

REAL-TIME OPTIMIZATION AS A GENERALIZED EQUATION

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Abstract. We establish results for the problem of tracking a time-dependent manifold arising in real-time optimization by casting this as a parametric generalized equation. We demonstrate that if points along a solution manifold are consistently strongly regular, it is possible to track the manifold approximately by solving a single linear complementarity problem (LCP) at each time step. We derive sufficient conditions guaranteeing that the tracking error remains bounded to second order with the size of the time step, even if the LCP is solved only approximately. We use these results to derive a fast, augmented Lagrangian tracking algorithm and demonstrate the developments through a numerical case study.

Key words. generalized equations, stability, nonlinear optimization, on-line, complementarity

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1. Introduction. Advanced real-time optimization, control, and estimation strategies rely on repetitive solutions of nonlinear optimization (NLO) problems. The structure of the NLO is normally fixed, but it depends on *time-dependent* data obtained at predefined sampling times (e.g., sensor measurements and model states).

Traditional on-line NLO strategies try to extend the sampling time (time step Δt) as much as possible in order to accommodate the solution of the NLO to a *fixed degree of accuracy*. A problem with this approach is that it neglects the fact that the NLO solver is implicitly tracking a time-dependent solution manifold. For instance, insisting on obtaining a high degree of accuracy can translate into long sampling times and increasing distances between subsequent problems. In turn, the number of iterations required by the NLO solver increases. This inconsistency limits the application scope of on-line NLO to systems with slow dynamics.

Approximate on-line NLO strategies, on the other hand, try to minimize the time step by computing a cheap approximate solution within a *fixed computational time*. Since shortening the time step reduces the distance between neighboring problems, this approach also tends to reduce the approximation (manifold tracking) error. These strategies are particularly attractive for systems with fast dynamics. However, an important issue is to ensure that the tracking error will remain stable.

Approximate strategies such as real-time iterations and continuation schemes have been studied previously in the context of model predictive control and state estimation. These strategies solve a single Newton-type step at each sampling time [21, 27, 9, 10, 26, 25]. In the real-time iteration strategy reported in [9, 10], the model is used to predict the data (e.g., states) at the next step, and a perturbed quadratic optimization (QO) problem is solved once the true data becomes available. In the absence of inequality constraints, the perturbed QO reduces to a perturbed Newton step obtained from the solution of a linear system. It has been demonstrated that, by computing a single Newton step per time step, the tracking error remains bounded to second order with respect to the error between the predicted and the actual data. In order to prove this result, a specialized discrete-time, shrinking-horizon control setting was used [10]. In [12], conditions for closed-loop stability of receding-horizon control were derived in the presence of approximation errors. A limitation of these analyzes is that the impact of the size of the time step gets lost and it is thus difficult to analyze behavior as $\Delta t \rightarrow 0$. In addition, the results cannot be applied directly in other applications. Furthermore, no error bounds have been provided for the case in which non smoothness effects are present along the manifold due to the presence of inequality constraints.

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The continuation scheme reported in [26, 25] is a manifold tracking strategy in which the optimality conditions of the NLO are formulated as a differential equation. This permits a detailed numerical analysis of the tracking error as a function of the size of the time step. Sufficient conditions for the stability of the tracking error are derived. However, no order results are established. For implementation, the differential equation is linearized and discretized to derive the Newton step. The resulting linear system is solved approximately by using an iterative scheme such as generalized minimum-residual (GMRES) [32]. The use of an iterative linear solver is particularly attractive because it can be terminated early, as opposed to direct solvers. This is important in an on-line environment since it can significantly reduce the size of the time step. However, a limitation of continuation schemes is that inequality constraints need to be handled indirectly using smoothing techniques (e.g., barrier functions [26, 34, 11]) which can introduce numerical instability.

In this work, we present a framework for the analysis of on-line NLO strategies based on generalized equation (GE) concepts. Our results are divided in two parts. First, we demonstrate that if points along a solution manifold are consistently strongly regular, it is possible to track the manifold approximately by solving a single linear complementarity problem (LCP) per time step. We derive sufficient conditions that guarantee that the tracking error remains bounded to second order with the size of the time step, even if the LCP is solved only approximately. These results generalize the approximation results in [10, 26] in the sense that we consider both equality and inequality constraints, with the possibility of changing the active-set along the manifold. In particular, the proposed approach does not require any smoothing, which makes it numerically more robust. Second, we derive an approximation approach where the NLO is reformulated using an augmented Lagrangian function. This permits the use of a matrix-free, projected successive over-relaxation (PSOR) algorithm to solve the LCP at each sampling time [22, 20, 3, 23]. We demonstrate that PSOR is particularly efficient because it can perform linear algebra and active-set identification tasks efficiently.

The paper is structured as follows. In the next section, we review basic concepts of parametric NLO and generalized equations. In Section 4 we will establish general approximation results and derive stability conditions for the tracking error. In Section 5 we will specialize these to the context of nonlinear optimization. The augmented Lagrangian tracking algorithm and associated stability properties are presented in Section 6. A numerical case study is provided in Section 7. The paper closes with conclusions and directions of future work.

2. Motivation. In this work, we analyze parametric NLO problems of the form

$$\min f(x, t), \quad \text{s.t.} \quad c(x, t) = 0, \quad x \geq 0. \quad (2.1)$$

Here, $x \in \Re^n$ are the decision variables, $t \in \Re^n$ is a scalar parameter, and the mappings $f : \Omega \times T \rightarrow \Re$, $c : \Omega \times T \rightarrow \Re^m$ are assumed to be continuously differentiable from the open sets $\Omega \subseteq \Re^n$ and $T \subseteq \Re$. To simplify our discussion and, without loss of generality, we consider only the case where all components of x are subject to inequality constraints. The first-order optimality conditions of this problem are

$$\nabla_x \mathcal{L}(w, t) - \nu = 0, \quad c(x, t) = 0, \quad x^T \nu = 0, \quad x \geq 0, \quad \nu \geq 0. \quad (2.2)$$

The Lagrange function is defined as

$$\mathcal{L}(w, t) = f(x, t) + \lambda^T c(x, t), \quad (2.3)$$

where $\lambda \in \Re^m$ are Lagrange multipliers and $w^T = [x^T, \lambda^T]$. Equivalently, (2.2) can be formulated without introducing the multipliers $\nu \in \Re^n$ as:

$$x^T \nabla_x \mathcal{L}(w, t) \geq 0, \quad c(x, t) = 0, \quad x \geq 0. \quad (2.4)$$

The optimality conditions can be posed as a parametric generalized equation (GE) of the form,

$$0 \in \nabla_x \mathcal{L}(w, t) + \mathcal{N}_{\mathbb{R}_+^n}(x) \quad (2.5a)$$

$$0 \in c(x, t) + \mathcal{N}_{\mathbb{R}^m}(\lambda), \quad (2.5b)$$

where \mathbb{R}_+^n is the non-negativity orthant. Given sets K, W and Z , the multifunction $\mathcal{N}_K : W \rightarrow 2^Z$ is the normal cone operator,

$$\mathcal{N}_K(w) = \begin{cases} \{\nu \in W \mid (w - y)^T \nu \geq 0, \forall y \in K\} & \text{if } w \in K \\ \emptyset & \text{if } w \notin K. \end{cases} \quad (2.6)$$

The above notation is used to analyze the optimal conditions using geometric arguments. Parametric NLO problems arise in on-line optimization applications such as state and parameter estimation [29], model predictive control [6], signal processing [19], on-line economic optimization [18, 37], American options pricing [14], multi-body rigid dynamics [2], among others. The decision variables x usually represent controls and states of the dynamic *model* of a system while the time-dependent data (represented by t) are observations generated by the *real* system. For instance, in state estimation, the decision variables are the initial conditions of the model while the data represents observations to be fitted. In model predictive control and on-line economic optimization, the decision variables are the controls fed to the system while the data are the current states and incoming price and disturbance (e.g., weather) information.

Under certain regularity conditions (see Section 5), the solution of the parametric NLO forms a non-smooth and continuous manifold [15]. In this work, we are interested in establishing approximate algorithms to track the solution manifold of parametric NLOs close to real-time. This will enable higher frequency solutions (as desired in most applications) and the consideration of more detailed models, longer prediction horizons, and more decision variables. We emphasize that our results are general and try to capture the basic essence of different time-dependent applications. This comes at the expense of sacrificing details arising in specific domains such as model predictive control.

3. Generalized Equations. In this section, we use the notation from [30, 7]. The optimality conditions (2.5) can be posed as a parametric GE problem of the form: For a given $t \in T \subseteq \mathbb{R}$, find $w \in W \subseteq \mathbb{R}^n$ such that

$$0 \in F(w, t) + \mathcal{N}_K(w). \quad (3.1)$$

Here, $F : W \times T \rightarrow Z$ is a continuously differentiable mapping in both arguments with

$$F(w, t) = \begin{bmatrix} \nabla_x \mathcal{L}(w, t) \\ c(x, t) \end{bmatrix} \quad (3.2)$$

and $K = \mathbb{R}_+^n \times \mathbb{R}^m \subseteq W$ is a polyhedral convex set. We denote the solution of (3.1) as w_t^* . In addition, we define the derivative mapping $F_w(w, t) := \nabla_w F(w, t)$ and assume that it is Lipschitz in both arguments with constant L_{F_w} , $\forall w \in W, t \in T$. Our final goal is to create a discrete-time tracking scheme \bar{w}_{t_k} providing a cheap but stable *approximation* of the solution of (3.1), $w_{t_k}^*$. To achieve this, we will perform a single *truncated* Newton iteration for the *generalized equation* per time step.

3.1. The Nonlinear Equation Case. A good intuition as to why a truncated Newton scheme is sufficient to track the solution manifold can be easily explained by considering the case without inequality constraints or, equivalently, when $K = \Re^n$ and $F(w, t) = 0$. In this case, the optimality conditions reduce to a set of nonlinear equations. Consequently, standard calculus and standard calculus results can be used to establish error bounds and stability conditions for approximate tracking schemes. This approach has been followed in [10, 26]. In this section, we perform a simple and informal analysis in order to motivate the results of later sections. In the absence of inequality constraints, the approximate tracking scheme \bar{w}_{t_k} , $k > 0$ can be obtained from the recursive solution of the truncated *linear* Newton system:

$$r_\epsilon = F(\bar{w}_{t_k}, t_{k+1}) + F_w(\bar{w}_{t_k}, t_k)(\bar{w}_{t_{k+1}} - \bar{w}_{t_k}) \quad (3.3)$$

where r_ϵ is the solution residual satisfying $\|r_\epsilon\| \leq \kappa_\epsilon > 0$. Assume by now that the linearization point \bar{w}_{t_k} satisfies $\|\bar{w}_{t_k} - w_{t_k}^*\| \leq \kappa_r$ where $F(w_{t_k}^*, t_k) = 0$. In addition, we assume that the solution manifold is Lipschitz continuous (see Theorem 4.1) such that $\|w_{t_{k+1}}^* - w_{t_k}^*\| \leq L_w \Delta t$ with $\Delta t = t_{k+1} - t_k$ and $\kappa_r, L_w > 0$. We need to establish conditions leading to stability of the tracking error in the sense that:

$$\|\bar{w}_{t_k} - w_{t_k}^*\| \leq \kappa_r \Rightarrow \|\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*\| \leq \kappa_r.$$

From the mean value theorem we have that,

$$0 = F(w_{t_{k+1}}^*, t_{k+1}) = F(w_{t_k}^*, t_{k+1}) + \int_0^1 F_w \left(w_{t_k}^* + \chi(w_{t_{k+1}}^* - w_{t_k}^*), t_{k+1} \right) (w_{t_{k+1}}^* - w_{t_k}^*) d\chi \quad (3.4)$$

and,

$$F(w_{t_k}^*, t_{k+1}) = F(\bar{w}_{t_k}, t_{k+1}) + \int_0^1 F_w \left(\bar{w}_{t_k} + \chi(w_{t_k}^* - \bar{w}_{t_k}), t_{k+1} \right) (w_{t_k}^* - \bar{w}_{t_k}) d\chi. \quad (3.5)$$

Plugging (3.3) in (3.5),

$$\begin{aligned} F(w_{t_k}^*, t_{k+1}) &= r_\epsilon - F_w(\bar{w}_{t_k}, t_k)(\bar{w}_{t_{k+1}} - \bar{w}_{t_k}) \\ &\quad + \int_0^1 F_w \left(\bar{w}_{t_k} + \chi(w_{t_k}^* - \bar{w}_{t_k}), t_{k+1} \right) (w_{t_k}^* - \bar{w}_{t_k}) d\chi. \end{aligned} \quad (3.6)$$

From (3.6) and (3.4) we obtain,

$$\begin{aligned} &F_w(\bar{w}_{t_k}, t_k)(\bar{w}_{t_{k+1}} - \bar{w}_{t_k}) \\ &= r_\epsilon + \int_0^1 F_w \left(w_{t_k}^* + \chi(w_{t_{k+1}}^* - w_{t_k}^*), t_{k+1} \right) (w_{t_{k+1}}^* - w_{t_k}^*) d\chi \\ &\quad + \int_0^1 F_w \left(\bar{w}_{t_k} + \chi(w_{t_k}^* - \bar{w}_{t_k}), t_{k+1} \right) (w_{t_k}^* - \bar{w}_{t_k}) d\chi \\ &F_w(\bar{w}_{t_k}, t_k)(\bar{w}_{t_{k+1}} - w_{t_{k+1}}^* + w_{t_{k+1}}^* - w_{t_k}^* + w_{t_k}^* - \bar{w}_{t_k}) \\ &= r_\epsilon + \int_0^1 F_w \left(w_{t_k}^* + \chi(w_{t_{k+1}}^* - w_{t_k}^*), t_{k+1} \right) (w_{t_{k+1}}^* - w_{t_k}^*) d\chi \\ &\quad + \int_0^1 F_w \left(\bar{w}_{t_k} + \chi(w_{t_k}^* - \bar{w}_{t_k}), t_{k+1} \right) (w_{t_k}^* - \bar{w}_{t_k}) d\chi \end{aligned}$$

$$\begin{aligned}
& F_w(\bar{w}_{t_k}, t_k)(\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*) \\
&= r_\epsilon + \int_0^1 \left(F_w \left(w_{t_k}^* + \chi(w_{t_{k+1}}^* - w_{t_k}^*), t_{k+1} \right) - F_w(\bar{w}_{t_k}, t_k) \right) (w_{t_{k+1}}^* - w_{t_k}^*) d\chi \\
&\quad + \int_0^1 \left(F_w \left(\bar{w}_{t_k} + \chi(w_{t_k}^* - \bar{w}_{t_k}), t_{k+1} \right) - F_w(\bar{w}_{t_k}, t_k) \right) (w_{t_k}^* - \bar{w}_{t_k}) d\chi.
\end{aligned}$$

Bounding terms,

$$\begin{aligned}
& \|F_w(\bar{w}_{t_k}, t_k)\| \|\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*\| \\
&\leq \kappa_\epsilon + L_{F_w} \|w_{t_{k+1}}^* - w_{t_k}^*\| \int_0^1 \left(\|w_{t_k}^* - \bar{w}_{t_k}\| + \chi \|w_{t_{k+1}}^* - w_{t_k}^*\| + \Delta t \right) d\chi \\
&\quad + L_{F_w} \|w_{t_k}^* - \bar{w}_{t_k}\| \int_0^1 (\chi \|w_{t_k}^* - \bar{w}_{t_k}\| + \Delta t) \\
&\leq \kappa_\epsilon + L_{F_w} \|w_{t_{k+1}}^* - w_{t_k}^*\| \left(\|w_{t_k}^* - \bar{w}_{t_k}\| + \frac{1}{2} \|w_{t_{k+1}}^* - w_{t_k}^*\| + \Delta t \right) \\
&\quad + L_{F_w} \|w_{t_k}^* - \bar{w}_{t_k}\| \left(\frac{1}{2} \|w_{t_k}^* - \bar{w}_{t_k}\| + \Delta t \right).
\end{aligned}$$

Then,

$$\begin{aligned}
& \|F_w(\bar{w}_{t_k}, t_k)\| \|\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*\| \leq \kappa_\epsilon + L_{F_w} L_w \Delta t \left(\kappa_r + \frac{1}{2} L_w \Delta t + \Delta t \right) + L_{F_w} \kappa_r \left(\frac{1}{2} \kappa_r + \Delta t \right) \\
& \|\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*\| \leq \kappa_\psi \kappa_\epsilon + \kappa_\psi L_{F_w} L_w \Delta t \left(\kappa_r + \frac{1}{2} L_w \Delta t + \Delta t \right) \\
&\quad + \kappa_\psi L_{F_w} \kappa_r \left(\frac{1}{2} \kappa_r + \Delta t \right),
\end{aligned}$$

where $\kappa_\psi = \frac{1}{\|F_w(\bar{w}_{t_k}, t_k)\|}$. For stability we require $\|\bar{w}_{t_{k+1}} - w_{t_{k+1}}^*\| \leq \kappa_r$. This implies,

$$\kappa_r \geq \kappa_\psi \kappa_\epsilon + \kappa_\psi L_{F_w} L_w \Delta t \left(\kappa_r + \frac{1}{2} L_w \Delta t + \Delta t \right) + \kappa_\psi L_{F_w} \kappa_r \left(\frac{1}{2} \kappa_r + \Delta t \right).$$

Rearranging,

$$\left(1 - \frac{1}{2} L_{F_w} \kappa_\psi \kappa_r \right) \kappa_r \geq \kappa_\psi \kappa_\epsilon + \kappa_\psi L_{F_w} (L_w + 1) \Delta t \kappa_r + L_{F_w} \kappa_\psi L_w \left(\frac{1}{2} L_w + 1 \right) \Delta t^2.$$

Stability follows if $\left(1 - \frac{1}{2} L_{F_w} \kappa_\psi \kappa_r \right) > 0$ and if there exist $\kappa \geq 0$ and Δt satisfying,

$$\alpha_1^{NLE} \Delta t \kappa_r \leq \kappa \Delta t^2 \tag{3.7a}$$

$$\alpha_2^{NLE} \Delta t^2 + \kappa_\psi \kappa_\epsilon \leq \alpha_3^{NLE} \kappa_r, \tag{3.7b}$$

where $\alpha_1^{NLE}, \alpha_2^{NLE}, \alpha_3^{NLE}$ are defined in the Appendix A. At every time t_k , $\bar{w}_{t_{k+1}}$ is obtained by solving (4.2). This is an approximation of $w_{t_{k+1}}^*$. We have thus created an algorithm that tracks the solution manifold of $F(w, t) = 0$ by solving (within κ_ϵ) a single *truncated* Newton step per time step. This allows us to use iterative linear algebra algorithms that can be terminated early. Note that the above conditions guarantee that if, $\kappa_r, \kappa_\epsilon = O(\Delta t^2)$ then, the tracking error remains $O(\Delta t^2)$ for all $k > 0$.

Stability results can also be established for the more general case including inequality constraints (i.e., the cone K is not trivial), but this task is not straightforward. The difficulties, as pointed out in [10, 26], are technical and include the fact that, in the presence of inequality constraints, we cannot algebraically invert the Newton system. In particular, this enables to compute $\kappa_\psi = \frac{1}{\|F_w(\bar{w}_{t_k}, t_k)\|}$ explicitly. In addition, nonsmoothness effects prevent the direct application of standard calculus results. These are the difficulties we resolve in the following sections through the use of GE concepts.

3.2. Linearized Generalized Equations. An important consequence of the structure of (3.1) is that it allows us to analyze the smooth and nonsmooth components independently. With this, theoretical properties can be established as in the nonlinear equation case of Section 3.1. We start by defining the linearized generalized equation (LGE) at a given solution $w_{t_0}^*$,

$$r \in F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w - w_{t_0}^*) + \mathcal{N}_K(w) \quad (3.8)$$

If $K = \mathbb{R}_+^n$, solving the above LGE is equivalent to solving the perturbed linear complementarity problem,

$$w \geq 0, \quad \nu = F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)\Delta w - r \geq 0, \quad w^T \nu = 0. \quad (3.9)$$

If F_w is a symmetric matrix then (3.9) are, in turn, the optimality conditions of the quadratic optimization (QO) problem,

$$\min_{\Delta w \geq -w_{t_0}^*} \frac{1}{2} \Delta w^T F_w(w_{t_0}^*, t_0) \Delta w + F(w_{t_0}^*, t_0)^T \Delta w - r^T \Delta w. \quad (3.10)$$

We can rewrite (3.1) at any point (w, t) in the neighborhood of $w_{t_0}^*$ in terms of (3.8) by defining the *residual*,

$$r(w, t) = F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w - w_{t_0}^*) - F(w, t). \quad (3.11)$$

This gives, for any point satisfying (3.1),

$$r(w, t) \in F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w - w_{t_0}^*) + \mathcal{N}_K(w). \quad (3.12)$$

The above formulation will allow us to bound the distance between $(w_{t_0}^*, t_0)$ and neighboring points (w, t) in terms of $r(w, t)$.

Central to this study is the inverse operator $\psi^{-1} : Z \rightarrow W$ of the perturbed LGE (3.12) which we define as

$$w \in \psi^{-1}[r] \iff r \in F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w - w_{t_0}^*) + \mathcal{N}_K(w). \quad (3.13)$$

In other words, the operator is a multifunction from the space of the residual (perturbation) of the LGE to the space of the solution. Note that the operator ψ^{-1} and the residual $r(w, t)$ depend implicitly on the linearization point $w_{t_0}^*$. This dependence will be made clear from the context, so we will not carry it in the notation. Some basic properties arising from the definition of the inverse operator are as follows:

$$w_{t_0}^* \in \psi^{-1}[r(w_{t_0}^*, t_0)] = \psi^{-1}[0], \quad w_t^* \in \psi^{-1}[r(w_t^*, t)].$$

DEFINITION 3.1. (*Strong Regularity [30]*). *It is said that the GE (3.1) is strongly regular at $w_{t_0}^*$ in the sense of Robinson if there exists a neighborhood $V_W \subseteq W$ of $w_{t_0}^*$ and a neighborhood $V_Z \subseteq Z$ of $r(w_{t_0}^*, t_0) = 0$, such that for every $r \in V_Z$, (3.12) has a unique solution*

$w = \psi^{-1}[r] \in V_W$, and the inverse mapping $\psi^{-1} : V_Z \rightarrow V_W$ is Lipschitz with constant L_ψ . That is, for any $r_1, r_2 \in V_Z$,

$$\|\psi^{-1}[r_1] - \psi^{-1}[r_2]\| \leq L_\psi \|r_1 - r_2\|.$$

Establishing conditions for strong regularity consists of seeking properties of the derivative matrix $F_w(w_{t_0}^*, t_0)$ guaranteeing that ψ^{-1} becomes a single-valued function. To explain this, we consider the case $K = \mathbb{R}_+^n$. At a given solution $w_{t_0}^*$, system (3.12) will have three different components,

$$(\mathbf{M}w_{t_0}^* + \mathbf{b})_j = 0, \quad (w_{t_0}^*)_j > 0, \quad j = 1 : n_a, \quad (3.14a)$$

$$(\mathbf{M}w_{t_0}^* + \mathbf{b})_j = 0, \quad (w_{t_0}^*)_j = 0, \quad j = n_a + 1 : n_s + n_a, \quad (3.14b)$$

$$(\mathbf{M}w_{t_0}^* + \mathbf{b})_j > 0, \quad (w_{t_0}^*)_j = 0, \quad j = n_s + n_a + 1 : n, \quad (3.14c)$$

where $n = n_a + n_s + n_i$, $\mathbf{M} := F_w(w_{t_0}^*, t_0)$, and $\mathbf{b} := F(w_{t_0}^*, t_0) - \mathbf{M}w_{t_0}^*$. By eliminating the last n_i inactive components from the system, \mathbf{M} can be reduced to

$$\hat{\mathbf{M}} = \begin{bmatrix} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \mathbf{M}_{21} & \mathbf{M}_{22} \end{bmatrix}, \quad (3.15)$$

and (3.12) can be expressed in the reduced form

$$r \in \hat{\mathbf{M}}y + \hat{\mathbf{b}} + \mathcal{N}_{\mathbb{R}^{n_a} \times \mathbb{R}_+^{n_s}}(y), \quad (3.16)$$

where $y \in \mathbb{R}^{n_a+n_s}$ and $\hat{\mathbf{b}}^T = [\mathbf{b}_1^T \ \mathbf{b}_2^T]$.

PROPOSITION 3.2. (*Theorem 3.1 in [30]*). Consider the system (3.16) and the operator

$$\psi y := \hat{\mathbf{M}}y + \mathbf{b} + \mathcal{N}_{\mathbb{R}^{n_a} \times \mathbb{R}_+^{n_s}}(y).$$

Necessary and sufficient conditions for ψ^{-1} to be Lipschitzian are (i) \mathbf{M}_{11} is nonsingular and (ii) $\mathbf{M}_{22} - \mathbf{M}_{21}\mathbf{M}_{11}^{-1}\mathbf{M}_{12}$ have positive principal minors.

In Section 5, we will interpret these conditions in the context of parametric NLO.

4. Bounds and Stability of Approximation Error. Using this basic set of tools, we now establish results that will allow us to construct algorithms able to track the solution manifold of (3.1) approximately.

THEOREM 4.1. (*Theorem 2.3 in [30] and Theorem 3.3.4 in [15]*) Assume (3.1) is strongly regular at $w_{t_0}^*$. Then, there exist neighborhoods V_W and V_T and a unique and Lipschitz continuous solution $w_t^* \in V_W$ of the GE (3.1) that satisfies, for each $t = t_0 + \Delta t \in V_T$,

$$(i) \quad \|w_t^* - w_{t_0}^*\| \leq L_w \Delta t \quad (4.1)$$

with $L_w > 0$. In addition, consider that \bar{w}_t solves the truncated system,

$$\delta_\epsilon \in F(w_{t_0}^*, t) + F_w(w_{t_0}^*, t_0)(\bar{w}_t - w_{t_0}^*) + \mathcal{N}_K(\bar{w}_t) \quad (4.2)$$

where r_ϵ is the solution residual satisfying $\|r_\epsilon\| \leq \delta_\epsilon > 0$. We have that \bar{w}_t satisfies

$$(ii) \quad \|w_t^* - \bar{w}_t\| \leq L_\psi (\delta_\epsilon + \gamma(\Delta t)\Delta t),$$

with $\gamma(\Delta t) \rightarrow 0$ as $\Delta t \rightarrow 0$ and, if F_w is Lipschitz continuous then,

$$(iii) \quad \|w_t^* - \bar{w}_t\| \leq L_\psi (\delta_\epsilon + \kappa \Delta t^2)$$

with $\kappa > 0$.

Proof. Result (i) follows from strong regularity (Def. 3.1) and Lipschitz continuity of ψ^{-1} . This can be established under a fixed-point argument for sufficiently small Δt , as shown in Theorem 2.1 in [30] and Theorem 5.13 in [7]. Result (ii) follows from strong regularity (Def. 3.1), by noticing that the truncated system (4.2) is equivalent to (3.12) with $r = r_\epsilon + F(w_{t_0}^*, t_0) - F(w_{t_0}^*, t)$, and from the definition of the residual (3.11) for w_t^* . With this, we have

$$\begin{aligned} \|\bar{w}_t - w_t^*\| &\leq L_\psi \|r - r(w_t^*, t)\| \\ &\leq L_\psi \| (r_\epsilon + F(w_{t_0}^*, t_0) - F(w_{t_0}^*, t)) - (F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) - F(w_t^*, t)) \| \\ &\leq L_\psi \|r_\epsilon + F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) + F(w_t^*, t) - F(w_{t_0}^*, t)\|. \end{aligned}$$

From the mean value theorem we have

$$F(w_t^*, t) - F(w_{t_0}^*, t) = \int_0^1 F_w(w_{t_0}^* + \chi(w_t^* - w_{t_0}^*), t)(w_t^* - w_{t_0}^*) d\chi, \quad (4.3)$$

so we obtain, after replacing (4.3) in the preceding inequality, that

$$\begin{aligned} \|\bar{w}_t - w_t^*\| &\leq \delta_\epsilon + L_\psi \|w_t^* - w_{t_0}^*\| \int_0^1 \|F_w(w_{t_0}^*, t_0) - F_w(w_{t_0}^* + \chi(w_t^* - w_{t_0}^*), t)\| d\chi \\ &\stackrel{(i)}{\leq} L_\psi \delta_\epsilon + L_\psi L_w \Delta t \int_0^1 \|F_w(w_{t_0}^*, t_0) - F_w(w_{t_0}^* + \chi(w_t^* - w_{t_0}^*), t)\| d\chi \\ &\leq L_\psi (\delta_\epsilon + \gamma(\Delta t) \Delta t). \end{aligned}$$

Result (iii) is a consequence of the Lipschitz continuity of F_w ,

$$\begin{aligned} \|w_t^* - \bar{w}_t\| &\leq L_\psi \delta_\epsilon + L_\psi L_w \Delta t \int_0^1 \|F_w(w_{t_0}^*, t_0) - F_w(w_{t_0}^* + \chi(w_t^* - w_{t_0}^*), t)\| d\chi \\ &\leq L_\psi \delta_\epsilon + L_\psi L_w \Delta t \int_0^1 L_{F_w}(\chi \|w_t^* - w_{t_0}^*\| + \Delta t) d\chi \\ &\stackrel{(i)}{\leq} L_\psi \delta_\epsilon + L_\psi L_w \Delta t L_{F_w} \left(\frac{1}{2} L_w \Delta t + \Delta t \right) \\ &\leq L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2. \end{aligned}$$

The result follows with $\kappa = L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right)$. \square

Having a reference solution $w_{t_0}^*$, we can compute the approximate solution \bar{w}_t by solving the LCP (3.9) or the QO (3.10) with $r = F(w_{t_0}^*, t_0) - F(w_{t_0}^*, t)$. From Theorem 4.1, we see that this approximation can be expected to be close to the optimal solution w_t^* even in the presence of active-set changes. In our approximate algorithm, however, we relax the requirement that $w_{t_0}^*$ be available. Instead, we consider a linearization point \bar{w}_{t_0} located in the neighborhood

of $w_{t_0}^*$. In addition, we assume that the LCP is not solved exactly. In other words, \bar{w}_t is the solution of the truncated system,

$$r_\epsilon \in F(\bar{w}_{t_0}, t) + F_w(\bar{w}_{t_0}, t_0)(w - \bar{w}_{t_0}) + \mathcal{N}_K(w), \quad (4.4)$$

where $r_\epsilon \in \Re^n$ is the solution residual. This system can be posed in form (3.12) using the following definition:

$$r = r_\epsilon + F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(w - w_{t_0}^*) - F(\bar{w}_{t_0}, t) - F_w(\bar{w}_{t_0}, t_0)(w - \bar{w}_{t_0}). \quad (4.5)$$

Note that, in this case, the perturbation r is an implicit function of the solution $w = \bar{w}_t$. In addition, we emphasize that (4.5) is used only as an analytical tool. This is needed in order to use the strongly regular solution $w_{t_0}^*$ as the reference point and thus use the approximation results of Section 3. This is a key difference with the nonlinear equation case. In practice, however, (4.4) is solved. In the following theorem we establish stability conditions for the tracking error $\|\bar{w}_t - w_t^*\|$.

THEOREM 4.2. (Stability of Tracking Error). *Assume (3.1) is strongly regular at $w_{t_0}^*$. Define \bar{w}_t as the solution of the perturbed LGE (4.4) where \bar{w}_{t_0} is a point in the neighborhood V_W of $w_{t_0}^*$. The associated residual $r(\bar{w}_{t_0}, t_0)$ is assumed to satisfy*

$$\|r(\bar{w}_{t_0}, t_0) - r(w_{t_0}^*, t_0)\| \leq \delta_r,$$

with $\delta_r > 0$. Assume there exists $\delta_\epsilon > 0$ such that $\|r_\epsilon\| \leq \delta_\epsilon$. If there exists $\kappa > 0$ and if Δt satisfies

$$\alpha_1^{GE} \Delta t \delta_r \leq \kappa \Delta t^2 \quad (4.6a)$$

$$(\alpha_2^{GE} + \kappa) \Delta t^2 + \delta_\epsilon \leq \alpha_3^{GE} \delta_r, \quad (4.6b)$$

with α_1^{GE} , α_2^{GE} and α_3^{GE} defined in Appendix A; then the tracking error remains stable:

$$\|\bar{w}_{t_0} - w_{t_0}^*\| \leq L_\psi \delta_r \Rightarrow \|\bar{w}_t - w_t^*\| \leq L_\psi \delta_r.$$

Proof. To bound $\|\bar{w}_t - w_t^*\|$ we need to bound the distance between the associated residuals. From (4.5) and (3.11) we have

$$\begin{aligned} r - r(w_t^*, t) &= r_\epsilon + F(w_{t_0}^*, t_0) + F_w(w_{t_0}^*, t_0)(\bar{w}_t - w_{t_0}^*) - F(\bar{w}_{t_0}, t) - F_w(\bar{w}_{t_0}, t_0)(\bar{w}_t - \bar{w}_{t_0}) \\ &\quad - F(w_{t_0}^*, t_0) - F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) + F(w_t^*, t) \\ &= r_\epsilon + F_w(w_{t_0}^*, t_0)(\bar{w}_t - w_{t_0}^*) - F(\bar{w}_{t_0}, t) - F_w(\bar{w}_{t_0}, t_0)(\bar{w}_t - \bar{w}_{t_0}) \\ &\quad - F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) + F(w_t^*, t) \\ &= r_\epsilon + F(w_t^*, t) - F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) - F(w_{t_0}^*, t) \\ &\quad + F(w_{t_0}^*, t) - F_w(\bar{w}_{t_0}, t_0)(w_{t_0}^* - \bar{w}_{t_0}) - F(\bar{w}_{t_0}, t) \\ &\quad + F_w(w_{t_0}^*, t_0)(\bar{w}_t - w_t^* + w_t^* - w_{t_0}^*) - F_w(\bar{w}_{t_0}, t_0)(\bar{w}_t - w_t^* + w_t^* - w_{t_0}^*). \end{aligned}$$

Bounding,

$$\begin{aligned}
& \|F(w_t^*, t) - F_w(w_{t_0}^*, t_0)(w_t^* - w_{t_0}^*) - F(w_{t_0}^*, t)\| \\
& \leq L_w \Delta t \int_0^1 \|F_w(w_{t_0}^* + \chi(w_t^* - w_{t_0}^*), t) - F_w(w_{t_0}^*, t_0)\| d\chi \\
& \leq L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2 \\
& \|F(w_{t_0}^*, t) - F_w(\bar{w}_{t_0}, t_0)(w_{t_0}^* - \bar{w}_{t_0}) - F(\bar{w}_{t_0}, t)\| \\
& \leq \|w_{t_0}^* - \bar{w}_{t_0}\| \int_0^1 \|F_w(\bar{w}_{t_0} + \chi(w_{t_0}^* - \bar{w}_{t_0}), t) - F_w(\bar{w}_{t_0}, t_0)\| d\chi \\
& \leq L_{F_w} \left(\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t \right).
\end{aligned}$$

We also have $\|r_\epsilon\| \leq \delta_\epsilon$. The remaining terms can be bounded as follows:

$$\begin{aligned}
& \|F_w(w_{t_0}^*, t_0)(\bar{w}_t - w_t^* + w_t^* - w_{t_0}^*) - F_w(\bar{w}_{t_0}, t_0)(\bar{w}_t - w_t^* + w_t^* - w_{t_0}^*)\| \\
& \leq L_{F_w} \|w_{t_0}^* - \bar{w}_{t_0}\| (\|\bar{w}_t - w_t^*\| + \|w_t^* - w_{t_0}^*\|) \\
& \leq L_{F_w} L_\psi \delta_r \|\bar{w}_t - w_t^*\| + L_{F_w} L_w L_\psi \delta_r \Delta t.
\end{aligned}$$

Merging terms, and moving all terms containing $\|\bar{w}_t - w_t^*\|$ to the left, we obtain

$$\begin{aligned}
& \|\bar{w}_t - w_t^*\| \leq L_\psi \|r - r(w_t^*, t)\| \\
& \leq L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2 + L_\psi L_{F_w} \left(\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t \right) \\
& \quad + L_\psi L_{F_w} L_\psi \delta_r \|\bar{w}_t - w_t^*\| + L_\psi L_{F_w} L_w L_\psi \delta_r \Delta t \\
& \implies \\
& \|\bar{w}_t - w_t^*\| \\
& \leq \frac{L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2 + L_\psi L_{F_w} \left(\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t \right) + L_\psi L_{F_w} L_w L_\psi \delta_r \Delta t}{1 - L_{F_w} L_\psi^2 \delta_r}.
\end{aligned}$$

To establish stability, we need to find conditions for Δt such that $\|\bar{w}_t - w_t^*\| \leq L_\psi \delta_r$. This implies,

$$L_\psi \delta_r \geq \frac{L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2 + L_\psi L_{F_w} \left(\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t \right) + L_\psi L_{F_w} L_w L_\psi \delta_r \Delta t}{1 - L_{F_w} L_\psi^2 \delta_r}.$$

Dividing through by L_ψ , multiplying with the denominator, and simplifying we have

$$\delta_r - \frac{3}{2} L_{F_w} L_\psi^2 \delta_r^2 \geq \delta_\epsilon + L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \Delta t^2 + L_{F_w} L_\psi (L_w + 1) \Delta t \delta_r.$$

This condition is satisfied if (4.6a)-(4.6b) and $1 - L_{F_w} L_\psi^2 \delta_r > 0$ hold. The proof is complete. \square

COROLLARY 4.3. *Assume conditions of Theorem 4.2 hold $\forall t_k \in [t_0, t_f]$. Then,*

$$\|\bar{w}_{t_k} - w_{t_k}^*\| \leq L_\psi \delta_r, \quad t_{k+1} = t_k + k \cdot \Delta t, \quad \forall k \leq \frac{t_f - t_0}{\Delta t}.$$

Discussion of Theorem 4.2. From Theorem 4.2, a condition for (4.6a)-(4.6b) to hold is that

$$\|r(\bar{w}_{t_k}, t_k) - r(w_{t_k}^*, t_k)\| = \|F(w_{t_k}^*, t_k) + F(w_{t_k}^*, t_k)(\bar{w}_{t_k} - w_{t_k}^*) - F(\bar{w}_{t_k}, t_k)\| \leq \delta_r, \quad (4.7)$$

where $r(w_{t_k}^*, t_k) = 0$. This condition gives a guideline for monitoring the progress of the algorithm. Condition (4.6a) can be satisfied for $\delta_r = o(\Delta t), O(\Delta t^2)$. Condition (4.6b) is stricter. If $\delta_r = o(\Delta t)$, this condition states that the solution error should be at least $\delta_\epsilon = o(\Delta t)$. The first term on the left-hand side represents the tracking error of \bar{w}_t if $w_{t_0}^*$ is used as linearization point. If we choose $\delta_r = O(\Delta t^2)$ at the initial point, and $\delta_\epsilon = O(\Delta t^2)$ at all subsequent iterations, there will exist κ such that for all Δt sufficiently small the tracking error is $O(\Delta t^2)$ as stated in Theorem 4.1. Note that a small L_ψ is beneficial because it relaxes both (4.6a) and (4.6b). As seen in Theorem 3.2, this Lipschitz constant can be related to the conditioning of the derivative matrix F_w .

We also note that the technique of proof for Theorem 4.2 is similar to the one concerning the geometrical infeasibility of a time-stepping method [1] for differential variational inequalities (DVI) [28]. Indeed, one can prove that the parameteric solution w_t^* satisfies a DVI. Nevertheless, the fact that the problem has no dynamics makes it easy to solve directly rather than casting it as a DVI.

5. On-Line nonlinear optimization. If we linearize the optimality conditions around a given solution $w_{t_0}^*$ we get,

$$0 \in \begin{bmatrix} H_{xx}(w_{t_0}^*, t_0) & J_x^T(x_{t_0}^*, t_0) & -\mathbb{I}_n \\ J_x(x_{t_0}^*, t_0) & \mathbb{I}_n \\ \mathbb{I}_n \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \\ \Delta \nu \end{bmatrix} + \begin{bmatrix} \nabla_x \mathcal{L}(w_{t_0}^*, t_0) - \nu_{t_0}^* \\ c(x_{t_0}^*, t_0) \\ x_{t_0}^* \end{bmatrix} + \begin{bmatrix} \mathcal{N}_{\mathbb{R}^n}(x) \\ \mathcal{N}_{\mathbb{R}^m}(\lambda) \\ \mathcal{N}_{\mathbb{R}_+^n}(\nu) \end{bmatrix}. \quad (5.1)$$

Here, $\Delta x := x - x_{t_0}^*$, $\Delta \lambda := \lambda - \lambda_{t_0}^*$, $\Delta \nu := \nu - \nu_{t_0}^*$, $J_x(x_{t_0}^*, t_0) := \nabla_x c(x_{t_0}^*, t_0)$, and $H_{xx}(w_{t_0}^*, t_0) := \nabla_{xx} \mathcal{L}(w_{t_0}^*, t_0)$. As shown in Section 3, to establish conditions for strong regularity, we eliminate the n_i components corresponding to the pair $(x_{t_0}^*)_j > 0, (\nu_{t_0}^*)_j = 0$. This gives a reduced matrix of the form

$$\left[\begin{array}{c|c} \mathbf{K}(w_{t_0}^*, t_0) & -\mathbb{E} \\ \hline \mathbb{E}^T & \end{array} \right] = \left[\begin{array}{ccc|c} H_{xx}(w_{t_0}^*, t_0) & J_x^T(x_{t_0}^*, t_0) & -\mathbb{I}_{n_a} & -\mathbb{I}_{n_s} \\ J_x(x_{t_0}^*, t_0) & \mathbb{I}_{n_a} & & \\ \hline \mathbb{I}_{n_a} & & & \mathbb{I}_{n_s} \end{array} \right], \quad (5.2)$$

where $\mathbb{E} = [\mathbb{I}_{n_s} | 0 | 0]$.

THEOREM 5.1. (*Strong Regularity of NLO - Theorem 4.1 in [30] and Theorem 6 in [13]*). Let $f(x, \cdot)$ and $c(x, \cdot)$ be functions from the open set $\Omega \in \mathbb{R}^n$ into \mathbb{R}, \mathbb{R}^m that are at least twice differentiable at a point $x_{t_0}^* \in \Omega$. Suppose that $w_{t_0}^*$ solves (2.5). If and only if, (i) for every nonzero vector $w \in \mathbb{R}^n$ satisfying $J_x(x_{t_0}^*, t_0)w = 0$, $\mathbb{I}_{n_a}w = 0$, one has $w^T H_{xx}(w_{t_0}^*, t_0)w > 0$, and (ii) $[J_x^T(x_{t_0}^*, t_0) | \mathbb{I}_{n_a} | \mathbb{I}_{n_s}]$ is full rank, then (5.1) is strongly regular at this point.

The conditions of Theorem 5.1 are the strong second-order conditions and the linear independence constraint qualification (LICQ) (Chapter 12 in [24]). As seen in Section 3, strong

regularity guarantees that there exist nonempty neighborhoods where the solution of the linearized GE is a Lipschitz continuous function of the data. A similar result has been obtained in [16] without resorting to GE results. In [31] it is shown that by weakening LICQ to the Mangasarian-Fromovitz constraint qualification (MFCQ), the Lipschitz continuity properties of the solution are lost (see discussion after Corollary 4.3 in [31]). The reason is that LICQ guarantees that the multifunction (2.5) becomes a single-valued function on a neighborhood of the solution (i.e., the multipliers are unique). Nevertheless, boundedness results still hold under MFCQ. We emphasize that strict complementarity slackness is not necessary to guarantee strong regularity. This property is crucial since, as t varies and the active-set change, points at which complementarity slackness does not hold will be encountered.

Consider the perturbed QO problem formed at $\bar{w}_{t_0}^T = [\bar{x}_{t_0}^T, \bar{\lambda}_{t_0}^T]$ in the neighborhood of $w_{t_0}^*$,

$$\min_{\Delta x \geq -\bar{x}_{t_0}} \nabla_x f(\bar{x}_{t_0}, t)^T \Delta x + \frac{1}{2} \Delta x^T H_{xx}(\bar{w}_{t_0}, t_0) \Delta x \quad (5.3a)$$

$$\text{s.t.} \quad c(\bar{x}_{t_0}, t) + J_x(\bar{x}_{t_0}, t_0) \Delta x = 0, \quad (5.3b)$$

where $\Delta x = x - \bar{x}_{t_0}$. Note the perturbation on the data $t_0 \leftarrow t$ in the equality constraints and in the gradient of the objective function. The solution of this problem is given by the step $\Delta \bar{w}_t$ toward w_t^* . The optimality conditions of this QO formulate an LGE of the form (4.4). Therefore, the results of Theorem 4.2 apply directly.

6. Augmented Lagrangian Strategy. The approximation results of the previous sections can be used to derive algorithms to track of the solution manifold of the NLO (2.1). For instance, as we have seen, solving a single QO (5.3) at each time step is sufficient. This property has been used in the context of model predictive control to derive fast solution algorithms [9, 26]. In our context, however, we assume that the QOs are large-scale and may contain many degrees of freedom and bounds. Therefore, it is crucial to have a fast solution strategy for the QO itself in order to keep Δt as small as possible. Here, we propose to reformulate the NLO using an augmented Lagrangian function and solve the underlying QO using a PSOR strategy. The justification of this approach is provided at the end of this section. To derive our strategy, we define the augmented Lagrangian function,

$$\mathcal{L}_A(x, \bar{\lambda}, t, \rho) = f(x, t) + \bar{\lambda}^T c(x, t) + \frac{\rho}{2} \|c(x, t)\|^2. \quad (6.1)$$

A strategy to solve the original NLO (2.1) consists of computing solutions of the augmented Lagrangian subproblem

$$\min_{x \geq 0} \mathcal{L}_A(x, \bar{\lambda}, t, \rho) \quad (6.2)$$

for a sequence of increasing ρ . In the following, we assume that the penalty parameter ρ is not updated but remains fixed to a sufficiently large value. Consequently, we drop from the notation any dependencies on this parameter. Note that the multipliers $\bar{\lambda}$ act as parameters of the augmented Lagrangian subproblem. The solution of the subproblem is defined as $x^*(\bar{\lambda}, t)$. The multipliers can be updated externally as

$$\bar{\lambda} \leftarrow \bar{\lambda} + \rho c(x^*(\bar{\lambda}, t), t). \quad (6.3)$$

We thus define the solution pair $x^*(\bar{\lambda}, t)$, $\Lambda^*(\bar{\lambda}, t) = \bar{\lambda} + \rho c(x^*(\bar{\lambda}, t), t)$. The first-order conditions of (6.2) can be posed as a GE of the form

$$0 \in \nabla_x \mathcal{L}_A(x, \bar{\lambda}, t) + \mathcal{N}_{\mathbb{R}_+^n}(x), \quad (6.4)$$

where

$$\nabla_x \mathcal{L}_A(x, \bar{\lambda}, t) = \nabla_x f(x, t) + (\bar{\lambda} + \rho c(x, t))^T \nabla_x c(x, t).$$

The linearized version of (6.4) defined at the NLO solution $x_{t_0}^*$, $\bar{\lambda} = \lambda_{t_0}^*$ is given by

$$r \in \nabla_x \mathcal{L}_A(x_{t_0}^*, \lambda_{t_0}^*, t_0) + \nabla_{xx} \mathcal{L}_A(x_{t_0}^*, \lambda_{t_0}^*, t_0)(x - x_{t_0}^*) + \mathcal{N}_{\mathbb{R}_+^n}(x) \quad (6.5)$$

for $r = 0$. To establish perturbation results for the augmented Lagrangian LGE in connection with those of the original NLO (2.1), we consider the following *equivalent* formulation of (6.4), proposed in [5]:

$$0 \in F(w, p(\bar{\lambda}), t) + \mathcal{N}_{\mathbb{R}_+^n \times \mathbb{R}^m}(w), \quad (6.6)$$

where

$$F(w, p(\bar{\lambda}), t) = \begin{bmatrix} \nabla_x f(x, t) + \Lambda^T \nabla_x c(x, t) \\ c(x, t) + p(\bar{\lambda}) + \frac{1}{\rho}(\lambda_{t_0}^* - \Lambda) \end{bmatrix}, \quad (6.7)$$

$w^T = [x^T \Lambda^T]$, and

$$p(\bar{\lambda}) = \frac{1}{\rho}(\bar{\lambda} - \lambda_{t_0}^*). \quad (6.8)$$

For $t = t_0$ and $\bar{\lambda} = \lambda_{t_0}^*$, we have $p(\bar{\lambda}) = 0$, $x^*(p(\bar{\lambda}), t) = x_{t_0}^*$, and $\Lambda^*(p(\bar{\lambda}), t) = \lambda_{t_0}^*$. The solution of GE (6.6) is denoted as $w^*(p(\bar{\lambda}), t)$. The linearized version of (6.6) at $w_{t_0}^*$ is

$$r \in F(w_{t_0}^*, 0, t_0) + F_w(w_{t_0}^*, 0, t_0)(w - w_{t_0}^*) + \mathcal{N}_{\mathbb{R}_+^n \times \mathbb{R}^m}(w), \quad (6.9)$$

where

$$F_w(w_{t_0}^*, 0, t_0) = \begin{bmatrix} \nabla_{xx} \mathcal{L}(w_{t_0}^*, t_0) & \nabla_x c(x_{t_0}^*, t_0) \\ \nabla_x^T c(x_{t_0}^*, t_0) & -\frac{1}{\rho} \mathbb{I}_m \end{bmatrix}. \quad (6.10)$$

After applying the reduction procedure of Section 3 to the derivative matrix (6.10) we can show that, for sufficiently large ρ , the reduced matrix satisfies conditions of Theorem 3.2 at a strongly regular solution $w_{t_0}^*$. The proof of this assertion is long and will be omitted here. It follows along the lines of the results of Section 5 and uses the results of Proposition 2.4 in [5]. In particular, one needs to show that the negative diagonal matrix in the bottom right-hand corner of (6.10) does not affect significantly the conditioning of the derivative matrix for sufficiently large ρ . Because of the equivalence between (6.4) and (6.6), the same can be argued for the Hessian matrix $\nabla_{xx} \mathcal{L}_A(x_{t_0}^*, \lambda_{t_0}^*, t_0)$. We emphasize that the reformulation (6.6) is considered only for theoretical purposes. In practice, (6.4) is solved.

We now establish the following approximation results in the context of the augmented Lagrangian framework.

LEMMA 6.1. *Assume (6.4) is strongly regular at $w_{t_0}^*$. Then, there exist neighborhoods V_W, V_T , and V_p where the solution of the augmented Lagrangian subproblem (6.2) satisfies, for each $t = t_0 + \Delta t \in V_T$, $p(\bar{\lambda}) \in V_p$,*

$$(i) \quad \|w^*(\bar{\lambda}, t) - w_{t_0}^*\| \leq \frac{L_w}{\rho} \|\bar{\lambda} - \lambda_{t_0}^*\| + L_w \Delta t. \quad (6.11)$$

Furthermore, consider the approximate solution $\bar{x}(\bar{\lambda}, t)$ obtained from the perturbed LGE (6.5) with

$$r = \nabla_x \mathcal{L}_A(x_{t_0}^*, \lambda_{t_0}^*, t_0) - \nabla_x \mathcal{L}_A(x_{t_0}^*, \bar{\lambda}, t), \quad (6.12)$$

and associated multiplier $\bar{\Lambda}(\bar{\lambda}, t) = \bar{\lambda} + \rho c(\bar{x}(\bar{\lambda}, t), t)$. The pair, denoted by $\bar{w}(\bar{\lambda}, t)$, satisfies

$$(ii) \quad \|\bar{w}(\bar{\lambda}, t) - w^*(\bar{\lambda}, t)\| = O\left(\left(\Delta t + \frac{1}{\rho}\|\bar{\lambda} - \lambda_{t_0}^*\|\right)^2\right). \quad (6.13)$$

Proof. The result follows from the equivalence between (6.4) and (6.6), by recalling that $p(\lambda_{t_0}^*) = 0$, $p(\bar{\lambda}) = \frac{1}{\rho}\|\bar{\lambda} - \lambda_{t_0}^*\|$, and by applying Theorem 4.1. \square

This result states that the solution of a perturbed augmented Lagrangian LGE formed at $w_{t_0}^*$ provides a second-order approximation of the subproblem solution $w^*(\bar{\lambda}, t)$. The impact of the multiplier error can be made arbitrarily small by fixing ρ to a sufficiently large value. Stability of the tracking error is established in the following theorem. Here, we relax the requirement of the availability of $w_{t_0}^*$. In addition, we establish conditions for the step size Δt and the penalty parameter ρ guaranteeing that, by solving a single augmented Lagrangian LGE per time step, the tracking error remains stable.

THEOREM 6.2. (Stability of Tracking Error for Augmented Lagrangian). Assume $w_{t_0}^*$ is a strongly regular solution of (6.5). Define $\bar{x}(\bar{\lambda}, t)$ as the solution of the LGE,

$$r_\epsilon \in \nabla_x \mathcal{L}_A(\bar{x}_{t_0}, \bar{\lambda}, t) + \nabla_{xx} \mathcal{L}_A(\bar{x}_{t_0}, \bar{\lambda}, t_0)(x - \bar{x}_{t_0}) + \mathcal{N}_{\mathbb{R}_+^n}(x), \quad (6.14)$$

with associated multiplier update $\bar{\Lambda}(\bar{\lambda}, t) = \bar{\lambda} + \rho c(\bar{x}(\bar{\lambda}, t), t)$. The pair is denoted by $\bar{w}(\bar{\lambda}, t)$. The reference linearization point $\bar{w}_{t_0}^T = [\bar{x}_{t_0}^T, \bar{\Lambda}_{t_0}^T]$ with $\bar{\Lambda}_{t_0} = \bar{\lambda} + \rho c(\bar{x}_{t_0}, t_0)$ is assumed to exist in the neighborhood V_W of $w_{t_0}^*$. The associated residual $r(\bar{w}_{t_0}, t_0)$ is assumed to satisfy $\|r(\bar{w}_{t_0}, t_0) - r(w_{t_0}^*, t_0)\| \leq \delta_r$ with $\delta_r > 0$. Furthermore, assume there exists $\delta_\epsilon > 0$ such that $\|r_\epsilon\| \leq \delta_\epsilon$. If there exists $\kappa > 0$, Δt and ρ satisfying

$$\alpha_1^{AL} \Delta t \delta_r + \frac{L_w}{\rho} \left(\delta_r + \frac{L_w}{L_\psi} \Delta t \right) \leq \kappa \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2 \quad (6.15a)$$

$$\alpha_2^{AL} \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2 + \delta_\epsilon \leq \alpha_3^{AL} \delta_r, \quad (6.15b)$$

where $\alpha_1^{AL}, \alpha_2^{AL}, \alpha_3^{AL}$ are defined in Appendix A; then the tracking error remains stable:

$$\|\bar{w}_{t_0} - w_{t_0}^*\| \leq L_\psi \delta_r \Rightarrow \|\bar{w}(\bar{\lambda}, t) - w_t^*\| \leq L_\psi \delta_r.$$

Proof. Using the equivalence between (6.4) and (6.6), we have $\bar{w}(\bar{\lambda}, t) = \bar{w}(p(\bar{\lambda}), t)$. Consequently, we need to bound

$$\begin{aligned} \|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| &= \|\bar{w}(p(\bar{\lambda}), t) - w^*(p(\bar{\lambda}), t) + w^*(p(\bar{\lambda}), t) - w_t^*\| \\ &\leq \|\bar{w}(p(\bar{\lambda}), t) - w^*(p(\bar{\lambda}), t)\| + \|w^*(p(\bar{\lambda}), t) - w_t^*\|. \end{aligned} \quad (6.16)$$

The second term, the distance between the solution of the augmented Lagrangian subproblem $w^*(p(\bar{\lambda}), t)$ and the NLO solution w_t^* , can be bounded by using the Lipschitz continuity property,

$$\begin{aligned} \|w^*(p(\bar{\lambda}), t) - w_t^*\| &= \|w^*(p(\bar{\lambda}), t) - w^*(p(\lambda_t^*), t)\| \\ &\leq L_w \|p(\bar{\lambda}) - p(\lambda_t^*)\| \\ &\leq L_w \|p(\bar{\lambda})\| + L_w \|p(\lambda_t^*)\|. \end{aligned} \quad (6.17)$$

The distance between $w^*(p(\bar{\lambda}), t)$ and the approximate solution of the LGE (6.14) follows from the definition of strong regularity.

$$\|\bar{w}(p(\bar{\lambda}), t) - w^*(p(\bar{\lambda}), t)\| \leq L_\psi \|r - r(w^*(p(\bar{\lambda}), t), t)\|.$$

From the equivalence between (6.4) and (6.6) we have that solving (6.14) is equivalent to solving

$$r_\epsilon \in F(\bar{w}_{t_0}, p(\bar{\lambda}), t) + F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(w - \bar{w}_{t_0}) + \mathcal{N}_{\mathbb{R}_+^n \times \mathbb{R}^m}(w).$$

Consequently, the perturbation r associated to $\bar{w}(p(\bar{\lambda}), t)$ is given by

$$\begin{aligned} r = r_\epsilon + F(w_{t_0}^*, 0, t_0) + F_w(w_{t_0}^*, 0, t_0)(w - w_{t_0}^*) - F(\bar{w}_{t_0}, p(\bar{\lambda}), t) \\ - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(w - \bar{w}_{t_0}), \end{aligned}$$

with $w = \bar{w}(p(\bar{\lambda}), t)$. The residual $r(w^*(p(\bar{\lambda}), t), t)$ is obtained from (3.11). We proceed by parts. First we have

$$\begin{aligned} \mathbf{A} &= r - r(w^*(p(\bar{\lambda}), t)) \\ &= r_\epsilon + F(w_{t_0}^*, 0, t_0) + F_w(w_{t_0}^*, 0, t_0)(\bar{w}(p(\bar{\lambda}), t) - w_{t_0}^*) \\ &\quad - F(\bar{w}_{t_0}, p(\bar{\lambda}), t) - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(\bar{w}(p(\bar{\lambda}), t) - \bar{w}_{t_0}) \\ &\quad - F(w_{t_0}^*, 0, t_0) - F_w(w_{t_0}^*, 0, t_0)(w^*(p(\bar{\lambda}), t) - w_{t_0}^*) + F(w^*(p(\bar{\lambda}), t), p(\bar{\lambda}), t) \\ &= r_\epsilon + F(w^*(p(\bar{\lambda}), t), p(\bar{\lambda}), t) - F_w(w_{t_0}^*, 0, t_0)(w^*(p(\bar{\lambda}), t) - w_{t_0}^*) - F(w_{t_0}^*, p(\bar{\lambda}), t) \\ &\quad + F(w_{t_0}^*, p(\bar{\lambda}), t) - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(w_{t_0}^* - \bar{w}_{t_0}) - F(\bar{w}_{t_0}, p(\bar{\lambda}), t) \\ &\quad + F_w(w_{t_0}^*, 0, t_0)(\bar{w}(p(\bar{\lambda}), t) - w_t^* + w_t^* - w_{t_0}^*) \\ &\quad - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(\bar{w}(p(\bar{\lambda}), t) - w_t^* + w_t^* - w_{t_0}^*). \end{aligned}$$

We use the mean value theorem,

$$\begin{aligned} &F(w^*(p(\bar{\lambda}), t), p(\bar{\lambda}), t) - F(w_{t_0}^*, p(\bar{\lambda}), t) \\ &= \int_0^1 F_w(w_{t_0}^* + \chi(w^*(p(\bar{\lambda}), t) - w_{t_0}^*), p(\bar{\lambda}), t)(w^*(p(\bar{\lambda}), t) - w_{t_0}^*) d\chi, \end{aligned}$$

to compute the following bound:

$$\begin{aligned} \mathbf{B} &= \|F(w^*(p(\bar{\lambda}), t), p(\bar{\lambda}), t) - F_w(w_{t_0}^*, 0, t_0)(w^*(p(\bar{\lambda}), t) - w_{t_0}^*) - F(w_{t_0}^*, p(\bar{\lambda}), t)\| \\ &\leq \int_0^1 \|(F_w(w_{t_0}^* + \chi(w^*(p(\bar{\lambda}), t) - w_{t_0}^*), p(\bar{\lambda}), t) - F_w(w_{t_0}^*, 0, t_0))(w^*(p(\bar{\lambda}), t) - w_{t_0}^*)\| d\chi \\ &\leq \frac{1}{2} L_{F_w} L_w^2 (\|p(\bar{\lambda})\| + \Delta t)^2 + L_{F_w} L_w (\|p(\bar{\lambda})\| + \Delta t) (\|p(\bar{\lambda})\| + \Delta t) \\ &\leq L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) (\Delta t + \|p(\bar{\lambda})\|)^2. \end{aligned}$$

Similarly,

$$\begin{aligned} \mathbf{C} &= \|F(w_{t_0}^*, p(\bar{\lambda}), t) - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(w_{t_0}^* - \bar{w}_{t_0}) - F(\bar{w}_{t_0}, p(\bar{\lambda}), t)\| \\ &\leq \frac{1}{2} L_{F_w} \|\bar{w}_{t_0} - w_{t_0}^*\|^2 + L_{F_w} \|\bar{w}_{t_0} - w_{t_0}^*\| \Delta t \\ &\leq \frac{1}{2} L_{F_w} L_\psi^2 \delta_r^2 + L_{F_w} L_\psi \delta_r \Delta t. \end{aligned}$$

The remaining terms can be bounded as

$$\begin{aligned}\mathbf{D} &= \|F_w(w_{t_0}^*, 0, t_0)(\bar{w}(p(\bar{\lambda}), t) - w_t^* + w_t^* - w_{t_0}^*) \\ &\quad - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)(\bar{w}(p(\bar{\lambda}), t) - w_t^* + w_t^* - w_{t_0}^*)\| \\ &\leq \|F_w(w_{t_0}^*, 0, t_0) - F_w(\bar{w}_{t_0}, p(\bar{\lambda}), t_0)\| \|\bar{w}(p(\bar{\lambda}), t) - w_t^* + w_t^* - w_{t_0}^*\| \\ &\leq L_{F_w} (\|w_{t_0}^* - \bar{w}_{t_0}\| + \|p(\bar{\lambda})\|) (\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| + \|w_t^* - w_{t_0}^*\|) \\ &\leq L_{F_w} (L_\psi \delta_r + \|p(\bar{\lambda})\|) (\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| + L_w \Delta t).\end{aligned}$$

Using $\|r_\epsilon\| \leq \delta_\epsilon$ and merging terms \mathbf{B} , \mathbf{C} , and \mathbf{D} into \mathbf{A} , we obtain

$$\begin{aligned}\|\bar{w}(p(\bar{\lambda}), t) - w_t^*(p(\bar{\lambda}), t)\| &\leq L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) (\Delta t + \|p(\bar{\lambda})\|)^2 \\ &\quad + L_\psi \frac{1}{2} L_{F_w} L_\psi^2 \delta_r^2 + L_\psi L_{F_w} L_\psi \delta_r \Delta t \\ &\quad + L_\psi L_{F_w} (L_\psi \delta_r + L_\psi \|p(\bar{\lambda})\|) (\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| + L_w \Delta t).\end{aligned}\tag{6.18}$$

We substitute (6.17) and (6.18) in (6.16) and apply,

$$\begin{aligned}\|p(\bar{\lambda})\| &\leq \frac{1}{\rho} \|\bar{\lambda} - \lambda_{t_0}^*\| \leq \frac{L_\psi}{\rho} \|r(\bar{w}_{t_0}, t_0) - r(w_{t_0}^*, t_0)\| \leq \frac{L_\psi}{\rho} \delta_r \\ \|p(\lambda_t^*)\| &\leq \frac{1}{\rho} \|\lambda_t^* - \lambda_{t_0}^*\| \leq \frac{L_w}{\rho} \Delta t\end{aligned}\tag{6.19}$$

to obtain

$$\begin{aligned}\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| &\leq L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) (\Delta t + \|p(\bar{\lambda})\|)^2 \\ &\quad + L_\psi \frac{1}{2} L_{F_w} L_\psi^2 \delta_r^2 + L_\psi L_{F_w} L_\psi \delta_r \Delta t \\ &\quad + L_\psi L_{F_w} (L_\psi \delta_r + L_\psi \|p(\bar{\lambda})\|) (\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| + L_w \Delta t) \\ &\quad + L_w \|p(\bar{\lambda})\| + L_w \|p(\lambda_t^*)\| \\ &\leq L_\psi \delta_\epsilon + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2 \\ &\quad + \frac{1}{2} L_\psi L_{F_w} L_\psi^2 \delta_r^2 + L_\psi L_{F_w} L_\psi \delta_r \Delta t \\ &\quad + L_{F_w} L_\psi^2 \delta_r \left(1 + \frac{L_\psi}{\rho} \right) (\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| + L_w \Delta t) \\ &\quad + L_w \frac{L_\psi \delta_r}{\rho} + L_w^2 \frac{\Delta t}{\rho}.\end{aligned}$$

For stability we require $\|\bar{w}(p(\bar{\lambda}), t) - w_t^*\| \leq L_\psi \delta_r$. This implies

$$\begin{aligned}L_\psi \delta_r &\geq \frac{L_\psi \delta_\epsilon + \frac{L_w}{\rho} (L_\psi^2 \delta_r + L_w \Delta t) + L_\psi L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2}{1 - L_{F_w} L_\psi^2 \delta_r \left(1 + \frac{L_\psi}{\rho} \right)} \\ &\quad + \frac{L_\psi L_{F_w} (\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t) + L_{F_w} L_\psi^2 \delta_r \left(1 + \frac{L_\psi}{\rho} \right) L_w \Delta t}{1 - L_{F_w} L_\psi^2 \delta_r \left(1 + \frac{L_\psi}{\rho} \right)}.\end{aligned}$$

Dividing through by L_ψ and rearranging we have,

$$\begin{aligned}
& \delta_r - L_{F_w} L_\psi^2 \delta_r^2 \left(1 + \frac{L_\psi}{\rho} \right) \\
& \geq \delta_\epsilon + \frac{L_w}{\rho} \left(\delta_r + \frac{L_w}{L_\psi} \Delta t \right) + L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2 \\
& \quad + L_{F_w} \left(\frac{1}{2} L_\psi^2 \delta_r^2 + L_\psi \delta_r \Delta t \right) + L_{F_w} L_\psi L_w \delta_r \left(1 + \frac{L_\psi}{\rho} \right) \Delta t \\
& \delta_r - \left(\frac{3}{2} + \frac{L_\psi}{\rho} \right) L_{F_w} L_\psi^2 \delta_r^2 \\
& \geq \delta_\epsilon + L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) \left(\Delta t + \frac{L_\psi \delta_r}{\rho} \right)^2 \\
& \quad + L_{F_w} L_\psi \left(L_w \left(1 + \frac{L_\psi}{\rho} \right) + 1 \right) \delta_r \Delta t + \frac{L_w}{\rho} \left(\delta_r + \frac{L_w}{L_\psi} \Delta t \right).
\end{aligned}$$

This last condition is satisfied if (6.15a)-(6.15b) and $1 - L_{F_w} L_\psi^2 \delta_r \left(1 + \frac{L_\psi}{\rho} \right) > 0$ hold. The proof is complete. \square

Discussion of Theorem 6.2. The recursive stability result of Corollary 4.3 also applies in this context. Note that, if $\rho \rightarrow \infty$, conditions (6.15a)-(6.15b) reduce to (4.6a)-(4.6b). Therefore, similar order results to those of Theorem 4.2 can be expected for sufficiently large ρ . In particular, (6.15a) reduces to $\delta_r \leq \frac{\kappa}{L_{F_w} L_\psi (1+L_w)}$ which can give a condition for δ_r . The initial multiplier error (bounded by δ_r) always appears divided by ρ . This indicates that relatively large initial multiplier errors can be tolerated by increasing ρ . Nevertheless, note that the second term on the left hand side of (6.15a) remains $o(\Delta t)$ even if $\delta_r = O(\Delta t^2)$. In other words, this condition is more restrictive than (4.6a). This difficulty is related to the fact that the multiplier update is only first-order [5].

As a final remark, we point out that the stability conditions can be satisfied for fixed and sufficiently large κ as long as $\rho = O(\frac{1}{\Delta t})$ and $\delta_r = O(\Delta t^2)$. This has the side effect of having ρ effectively as a penalty parameter, a situation that resembles the use of a smoothing barrier function for inequalities and that may raise stability problems. While both penalizations arise in different contexts, an important question is whether the augmented Lagrangian penalization is more stable than that obtained by using smoothing penalty functions. In our scheme, the penalty parameter is *finite* for every fixed Δt , and the scheme is guaranteed to be stable. Stability results for continuation schemes incorporating smoothing functions are currently lacking. A simple numerical comparison will be presented in the next section.

In order to solve the QO associated to the LGE (6.14), we follow a PSOR approach. The QO has the form,

$$\min_{z \geq \alpha} \quad \frac{1}{2} z^T \mathbf{M} z + \mathbf{b}^T z. \quad (6.20)$$

Any solution of this QO solves the LCP,

$$\mathbf{M} z + \mathbf{b} \geq 0, \quad z - \alpha \geq 0, \quad (z - \alpha)^T (\mathbf{M} z + \mathbf{b}) = 0. \quad (6.21)$$

Consider the following PSOR algorithm adapted from [20, 22]:

PSOR Algorithm.

Given $z^0 \geq \alpha$, compute for $k = 0, 1, \dots, n_{iter}$,

$$\begin{aligned} z_i^{k+1} &= (1 - \omega)z_i^k - \frac{\omega}{\mathbf{M}_{ii}} \left(\sum_{j < i} \mathbf{M}_{ij} z_j^{k+1} + \sum_{j > i} \mathbf{M}_{ij} z_j^k - \mathbf{b}_i \right) \\ z_i^{k+1} &= \max(z_i^{k+1}, \alpha_i), \quad i = 1, \dots, n, \end{aligned} \quad (6.22)$$

where $\omega \in (0, 2)$ is the relaxation factor.

THEOREM 6.3. (*Theorem 2.1 in [22]*). *Let \mathbf{M} be symmetric positive definite. Then, each accumulation point of the sequence $\{z^k\}$ generated by (6.22) converges to a solution of the LCP (3.9). The rate of convergence is R-linear.*

Estimating the contraction rate for PSOR is difficult as it depends on the *optimal* choice of ω which is problem-dependent. However, it is known that, for the SOR method for linear systems, in order to reduce the error by a factor of $1/10$, SOR with non-optimal parameter ω requires $O(n)$ iterations, while with optimal ω only $O(n^{0.5})$ iterations are needed [20]. Here, $n = \dim(z)$. A suitable measure of progress of the PSOR algorithm is the projected gradient (or residual) $P_K(\mathbf{M}z + \mathbf{b})$, where $K := \{z \mid z \geq \alpha\}$ and

$$(P_K(g))_j = \begin{cases} \min\{0, g_j\} & \text{if } z_j = \alpha_j \\ g_j & \text{if } z_j > \alpha_j. \end{cases}$$

This is based on the fact that a solution of (6.20) satisfies $P_K(\mathbf{M}z + \mathbf{b}) = 0$. Similarly, the progress of the algorithm can be monitored by using the projected gradient of the augmented Lagrangian function $P_{\mathfrak{R}_+^n}(\nabla_x \mathcal{L}_A(\bar{x}_{t_k}, \bar{\lambda}_{t_k}, t_k, \rho))$. This is a more direct convergence check of (3.1), as opposed to (4.7). The computational complexity of PSOR is at most $O(n^2)$. We can now establish our tracking algorithm (2.1), which we refer to as AugLag:

AugLag Tracking Algorithm.

Given $\bar{x}_{t_0}, \bar{\lambda}_{t_0}, \Delta t, \rho, n_{iter}$,

1. Evaluate $\nabla_x \mathcal{L}_A(\bar{x}_{t_k}, \bar{\lambda}_{t_k}, t_{k+1}, \rho)$ and $\nabla_{xx} \mathcal{L}_A(\bar{x}_{t_k}, \bar{\lambda}_{t_k}, t_k, \rho)$.
2. Compute step $\Delta \bar{x}_{t_{k+1}}$ by applying n_{iter} PSOR iterations to (6.20) with:

$$\mathbf{M} = \nabla_{xx} \mathcal{L}_A(\bar{x}_{t_k}, \bar{\lambda}_{t_k}, t_k, \rho), \quad \mathbf{b} = \nabla_x \mathcal{L}_A(\bar{x}_{t_k}, \bar{\lambda}_{t_k}, t_{k+1}, \rho)$$

3. Update variables $\bar{x}_{t_{k+1}} = \bar{x}_{t_k} + \Delta \bar{x}_{t_{k+1}}$ and $\bar{\lambda}_{t_{k+1}} = \bar{\lambda}_{t_k} + \rho c(\bar{x}_{t_{k+1}}, t_{k+1})$.
4. Set $k \leftarrow k + 1$.

Justification of Augmented Lagrangian Framework. If the QO (5.3) is sparse, full-space active-set and interior-point solvers are the most efficient alternatives [4, 36]. In on-line applications, active-set strategies have been preferred because warm-start information can be used efficiently, as opposed to interior-point methods. However, the time per iteration in an interior-point solver tends to be smaller because the structure of the Karush-Kuhn-Tucker matrix is fixed and, consequently, symbolic factorizations need to be applied only once. In most active-set and interior-point implementations direct indefinite linear solvers are used to compute the search step. The accuracy of these steps is high. However, the computational overhead of a single factorization can be very high as well. As an alternative, one could consider the use of iterative linear solvers such as QMR, GMRES, or PCG in an interior-point framework [8]. A problem with this approach is that multiple linear systems still need to

be solved because of the barrier parameter update. This situation can be avoided by fixing the barrier parameter. However, as we will see in the next section, this approach is not very robust. Based on these observations, we argue that the AugLag strategy is attractive because: (i) the iteration matrix (Hessian of the augmented Lagrangian) remains at least positive semi-definite close to the solution manifold [5, 24], (ii) it performs linear algebra and active-set identification tasks simultaneously, (iii) it can exploit warm-start information, and (iv) it has a favorable computational complexity. We emphasize that achieving a high accuracy with PSOR might require a very large number of iterations. As demonstrated by Theorem 6.2, however, this does not represent an important limitation in an on-line setting.

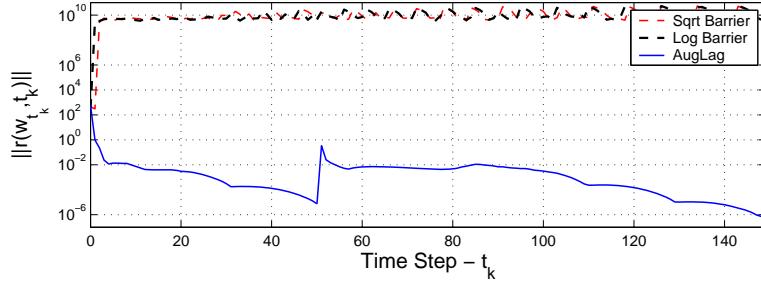
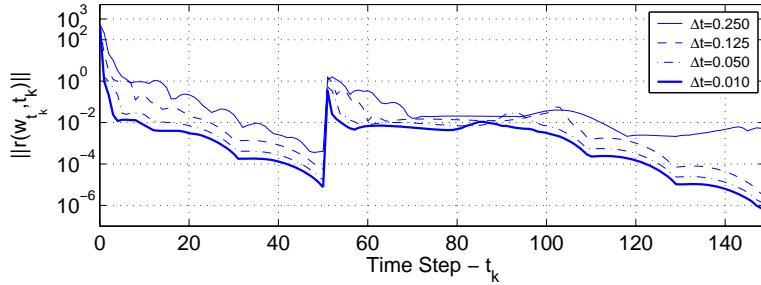
7. Numerical Example. To illustrate the developments, we consider the model predictive control of a nonlinear CSTR [17]. The optimal control formulation is given by

$$\begin{aligned} \min_{u(\tau)} & \int_t^{t+T} (w_T(z_T - z_T^{sp})^2 + w_C(z_C - z_C^{sp})^2 + w_u(u - u^{sp})^2) d\tau \\ \text{s.t. } & \frac{dz_C}{d\tau} = \frac{z_C - 1}{\theta} + k_0 \cdot z_C \cdot \exp\left[\frac{-E_a}{z_T}\right], \quad z_C(0) = \tilde{z}_C(t) \\ & \frac{dz_T}{d\tau} = \frac{z_T - z_T^f}{\theta} - k_0 \cdot z_C \cdot \exp\left[\frac{-E_a}{z_T}\right] + \alpha \cdot u \cdot (z_T - z_T^{cw}), \quad z_T(0) = \tilde{z}_T(t) \\ & z_C^{\min} \leq z_C \leq z_C^{\max}, \quad z_T^{\min} \leq z_T \leq z_T^{\max}, \quad u^{\min} \leq u \leq u^{\max}. \end{aligned}$$

The system involves two states, $z(\tau) = [z_C(\tau), z_T(\tau)]$, corresponding to dimensionless concentration and temperature, and one control, $u(\tau)$, corresponding to the cooling water flow rate. The model parameters are $z_T^{cw} = 0.38$, $z_T^f = 0.395$, $E_a = 5$, $\alpha = 1.95 \times 10^4$, $\theta = 20$, $k_0 = 300$, $w_C = 1 \times 10^6$, $w_T = 1 \times 10^3$, and $w_u = 1 \times 10^{-3}$. The bounds are set to $z_C^{\min} = 0$, $z_C^{\max} = 0.5$, $z_T^{\min} = 0.5$, $z_T^{\max} = 1.0$, $u^{\min} = 0.25$, and $u^{\max} = 0.45$. The set-points are denoted by the superscript sp . The *model* time dimension is denoted by τ , and the *real* time dimension is denoted by t . Accordingly, the moving horizon is defined as $\tau \in [t, t+T]$. For implementation, the optimal control problem is converted into an NLO of the form in (2.1) by applying an implicit Euler discretization scheme with $N = 100$ grid points and $\Delta\tau = 0.25$. The NLO is parametric in the initial conditions, which are implicit functions of t . The initial conditions are denoted by $\tilde{z}_T(t)$ and $\tilde{z}_C(t)$. Note that these states do not match the states predicted by the model (due to the use of a different discretization mesh). To apply the AugLag tracking algorithm, we define a simulation horizon $t \in [t_0, t_f]$ which is divided into N_s points with states $z(t_k)$, $k = 0, \dots, N_s$ and $\Delta t = t_{k+1} - t_k$. We set the augmented Lagrangian penalty parameter to $\rho = 100$. To solve the augmented Lagrangian QO at each step, we fix the number of PSOR iterations to 25. To illustrate the effectiveness of handling non smoothness effects with projection, we compare the performance AugLag with two continuation algorithms incorporating different smoothing barrier functions. The first algorithm (Log Barrier) eliminates the equality constraints with an augmented Lagrangian penalty and smooths out the inequality constraints by using terms of the form $\mu \cdot \log(x - x^{\min}) + \mu \cdot \log(x^{\max} - x)$, $\mu = 1.0$ [34, 33]. The second algorithm (Sqrt Barrier) also used an augmented Lagrangian penalty but incorporates smoothing terms of the form $\mu \cdot \sqrt{x - x^{\min}} + \mu \cdot \sqrt{x^{\max} - x}$, $\mu = 100$ [26, 11]. To prevent indefiniteness of the barrier functions near the boundaries of the feasible region, we incorporate a fraction to the boundary rule of the form,

$$x = \min(\max(x, x^{\min} + \epsilon), x^{\max} - \epsilon), \quad \epsilon = 1 \times 10^{-3}.$$

We initialize the three algorithms by perturbing an initial solution $w_{t_0}^*$ as $\bar{w}_{t_0} \leftarrow w_{t_0}^* \cdot \delta_w$ where $\delta_w > 0$ is a perturbation parameter. This perturbation generates the initial residual

FIG. 7.1. Residual trajectories for Barrier and AugLag continuation algorithms with $\delta_w = 1.25$.FIG. 7.2. Residual trajectories for AugLag with increasing Δt .

$r(\bar{w}_{t_0}, t_0)$. An additional perturbation, in the form of a set-point change, is introduced at $t_k = 50$. The residuals along the manifold $r(\bar{w}_{t_k}, t_k)$ are computed from (4.7). Log Barrier destabilizes at $\delta_w = 1.20$ while Sqrt Barrier destabilizes at $\delta_w = 1.25$. The errors accumulate and grow to $O(10^{10})$. The magnitude of the errors is due to the large magnitude of the Lagrange multipliers. AugLag remains stable in both cases, tolerating perturbations as large as $\delta_w = 5.0$. In Figure 7.1, we present the norm of the residuals along the simulation horizon with $\Delta t = 0.025$ and for an initial perturbation of $\delta_w = 1.25$. As can be seen, even if the initial residual is large, $O(10^2)$, AugLag remains stable. In addition, the use of smoothing functions introduces numerical instability. We now illustrate the effect of Δt on the residual of AugLag. Here, the initial residual is generated by using $\delta_w = 5.0$ and can go as high as $O(10^3)$. In Figure 7.2, note that the residual levels remain stable, implying that δ_r is at least $O(10^3)$. The set-point change generates a residual that is only $O(10^0)$ and can be tolerated with no problems. The PSOR residuals r_ϵ at the beginning of the horizon and at $t_k = 50$ are $O(10^{-1})$ and go down to $O(10^{-6})$ when the system reaches the set-points. In Figure 7.3, we present control and temperature profiles for $\Delta t = 0.25$ and $\Delta t = 0.01$. As expected, the tracking error decreases with the step size. We note that the PSOR strategy does a good job at identifying the active-set changes in subsequent steps. At a single step, up to 100 changes were observed. For the larger step size, note that even if the active-sets do not match, the residuals remain bounded and the system eventually converges to the optimal trajectories.

In our numerical experiments, the smoothing algorithms are able to tolerate relatively large initial perturbations, maintaining the residuals stable along the entire time horizon. However, the stability thresholds of smoothing approaches are smaller than that of the augmented Lagrangian approach with PSOR. The fixed logarithmic barrier function has been used in the model predictive control literature by Heath [34] and Boyd [33]. The problem

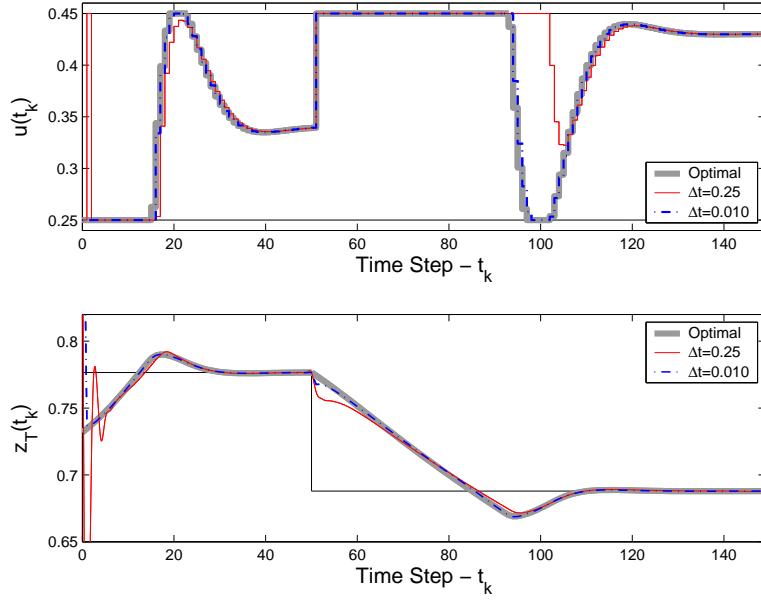


FIG. 7.3. *AugLag and optimal trajectories for the control (top) and temperature (bottom).*

with fixing the logarithmic barrier function is that, if an active-set change occurs, the Newton steps will tend to take the iterates outside of the feasible region (See Chapter 3 in [35]). In addition, the approximation of the logarithmic barrier function becomes poor, introducing large numerical errors. The results presented in [33] do not involve active-set changes while the results presented in [34] solve the NLO to optimality. This explains the good performance observed in those reports. The smoothing approach using squared root penalties is a variant of the original quadratic slacks relaxation approach discussed in [5, 26, 10]. In our numerical experiments we have observed that adding the squared root penalties directly into the objective (as opposed to relaxing the bounds with quadratic slacks [11]) gives much better performance. This is attributed to the fact that the first-order multiplier update is not efficient for the additional equality constraints.

8. Conclusions and Future Work. We have presented a framework for the analysis of parametric nonlinear optimization (NLO) problems based on generalized equation concepts. The framework allows us to derive approximate algorithms for on-line NLO. We demonstrate that if points along a solution manifold are consistently strongly regular, it is possible to track the manifold approximately by solving a single linear complementarity problem (LCP) per time step. We established sufficient conditions that guarantee that the tracking error remains bounded to second order with the size of the time step, even if the LCP is solved only to first-order accuracy. We present a tracking algorithm based on an augmented Lagrangian reformulation and a projected successive overrelaxation strategy to solve the LCPs. We demonstrate that the algorithm is able to identify multiple active-set changes and reduce the tracking errors efficiently. As part of our future work, we will establish a more rigorous comparison between the stability properties of the augmented Lagrangian penalization and of smoothing approaches. In addition, we are interested in exploring a strategy able to adapt the number of PSOR iterations (and thus the step size) along the manifold by monitoring the generalized equation residuals.

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Appendix A. Constants.

$$\alpha_1^{NLE} = L_{F_w} \kappa_\psi (L_w + 1) \quad (\text{A.1a})$$

$$\alpha_2^{NLE} = L_w L_{F_w} \kappa_\psi \left(\frac{1}{2} L_w + 1 \right) \quad (\text{A.1b})$$

$$\alpha_3^{NLE} = 1 - \frac{1}{2} L_{F_w} \kappa_\psi \kappa_r \quad (\text{A.1c})$$

$$\alpha_1^{GE} = L_{F_w} L_\psi (L_w + 1) \quad (\text{A.1d})$$

$$\alpha_2^{GE} = L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) + \kappa \quad (\text{A.1e})$$

$$\alpha_3^{GE} = 1 - \frac{3}{2} L_{F_w} L_\psi^2 \delta_r \quad (\text{A.1f})$$

$$\alpha_1^{AL} = L_{F_w} L_\psi \left(L_w \left(1 + \frac{L_\psi}{\rho} \right) + 1 \right) \quad (\text{A.1g})$$

$$\alpha_2^{AL} = L_w L_{F_w} \left(\frac{1}{2} L_w + 1 \right) + \kappa \quad (\text{A.1h})$$

$$\alpha_3^{AL} = 1 - \left(\frac{3}{2} + \frac{L_\psi}{\rho} \right) L_{F_w} L_\psi^2 \delta_r \quad (\text{A.1i})$$

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