence of positive scalars $\epsilon^k \to 0$, apply the Bounding Algorithm to $BA(\epsilon^k)$, such that the parameters p^k are updated whenever ϵ^k is updated.

- Assume this generates a sequence $\{z^k\} \to \bar{z}$, where every z^k is a KKT point of $BA(\epsilon^k)$ 422
- and the associated multipliers are bounded. Then \bar{z} is a C-stationary point of MPCC 423
- 424
- *Proof.* When $\epsilon^k > 0$, at every KKT point z^k of $BA(\epsilon^k)$, there exist multipliers 425
- $u^{k} = (u^{g,k}, u^{h,k}, u^{\Phi,k})$ with $u^{g,k} > 0$, such that

427 (4.5)
$$0 = \nabla f(z^k) + \sum_{i \in I_\sigma(z^k)} u_i^{g,k} \nabla g_i(z^k) + \sum_{i=1}^{n_h} u_i^{h,k} \nabla h_i(z^k) - \sum_{i=1}^m u_i^{\Phi,k} \nabla \Phi_i^{\epsilon}(z^k),$$

where the gradient of Φ_i^{ϵ} is given by 428

$$\nabla \Phi_{i}^{\epsilon}(z^{k}) = \nabla_{G} \Phi_{i}^{\epsilon}(z^{k}) \nabla G_{i}(z^{k}) + \nabla_{H} \Phi_{i}^{\epsilon}(z^{k}) \nabla H_{i}(z^{k})$$

$$= \frac{H_{i}(z^{k}) + p_{i}^{k}}{G_{i}(z^{k}) + H_{i}(z^{k}) + 2p_{i}^{k}} \nabla G_{i}(z^{k}) + \frac{G_{i}(z^{k}) + p_{i}^{k}}{G_{i}(z^{k}) + H_{i}(z^{k}) + 2p_{i}^{k}} \nabla H_{i}(z^{k}).$$
⁴²⁹

- Derivatives in the limit. In the limit $\epsilon^k \to 0$, the function Φ_i^0 is in general not 430
- differentiable for $i \in \beta(\bar{z})$. However, if $\Phi_i^0(z)$ is locally Lipschitz [6, Section 1.2] near \bar{z} , 431
- the generalized gradient $\partial \Phi_i^0(\bar{z})$ is generated by a convex hull (see [6, Theorem 2.5.1] 432
- [7, Eq.(3.1.5)]433

$$\partial \Phi_i^0(\bar{z}) = \operatorname{conv} \left\{ \lim_{s^K \to \bar{z}} \nabla \Phi_i^0(s^K) \, | \, \nabla \Phi_i^0(s^K) \, \operatorname{exists} \right\},\,$$

- where $\{s^K\}$ is any sequence that converges to \bar{z} while avoiding the points where Φ_i^0 435
- is not differentiable. (Locally Lipschitz function is differentiable almost everywhere. 436
- Therefore, there are "plenty" of sequences which converge to \bar{z} and avoid the set of 437
- points where $\nabla \Phi_i^0$ is not differentiable, since the latter is of measure zero.) Noting 438
- that $\Phi_i^0(\bar{z}) = \min\{G_i(\bar{z}), H_i(\bar{z})\} = 0 \text{ for } i = 1 \dots m, \text{ we have } i = 1 \dots m \}$ 439

$$\partial \Phi_i^0(\bar{z}) = \partial \min\{G_i(\bar{z}), H_i(\bar{z})\} = \operatorname{conv}\{\nabla G_i(\bar{z}), \nabla H_i(\bar{z})\}.$$

For $\delta_i \in \partial \Phi_i^0(\bar{z})$, it follows that (see [25, Lemma 1]) 441

$$\delta_i = \theta_i \nabla G_i(\bar{z}) + (1 - \theta_i) \nabla H_i(\bar{z}), \quad \theta_i \in [0, 1],$$

$$\theta_i G_i(\bar{z}) = 0,$$

$$(1 - \theta_i) H_i(\bar{z}) = 0.$$

Therefore, as $\epsilon^k \to 0$, the gradient of Φ_i^{ϵ} tends to

$$\delta_{i} = \begin{cases} \nabla G_{i}(\bar{z}), & i \in \alpha(\bar{z}), \\ \nabla H_{i}(\bar{z}), & i \in \gamma(\bar{z}), \\ \theta_{i} \nabla G_{i}(\bar{z}) + (1 - \theta_{i}) \nabla H_{i}(\bar{z}), & i \in \beta(\bar{z}), \end{cases}$$

where $\theta_i \in [0, 1]$. 445

- Existence of multipliers in the limit. Without loss of generality, we have the vector 446
- of the multipliers $u^k \neq 0$ (otherwise z^k is an unconstrained local minimum). Let 447

$$\Delta^{k} = \sqrt{1 + \sum_{i \in I_{g}(z^{k})} (u_{i}^{g,k})^{2} + \sum_{i=1}^{n_{h}} (u_{i}^{h,k})^{2} + \sum_{i=1}^{m} (u_{i}^{\Phi,k})^{2}},$$

$$\mu^{k} = \frac{1}{\Delta^{k}}, \quad \nu_{i}^{g,k} = \frac{u_{i}^{g,k}}{\Delta^{k}}, \quad \nu_{i}^{h,k} = \frac{u_{i}^{h,k}}{\Delta^{k}}, \quad \nu_{i}^{\Phi,k} = \frac{u_{i}^{\Phi,k}}{\Delta^{k}}.$$
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Dividing (4.5) by Δ^k , we obtain

$$0 = \mu^{k} \nabla f(z^{k}) + \sum_{i \in I_{g}(z^{k})} \nu_{i}^{g,k} \nabla g_{i}(z^{k}) + \sum_{i=1}^{n_{h}} \nu_{i}^{h,k} \nabla h_{i}(z^{k})$$

$$- \sum_{i \in \alpha(\bar{z})} \nu_{i}^{\Phi,k} \nabla \Phi_{i}^{\epsilon}(z^{k}) - \sum_{i \in \gamma(\bar{z})} \nu_{i}^{\Phi,k} \nabla \Phi_{i}^{\epsilon}(z^{k}) - \sum_{i \in \beta(\bar{z})} \nu_{i}^{\Phi,k} \nabla \Phi_{i}^{\epsilon}(z^{k}).$$

451 Since we have

$$(\mu^k)^2 + \sum_{i \in I_g(z^k)} (\nu_i^{g,k})^2 + \sum_{i=1}^{n_h} (\nu_i^{h,k})^2 + \sum_{i=1}^m (\nu_i^{\Phi,k})^2 = 1,$$

the sequence $\{(\mu^k, \nu^{g,k}, \nu^{h,k}, \nu^{\Phi,k})\}$ is bounded and must converge to some limit $(\bar{\mu}, \bar{\nu}^g, \bar{\nu}^h, \bar{\nu}^\Phi)$. It follows from (4.8) that this limit must satisfy

$$0 = \bar{\mu} \nabla f(\bar{z}) + \sum_{i \in I_g(\bar{z})} \bar{\nu}_i^g \nabla g_i(\bar{z}) + \sum_{i=1}^{n_h} \bar{\nu}_i^h \nabla h_i(\bar{z})$$

$$- \sum_{i \in \alpha(\bar{z})} \bar{\nu}_i^{\Phi} \nabla G_i(\bar{z}) - \sum_{i \in \gamma(\bar{z})} \bar{\nu}_i^{\Phi} \nabla H_i(\bar{z}) - \sum_{i \in \beta(\bar{z})} \bar{\nu}_i^{\Phi} \left[\theta_i \nabla G_i(\bar{z}) + (1 - \theta_i) \nabla H_i(\bar{z})\right],$$

- where (4.6) has been used to characterize the derivatives at \bar{z} , and $\bar{\mu}, \bar{\nu}^g \geq 0$ because of (4.7).
- Now suppose that μ^k vanishes in the limit, namely, $\bar{\mu} = 0$. Then for every small positive number $\sigma > 0$, there exists K > 0, such that $\mu^k = \frac{1}{\Delta^k} < \sigma$ for all k > K.

 This implies that $\{\Delta^k\}$ is unbounded above, in contradiction with the assumption of bounded KKT multipliers $\{(u^{g,k}, u^{h,k}, u^{\Phi,k})\}$. Therefore, $\bar{\mu} > 0$ and Lagrange multipliers exist at the limit point \bar{z} .
- Weak and C- stationarity. Without loss of generality, letting $\bar{\mu}=1$ and $\bar{u}=464$ $(\bar{u}^g,\bar{u}^h,\bar{u}^\Phi)$ with $\bar{u}^g\geq 0$ be the multipliers associated with \bar{z} , we obtain

$$0 = \nabla f(\bar{z}) + \sum_{i \in I_g(\bar{z})} \bar{u}_i^g \nabla g_i(\bar{z}) + \sum_{i=1}^{n_h} \bar{u}_i^h \nabla h_i(\bar{z})$$

$$- \sum_{i \in \alpha(\bar{z})} \bar{u}_i^{\Phi} \nabla G_i(\bar{z}) - \sum_{i \in \gamma(\bar{z})} \bar{u}_i^{\Phi} \nabla H_i(\bar{z}) - \sum_{i \in \beta(\bar{z})} \bar{u}_i^{\Phi} \left[\theta_i \nabla G_i(\bar{z}) + (1 - \theta_i) \nabla H_i(\bar{z})\right],$$

for some $\theta_i \in [0, 1]$. Thus \bar{z} satisfies the weak stationarity conditions (1.3), with the MPCC multipliers given by

$$\bar{\lambda}^{g} = \bar{u}^{g} = \lim_{k \to \infty} u^{g,k},$$

$$\bar{\lambda}^{h} = \bar{u}^{h} = \lim_{k \to \infty} u^{h,k},$$

$$\bar{\lambda}^{i} = \begin{cases} \bar{u}_{i}^{\Phi} = \lim_{k \to \infty} u_{i}^{\Phi,k}, & i \in \alpha(\bar{z}) \\ \bar{u}_{i}^{\Phi}\theta_{i}, & i \in \beta(\bar{z}), \end{cases}$$

$$\bar{\lambda}_{i}^{H} = \begin{cases} \bar{u}_{i}^{\Phi} = \lim_{k \to \infty} u_{i}^{\Phi,k}, & i \in \gamma(\bar{z}) \\ \bar{u}_{i}^{\Phi}(1 - \theta_{i}), & i \in \beta(\bar{z}). \end{cases}$$

469 Moreover, \bar{z} is C-stationary because

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470 (4.10)
$$\bar{\lambda}_i^G \cdot \bar{\lambda}_i^H = (\bar{u}_i^{\Phi})^2 \theta_i (1 - \theta_i) \ge 0, \quad \forall i \in \beta(\bar{z}).$$

471 **4.5. M-stationarity.** The property (4.10) allows for two possibilities. One is that $\bar{u}_i^{\Phi} \geq 0$ for all $i \in \beta(\bar{z})$. Then $\bar{\lambda}_i^G, \bar{\lambda}_i^H \geq 0$ for all $i \in \beta(\bar{z})$, and \bar{z} is S-stationary and obviously a B-stationary point of the MPCC. It is also possible that there exist indices $i \in \beta(\bar{z})$ such that $\bar{u}_i^{\Phi} < 0$. For these indices $i, \bar{\lambda}_i^G, \bar{\lambda}_i^H \leq 0$. In the following, we analyze stationarity of \bar{z} further under an additional assumption that z^k is a strict local minimizer of $BA(\epsilon^k)$ (see, for example, scholtes4 in Section 3.1 and ex9.2.2 in Section 5.1).

THEOREM 4.2. Suppose that \bar{z} is generated from the sequence described in Theorem 4.1. In addition to the assumptions of Theorem 4.1, suppose that for every sufficiently large k, at z^k the collection of vectors

$$\nabla g_i(z^k), \quad i \in \{i \in I_g(z^k) \mid u_i^{g,k} > 0\},$$

$$\nabla h_i(z^k), \quad i = 1, \dots, n_h,$$

$$\nabla \Phi_i(z^k), \quad i = 1, \dots, m,$$

contains a set of n linearly independent vectors. Then \bar{z} is an M-stationary point of MPCC (1.1).

484 *Proof.* Denote C^k as the set at z^k of n linearly independent vectors. For the
485 gradient vectors in C^k coming from constraints g, h, and Φ , denote the sets of their
486 indices as J_q^+, J_h , and J_{Φ} , respectively. Then, the limit of C^k can be expressed as:

$$\bar{\mathcal{C}} = \begin{cases}
\nabla g_j(\bar{z}), & j \in J_g^+ = \{j \in I_g(\bar{z}) \mid \bar{\lambda}^g > 0\} \\
\nabla h_j(\bar{z}), & j \in J_h \\
\nabla G_j(\bar{z}), & j \in J_\Phi \cap \alpha(\bar{z}) \\
\nabla H_j(\bar{z}), & j \in J_\Phi \cap \gamma(\bar{z}) \\
\xi_j = \theta_j \nabla G_j(\bar{z}) + (1 - \theta_j) \nabla H_j(\bar{z}), & j \in J_\Phi \cap \beta(\bar{z})
\end{cases},$$

where every $\theta_j \in [0,1]$. The vectors in $\bar{\mathcal{C}}$ are linearly independent, which is a consequence of linear independence of the vectors in \mathcal{C}^k . The constraint gradients involved in the set $\bar{\mathcal{C}}$ form the basis for all of the other constraint gradients at \bar{z} , and Theorem 4.1 ensures that based on these constraints \bar{z} is C-stationary.

We show that there exists a partition $(\beta_1, \beta_2) \in \mathcal{P}(J_{\Phi} \cap \beta(\bar{z}))$ such that the multipliers suitable for $NLP_{(\beta_1,\beta_2)}$ also satisfy M-stationarity. Consider partition of the set $J_{\Phi} \cap \beta(\bar{z})$. Let

$$S_1 = \{ j \in J_{\Phi} \cap \beta(\bar{z}) \mid \theta_j = 1 \},$$

$$S_2 = \{ j \in J_{\Phi} \cap \beta(\bar{z}) \mid \theta_j = 0 \},$$

$$S_3 = \{ j \in J_{\Phi} \cap \beta(\bar{z}) \mid 0 < \theta_i < 1 \}.$$

For every $j \in \mathcal{S}_3$, since ξ_j is independent from all the vectors in $\overline{\mathcal{C}} \setminus \{\xi_j\}$, either $\nabla G_j(\overline{z})$ or $\nabla H_j(\overline{z})$ (or both) are linearly independent from all the vectors in $\overline{\mathcal{C}} \setminus \{\xi_j\}$. Hence, there exist the following sets:

$$S_{31} = \{ j \in S_3 \mid \nabla G_j \text{ is independent from } \bar{\mathcal{C}} \setminus \{\xi_j\} \},$$

 $S_{32} = S_3 \setminus S_{31},$

such that 500

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$$\operatorname{rank} \left(\begin{bmatrix} \nabla g_{j}(\bar{z})^{T}, & \forall j \in J_{g}^{+} \\ \nabla h_{j}(\bar{z})^{T}, & \forall j \in J_{h} \\ \nabla G_{j}(\bar{z})^{T}, & \forall j \in J_{\Phi} \cap \alpha(\bar{z}) \\ \nabla H_{j}(\bar{z})^{T}, & \forall j \in J_{\Phi} \cap \gamma(\bar{z}) \\ \nabla G_{j}(\bar{z})^{T}, & \forall j \in \mathcal{S}_{1} \\ \nabla H_{j}(\bar{z})^{T}, & \forall j \in \mathcal{S}_{2} \\ \nabla G_{j}(\bar{z})^{T}, & \forall j \in \mathcal{S}_{31} \\ \nabla H_{j}(\bar{z})^{T}, & \forall j \in \mathcal{S}_{32} \end{bmatrix} \right) = n,$$

and d = 0 is the only solution to the following problem:

$$\min \quad \nabla f(\bar{z})^T d$$
s.t.
$$\nabla g_{J^+}(\bar{z})^T d \leq 0,$$

$$\nabla h_{J_h}(\bar{z})^T d = 0,$$

$$\nabla G_{J_\Phi \cap \alpha}(\bar{z})^T d = 0,$$

$$\nabla H_{J_\Phi \cap \gamma}(\bar{z})^T d = 0,$$

$$\nabla G_{S_1}(\bar{z})^T d = 0,$$

$$\nabla H_{S_2}(\bar{z})^T d = 0,$$

$$\nabla G_{S_{31}}(\bar{z})^T d = 0,$$

$$\nabla G_{S_{32}}(\bar{z})^T d \geq 0,$$

with $\nabla g_{J^+}(\bar{z})^T d \leq 0$ strongly active. It follows that \bar{z} is a strict local minimizer of $NLP_{(\beta_1,\beta_2)}$ [3, Corollary in Section 4.4.2] with $(\beta_1,\beta_2) \in \mathcal{P}(J_{\Phi} \cap \beta(\bar{z}))$ given by 505

$$\beta_1 = \mathcal{S}_1 \cup \mathcal{S}_{31}, \quad \beta_2 = \mathcal{S}_2 \cup \mathcal{S}_{32}.$$

Since the KKT multipliers of $NLP_{(\beta_1,\beta_2)}$ must satisfy A-stationarity, which together 507 508 with C-stationarity shown by Theorem 4.1, implies that the multipliers satisfy Mstationarity (intersection of A- and C- stationarities). 509

4.6. Inequality variant of BA. To further understand and explore conver-510 511 gence properties of the Bounding Algorithm, it is beneficial to take advantage of an inequality variant of the problem $BA(\epsilon)$, which is given by 512

$$\text{MLF}(\epsilon): \quad \text{min} \quad f(z) \qquad \qquad \text{multipliers}$$
 s.t. $g(z) \leq 0, \qquad \qquad u^g$
$$h(z) = 0, \qquad \qquad u^h$$

$$-\epsilon/2 \leq \Phi_i^\epsilon(z) \leq 0, \; i = 1 \dots m. \quad u_{L,i}^\Phi, u_{U,i}^\Phi$$

For a sequence of positive scalars $\epsilon^k \to 0$, solving problems $\mathrm{MLF}(\epsilon^k)$ generates a

sequence $\{z^k\} \to \bar{z}$, where every z^k is a KKT point of MLF(ϵ^k). At every point z^k we have multipliers $u^k = (u^{g,k}, u^{h,k}, u^{\Phi,k}_L, u^{\Phi,k}_U)$ with $u^{g,k} \geq 0$ and $0 \leq u^{\Phi,k}_{L,i} \perp u^{\Phi,k}_{U,i} \geq 0$

for $i = 1 \dots m$, such that

518 (4.12)
$$0 = \nabla f(z^k) + \sum_{i \in I_g(z^k)} u_i^{g,k} \nabla g_i(z^k) + \sum_{i=1}^{n_h} u_i^{h,k} \nabla h_i(z^k) - \sum_{i=1}^m (u_{L,i}^{\Phi,k} - u_{U,i}^{\Phi,k}) \nabla \Phi_i^{\epsilon}(z^k).$$

- Under the assumption that the multipliers associated with every z^k are bounded, 519
- the existence of the multipliers in the limit can be proved as before. Comparing the 520
- problem formulations (4.1) and (4.11), and the KKT conditions (4.5) and (4.12), gives
- the relations between $BA(\epsilon^k)$ and $MLF(\epsilon^k)$:

$$p_i^k = \epsilon^k/2 \Leftrightarrow \text{lower bound of } \Phi_i^{\epsilon}(z^k) \text{ is active, and } u_{L,i}^{\Phi,k} \geq 0,$$
523 (4.13)
$$p_i^k = 0 \Leftrightarrow \text{upper bound of } \Phi_i^{\epsilon}(z^k) \text{ is active, and } u_{U,i}^{\Phi,k} \geq 0,$$

$$u^{\Phi,k} = u_L^{\Phi,k} - u_U^{\Phi,k}.$$

Substituting the last relation into (4.9) gives the MPCC multipliers at \bar{z} : 524

$$\bar{\lambda}^{g} = \bar{u}^{g} = \lim_{k \to \infty} u^{g,k},
\bar{\lambda}^{h} = \bar{u}^{h} = \lim_{k \to \infty} u^{h,k},
\bar{\lambda}^{i}_{i} = \begin{cases}
\bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi} = \lim_{k \to \infty} (u_{L,i}^{\Phi,k} - u_{U,i}^{\Phi,k}), & i \in \alpha(\bar{z}) \\
(\bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi})\theta_{i}, & i \in \beta(\bar{z}),
\end{cases}$$

$$\bar{\lambda}^{H}_{i} = \begin{cases}
\bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi} = \lim_{k \to \infty} (u_{L,i}^{\Phi,k} - u_{U,i}^{\Phi,k}), & i \in \gamma(\bar{z}) \\
(\bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi})(1 - \theta_{i}), & i \in \beta(\bar{z}).
\end{cases}$$

Stationarity of \bar{z} established in the previous subsections for BA can be extended 526 directly to MLF. 527

Numerical experience demonstrates the feature that when \bar{z} is not S-stationary, 528 namely, there exists a subset 529

530 (4.15)
$$\Omega \subseteq \beta(\bar{z}), \text{ such that } \bar{\lambda}_i^G, \bar{\lambda}_i^H \leq 0 \text{ for all } i \in \Omega,$$

a sequence $\{z^k\}$ converges to \bar{z} from the upper bounds of the constraints $-\epsilon^k/2 \leq$

 $\Phi_{\Omega}^{\epsilon}(z) \leq 0$, thus $u_{L,\Omega}^{\Phi,k} - u_{U,\Omega}^{\Phi,k} < 0$ for every k sufficiently large, and $(\bar{u}_{L,\Omega}^{\Phi} - \bar{u}_{U,\Omega}^{\Phi}) < 0$ 532

in the limit. In parallel with this observation, a sequence $\{z^k\}$ generated by the Bounding Algorithm converges to \bar{z} with $p_{\Omega}^k=0$ for constraints $\Phi_{\Omega}^\epsilon(z)+p_{\Omega}^k=0$, thus the corresponding multipliers $u_{\Omega}^{\Phi,k}<0$ (as implied by (4.13)), and $\bar{u}_{\Omega}^{\Phi}<0$ in the limit. Behind these observations lies a fundamental justification, which explains why 533

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MLF and BA identify a non-strongly stationary point in such a way, or why approaching to a non-strongly stationary point makes these methods behave like this. 538

539 To be specific, at a feasible point z of $MLF(\epsilon^k)$, define the index sets

$$I_L^{\Phi}(z) = \{i \mid \Phi_i^{\epsilon}(z) = -\epsilon^k/2\},\$$

$$I_U^{\Phi}(z) = \{i \mid \Phi_i^{\epsilon}(z) = 0\}.$$

The constraint $-\epsilon^k/2 \le \Phi_i^{\epsilon}(z) \le 0$ requires that

$$(G_i(z) + \frac{\epsilon^k}{2})(H_i(z) + \frac{\epsilon^k}{2}) \ge (\epsilon^k)^2 / 4,$$

$$G_i(z)H_i(z) \le (\epsilon^k)^2 / 4,$$

and at the lower and upper bounds we have

$$G_i(z) + \frac{\epsilon^k}{2} > 0, \ H_i(z) + \frac{\epsilon^k}{2} > 0, \ (G_i(z) + \frac{\epsilon^k}{2})(H_i(z) + \frac{\epsilon^k}{2}) = (\epsilon^k)^2/4, \quad \forall i \in I_L^{\Phi}(z)$$

$$G_i(z) > 0, \ H_i(z) > 0, \ G_i(z)H_i(z) = (\epsilon^k)^2/4, \quad \forall i \in I_U^{\Phi}(z).$$

Therefore, the feasible region of MLF(ϵ^k) includes the feasible region of MPCC (1.1), while it restricts the feasible region of RNLP (1.6) from above by enforcing $\Phi_i^{\epsilon}(z) \leq 0$ and extends the region a little below by using the relaxed lower bounds $\Phi_i^{\epsilon}(z) \geq -\epsilon^k/2$ to allow for small perturbations $G_i(z) < 0$ or $H_i(z) < 0$.

Suppose that there exists a subset $\Omega \subseteq \{1 \dots m\}$, such that RNLP (1.6) is minimized at $G_{\Omega}(z) > 0$ and $H_{\Omega}(z) > 0$. As the solutions of RNLP locate outside of the feasible region of the MPCC, no local minimizer of the MPCC can be S-stationary. In such circumstance, the RNLP constrained additionally by $\Phi_{\Omega}^{\epsilon}(z) \leq 0$ achieves the minimal cost on the boundaries of $\Phi_{\Omega}^{\epsilon}(z) \leq 0$ for every $\epsilon^k > 0$. For MLF (ϵ^k) , it may have the same minimizer as the additionally constrained RNLP, or have a better solution on the lower bound of $\Phi_i^{\epsilon}(z)$ for some $i \in \Omega$ and every $\epsilon^k > 0$ suitably small. In the latter case, for those $i \in \Omega$, we have that in the limit $\bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi} \geq 0$ and therefore $\bar{\lambda}_i^G, \bar{\lambda}_i^H \geq 0$ (as indicated by (4.14)), which contradicts the assumption that RNLP is minimized at $G_i(z), H_i(z) > 0$.

Therefore, for every $\epsilon^k > 0$ suitably small, a local minimizer of $\mathrm{MLF}(\epsilon^k)$ is also a local minimizer of the RNLP constrained additionally by $\Phi_\Omega^\epsilon(z) \leq 0$. This gives rise to the phenomenon that the upper bounds of the constraints $-\epsilon^k/2 \leq \Phi_\Omega^\epsilon(z) \leq 0$ are active at every z^k as $\epsilon^k \to 0$. Moreover, we have $\Omega \subseteq \beta(\bar{z})$ because the constantly active upper bounds as $\epsilon^k \to 0$ means that $G_\Omega(z^k) > 0$, $H_\Omega(z^k) > 0$, and $G_\Omega(z^k)H_\Omega(z^k) = (\epsilon^k)^2/4$ (componentwise product) for infinitely many k.

Now we reconsider a limit point \bar{z} of BA or MLF, at which there exists a subset

$$\Omega \subseteq \beta(\bar{z})$$
, such that $\bar{u}_{\Omega}^{\Phi} < 0$ (BA) or $\bar{u}_{L,\Omega}^{\Phi} - \bar{u}_{U,\Omega}^{\Phi} < 0$ (MLF).

According to (4.9) and (4.14), the MPCC multipliers have non-positive components for the subset Ω , as shown by (4.15). We aim to verify whether such \bar{z} is B-stationary. Suppose that MPCC-ACQ holds at \bar{z} . According to Theorem 3.2, B-stationarity of MPCC (1.1) can be established from piecewise M-stationarity under MPCC-ACQ. The above discussion has shown that the existence of the subset Ω usually signifies the absence of S-stationary solutions. So, for every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, piecewise M-stationarity can be satisfied by the MPCC multipliers (4.15) only if

574 (4.16)
$$\bar{\lambda}_i^G < 0, \ \bar{\lambda}_i^H = 0, \quad \forall i \in \beta_1 \cap \Omega,$$
$$\bar{\lambda}_i^G = 0, \ \bar{\lambda}_i^H < 0, \quad \forall i \in \beta_2 \cap \Omega.$$

75 In this case, the LPs comprising LPCC (3.1) have the same solution as

min
$$obj(d) = \nabla f(\bar{z})^T d$$

s.t. $\nabla g_I(\bar{z})^T d \leq 0$,
 $\nabla h(\bar{z})^T d = 0$,
 $\nabla G_{\alpha}(\bar{z})^T d = 0$,
 $\nabla H_{\gamma}(\bar{z})^T d = 0$,
 $\nabla G_{\beta_1}(\bar{z})^T d = 0$, $\nabla H_{\beta_1 \setminus \Omega}(\bar{z})^T d \geq 0$,
 $\nabla G_{\beta_2 \setminus \Omega}(\bar{z})^T d \geq 0$, $\nabla H_{\beta_2}(\bar{z})^T d = 0$.

Here the constraints corresponding to the subset Ω can be excluded from the inequality constraints, because (4.16) implies that for every partition $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, the constraints corresponding to $\bar{\lambda}_i^H$ for all $i \in \beta_1 \cap \Omega$, and corresponding to $\bar{\lambda}_i^G$ for all $i \in \beta_2 \cap \Omega$, must be locally inactive. Hence, the LPs with partitions drawn from the subset Ω are already known to be piecewise M-stationary; and provided that the problem (4.17) is bounded below for every $(\beta_1, \beta_2) \in \mathcal{P}(\beta(\bar{z}))$, \bar{z} is B-stationary.

5. Practical issues. Numerical results of the NCP-based bounding methods (BA and MLF) applied to the MacMPEC collection [21] as well as large-scale MPCCs drawn from real-world chemical engineering examples can be found in [29]. In that study, we considered a selection of problems from the MacMPEC collection, which have solutions with biactive complementary components, as well as seven MPCC problems constructed from distillation models with up to 1264 variables and 48 complementarity constraints. The numerical comparison includes the typical regularization scheme proposed in [26], the regularization method proposed in [23] and closely related to MLF, and three NCP-based methods, namely, BA, MLF, and a standard NCP-based method (without bounding scheme). This demonstrates that the NCP-based methods are the most efficient of these methods, especially on examples without S-stationary solutions, and that, in general, the BA method performs well among these methods.

In this section, we take a closer look at the behaviors of MPCC methods, when converging to a limit point \bar{z} which is not S-stationary. By examples, we first show the course of convergence of multipliers produced by the NCP-based bounding methods with vanishing ϵ . Then we show that the Lagrange multipliers generated by these methods are bounded, as a benefit of the generalized gradients of the underlying NCP functions. This allows the convergence results in Section 4, which are developed under the assumption of the boundedness of the multipliers, to be applicable in practice.

5.1. MPCC multipliers by NCP-based bounding methods. We observe convergence of the multipliers produced by the NCP-based bounding methods.

Example: ex9.2.2. This example shows that in the course of approaching a non-strongly stationary local minimizer, the solutions of the NCP-based bounding methods (BA and MLF) provide MPCC multipliers satisfying C-stationarity when the smoothing factor ϵ is not very small, and provide MPCC multipliers satisfying M-stationarity as ϵ vanishes.

Problem ex9.2.2 from the MacMPEC collection [21] is given by

$$\begin{array}{lll} & \min & x^2 + (y-10)^2 & \text{multipliers} \\ & \text{s.t.} & x \leq 15, & \text{(inactive)} \\ & -x + y \leq 0, & \lambda_1 \\ & -x \leq 0, & \text{(inactive)} \\ & x + y + s_1 = 20, & \lambda_2 \\ & -y + s_2 = 0, & \lambda_3 \\ & y + s_3 = 20, & \lambda_4 \\ & 2x + 4y + l_1 - l_2 + l_3 = 60, & \lambda_5 \\ & 0 \leq s_i \perp l_i \geq 0, \ i = 1 \dots 3. & \sigma^{si}, \sigma^{li} \end{array}$$

The NCP-based bounding methods converge to the point $\bar{z} = (\bar{x}, \bar{y}, \bar{s}, \bar{l})$ with

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$$\bar{x} = 10, \ \bar{y} = 10, \ \bar{s} = (0, 10, 10), \ \bar{l} = (0, 0, 0).$$

Since the constraint functions are linear, MPCC-ACQ holds at every feasible point of the problem. The weak stationarity conditions (1.3) at \bar{z} require that

$$2\bar{x} - \lambda_1 + \lambda_2 + 2\lambda_5 = 0,$$

$$2(\bar{y} - 10) + \lambda_1 + \lambda_2 - \lambda_3 + \lambda_4 + 4\lambda_5 = 0,$$

$$\lambda_2 - \sigma^{s1} = 0,$$

$$\lambda_3 = 0,$$

$$\lambda_4 = 0,$$

$$\lambda_5 - \sigma^{l1} = 0,$$

$$-\lambda_5 - \sigma^{l2} = 0,$$

$$\lambda_5 - \sigma^{l3} = 0,$$

617 which implies

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$$\sigma^{s1} = -3\lambda_5 - 10,$$

$$\sigma^{l1} = \lambda_5.$$

The multipliers σ^{s1} , σ^{l1} for the biactive complementary components s_1, l_1 cannot be both nonnegative, hence \bar{z} cannot be S-stationary. Let $\sigma^{s1} = 0$ or $\sigma^{l1} = 0$, then we obtain $(\sigma^{s1}, \sigma^{l1}) = (0, -10/3)$ or $(\sigma^{s1}, \sigma^{l1}) = (-10, 0)$, indicating that \bar{z} is piecewise M-stationary. These two sets of multipliers reflect stationarity of \bar{z} for NLPs on their respective partitions.

Now we check the multipliers given by the NCP-based bounding methods. For the set $\beta(\bar{z}) = \{1\}$, solutions of the NCP-based bounding methods give the corresponding NLP multipliers shown in Table 1. According to (4.9) and (4.14),

627 (5.2)
$$\bar{\lambda}_{i}^{G} + \bar{\lambda}_{i}^{H} = \bar{u}_{i}^{\Phi} = \bar{u}_{L,i}^{\Phi} - \bar{u}_{U,i}^{\Phi}, \quad \forall i \in \beta(\bar{z}).$$

At $\epsilon = 10^{-6}$, by enforcing $\sigma^{s1} + \sigma^{l1} = -5.74$, we obtain from (5.1) the MPCC multipliers at \bar{z} , that is, $(\sigma^{s1}, \sigma^{l1}) = (-3.61, -2.13)$, satisfying C-stationarity. With further decrease of ϵ , the multipliers in Table 1 reflect that they are converging to MPCC multipliers that satisfy M-stationarity at \bar{z} . According to (4.9) and (4.14), the value of θ is 1 in BA and 0 in MLF, corresponding to different partitions of $\beta(\bar{z})$.

Table 1

NLP multipliers of NCP-based bounding methods.

ϵ		10^{-6}	10^{-9} 10^{-10}		10^{-11}	10^{-12}	10^{-15}
BA	u^{Φ}	-5.74	-4.78	-5.23	-7.45	-9.94	-10.00
MLF	u_L^{Φ}	0	0	0	0	0	0
MILI	u_U^{Φ}	5.74	5.63	4.78	3.72	3.34	3.33

5.2. Unbounded NLP multipliers and inaccurate solution. In the course of seeking for a solution of an MPCC, NLP subproblems may encounter unbounded multipliers when approaching a limit point which is not S-stationary. Our numerical experience to date indicates that NCP-based reformulations $BA(\epsilon)$ and $MLF(\epsilon)$ avoid

unbounded NLP multipliers. The following confirms this observation, by comparing BA(ϵ) and MLF(ϵ) with the typical regularization scheme proposed in [26]:

REG(
$$\epsilon$$
): min $f(z)$ multipliers s.t. $g(z) \leq 0$, v^g
$$h(z) = 0, \qquad v^h$$

$$G(z) \geq 0, \qquad v^G$$

$$H(z) \geq 0, \qquad v^H$$

$$G_i(z)H_i(z) \leq \epsilon, \ i = 1 \dots m. \qquad v_i^{REG}$$

Solving a sequence of programs REG(ϵ^k) with the positive scalars $\epsilon^k \to 0$, generates a sequence $\{z^k\} \to \bar{z}$. Based on stationarity of z^k for REG(ϵ^k), namely,

$$0 = \nabla f(z^{k}) + \sum_{i \in I_{g}(z^{k})} v_{i}^{g,k} \nabla g_{i}(z^{k}) + \sum_{i=1}^{n_{h}} v_{i}^{h,k} \nabla h_{i}(z^{k})$$

$$- \sum_{i=1}^{m} v_{i}^{G,k} \nabla G_{i}(z^{k}) - \sum_{i=1}^{m} v_{i}^{H,k} \nabla H_{i}(z^{k}) + \sum_{i=1}^{m} v_{i}^{REG,k} \left[H_{i}(z^{k}) \nabla G_{i}(z^{k}) + G_{i}(z^{k}) \nabla H_{i}(z^{k}) \right],$$

the relations between the NLP multipliers $v^k = (v^{g,k}, v^{h,k}, v^{G,k}, v^{H,k}, v^{REG,k})$ at z^k and the MPCC multipliers $\bar{\lambda} = (\bar{\lambda}^g, \bar{\lambda}^h, \bar{\lambda}^G, \bar{\lambda}^H)$ at \bar{z} can be expressed by (see also [26, Eq.(6) and Theorem 3.1])

$$\bar{\lambda}^{g} = \bar{v}^{g} = \lim_{k \to \infty} v^{g,k},$$

$$\bar{\lambda}^{h} = \bar{v}^{h} = \lim_{k \to \infty} v^{h,k},$$

$$\bar{\lambda}^{G}_{i} = \lim_{k \to \infty} \left[v_{i}^{G,k} - v_{i}^{REG,k} H_{i}(z^{k}) \right], \ i = 1, \dots, m,$$

$$\bar{\lambda}^{H}_{i} = \lim_{k \to \infty} \left[v_{i}^{H,k} - v_{i}^{REG,k} G_{i}(z^{k}) \right], \ i = 1, \dots, m.$$

It has been proved that \bar{z} is a strongly stationary point of MPCC (1.1) if and only if it is a stationary point of REG(0) [11, Proposition 4.1].

Consider the case where \bar{z} is not S-stationary. Then \bar{z} is not a stationary point of REG(0). In the case \bar{z} is no better than C-stationary, then there exist indices $i \in \beta(\bar{z})$ such that $\bar{\lambda}_i^G < 0, \bar{\lambda}_i^H < 0$. According to (5.3), the NLP multipliers $v_i^{G,k}$ and $v_i^{H,k}$ have a tendency to be less than zero for k sufficiently large, which are not allowed in REG(ϵ^k). Since

$$\lim_{k \to \infty} v_i^{G,k} = \bar{\lambda}_i^G + \lim_{k \to \infty} v_i^{REG,k} H_i(z^k),$$

$$\lim_{k \to \infty} v_i^{H,k} = \bar{\lambda}_i^H + \lim_{k \to \infty} v_i^{REG,k} G_i(z^k),$$

the multipliers $v_i^{REG,k}$ become very large to enforce $v_i^{G,k}$ and $v_i^{H,k}$ nonnegative. At the same time, $G_i(z^k)$ and $H_i(z^k)$ are prevented from being very close to zero, otherwise $v_i^{REG,k}G_i(z^k)$ and $v_i^{REG,k}H_i(z^k)$ would be ineffective. As a consequence, it can be observed for k sufficiently large that $v_i^{G,k} = 0, v_i^{H,k} = 0, v_i^{REG,k} \to \infty$, and $G_i(z^k)$ and $H_i(z^k)$ cannot converge accurately to zero.

In the case \bar{z} is no better than M-stationary, there exist indices $i \in \beta(\bar{z})$ such that $\bar{\lambda}_i^G = 0, \bar{\lambda}_i^H < 0$ (or the reverse). The relations (5.3) imply that for k sufficiently large $v_i^{H,k}$ has a tendency to be less than zero, which is not a suitable NLP multiplier. We also use (5.4) to predict the behavior of the REG method. In order to enforce $v_i^{H,k}$ nonnegative, the multipliers $v_i^{REG,k}$ get to be very large, and at the same time, $G_i(z^k)$ cannot be very close to zero. The components $H_i(z^k)$ cannot approach zero quickly either, because the constraints $G_i(z^k)H_i(z^k) \leq \epsilon^k$ must be kept active for every $\epsilon^k > 0$. As a result, the observation for k sufficiently large should be the same as the above case.

On the other hand, the multipliers for the programs $\mathrm{BA}(\epsilon^k)$ and $\mathrm{MLF}(\epsilon^k)$ do not have this difficulty. As indicated by the relations (4.9) and (4.14), there is no contradiction between the signs of the MPCC multipliers $\bar{\lambda}_i^G, \bar{\lambda}_i^H$ and of the NLP multipliers $u_i^{\Phi,k}$ and $u_{L,i}^{\Phi,k} - u_{U,i}^{\Phi,k}$. In addition, the underlying relation (5.2) indicates that the NLP multipliers exist whenever the MPCC multipliers do. Therefore, whether \bar{z} is S-stationary or not has little influence on the performance of BA and MLF methods, which is an important difference from the REG method.

Examples: Multiplier comparison. We review the examples in Sections 3.1 and 5.1 to illustrate the difference in behavior between the NCP-based bounding methods (BA and MLF) and REG regularization method.

As we showed in the previous sections, the examples scholtes4 and ex9.2.2 have non-strongly stationary local minimizers. Numerical results of these two examples are presented in Tables 2 and 3. The results indicate that REG method gives rise to large NLP multipliers for the constraints corresponding to the biactive complementary components, and the multipliers get even larger when the regularization parameter ϵ becomes smaller. At the same time, the convergence is slow and inaccurate, compared to the magnitude of ϵ .

On the other hand, the multipliers of the NCP-based bounding methods are well behaved. According to (5.2), their multipliers can be used to derive the MPCC multipliers at a limit point and vice versa. In addition, the accuracy of their solutions (to the program variables and multipliers) is comparable to ϵ .

Table 2
Results of problem scholtes4.

ϵ	scholtes4	BA		MLF		REG			
		p	u^{Φ}	u_L^{Φ}	u_U^{Φ}	v^{z_1}	v^{z_2}	v^{REG}	
	multipliers	0	-2	0	2	0	0	1.00E + 3	
10^{-6}	z_1	5E-7		5E-7		0.001000			
	z_2	5E-7		5E-7		0.001000			
	z_3	2E-6		2E-6		0.003999			
		p	u^{Φ}	u_L^{Φ}	u_U^{Φ}	v^{z_1}	v^{z_2}	v^{REG}	
	multipliers	0	-2	0	2	0	0	2.69E+4	
10^{-9}	z_1	5E-10		5E-10		0.000037			
	z_2	5E-1		5E-10		0.000037			
	z_3	2E-9		2E-9		0.000149			
		p	u^{Φ}	u_L^{Φ}	u_U^{Φ}	v^{z_1}	v^{z_2}	v^{REG}	
	multipliers	0	-2	0	2	0	0	5.02E + 4	
10^{-12}	z_1	5E-11		5E-11		0.000020			
	z_2	5E-11		5E-11		0.000020			
	z_3	2E-10		2E-10		0.000080			

6. Conclusions. This study explores characteristics of local minimizers of MPCCs and their influence on convergence behavior of NLP-based MPCC algorithms. First,

Table 3
Results of problem ex9.2.2.

ϵ	ex9.2.2	BA		MLF		REG		
		$p u^{4}$	•	u_L^{Φ}	u_U^Φ	v^{s_1}	v^{l_1}	v^{REG}
	multipliers	0 -5.7	4	0	5.74	0	0	2.89E + 3
10^{-6}	s_1	3.8E-7		3.8E-7		0.000577		
	l_1	6.5E-7		6.5E-7		0.001732		
		$p u^{\Phi}$	•	u_L^{Φ}	u_U^Φ	v^{s_1}	v^{l_1}	v^{REG}
	multipliers	0 -4.7	78	0	5.63	0	0	7.85E+4
10^{-9}	s_1	2.04E-1	04E-10 3.65E-10		0.000021			
	l_1	1.11E-10		5.96E-10		0.000064		
		$p u^{\Phi}$	•	u_L^{Φ}	u_U^Φ	v^{s_1}	v^{l_1}	v^{REG}
	multipliers	0 -9.9	94	0	3.34	0	0	1.46E + 5
10^{-12}	s_1	s_1 2.94E-11		2.03E-11		0.000011		
	l_1	3.81E-11		1.09E-11		0.000034		

we derive M-stationarity of a local minimizer of an MPCC under MPCC-ACQ (Theorem 2.2). A key point is that the M-stationarity is a piecewise property. For a local minimizer \bar{z} which is not S-stationary, there exist multiple sets of MPCC multipliers, each corresponding to one partition of $\beta(\bar{z})$ and satisfying M-stationarity on that partition.

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Second, we aim to capture conditions that guarantee a feasible point of an MPCC to be B-stationary. By applying the main results (D1), (D2), and (D3) of duality theory to the LPCC at a weakly stationary point of an MPCC, we prove under MPCC-ACQ that either a weakly stationary point is B-stationary, or there exists a component LP of the LPCC, which is unbounded below (Theorem 3.1). The link between the optimality of the LPs comprising the LPCC and the first-order optimality of the NLPs comprising the MPCC, allows to establish B-stationarity from piecewise M-stationarity under MPCC-ACQ (Theorem 3.2). In addition, a method to detect unbounded LPs is proposed, which is applicable when n out of the active constraints are linearly independent (Section 3.3).

To investigate convergence properties of the Bounding Algorithm we proposed in [29] in the absence of MPCC-LICQ, we consider stationarity of a limit point of this method, based on stationarity of a sequence of NLP solutions approaching to it. We establish C-stationarity of a limit point by using attributes of the NCP function involved (Theorem 4.1), and M-stationarity by introducing an additional assumption on active constraint gradients (Theorem 4.2). Further investigation from the perspective of an inequality variant of this algorithm leads to a simplification of the LPCC when verifying B-stationarity of a limit point.

Finally, we discuss a few practical issues related to local minimizers of MPCCs which are not S-stationary. It is illustrated that the NCP-based bounding methods (BA and MLF) usually produce MPCC multipliers that satisfy C-stationarity at a non-strongly stationary solution when the smoothing factor ϵ is not sufficiently small, and satisfy M-stationarity as ϵ vanishes (Section 5.1). Moreover, the sequence of NLP multipliers is bounded, even if the methods are approaching a non-strongly stationary MPCC solution. On the other hand, the REG method, which is a typical regularization method, usually encounters unbounded NLP multipliers and inaccurate convergence when approaching a non-strongly stationary solution (Section 5.2). This analysis shows an advantage of NCP-based reformulation of complementarity constraints. Namely, the structure of the generalized gradients of the NCP functions corresponding to the degenerate complementarity constraints, can prevent the NLP

multipliers from blowing up, provided that the MPCC multipliers are well defined at a limit point.

729 REFERENCES

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- 730 [1] R Andreani, L D Secchin, P J S Silva. Convergence properties of a second order augmented
 731 Lagrangian method for mathematical programs with complementarity constraints. SIAM
 732 Journal on Optimization (2018), 28(3): 2574-2600
 - M Anitescu. On using the elastic mode in nonlinear programming approaches to mathematical programs with complementarity constraints. SIAM Journal on Optimization (2005), 15(4): 1203-1236
 - [3] M S Bazaraa, H D Sherali, C M Shetty. Nonlinear Programming: Theory and Algorithms (3rd edition). Wiley, Hoboken, New Jersey (2006)
 - [4] D P Bertsekas, A E Ozdaglar. Pseudonormality and a Lagrange multiplier theory for constrained optimization. Journal of Optimization Theory and Applications (2002), 114: 287-343
 - [5] D Bertsimas, J N Tsitsiklis. Introduction to Linear Optimization. Athena Scientific, Belmont, MA (1997)
 - [6] F H Clarke. Optimization and Nonsmooth Analysis. Wiley, New York, NY (1983)
 - [7] A R Conn, N I M Gould. Trust-Region Methods. SIAM, Philadelphia, PA (2000)
 - [8] M L Flegel, C Kanzow. An Abadie-type constraint qualification for mathematical programs with equilibrium constraints. Journal of Optimization Theory and Applications (2005), 124: 595-614
 - [9] M L Flegel, C Kanzow. On the Guignard constraint qualification for mathematical programs with equilibrium constraints. Optimization (2005), 54(6): 517-534
 - [10] M L Flegel, C Kanzow. A direct proof for M-stationarity under MPEC-GCQ for mathematical programs with equilibrium constraints. In: S Dempe, V Kalashnikov (eds.) Optimization with Multivalued Mappings: Theory, Applications and Algorithms, 111–122. Springer, New York, NY (2006)
 - [11] R Fletcher, S Leyffer, D Ralph, S Scholtes. Local convergence of SQP methods for mathematical programs with equilibrium constraints. SIAM Journal on Optimization (2006), 17(1): 259-286
 - [12] M Fukushima, J-S Pang. Convergence of a smoothing continuation method for mathematical progams with complementarity constraints. In: M Thera, R Tichatschke (eds.) Ill-posed Variational Problems and Regularization Techniques, 99-110. Springer-Verlag, Berlin Heidelberg, (1999)
 - [13] F J Gould, J W Tolle. A necessary and sufficient qualification for constrained optimization. SIAM Journal on Applied Mathematics (1971), 20(2): 164-172
 - [14] L Guo, Z Deng. A new augmented Lagrangian method for MPCCs Theoretical and numerical comparison with existing augmented Lagrangian methods. Mathematics of Operations Research (2022), 47(2), 1229-1246
 - [15] T Hoheisel, C Kanzow, A Schwartz. Convergence of a local regularization approach for mathematical programs with complementarity or vanishing constraints. Optimization Methods and Software (2012), 27(3): 483-512
 - [16] T Hoheisel, C Kanzow, A Schwartz. Theoretical and numerical comparison of relaxation methods for mathematical programs with complementarity constraints. Mathematical Programming (2013), 137: 257–288
 - [17] A F Izmailov, M V Solodov, E I Uskov. Global convergence of augmented Lagrangian methods applied to optimization problems with degenerate constraints, including problems with complementarity constraints. SIAM Journal on Optimization (2012), 22(4): 1579-1606
 - [18] A Kadrani, J P Dussault, A Benchakroun. A new regularization scheme for mathematical programs with complementarity constraints. SIAM Journal on Optimization (2009), 20(1): 78-103
 - [19] C Kanzow, A Schwartz. A new regularization method for mathematical programs with complementarity constraints with strong convergence properties. SIAM Journal on Optimization (2013), 23(2): 770–798
- 781 [20] C Kanzow, A Schwartz. Mathematical programs with complementarity constraints: Enhanced 782 Fritz John conditions, new constraint qualifications, and improved exact penalty results. 783 SIAM Journal on Optimization (2010), 20(5): 2730-2753
- 784 [21] S Leyffer MacMPEC: AMPL collection of MPECs, (2000).
 785 https://wiki.mcs.anl.gov/leyffer/index.php/MacMPEC

- 786 [22] S Leyffer, G López-Calva, J Nocedal. Interior methods for mathematical programs with complementarity constraints. SIAM Journal on Optimization (2006), 17(1): 52-77
 - [23] G Lin, M Fukushima. A modified relaxation scheme for mathematical programs with complementarity constraints. Annals of Operations Research (2005), 133: 63-84
- 790 [24] R T Rockafellar, R J-B Wets. Variational Analysis. Springer, Berlin, Heidelberg (2009)

788

789

794

795

796

797 798

- 791 [25] H Scheel, S Scholtes. Mathematical programs with complementarity constraints: Stationarity, 792 optimality, and sensitivity. Mathematics of Operations Research (2000), 25(1): 1–22 793 [26] S Scholtes. Convergence properties of a regularization scheme for mathematical programs with
 - [26] S Scholtes. Convergence properties of a regularization scheme for mathematical programs with complementarity constraints. SIAM Journal on Optimization (2001), 11(4): 918-936
 - [27] A Schwartz. Mathematical programs with complementarity constraints and related problems, (2018). https://ifm.mathematik.uni-wuerzburg.de/schools/archive/540-2018Winter/img/LectureNotes_ASchwartz.pdf
 - [28] S Steffensen, M Ulbrich. A new regularization scheme for mathematical programs with equilibrium constraints. SIAM Journal on Optimization (2010), 20(5): 2504-2539
- 800 [29] K Wang, L T Biegler. MPCC strategies for nonsmooth nonlinear programs. Optimization and 801 Engineering (2023), 24: 1883-1929