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Filter-based Additional Constraints to Relax the Model Adequacy Conditions in Modifier Adaptation

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Abstract: Modifier adaptation (MA) is a real-time optimization (RTO) method with the built-in guarantee to reach the plant optimal operating conditions upon convergence despite disturbances and modeling uncertainties. MA requires a model that (i) is adequate, i.e., the reduced Hessian of the Lagrangian is positive definite at the plant optimum, and (ii) with the same inputs variable as the plant. In this paper, we consider the cases where (i) is not satisfied. The contribution of this article is to propose to merge two steps of the standard MA implementation, i.e., the model-based optimization and the filtering steps by the adding of constraints in the problem formulation. It is shown than the suggested addition of constraints does not require any additional assumption compared to standard MA, and that the resulting model adequacy conditions are less stringent. Indeed, strict convexity is only required for the cost function and therefore, there is no need for the convexification or linearisation of the contraints. The successful application and the advantages of this new method are illustrated by means of a standard benchmark case study for RTO algorithms and a numerical example.

Keywords: Real-time optimization, modifier adaptation, model adequacy.

1. INTRODUCTION

Industrial processes are operated via the manipulation of input variables. Process-optimization methods like (i) evolutionary techniques and (ii) model-based optimization, are methods of choice for their systematic manipulation with the potential to maximize performances and enforce the satisfaction of operational constraints. Methods of type (i) such as steepest-decent methods, heuristic search methods (such as the Nelder-Mead method (Conn et al., 2009)), or evolutionary optimization (Box and Draper, 1969) use past and current plant measurements for choosing the next set of inputs. Methods of type (ii) make an explicit use of a model of the plant and are thus more suited to complex and constrained optimization problems, when the number of inputs is large. However, the fact that the available models are often inaccurate generally leads to suboptimal operation and constraints violations.

Model-based real-time optimization (RTO) integrate both the model and measurements in the decision-making procedure. The most used RTO approach is undoubtedly the two-step approach (TS), i.e. repeated parameter estimation and optimization (Jang et al., 1987). At each iteration, measurements are used to refine the parameters of a first-principles model and the updated model is used for the subsequent model-based optimization. This approach, however, is prone to not converge to the plant optimal inputs in the presence of structural plant-model mismatch (Tatjewski, 2002), unless stringent model adequacy conditions are met (Forbes et al., 1994).

On the other hand, modifier-adaptation (MA) has the mathematically proven ability to reach the plant optimum upon convergence despite structural model mismatch (Tatjewski, 2002; Gao and Engell, 2005; Marchetti et al., 2009). With standard MA, the model is kept unchanged and measurements are used to build and add affine corrections to the cost and constraint functions, leading to a reconciliation of the conditions of optimality of the plant and of the modified model upon convergence.

Output modifier adaptation (MAy) suggests to incorporate these correction terms at the level of the input-output mapping (Marchetti et al., 2016), which induces simultaneous modifications of the modelled cost and constraints. This way, more corrections are brought to the optimization problem at no extra experimental cost (Papasavvas et al., 2018). Similarly to TS, MA and MAy require the satisfaction of model adequacy conditions (Marchetti et al., 2009), but these conditions are much easier to satisfy with MA since they reduce to the positive definiteness of the reduced Hessian of the Lagrangian function at the plant optimum. Indeed, these conditions can easily be enforced by the use of convex model approximations (François and Bonvin, 2013), or by the application of second order corrections, when measurements or estimates of the gradients and *Hessians* of the plant are accessible (Faulwasser and Bonvin, 2014) – which is unfortunately rarely the case.

This article proposes and discusses, at the methodological level, a new development of MAy that provides a new solution to the model adequacy issue. While MA suggests to add an exponential filter to the newly computed model-based optimal inputs before they are applied to the plant (or to the modifier terms before the optimisation problem is modified), it is proposed in this article to implement the input filter as a set of additional constraints to the problem formulation. This way, model-based feasibility is ensured at both the optimal and the filtered inputs. It is shown for the proposed improved MAy framework (KMAy) that (i) the Karush-Kuhn-Tucker (KKT) optimality conditions of the modified model matches the ones of the plant upon convergence, (ii) the model adequacy conditions are relaxed compared to MAy and (iii) no additional assumptions or measurements are required.

The paper is organized as follows. After a brief review of MAy in Section 2, the proposed extension to MAy is presented and analyzed in Section 3. Section 4 illustrates the successful application of KMAy for the optimization of a simulated Williams-Otto benchmark chemical reactor – with a model inadequate for MA and MAy – and to a numerical example. Finally, Section 5 concludes the paper.

2. REAL-TIME OPTIMIZATION VIA MODIFIER ADAPTATION

2.1 Optimization Problem

Hereafter, the subscript $(.)_p$ indicates a quantity related to the plant. The problem of finding the optimal operating conditions of the plant can be formulated mathematically as a nonlinear program (NLP):

$$\begin{aligned} \boldsymbol{u}_p^\star := \arg\min_{\boldsymbol{u}} \quad & \Phi_p(\boldsymbol{u}) := \phi(\boldsymbol{u}, \boldsymbol{y}_p(\boldsymbol{u})) \\ \text{s.t.} \quad & \boldsymbol{G}_p(\boldsymbol{u}) := \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{y}_p(\boldsymbol{u})) \leq \boldsymbol{0}, \end{aligned} \tag{2.1}$$

where $\boldsymbol{u} \in \mathbb{R}^{n_u}$ are the input variables, $\boldsymbol{y}_p \in \mathbb{R}^{n_y}$ are the measured outputs of the plant, $\phi \in \mathbb{R}$ is the cost function, and $\boldsymbol{g} \in \mathbb{R}^{n_g}$ is the vector of constraint functions. The optimal solution to Problem(2.1) is the plant optimum $\boldsymbol{u}_p^\star$.

Definition 1. Let $\mathcal{F}_p \subseteq \mathbb{R}^{n_u}$ denote the set of feasible inputs for the plant and $\mathcal{U} \subseteq \mathbb{R}^{n_u}$ denote the set of feasible inputs for the subset of known (i.e., not subject to plant-model mismatch) constraints functions. Note that $\mathcal{F}_p \subseteq \mathcal{U}$. The *known* constraints functions typically only depend of $\boldsymbol{u}$ and generally correspond to the lower ($\boldsymbol{u}^{\mathrm{L}}$) and upper bounds ($\boldsymbol{u}^{\mathrm{U}}$) on the inputs, i.e., $\mathcal{U} := \{\boldsymbol{u} \in \mathbb{R}^{n_u} \mid \boldsymbol{u}^{\mathrm{L}} \leq \boldsymbol{u} \leq \boldsymbol{u}^{\mathrm{U}}\}$ with $\boldsymbol{u}^{\mathrm{L}}$ and $\boldsymbol{u}^{\mathrm{U}}$.

Assumption 1. (Plant properties). Problem (2.1) is such that: (a) $\forall \boldsymbol{u} \in \mathcal{F}_p$, there are no steady-state output multiplicities, (b) Φ_p and $G_{i,p}$, $i = 1, ..., n_g$, are twice continuously differentiable ($\mathcal{C}^2$) on $\mathcal{F}_p$, (c) $\mathcal{F}_p$ is a non-empty compact set, (d) the linear independence constraint qualification (LICQ) holds $\forall \boldsymbol{u} \in \mathcal{F}_p$, and (e) ϕ and g_i, $i = 1, ..., n_g$, are known functions of $\boldsymbol{u}$ and $\boldsymbol{y}_p$.

In practice $\boldsymbol{y}_p(\boldsymbol{u})$ is not perfectly known, and only an approximate model of the input-output mapping $\boldsymbol{y}(\boldsymbol{u})$ is available. Using this model, the solution to Problem (2.1) can be approached by solving the following NLP:

$$\begin{aligned} \boldsymbol{u}^\star := \arg\min_{\boldsymbol{u}} \quad & \Phi(\boldsymbol{u}) := \phi(\boldsymbol{u}, \boldsymbol{y}(\boldsymbol{u})) \\ \text{s.t.} \quad & \boldsymbol{G}(\boldsymbol{u}) := \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{y}(\boldsymbol{u})) \leq \boldsymbol{0}. \end{aligned} \tag{2.2}$$

Due to plant-model mismatch $\boldsymbol{u}^\star$ does not generally match $\boldsymbol{u}_p^\star$, hence the need for RTO methods.

Assumption 2. (Model properties). The model is such that: (a) $\forall \boldsymbol{u} \in \mathcal{U}$, the steady-state nonlinear model equation $\boldsymbol{y}(\boldsymbol{u})$ has a unique solution and (b) Φ and $G_i, \forall i$, are twice continuously differentiable functions on $\mathcal{U}$.

2.2 Output Modifier Adaptation (MAy)

With MAy, the input-output mapping $\boldsymbol{y}(\boldsymbol{u})$ is modified by the addition of affine-in-input, measurement-based, correction terms, which leads to the simultaneous modification of the cost and constraints of Problem (2.2), while similar modifications are made directly (i.e. not through $\boldsymbol{y}(\boldsymbol{u})$) to the cost and constraint functions with standard MA. Still, it can be shown that the KKT matching property is preserved upon convergence (Papasavvas et al., 2018). For both MA and MAy, filtering the inputs (or the modifiers) is highly recommended to easier asymptotic convergence. Since this study is in essence methodological, we perform the following assumption:

Assumption 3. The output values and gradients are perfectly known for the plant at each RTO iteration. Note that perfect gradients of the cost and constraints for the plant are also required with MA or MAy for similar analyses.

The MAy algorithm, with input filtering, is summarized as follows:

Output Modifier Adaptation (MAy)

At the k^{th} iteration, $\boldsymbol{u}_k$ is applied to the plant until steady state is reached, and the modified output functions are constructed as follows:

$$y_{i,m,k}(\boldsymbol{u}) := y_i(\boldsymbol{u}) + \varepsilon_k^{y_i} + (\boldsymbol{\lambda}_k^{y_i})^{\mathsf{T}}(\boldsymbol{u} - \boldsymbol{u}_k), \tag{2.3}$$

where $\varepsilon_k^{y_i} \in \mathbb{R}$ and $\boldsymbol{\lambda}_k^{y_i} \in \mathbb{R}^{n_u}$ are the zeroth and first-order modifiers of the outputs. These modifiers are defined as follows:

$$\boldsymbol{\varepsilon}_k^{y_i} := y_{i,p}(\boldsymbol{u}_k) - y_i(\boldsymbol{u}_k), \tag{2.4}$$

$$\boldsymbol{\lambda}_k^{y_i} := \nabla_{\boldsymbol{u}} y_{i,p}|_{\boldsymbol{u}_k} - \nabla_{\boldsymbol{u}} y_i|_{\boldsymbol{u}_k}, \tag{2.5}$$

Note that estimates of the plant output gradients $\nabla_{\boldsymbol{u}} \boldsymbol{y}_p|_{\boldsymbol{u}_k}$ are used, while standard MA requires the cost and constraints gradients for the plant. Using the modified output functions (2.3), the cost and constraint functions at the k^{th} RTO iteration read:

$$\Phi_{\mathrm{MAy},k}(\boldsymbol{u}) := \phi(\boldsymbol{u}, \boldsymbol{y}_{m,k}(\boldsymbol{u})), \tag{2.6}$$

$$\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}) := \boldsymbol{g}(\boldsymbol{u}, \boldsymbol{y}_{m,k}(\boldsymbol{u})). \tag{2.7}$$

The following modified model-based optimization problem is then solved to determine the next optimal inputs:

$$\begin{aligned} \boldsymbol{u}_{k+1}^\star := \arg\min_{\boldsymbol{u}} \quad & \Phi_{\mathrm{MAy},k}(\boldsymbol{u}) \\ \text{s.t.} \quad & \boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}) \leq \boldsymbol{0}, \end{aligned} \tag{2.8}$$

The next operating point $\boldsymbol{u}_{k+1}$ is determined by applying a first-order filter:

$$\boldsymbol{u}_{k+1} = \boldsymbol{u}_k + \boldsymbol{K}(\boldsymbol{u}_{k+1}^\star - \boldsymbol{u}_k), \tag{2.9}$$

where $\boldsymbol{K} \in \mathbb{R}^{n_u \times n_u}$ is a gain matrix, typically diagonal, with diagonal elements $K_i \in (0, 1]$, $\forall i \in [1, n_g]$.

Remark 1. (KKT matching). Assumption 3 implies that:

$$\boldsymbol{y}_{m,k}(\boldsymbol{u}_k) = \boldsymbol{y}_p(\boldsymbol{u}_k), \quad \nabla_{\boldsymbol{u}} \boldsymbol{y}_{m,k}|_{\boldsymbol{u}_k} = \nabla_{\boldsymbol{u}} \boldsymbol{y}_p|_{\boldsymbol{u}_k}. \tag{2.10}$$

Together with Assumption 1, it follows straightforwardly that (Papasavvas et al., 2018):

$$X_{\mathrm{MAy},k}(\boldsymbol{u}_k) = X_p(\boldsymbol{u}_k), \;\; \nabla_{\boldsymbol{u}} X_{\mathrm{MAy},k}|_{\boldsymbol{u}_k} = \nabla_{\boldsymbol{u}} X_p|_{\boldsymbol{u}_k} \tag{2.11}$$

for $X := \{\Phi, G_i \text{ with } i = 1, ..., n_g\}$. All together, the fact that the KKT conditions of MAy upon convergence match those of the plant can be easily established (Papasavvas et al., 2018).

Remark 2. $\Phi_{\mathrm{MAy,k}}$ and $G_{i,\mathrm{MAy,k}}, \forall i$, are twice continuously differentiable since they are composed functions of Φ and $G_i, \forall i$, respectively (which are $\mathcal{C}^2$ from assumption 2)) with the linear function (2.3) (also $\mathcal{C}^2$).

3. FILTER-INSPIRED ADDITIONAL CONSTRAINTS FOR AN EASIER MODEL ADEQUACY SATISFACTION

3.1 Improved MAy (KMAy)

We propose to embed the filter (2.9) into problem (2.8) by duplicating the constraints $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u})$ and force the satisfaction of the constraints at $\boldsymbol{u}$ and $\boldsymbol{v}_k(\boldsymbol{u})$ simultaneously, where:

$$\boldsymbol{v}_k(\boldsymbol{u}) := (\boldsymbol{K})^{-1}(\boldsymbol{u}-\boldsymbol{u}_k)+\boldsymbol{u}_k \tag{3.1}$$

In other words, we force the constraints to be also satisfied at what would be the filtered point. Then, Problem (2.8) and equation (2.9) are replaced by the following NLP:

$$\boldsymbol{u}_{k+1} := \arg\min_{\boldsymbol{u}} \quad \Phi_{\mathrm{KMAy},k}(\boldsymbol{u}) := \Phi_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u})) \tag{3.2}$$

$$\text{s.t. } \boldsymbol{G}_{\mathrm{KMAy},k}(\boldsymbol{u}) := \begin{bmatrix} \boldsymbol{G}^{(1)}_{\mathrm{KMAy},k}(\boldsymbol{u}) := \boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u})) \\ \boldsymbol{G}^{(2)}_{\mathrm{KMAy},k}(\boldsymbol{u}) := \boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}) \end{bmatrix} \leq \boldsymbol{0}.$$

Adding constraints can change the properties of the model-based optimization problem. It is argued in the following lemmas that a simple choice for the matrix $\boldsymbol{K}$ ensures that it does not have any detrimental effect.

Lemma 1. The following properties hold $\forall k$:

(1) $\forall i \in [1, n_g]$ and $\forall k$, if $G_{i,p}(\boldsymbol{u}_k)$ is active (resp. inactive) at $\boldsymbol{u}_k$, so are the corresponding $G_{i,\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $G_{i,\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ and vice-versa.
(2) The cones of feasible directions[1] of $\boldsymbol{G}_p(\boldsymbol{u}_k)$ and $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ are identical. The same remark holds for their null spaces.
(3) Consider (3.1). If $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$, $\boldsymbol{I}_{n_u}$ being the $n_u \times n_u$ identity matrix and $K \in (0,1]$, then $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ share the same descent directions at any $\boldsymbol{u}_k$ – and the same null spaces. It follows that the cones of feasible directions of Problems (3.2) and (2.1) are identical at any $\boldsymbol{u}_k \in \mathcal{F}_p$.

Proof. First of all, it is worth noticing that:

$$\boldsymbol{v}_k(\boldsymbol{u}_k) = \boldsymbol{u}_k, \qquad \boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k)) = \boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k). \tag{3.3}$$

Property (1) results from Equation (3.3): the values of $\boldsymbol{G}_p(\boldsymbol{u}_k)$, $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ being the same so are their activities or inactivities. Property (2) results from Equation (2.11): since the gradients of $\boldsymbol{G}_p(\boldsymbol{u}_k)$ and $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ are the same, so are their respective descent directions (and thus the feasible directions for active constraints) and null spaces. Property (3) results from (3.3) and the chain rule:

$$\nabla_{\boldsymbol{u}} X_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}))\big|_{\boldsymbol{u}_k} = \nabla_{\boldsymbol{u}} X_{\mathrm{MAy},k}(\boldsymbol{u})\big|_{\boldsymbol{u}_k} \boldsymbol{K}^{-1}, \tag{3.4}$$

for $X := \{\Phi, G_i \text{ with } i = 1, ..., n_g\}$. Because $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$ and $K \in (0,1]$, $\boldsymbol{K}^{-1}$ exists. Thus, gradients are proportional and the null spaces and descent directions of each $G_{i,\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $G_{i,\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ taken individually are the same. Since from property (1), the values of i for which $G_{i,\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $G_{i,\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ are active are the same, $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ and $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$ have the same cones of feasible directions. Said differently, the cone of feasible directions for Problem (3.2) is defined by the constraints $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{u}_k)$ alone (as it is not affected by $\boldsymbol{G}_{\mathrm{MAy},k}(\boldsymbol{v}_k(\boldsymbol{u}_k))$) and matches therefore, according to property (2), the cone of feasible directions of (2.1) at any $\boldsymbol{u}_k \in \mathcal{F}_p$ □

Equation (3.4) also implies that LICQ cannot hold since the gradients of several constraints are proportional. Indeed, another constraint qualification holds:

Lemma 2. If the LICQ holds at any $\boldsymbol{u} \in \mathcal{F}_p$ for Problem (2.1), then the Mangasarian-Fromovitz constraint qualification (MFCQ) holds for the Problem (3.2) at $\boldsymbol{u}_k$, $\forall k$, provided $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$ and $K \in (0,1]$.

Proof. To prove that MFCQ holds, we need to show that there exists a direction $\boldsymbol{d} \in \mathbb{R}^{n_u}$ for each active constraint $G_{i,\mathrm{KMAy},k}$ at $\boldsymbol{u}_k$, such that $\nabla_{\boldsymbol{u}} G_{i,\mathrm{KMAy},k}|_{\boldsymbol{u}_k}^{\mathsf{T}} \boldsymbol{d} < 0$. Lemma 1 holds since $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$ and $K \in (0,1]$. Thus, $\forall k$, the cones of feasible directions for Problems (2.1) and (3.2) at $\boldsymbol{u}_k$ are identical. Since LICQ holds for Problem (2.1) $\forall \boldsymbol{u} \in \mathcal{F}_p$, its cone of feasible directions is never empty and MFCQ holds for Problem (3.2) at $\boldsymbol{u}_k$. □

Therefore, the standard LICQ assumption for the plant is sufficient to guarantee a constraint qualification at any $\boldsymbol{u}_k, \forall k$, and, thus, upon convergence and the proposed KMAy algorithm can now be stated:

Modifier Adaptation Updated (KMAy)

Initialization. Provide $\boldsymbol{u}_0$. Choose $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$ with $K \in (0,1]$.

for $k = 0 \to \infty$

(1) Apply the inputs $\boldsymbol{u}_k$ to the plant and wait for steady state.
(2) Measure the plant outputs to estimate the plant input-output mapping $\boldsymbol{y}_p(\boldsymbol{u}_k)$, and its gradient $\nabla_{\boldsymbol{u}}\boldsymbol{y}_p$ at $\boldsymbol{u}_k$. These estimates require data from perturbed operating points in the neighborhood of $\boldsymbol{u}_k$.
(3) Evaluate the modifiers (2.4)-(2.5).
(4) Compute $\boldsymbol{u}_{k+1}$ by solving Problem (3.2).

end

Hereafter, the convergence properties of KMAy are analyzed through two main theorems.

Theorem 1. (1st-order NCO matching upon convergence). If the input sequence $\{\boldsymbol{u}_k\}$ generated by KMAy converges to a limit value $\boldsymbol{u}_\infty = \lim_{k\to\infty} \boldsymbol{u}_k$ and if $\boldsymbol{K} = K\boldsymbol{I}_{n_u}$ with $K \in (0,1]$, then $\boldsymbol{u}_\infty$ is a KKT-point of Problem (2.1).

Proof. Since upon convergence, Problem (3.2) satisfies the MFCQ regularity condition, there exist KKT-multipliers $\boldsymbol{\mu} := [\boldsymbol{\mu}^{(1)\mathsf{T}}, \boldsymbol{\mu}^{(2)\mathsf{T}}]^{\mathsf{T}} \in \mathbb{R}^{2n_g}$ such that the KKT-conditions are satisfied at $\boldsymbol{u}_\infty$, i.e.,

$$\boldsymbol{G}_{\mathrm{KMAy},\infty}(\boldsymbol{u}_\infty) \leq \boldsymbol{0}, \tag{3.5}$$

$$\boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{G}_{\mathrm{KMAy},\infty}(\boldsymbol{u}_\infty) = 0, \tag{3.6}$$

$$\boldsymbol{\mu} \geq \boldsymbol{0}, \tag{3.7}$$

$$\nabla_{\boldsymbol{u}} \Phi_{\mathrm{KMAy},\infty}\big|_{\boldsymbol{u}_\infty} + \boldsymbol{\mu}^{\mathsf{T}} \nabla_{\boldsymbol{u}} \boldsymbol{G}_{\mathrm{KMAy},\infty}\big|_{\boldsymbol{u}_\infty} = \boldsymbol{0}. \tag{3.8}$$

[1] The cone of feasible directions of an active constraint G_i at a feasible point $\boldsymbol{u}_k$ is the set of vectors $\boldsymbol{d}$ such that $\nabla_{\boldsymbol{u}} G_i|_{\boldsymbol{u}_k}^{\mathsf{T}} \boldsymbol{d} < 0$.

From the definition of $\boldsymbol{G}_{\text{KMAy},k}$ and (3.4), equation (3.8) can be rewritten as:

$$\nabla_{\boldsymbol{u}}\Phi_{\text{MAy},\infty}|_{\boldsymbol{u}_\infty}+\left(\boldsymbol{\mu}^{(1)}+K\boldsymbol{\mu}^{(2)}\right)^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_{\text{MAy},\infty}|_{\boldsymbol{u}_\infty}=\mathbf{0}. \tag{3.9}$$

Equations (2.11), (3.3) and (3.4) holding at any k, they also hold upon convergence. From Equations (2.11) and (3.5), it follows that (i) $\boldsymbol{G}_p(\boldsymbol{u}_\infty)\leq\mathbf{0}$.

Noticing that $\boldsymbol{\mu}^{\mathsf{T}}\boldsymbol{G}_{\text{KMAy},\infty}(\boldsymbol{u}_\infty)=0$ implies both:

- ${\boldsymbol{\mu}^{(1)}}^{\mathsf{T}}\boldsymbol{G}_{\text{MAy},\infty}(\boldsymbol{u}_\infty)=0$, and
- ${\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\boldsymbol{G}_{\text{MAy},\infty}(\boldsymbol{v}_k(\boldsymbol{u}_\infty))={\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\boldsymbol{G}_{\text{MAy},\infty}(\boldsymbol{u}_\infty)=0.$

Multiplying the second equation by K, summing and regrouping leads to (iii):

$$\left({\boldsymbol{\mu}^{(1)}}^{\mathsf{T}}+K{\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\right)\boldsymbol{G}_{\text{MAy},\infty}(\boldsymbol{u}_\infty)=0$$

Defining (ii): $\boldsymbol{\mu}_p:=\boldsymbol{\mu}^{(1)}+K\boldsymbol{\mu}^{(2)}\geq\mathbf{0}$ and noticing that $\boldsymbol{G}_{\text{MAy},\infty}(\boldsymbol{u}_\infty)=\boldsymbol{G}_p(\boldsymbol{u}_\infty)$ yields (iii):

$$\boldsymbol{\mu}_p^{\mathsf{T}}\boldsymbol{G}_p(\boldsymbol{u}_\infty)=0$$

Finally combining (2.11), (3.9) and (ii) yields (iv):

$$\nabla_{\boldsymbol{u}}\Phi_p|_{\boldsymbol{u}_\infty}+\boldsymbol{\mu}_p^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_p|_{\boldsymbol{u}_\infty}=\mathbf{0}.$$

Writing down (i), (ii), (iii) and (iv) in matrix form yields:

$$\boldsymbol{G}_p(\boldsymbol{u}_\infty)\leq\mathbf{0}, \tag{3.10}$$
$$\boldsymbol{\mu}_p^{\mathsf{T}}\boldsymbol{G}_p(\boldsymbol{u}_\infty)=0, \tag{3.11}$$
$$\boldsymbol{\mu}_p\geq\mathbf{0} \tag{3.12}$$
$$\nabla_{\boldsymbol{u}}\Phi_p|_{\boldsymbol{u}_\infty}+\boldsymbol{\mu}_p^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_p|_{\boldsymbol{u}_\infty}=\mathbf{0}. \tag{3.13}$$

Equations (3.10) to (3.13) are indeed the KKT conditions for Problem (2.1), and therefore, we have shown that if $(\boldsymbol{u}_\infty,\boldsymbol{\mu})$ is a KKT-point of Problem (3.2), then $(\boldsymbol{u}_\infty,\boldsymbol{\mu}_p)$ is a KKT-point of Problem (2.1) with $\boldsymbol{\mu}_p:=\boldsymbol{\mu}^{(1)}+K\boldsymbol{\mu}^{(2)}$. □

Before moving to the second theorem, which discusses second-order properties, the following lemma is required.

Lemma 3. Let $\boldsymbol{A}\in\mathbb{R}^{n\times n}$ a positive definite matrix and $\boldsymbol{B}\in\mathbb{R}^{n\times n}$. Then, there always exists a scalar $K>0$, such that $\boldsymbol{A}+K\boldsymbol{B}$ is positive definite.

Proof. For any vector $\boldsymbol{d}\in\mathbb{R}^n$ and any matrix $\boldsymbol{X}\in\mathbb{R}^{n\times n}$:

$$\begin{aligned}\boldsymbol{d}^{\mathsf{T}}\boldsymbol{X}\boldsymbol{d}=\boldsymbol{d}^{\mathsf{T}}\boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{-1}\boldsymbol{d}&\geq\boldsymbol{d}^{\mathsf{T}}\boldsymbol{P}\boldsymbol{P}^{-1}\boldsymbol{d}\,\min\{\sigma(\boldsymbol{X})\}\\&\geq||\boldsymbol{d}||_2^2\min\{\sigma(\boldsymbol{X})\},\end{aligned} \tag{3.14}$$

where $\boldsymbol{P}$ and $\boldsymbol{D}$ are matrices of eigenvectors and eigenvalues of $\boldsymbol{X}$, respectively, and $\sigma(\boldsymbol{X})$ are the eigenvalues of $\boldsymbol{X}$. Applying (3.14) to the matrices $\boldsymbol{A}$ and $\boldsymbol{K}\boldsymbol{B}$, summing and rearranging, yields:

$$\boldsymbol{d}^{\mathsf{T}}\left(\boldsymbol{A}+K\boldsymbol{B}\right)\boldsymbol{d}\geq||\boldsymbol{d}||_2^2\left(\min\{\sigma(\boldsymbol{A})\}+K\min\{\sigma(\boldsymbol{B})\}\right). \tag{3.15}$$

$\boldsymbol{A}$ being positive definite, $\min\sigma(\boldsymbol{A})>0$ and $K>0$ can always be chosen small enough so that $\boldsymbol{A}+K\boldsymbol{B}>0$. □

Theorem 2. Consider Problem (2.8) modified at $\boldsymbol{u}_p^\star$ and denote $\boldsymbol{N}_{\text{MAy},\star}$ the null space of the strongly active constraints[2] of Problem (2.8) at $\boldsymbol{u}_p^\star$, with the subscript $\star$ denoting that modification is thought at $\boldsymbol{u}_p^\star$. If the reduced Hessian of the cost function of Problem (2.8) modified at $\boldsymbol{u}_p^\star$ is positive definite at $\boldsymbol{u}_p^\star$, i.e. if $\boldsymbol{N}_{\text{MAy},\star}^{\mathsf{T}}\nabla^2_{\boldsymbol{uu}}\Phi_{\text{MAy},\star}(\boldsymbol{u}))|_{\boldsymbol{u}_p^\star}\boldsymbol{N}_{\text{MAy},\star}>0$ (condition A), then there exists a filter $\boldsymbol{K}=K\boldsymbol{I}_{n_u}$, with $K\in(0,1]$ such that the second order sufficient conditions for optimality (SCO) of Problem (3.2) are satisfied at $\boldsymbol{u}_p^\star$.

Proof. According to the Theorem 20.3 in Chong and Zak (2001), a sufficient condition for $\boldsymbol{u}_p^\star$ to be a local optimum of Problem (3.2) is the existence of KKT-multipliers $\boldsymbol{\mu}:=[{\boldsymbol{\mu}^{(1)}}^{\mathsf{T}},{\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}]^{\mathsf{T}}\in\mathbb{R}^{2n_g}$ such that:

(i) $(\boldsymbol{u}_p^\star,\boldsymbol{\mu})$ is a KKT-point of the Problem (3.2) modified at $\boldsymbol{u}_p^\star$,

(ii) the reduced Hessian of the Lagrangian of the Problem (3.2) modified and evaluated at $\boldsymbol{u}_p^\star$ satisfies:

$$\boldsymbol{N}_{\text{KMAy},\star}^{\mathsf{T}}\nabla^2_{\boldsymbol{uu}}\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu})\big|_{\boldsymbol{u}_p^\star}\boldsymbol{N}_{\text{KMAy},\star}>0, \tag{3.16}$$

where $\boldsymbol{N}_{\text{KMAy},\star}$ is the null space the strongly active constraints for Problem (3.2) at $\boldsymbol{u}_p^\star$ and $\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu})$ is the Lagrangian of Problem (3.2), i.e. $\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu}):=\Phi_{\text{KMAy},\star}(\boldsymbol{u})+\boldsymbol{\mu}^{\mathsf{T}}\boldsymbol{G}_{\text{KMAy},\star}(\boldsymbol{u})$.

It is next shown that $(\boldsymbol{\mu}^{(1)},\boldsymbol{\mu}^{(2)}):=(\mathbf{0},\boldsymbol{\mu}_p/K)$ validates both conditions when K is appropriately chosen.

(i): Noticing that $\boldsymbol{u}_p^\star$ being a KKT point for the plant and applying (2.11) at $\boldsymbol{u}_p^\star$ leads to:

$$\boldsymbol{G}_p(\boldsymbol{u}_p^\star)\leq0\;\Rightarrow\;\boldsymbol{G}^{(1)}_{\text{KMAy},\star}(\boldsymbol{u}_p^\star)\leq0, \tag{3.17}$$
$$\boldsymbol{G}_p(\boldsymbol{u}_p^\star)\leq0\;\Rightarrow\;\boldsymbol{G}^{(2)}_{\text{KMAy},\star}(\boldsymbol{u}_p^\star)\leq0, \tag{3.18}$$
$$\boldsymbol{\mu}^{(1)}=0\;\Rightarrow\;{\boldsymbol{\mu}^{(1)}}^{\mathsf{T}}\boldsymbol{G}^{(1)}_{\text{KMAy},\star}(\boldsymbol{u}_p^\star)=0, \tag{3.19}$$
$$\boldsymbol{\mu}_p^{\mathsf{T}}\boldsymbol{G}_p(\boldsymbol{u}_p^\star)=0\;\Rightarrow\;{\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\boldsymbol{G}^{(2)}_{\text{KMAy},\star}(\boldsymbol{u}_p^\star)=0, \tag{3.20}$$
$$\boldsymbol{\mu}_p\geq0\;\Rightarrow\;\boldsymbol{\mu}\geq0. \tag{3.21}$$

From: (2.11) at $\boldsymbol{u}_p^\star$, $(\boldsymbol{\mu}^{(1)},\boldsymbol{\mu}^{(2)})=(\mathbf{0},\boldsymbol{\mu}_p/K)$, and(3.4), we have for the remaining KKT condition of Problem (2.1):

$$\nabla_{\boldsymbol{u}}\Phi_p|_{\boldsymbol{u}_p^\star}+\boldsymbol{\mu}_p^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_p|_{\boldsymbol{u}_p^\star}=\mathbf{0}$$
$$\nabla_{\boldsymbol{u}}\Phi_{\text{MAy},\star}|_{\boldsymbol{u}_p^\star}+\boldsymbol{\mu}_p^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_{\text{MAy},\star}\big|_{\boldsymbol{u}_p^\star}=\mathbf{0}$$
$$\nabla_{\boldsymbol{u}}\Phi_{\text{MAy},\star}|_{\boldsymbol{u}_p^\star}+{\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_{\text{MAy},\star}\big|_{\boldsymbol{u}_p^\star}=\mathbf{0}$$
$$K\,\nabla_{\boldsymbol{u}}\Phi_{\text{KMAy},\star}|_{\boldsymbol{u}_p^\star}+K{\boldsymbol{\mu}^{(2)}}^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}^{(2)}_{\text{KMAy},\star}\big|_{\boldsymbol{u}_p^\star}=\mathbf{0}$$

We can now add K times equation (3.19) to the left hand side, as it equals zero, regroup and divide by K to derive:

$$\nabla_{\boldsymbol{u}}\Phi_{\text{KMAy},\star}|_{\boldsymbol{u}_p^\star}+\boldsymbol{\mu}^{\mathsf{T}}\nabla_{\boldsymbol{u}}\boldsymbol{G}_{\text{KMAy},\star}|_{\boldsymbol{u}_p^\star}=\mathbf{0} \tag{3.22}$$

Implication (3.17) holds because $\boldsymbol{v}_\star(\boldsymbol{u}_p^\star):=(\boldsymbol{u}_p^\star-\boldsymbol{u}_p^\star)/K+\boldsymbol{u}_p^\star=\boldsymbol{u}_p^\star$, and from (3.3) $\boldsymbol{G}_{\text{MAy},\star}(\boldsymbol{v}_\star(\boldsymbol{u}_p^\star))=\boldsymbol{G}_{\text{MAy},\star}(\boldsymbol{u}_p^\star)$.

Equations (3.17)-(3.22) show that $(\boldsymbol{u}_p^\star,[\mathbf{0}^{\mathsf{T}},\boldsymbol{\mu}_p^{\mathsf{T}}/K]^{\mathsf{T}})$ is a KKT-point of the Problem (3.2), which concludes the first part of the proof.

(ii): From the definition of the Hessian, of the Lagrangian and since $\boldsymbol{\mu}^{(1)}=\mathbf{0}$, we have:

$$\nabla^2_{\boldsymbol{uu}}\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu})\big|_{\boldsymbol{u}_p^\star}=\nabla^2_{\boldsymbol{uu}}\Phi_{\text{KMAy},\star}\big|_{\boldsymbol{u}_p^\star}+\sum_{i=1}^{n_g}\left(\mu_i^{(2)}\nabla^2_{\boldsymbol{uu}}G^{(2)}_{i,\text{KMAy}}\big|_{\boldsymbol{u}_p^\star}\right)$$

[2] Strongly active constraints are such that their values are zero while their associated Lagrange multipliers are not.

Applying the chain rule twice leads to:

$$\nabla^2_{\boldsymbol{uu}}\Phi_{\text{MAy},\star}(\boldsymbol{v}_\star(\boldsymbol{u}))\big|_{\boldsymbol{u}_p^\star} = \nabla^2_{\boldsymbol{uu}}\Phi_{\text{MAy},\star}(\boldsymbol{u})\big|_{\boldsymbol{u}_p^\star} K^{-2}\boldsymbol{I}_{n_u}.$$

Thus,

$$\nabla^2_{\boldsymbol{uu}}\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu})\big|_{\boldsymbol{u}_p^\star} = K^{-2}\nabla^2_{\boldsymbol{uu}}\Phi_{\text{MAy},\star}\big|_{\boldsymbol{u}_p^\star} + \sum_{i=1}^{n_g}\left(\frac{\mu_{i,p}}{K}\nabla^2_{\boldsymbol{uu}}G_{i,\text{MAy}}\big|_{\boldsymbol{u}_p^\star}\right).$$

Multiplying both sides by $K^2\boldsymbol{N}_{\text{KMAy},\star}{}^{\mathsf{T}}(\cdot)\boldsymbol{N}_{\text{KMAy},\star}$, and noticing that $\boldsymbol{N}_{\text{KMAy},\star} = \boldsymbol{N}_{\text{MAy},\star} = \boldsymbol{N}_p$, where $\boldsymbol{N}_p$ is the nullspace of the active constraints for the plant at $\boldsymbol{u}_p^\star$, as discussed in Lemma 1, yields:

$$\begin{aligned} &K^2\boldsymbol{N}^{\mathsf{T}}_{\text{KMAy},\star}\nabla^2_{\boldsymbol{uu}}\mathcal{L}_{\text{KMAy},\star}(\boldsymbol{u},\boldsymbol{\mu})\big|_{\boldsymbol{u}_p^\star}\boldsymbol{N}_{\text{KMAy},\star} \\ &= \boldsymbol{N}^{\mathsf{T}}_{\text{KMAy},\star}\boldsymbol{A}\boldsymbol{N}_{\text{KMAy},\star} + K\boldsymbol{N}^{\mathsf{T}}_{\text{KMAy},\star}\boldsymbol{B}\boldsymbol{N}_{\text{KMAy},\star}, \\ &= \boldsymbol{N}^{\mathsf{T}}_{\text{MAy},\star}\boldsymbol{A}\boldsymbol{N}_{\text{MAy},\star} + K\boldsymbol{N}^{\mathsf{T}}_{\text{MAy},\star}\boldsymbol{B}\boldsymbol{N}_{\text{MAy},\star}, \end{aligned} \tag{3.23}$$

where the matrices $\boldsymbol{A} = \nabla^2_{\boldsymbol{uu}}\Phi_{\text{KMAy},\star}|_{\boldsymbol{u}_p^\star}$ and $\boldsymbol{B} = \sum_{i=1}^{n_g}(\mu_{i,p}\nabla^2_{\boldsymbol{uu}}G^{(2)}_{i,\text{KMAy}}|_{\boldsymbol{u}_p^\star})$ are introduced to keep the notations compact. The first term on the right-hand side of the bottom equation in (3.23) being positive definite by virtue of condition A, Lemma 3 applies and there always exist values for $K > 0$ such that $(3.23) > 0$. Thus, there exist values for $K > 0$ such that(3.16) holds. Also, since the functions $\Phi_{\text{MAy},\star}$ and $G_{i,\text{MAy},\star}, \forall i$, are $\mathcal{C}^2$ (Remark 2), the existence of $K > 0$ is ensured.

In summary: there always exist KKT-multipliers $\boldsymbol{\mu} \in \mathbb{R}^{2n_g}$, e.g., $\boldsymbol{\mu} := [\boldsymbol{\mu}^{(1)\mathsf{T}}, \boldsymbol{\mu}^{(2)\mathsf{T}}]^{\mathsf{T}} = [\boldsymbol{0}^{\mathsf{T}}, \boldsymbol{\mu}_p^{\mathsf{T}}/K]^{\mathsf{T}}$, such that conditions (i) and (ii) are met simultaneously at $\boldsymbol{u}_p^\star$, provided K is chosen small enough. Therefore, the conditions of Theorem 20.3 in Chong and Zak (2001) are met, which concludes the proof. □

Remark 3. Inspecting Theorem 2, it is clear that the model adequacy condition for KMAy is indeed condition A. It is interesting to note that this condition is on the cost function only and is therefore not the same as the model adequacy condition for MAy, which would be a similar condition on the Hessian of the Lagrangian (Marchetti et al., 2016) of the MAy problem. In other words, the model adequacy condition for KMAy is less restrictive than for MAy, thanks to the additional constraints and to the appropriate choice of the gain matrix $\boldsymbol{K}$.

4. ILLUSTRATIVE EXAMPLES

4.1 Williams-Otto Reactor

The standard benchmark case study for RTO considered is the continuous stirred-tank reactor of Williams and Otto (1960). Three following reactions take place (for the plant):

$$\text{A} + \text{B} \xrightarrow{k_{p,1}} \text{C}, \qquad k_{p,1} = A_{p,1}e^{-B_{p,1}/(T_R+273.15)} \tag{4.1}$$

$$\text{C} + \text{B} \xrightarrow{k_{p,2}} \text{P} + \text{E}, \qquad k_{p,2} = A_{p,2}e^{-B_{p,2}/(T_R+273.15)} \tag{4.2}$$

$$\text{P} + \text{C} \xrightarrow{k_{p,3}} \text{G}. \qquad k_{p,3} = A_{p,3}e^{-B_{p,3}/(T_R+273.15)}, \tag{4.3}$$

The reactants A and B are fed separately, with mass flowrates of F_A and F_B, respectively. P and E are the desired products, C is an intermediate product and G is an undesired by-product. The reactor is operated isothermally at a controlled temperature T_R. Steady-state mass balances can be found in Zhang and Forbes (2000). The optimization problem of (Marchetti et al., 2017) is considered, wherein the input variables are $\boldsymbol{u} = [F_A, F_B, T_R]^{\mathsf{T}}$ and the outputs are $\boldsymbol{y} = [X_E, X_P, X_G]^{\mathsf{T}}$ with X_i denoting the concentration of species i. There is significant plant-model mismatch since the available model only considers two reactions (Marchetti et al., 2017; Forbes et al., 1994). The objective is to maximize profit at steady-state, while satisfying an upper bound on X_G and input bounds:

$$\max_{\boldsymbol{u}} \quad \phi(\boldsymbol{u},\boldsymbol{y}) = (1143.38X_P + 25.92X_E)(F_A + F_B) - 76.23F_A - 114.34F_B \tag{4.4}$$

$$\text{s.t.} \quad g(\boldsymbol{y}) = X_G - 0.08 \le 0, \tag{4.5}$$

$$F_A \in [3,\ 4.5] \ \ (\text{kg/s}), \qquad F_B \in [6,\ 11] \ \ (\text{kg/s}), \qquad T_R \in [80,\ 105] \ \ (°\text{C}).$$

At the plant optimum $\boldsymbol{u}_p^\star = [3.887, 9.369, 91.2]^{\mathsf{T}}$, the constraint (4.5) is active.

MAc, MAy and KMAy are applied, starting from a quite conservative initial point $\boldsymbol{u}_0 = [3.5, 9, 90]^{\mathsf{T}}$, with two 2 different filters, $\boldsymbol{K} = 0.5\boldsymbol{I}_{n_u}$ and $\boldsymbol{K} = 0.8\boldsymbol{I}_{n_u}$. The simulation results are shown on Figures 1 and 2, respectively.

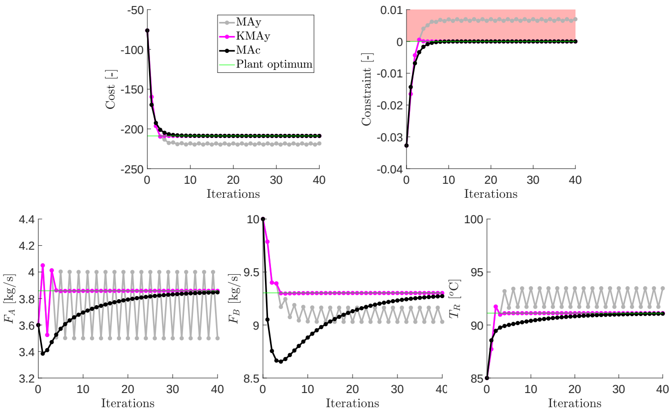

Fig. 1. Simulation results for $\boldsymbol{K} = 0.5\boldsymbol{I}_{n_u}$.

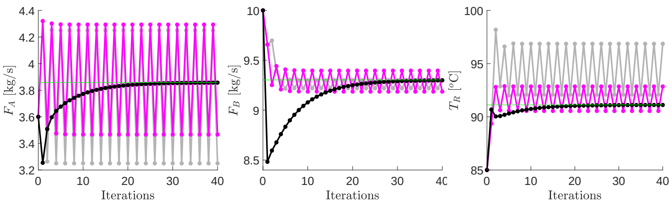

Fig. 2. Simulation results for $\boldsymbol{K} = 0.8\boldsymbol{I}_{n_u}$.

It is easy to verify (in simulation) that the model is not adequate for MAy. But it is also easy to check that condition A, i.e. the reduced Hessian of the modified model of the cost function is indeed positive definite at the plant optimum. Thus, we know that small enough values of K. e.g., $\boldsymbol{K} = 0.5\boldsymbol{I}_{n_u}$ enforce model adequacy for KMAy, which is confirmed in Figure 1. But, when K is chosen too high, e.g., $\boldsymbol{K} = 0.8\boldsymbol{I}_{n_u}$, model adequacy may not hold, as illustrated with the sustained oscillations of the inputs in Figure 2. Figure 1 also illustrates that KMAy has the potential to converge faster than MAc, with 4 vs. 40 iterations. This difference is certainly due to the linearization of the concave constraints with MAc, which results into a loss of accuracy and into of "spreading" of the concave constraints throughout the input space, affecting convergence rate even when the concave constraints are far from the iterates.

4.2 Numerical Example

To support the latter statement, we consider next a simple 2D numerical optimization example.

$$\min_{\boldsymbol{u}} \quad \phi(\boldsymbol{u}, \boldsymbol{y}_p(\boldsymbol{u})) := y_{1,p} \tag{4.6}$$
$$\text{s.t.} \quad g(\boldsymbol{u}, \boldsymbol{y}_p(\boldsymbol{u})) := y_{2,p} \leq \boldsymbol{0}, \text{ and } \boldsymbol{u} \in [0,1] \times [0,1],$$

where $\boldsymbol{u} \in \mathbb{R}^2$, $\boldsymbol{y}_p \in \mathbb{R}^2$, and:

$$y_{1,p} := a - \boldsymbol{b}^\mathsf{T}\,\boldsymbol{u} + \frac{1}{2}\boldsymbol{u}^\mathsf{T}\boldsymbol{C}\boldsymbol{u}, \tag{4.7}$$

$$y_{2,p} := d + \boldsymbol{e}^\mathsf{T}\,\boldsymbol{u} - \frac{1}{2}\boldsymbol{u}^\mathsf{T}\boldsymbol{F}\boldsymbol{u}. \tag{4.8}$$

The plant is such that $a = 1$, $\boldsymbol{b}^\mathsf{T} = [1,\ 10]$, $d = 1.3$, $\boldsymbol{e}^\mathsf{T} = [3,\ 5]$. $\boldsymbol{C}$ and $\boldsymbol{F}$ are diagonal 2×2 matrices, with (i) 1 and 10 and (ii) 5 and 9 as diagonal elements, respectively.

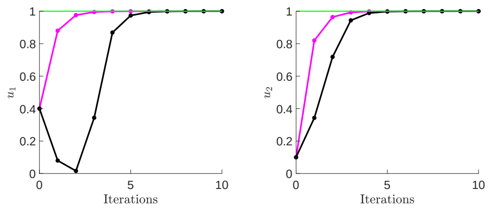

Fig. 3. Simulation results for the 2D optimization problem.

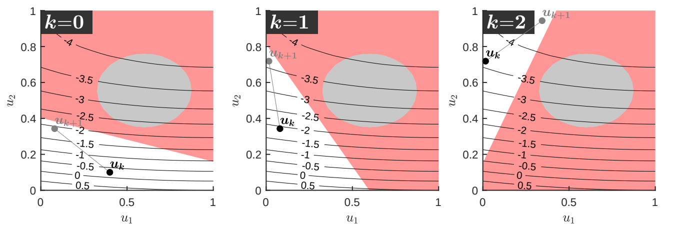

Fig. 4. Unfeasible regions for the linearized (red area) and plant contraints (grey area), for the 3 first MAc iterations; Points: RTO iterations.

The optimal solution of Problem (4.6) is $\boldsymbol{u}_p^\star = [1,1]^\mathsf{T}$ and MAc and KMAy are both initialized at the conservative inputs $\boldsymbol{u}_0 = [0.4, 0.1]^\mathsf{T}$. Figure 3 shows that KMAy converges in 4 iterations with $\boldsymbol{K} = 0.8\boldsymbol{I}_{n_u}$, while it takes more than 6 iterations for MAc (that uses same gain for input filtering). Figure 4 depicts the location of the linearized constraints vs. the plant constraints for the 3 first RTO iterations of MAc. It is clear that the linearization of the concave constraints and their spreading into the input space is detrimental to the convergence of MAc.

5. CONCLUSIONS

In this article KMAy has been introduced. It is shown that embedding the classical input filtering step of MA schemes into the problem formulation, in the form of additional constraints that force the satisfaction of the model-based constraints also at the filtered inputs: (i) preserves the KKT-matching property upon convergence of MA schemes, (ii) is not detrimental to constraint qualification and (iii) relaxes the model adequacy condition compared to MAy, since the reduced Hessian of the cost function alone must be positive definite rather than of the Lagrangian function as with MAy. By decreasing the KMAy gain, it is always possible to force the satisfaction of the second-order sufficient conditions of optimality at the (unknown) plant optimal inputs, irrespective of the Hessian of the constraints. KMAy is also shown to potentially lead to better performances than MAc, since model constraints are not convexified or linearized, which often results in a loss of information that penalizes convergence. KMAy has been successfully applied to a benchmark chemical engineering optimization problem, with an inadequate model for MA and MAy. KMAy converges to the plant optimal inputs when MAy fails and converges faster than MAc due to a better prediction of the constraints. Future research should focus practical and methodological aspects of KMAy, e.g. the effect of measurement noise, enforcing plant feasibility at each iteration or model adequacy and application to a large-scale system with several non-convex constraints, where a larger difference with MAc in favor of KMAy can be expected.

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