A Globally Convergent Composite-Step Trust-Region Framework for Real-Time Optimization with Plant-Model Mismatch

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Abstract

Inaccurate models limit the performance of model-based real-time optimization (RTO) and even cause system instability. Therefore, a RTO framework that can guarantee global convergence with the presence of plant-model mismatch is desired. In this regard, the trust-region framework is simple to implement and guarantees globally convergent for unconstrained problems. However, it remains to be seen if the trust-region strategy can handle inequality constraints directly with the common model adaptation method. This paper addresses this issue and proposes a novel composite-step trust-region framework that guarantees global convergence for constrained RTO problems. The trial step is decomposed into a normal step that improves feasibility and a tangential step that reduces the cost function. In each iteration, the model optimization problem with relaxed constraints is solved. The proof of the global convergence property under structural plant-model mismatch is given.

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Process System Engineering

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Inaccurate models limit the performance of model-based real-time optimization (RTO) and even cause system instability. Therefore, a RTO framework that can guarantee global convergence with the presence of plant-model mismatch is desired. In this regard, the trust-region framework is simple to implement and guarantees globally convergent for unconstrained problems. However, it remains to be seen if the trust-region strategy can handle inequality constraints directly with the common model adaptation method. This paper addresses this issue and proposes a novel composite-step trust-region framework that guarantees global convergence for constrained RTO problems. The trial step is decomposed into a normal step that improves feasibility and a tangential step that reduces the cost function. In each iteration, the model optimization problem with relaxed constraints is solved. The proof of the global convergence property under structural plant-model mismatch is given.

Keywords — trust region, real-time optimization, composite step, global convergence, plant-model mismatch

Abbreviations: RTO, real-time optimization; TR, trust region.

1 | INTRODUCTION

Industrial enterprises increasingly demand higher quality and stricter cost control to cope with fierce market competition. Model-based optimal decision-making is an important enabler. In the process industry, first-principle models have been widely used in real-time optimization (RTO) because of their advantages in interpretability and extrapolation performance [30]. However, due to model simplifications, parameter uncertainty, and limited knowledge about the process, there is often a mismatch between the model and the actual plant, which affects the performance of RTO and even causes convergence problems.

Handling mismatches by reliable optimization algorithms aroused great interest. In static model-based optimization, structural plant-model mismatch is successfully handled by algorithms based on gradient matching ideas, e.g., integrated system optimization and parameter estimation [26], modifier adaptation [20] and generalized parameter estimation [34]. In each RTO iteration, the gradient of the plant is approximated, and the model is adapted so that its first-order necessary condition of optimality (FNCO) matches the FNCO of the plant. These methods guarantee upon-convergence optimality in the presence of structural plant-model mismatch.

However, they do not guarantee global convergence, and oscillation could arise due to an inadequate model or optimization overshoot. In the first case, the plant optimum does not satisfy the second-order optimality condition of the model optimization problem due to the model's wrong curvature [16, 17]. As a result, the algorithm diverges even starting from the actual optimum. The model is either directly convexified [17, 23] or adapted properly in each iteration [2] to avoid oscillation. In the second case, the trial step size calculated according to the mismatched model is too aggressive for the plant that the plant cost fails to decrease [22, 34]. Similar situations also occur in nonlinear optimization (see Section 2.2 in [24]). A simple solution to this problem is damping the input [22]. However, it only reduces the risk of divergence and lacks a theoretical convergence guarantee.

There are two ways to achieve global convergence and make RTO more reliable. First, global convergence is ensured by feasible-side convergence. In this case, not only does the algorithm converge from any feasible starting point, but all the iterates also satisfy the plant constraints. Feasible-side convergence is hard to guarantee in practice [5] unless additional global information about the plant is available. [5] analyzed the sufficient condition for feasibility and optimality (SCFO) of RTO. According to this condition, feasible-side convergence is achieved by projecting the model's optimal solution onto a cone of feasible descent directions. [21] proposed another algorithm using convex majorization functions of the plant objective and constraints. The nonconvex model is replaced by convex inner approximations, which results in interior-side monotone convergence. These two algorithms guarantee feasible-side global convergence to a KKT point of the plant.

Second, globalization strategies like line search and trust-region optimization in nonlinear optimization are exploited [24]. Trust-region method is the most natural for model-based RTO problems for many reasons. It has several advantages. (1) the trust-region framework is attractive because it can be extended to deal with inaccurate derivatives and function values [7]. (2) it is more efficient in RTO because it makes fuller use of the model. (3) the trust-region idea is simple and intuitive in practice.

In the process engineering community, trust-region optimization is applied to RTO [28, 19, 32, 12], black-box optimization problems [13, 8], as well as nonlinear model predictive control [11, 31]. The trust-region technique helps control the update step length based on the local quality of the model. In each iteration, the next input is restricted to the trust region, where plant-model mismatches are small. The trust-region radius is then adjusted according to the plant feedback data. For unconstrained RTO problems, the trust-region algorithm is straightforward. [3] showed the global convergence property using the trust-region framework. [4] showed that the modifier adaptation framework is equivalent to trust-region methods in certain cases.

However, constrained problems are more complicated because two goals must be considered simultaneously: reducing the cost and maintaining the iteration feasible. Several trust region algorithms have been proposed with or without theoretical global convergence guarantee. (1) Using Lagrangian. The trust radius is adjusted based on the agreement between the plant Lagrangian and the Lagrangian of the modified model [19]. The Lagrange multiplier acts as a weighting factor to reconcile the two goals. However, this is a heuristic approach that lacks a theoretical convergence guarantee. (2) Infeasibility-averse approach. The original model optimization problem with trust-region constraint is considered whenever the iterates are feasible. When an infeasible point occurs, the trust radius keeps shrinking to build a better model until a feasible point is found [12]. Global convergence is certified using results in derivative-free optimization. This method relies on a progressively refined global surrogate model, e.g., Gaussian process. For a general model, the algorithm may fail to find a feasible point. (3) Penalty approach. The constrained RTO problem is cast as an unconstrained one with a penalty for constraint violations included in the augmented cost function [3, 4]. If the penalty coefficient is large enough, the first-order criticality condition of these two problems are equivalent. Global convergence of the unconstrained problem then implies the convergence of the constrained problem under certain assumptions. (4) Filter approach. This approach is mostly applied to black-box/gray-box optimization[13, 14]. At each iteration, the acceptance of the solution to the optimization subproblem is controlled by a filter, which memorizes history iteration information. A step is accepted if it improves feasibility or reduces the objective function of the local surrogate model. If a point is rejected, the trust radius shrinks, and a better local surrogate is built based on sampling points in a smaller neighborhood. This method guarantees global convergence without the need to specify the penalty coefficient. However, it still needs further investigation on how to use the method to handle plant-model mismatch in RTO problems.

With the existing RTO literature, it is interesting whether the trust-region strategy can handle constrained RTO problems directly with a general mismatched model and guarantee optimality in theory. It has several benefits. On the one hand, it is more intuitive and compatible with existing model-based RTO algorithms. On the other hand, it is also more reliable since the physical model to preserving physical inequality constraints. This paper addresses this issue and proposes a novel composite-step trust-region framework for constrained RTO problems.

The rest of the paper is structured as follows. Previous trust-region methods in real-time optimization are described in Section 2. Section 3 presents the composite-step trust-region framework. Section 4 discusses the global convergence of the proposed algorithm and its link to the penalty methods. Section 5 demonstrated the algorithm's performance with two examples. Section 6 concludes the paper.

2 | PRELIMINARIES

2.1 | Model-based static real-time optimization

We consider the optimization of a continuous process operating at steady states. The plant optimization problem can be stated as problem (1). u is the input variable, y is the output variable, ϕ is the cost function, g is the inequality constraints, and $y = h(u)$ is the input-output mapping or the first principle model. The subscript p denotes the plant.

$$
\begin{aligned}
\min_{u} \quad & \phi_p(u, y) \\
s.t. \quad & g_p(u, y) \leq 0 \\
& y = h_p(u)
\end{aligned}
\tag{1}
$$

The equality constraint is a square system whose input is u and output is y. Therefore, it can eliminated by substituting y with $h(u)$. Then we have a neater representation of the plant optimization problem (2).

$$\begin{aligned} \min_{u} \quad & \phi_p(u) \\ s.t. \quad & g_p(u) \leq 0 \end{aligned} \tag{2}$$

The mathematical representation of the plant is unknown, so the model optimization problem (3) with subscript m is solved in each RTO iteration to calculate optimal u.

$$\begin{aligned} \min_{u} \quad & \phi_m(u) \\ s.t. \quad & g_m(u) \leq 0 \end{aligned} \tag{3}$$

However, plant-model mismatches exist, i.e., $\phi_p \neq \phi_m$ and $g_p \neq g_m$, and may lead to suboptimal or even infeasible input. Therefore, the model needs to be adapted based on the local information around u_k at each iteration. The model optimization problem (4) then uses this adapted model, where subscript k indicates the kth RTO iteration.

$$\begin{aligned} \min_{u} \quad & \phi_{m,k}(u) \\ s.t. \quad & g_{m,k}(u) \leq 0 \end{aligned} \tag{4}$$

To deal with structural plant-model mismatch and guarantee local convergence, the functions $\phi_{m,k}$ and $g_{m,k}$ in problem (4) should satisfy condition (5) given the information of plant output (ϕ_p and g_p) and plant derivatives ($\nabla\phi_p$ and ∇g_p) at the current input value u_k. Condition (5) implies gradient matching between the model and the plant and leads to KKT matching upon convergence. n_g is the number of constraints.

$$\begin{aligned} \phi_{m,k}(u_k) &= \phi_p(u_k) \\ g_{m,k}(u_k) &= g_p(u_k) \\ \nabla\phi_{m,k}(u_k) &= \nabla\phi_p(u_k) \\ \nabla g_{m,k,i}(u_k) &= \nabla g_{p,i}(u_k), \quad i = 1, \cdots, n_g \end{aligned} \tag{5}$$

There are various ways to achieve Eqs. (5), such as modifier adaptation [20]. In modifier adaptation, the adapted model optimization problem in iteration k is problem (6).

$$\begin{aligned} \min_{u} \quad & \phi_{m,k}(u) = \phi_m(u) + \phi_p(u_k) - \phi_m(u_k) + (u - u_k)^T \left(\nabla\phi_p(u_k) - \nabla\phi_m(u_k)\right) \\ s.t. \quad & g_{m,k,i}(u) = g_{m,i}(u) + g_{p,i}(u_k) - g_{m,i}(u_k) + (u - u_k)^T \left(\nabla g_{p,i}(u_k) - \nabla g_{m,i}(u_k)\right) \leq 0, \quad i = 1, \cdots, n_g \end{aligned} \tag{6}$$

To improve convergence of the RTO algorithm, a simple way is filtering the input in each step. Modifier adaptation algorithm with input filtering is described in Algorithm 1.

| Algorithm 1: Modifier adaptation with input filtering

Step 0: Initialization. Choose an initial point u_0 and filter coefficient $0 < K < 1$. $k \leftarrow 0$.

Step 1: Model adaptation. Implement u_k to the plant and obtain $\phi_p(u_k), \nabla\phi_p(u_k), g_p(u_k), \nabla g_p(u_k)$. Adapt the model optimization problem according to Eq. (6).

Step 2: Step calculation. Minimize the adapted model optimization problem (6) and denote the solution as u_k^*.

Step 3: Input filtering. Filter the input by Eq. (7).

$$u_{k+1} = u_k + K(u_k^* - u_k) \tag{7}$$

$k \leftarrow k + 1$. Go back to Step 1.

2.2 | Trust-region framework for unconstrained problems

Algorithms that solve problem (4) repeatedly based on local models only guarantee upon-convergence optimality. Inadequate models [16] and improper algorithm parameters [34] could lead to oscillation. To address this, [3, 4] proposed unconstrained RTO algorithms in the trust-region framework.

| Algorithm 2: Trust-Region Algorithm for Unconstrained Problems

Step 0: Initialization. Choose an initial point u_0, an initial trust-region radius $0 < \Delta_0 < \Delta_{\max}$. Choose constants $0 < \eta_1 \leq \eta_2 < 1, 0 < \gamma_1 < 1 < \gamma_2$. $k \leftarrow 0$.

Step 1: Model adaptation. Build a model satisfying Eqs. (5).

Step 2: Step calculation. Minimize the cost function of the model to obtain the step s_k.

$$\begin{aligned} s_k = \arg\min_s \quad & \phi_{m,k}\,(u_k + s) \\ s.t. \quad & \|s\| \leq \Delta_k \end{aligned} \tag{8}$$

Step 3: Acceptance of the trial point. Compute the ratio

$$\rho_k = \frac{\phi_p\,(u_k) - \phi_p\,(u_k + s_k)}{\phi_{m,k}\,(u_k) - \phi_{m,k}\,(u_k + s_k)} \tag{9}$$

If $\rho_k \geq \eta_1$, then define $u_{k+1} = u_k + s_k$; otherwise define $u_{k+1} = u_k$.

Step 4: Trust-region radius update. Set

$$\Delta_{k+1} = \begin{cases} \min\,(\gamma_2\Delta_k, \Delta_{max}) & if\ \rho_k > \eta_2, \\ \Delta_k & if\ \rho_k \in [\eta_1, \eta_2]\,, \\ \gamma_1\Delta_k & if\ \rho_k < \eta_1. \end{cases} \tag{10}$$

$k \leftarrow k + 1$. Go back to Step 1.

Step 2 determines the trial step by minimizing the adapted model cost within the trust-region constraint. Throughout this paper, if a optimization problem has multiple minima/maxima, then the "arg min/max" operator means to pick arbitrary one of them. After applying the trial step to the plant and getting new measurements, we compare the actual improvement to the value predicted by the model in Step 3. The trial point is accepted as the next iterate if sufficient improvement is made, and this iteration is said to be successful. Otherwise, u_{k+1} is rejected and the trust region shrinks; hopefully, the model provides a better prediction in a smaller region.

2.3 | Handling constraints by penalty function

Constrained RTO problems are more complicated because there are two often contradicting aims: minimizing the cost function and reducing infeasibility. The penalty trust-region algorithm [3] converts the constrained problem to an unconstrained one by the penalty functions (11), where $\|\cdot\|$ is L2-norm, $c(u)$ is the overall infeasibility calculated by Eqs. (12), and $\sigma > 0$ is the penalty coefficient.

$$\begin{aligned} f_p(u,\sigma) &= \phi_p(u) + \sigma c_p(u) \\ f_{m,k}(u,\sigma) &= \phi_{m,k}(u) + \sigma c_{m,k}(u) \end{aligned} \tag{11}$$

$$\begin{aligned} c_p(u) &= \left\| \max\left(g_p(u), 0\right) \right\| \\ c_{m,k}(u) &= \left\| \max\left(g_{m,k}(u), 0\right) \right\| \end{aligned} \tag{12}$$

The penalty trust-region algorithm is then similar to Algorithm 2 with $\phi(u)$ replaced by $f(u,\sigma)$. The difference between the two algorithms reads,

| Algorithm 3: Penalty Trust-Region Method

Step 2: Step calculation. Minimize the cost function of the model to obtain the step s_k.

$$\begin{aligned} s_k = \arg\min_s \quad & f_{m,k}(u_k + s, \sigma) \\ s.t. \quad & \|s\| \le \Delta_k \end{aligned} \tag{13}$$

Step 3: Acceptance of the trial point. Compute the ratio

$$\rho_k = \frac{f_p(u_k,\sigma) - f_p(u_k + s_k, \sigma)}{f_{m,k}(u_k,\sigma) - f_{m,k}(u_k + s_k, \sigma)} \tag{14}$$

If $\rho_k > \eta_1$, then define $u_{k+1} = u_k + s_k$; otherwise define $u_{k+1} = u_k$.

If the penalty coefficient σ is large enough, Algorithm 3 is globally convergent [3] under reasonable assumptions. However, determining σ is not easy because it depends on the specific problem, and a too large σ causes numerical difficulties.

3 | COMPOSITE-STEP TRUST-REGION FRAMEWORK

In this section, we propose a novel trust-region algorithm for constrained RTO problems with structural plant-model mismatch that deals with inequality constraints directly.

3.1 | Algorithm description

| Algorithm 4: Composition-Step Trust-Region Method

Step 0: Initialization. Choose an initial point u_0, an initial trust-region radius $0 < \Delta_0 < \Delta_{\max}$, and a sufficient large penalty coefficient $\sigma > 0$. Choose constants $0 < \eta_1 \le \eta_2 < 1$, $0 < \gamma_1 < 1 < \gamma_2$, $0 < \xi < 1$. $k \leftarrow 0$.

Step 1: Model adaptation. Build a model satisfying Eqs. (5).

Step 2: Normal step calculation. If u_k is feasible for the model, set $n_k \leftarrow 0$. Otherwise, move towards feasibility by solving problem (15).

$$\begin{aligned} n_k &= \arg\min_n c_{m,k}\left(u_k + n\right) \\ s.t. &\quad \|n\| \le \xi \Delta_k \end{aligned} \tag{15}$$

Step 3: Tangential step calculation. Compute a step t_k by problem (16)

$$\begin{aligned} t_k &= \arg\min_t \phi_{m,k}(u_k + n_k + t) \\ s.t. &\quad c_{m,k}\left(u_k + n_k + t\right) \le c_{m,k}\left(u_k + n_k\right) \\ &\quad \|n_k + t\| \le \Delta_k \end{aligned} \tag{16}$$

Step 4: Acceptance of the trial point. The composite step is $s_k = n_k + t_k$. Compute the ratio

$$\rho_k = \frac{f_p\left(u_k, \sigma\right) - f_p\left(u_k + s_k, \sigma\right)}{f_{m,k}\left(u_k, \sigma\right) - f_{m,k}\left(u_k + s_k, \sigma\right)} \tag{17}$$

If $\rho_k > \eta_1$, then define $u_{k+1} = u_k + s_k$; otherwise define $u_{k+1} = u_k$.

Step 5: Trust-region radius update. Set Δ_{k+1} according to Eq. (10). $k \leftarrow k + 1$. Go back to Step 1.

An earlier version of Algorithm 4 was reported in our conference paper[33]. One difficulty in imposing a trust region on a constrained optimization problem is that the feasible region of the original problem may not intersect with the trust region. Therefore, we have to allow some infeasibility in each iteration as long as there is a trend toward feasibility. In light of this, the composite-step method decomposes the overall step into a normal step that improves feasibility and a tangential step that reduces the cost function. The earliest composite-step ideas can be found in [6, 25]. A summary of trust-region composite-step methods in nonlinear programming is available in Section 15.4 of [10]. The tangential step is chosen not to increase infeasibility. It is called ”tangential” because it is usually tangential to the feasibility contour. It is often nearly orthogonal to (but not necessarily precisely orthogonal to) the normal step. By adjusting ξ, we change the step size for cost reduction and infeasibility reduction, and the overall step size is bounded by Δ_k.

In Step 1, any model adaptation approach satisfying Eqs. (5) can be used. Steps 2 and 3 solve the inequality-constrained subproblem with the updated model. The nonsmoothness in $c_{m,k}$ is not a problem for implementation because the subproblem can be converted to a smooth one by introducing slack variables. In Step 4, the progress towards a critical point is measured by the decrease of the merit function $f(u, \sigma)$, which is also a nonsmooth exact penalty function. Similar to the situation in Algorithm 3, if σ is large enough, the first-order criticality condition for this merit function will match the condition for the original constrained optimization problem.

The most crucial difference between the composite-step approach and the penalty approach lies in Steps 2 and 3. In the proposed algorithm, the overall step comprises the normal step that reduces infeasibility and the tangential step that improves the objective function while maintaining feasibility. The penalty approach calculates the overall step directly by solving the penalized optimization problem.

3.2 | Implementation issues

Scaling is very important for the trust-region method to avoid ill-conditioned problems and ensure the solution reaches desired precision [24]. For practical RTO problems, input and output variables usually have quite different orders of magnitude, so they must be normalized by their range before solving problems (15) and (16).

Furthermore, the nonsmooth optimization subproblems due to the maximum operator in $c_{m,k}(\cdot)$ are transformed into their equivalent smooth form by adding the slack variable z [1]. For problem (15), the equivalent formulation is problem (18), where i denotes constraint index.

$$\begin{aligned} n_k &= \arg\min_{n} \sum_{i=1}^{n_g} z_i^2 \\ s.t.\ & \|n\| \leq \xi \Delta_k \\ g_{m,k,i}(u_k + n) - z_i &\leq 0,\ i = 1, \cdots, n_g \\ z_i &\geq 0,\ i = 1, \cdots, n_g \end{aligned} \tag{18}$$

Likewise, (16) is replaced by problem (19).

$$\begin{aligned} t_k &= \arg\min_{t} \phi_{m,k}(u_k + n_k + t) \\ s.t.\ & \sum_{i=1}^{n_g} z_i^2 \leq c_{m,k}(u_k + n_k)^2 \\ & \|n_k + t\| \leq \Delta_k \\ g_{m,k,i}(u_k + n_k + t) - z_i &\leq 0,\ i = 1, \cdots, n_g \\ z_i &\geq 0,\ i = 1, \cdots, n_g \end{aligned} \tag{19}$$

4 | GLOBAL CONVERGENCE

In this section, we will prove the global convergence property of the proposed composite-step trust-region method and discuss its link to the penalty trust-region method. We shall show that the bounded merit function f decreases at successful iterations. Then, we can obtain that f and the optimality error are convergent according to the monotone convergence theorem. The proof outline is as follows.

The optimality improvement can be measured in each iteration by observing the merit function f. We define the optimality improvement of the plant problem and the model problem by Eqs. (20) and (21).

$$\delta f_p = f_p(u_k, \sigma) - f_p(u_k + s_k, \sigma) \tag{20}$$

$$\delta f_{m,k} = f_{m,k}(u_k, \sigma) - f_{m,k}(u_k + s_k, \sigma) \tag{21}$$

If iteration k is successful, i.e., $\rho_k > \eta_1$, then $\delta f_p > \eta_1 \delta f_{m,k} \geq 0$. In other words, if we focus on successful iterations, f_p decreases strictly monotonically. Because f_p is bounded below by the assumption, we expect that f_p converges by the monotone convergence theorem. Thus, δf_p and $\delta f_{m,k}$ converge to zero when $k \to \infty$.

However, one risk here is that the algorithm fails to find an acceptable point and the trust radius shrinks to zero. In this case, the algorithm terminates at a point that is not locally optimal . So our first task is to exclude this possibility. Fortunately, we can always make ρ_k close to 1 if the trust-radius is small enough if the currently point is not locally optimal. The reason is that, by Eq. (22)

$$|\rho_k - 1| = \left| \frac{f_p\,(u_k + s_k, \sigma) - f_{m,k}\,(u_k + s_k, \sigma)}{\delta f_{m,k}} \right| \tag{22}$$

,$|\rho_k - 1|$ equals the ratio of plant-model mismatch and model optimality improvement. When the trust-radius is small, plant-model mismatch$\sim O(\Delta_k^2)$, and $\delta f_{m,k} \sim O(\Delta_k)$. Therefore, ρ_k will be close to 1 and the next acceptable point always exists.

Next, we shall show that $\delta f_{m,k} = 0$ implies that the system is at a KKT point. On the one hand, $\delta f_{m,k}$ can be decomposed into three terms in Eq. (23), which can be called feasibility improvement, tangential step cost improvement and residue, respectively.

$$\delta f_{m,k} = \sigma \delta f_{m,k}^N + \delta f_{m,k}^T + \delta q_k \tag{23}$$

$$\delta f_{m,k}^N = c_{m,k}(u_k) - c_{m,k}(u_k + n_k + t_k) \tag{24}$$

$$\delta f_{m,k}^T = \phi_{m,k}(u_k + n_k) - \phi_{m,k}(u_k + n_k + t_k) \tag{25}$$

$$\delta q_k = \phi_{m,k}(u_k) - \phi_{m,k}(u_k + n_k) \tag{26}$$

The superscripts N and T stand for normal and tangential. Note that $\delta f_{m,k}^N$ and $\delta f_{m,k}^T$ are nonnegative because of the problem formulation in Steps 2 and 3 in Algorithm 4. As for the residue term δq, we shall show that it is not important if σ is large enough, which helps us to establish the correlation between $\delta f_{m,k}$ and $\delta f_{m,k}^N$ or $\delta f_{m,k}^T$. On the other hand, being an optimum of a constrained problem means stationarity and feasibility, which can be quantified by criticality measure π_p, π_m and constraint violation c_p, c_m. The subscripts p and m indicate plant and model respectively. A local optimum can be verified by checking whether π_p and c_p are zero.

On that account, our second task in this proof is to show that when the trust radius is small, the model optimality improvement $\delta f_{m,k}$ is lower bounded by the optimality error π_p and c_p. More specifically, we shall show Eqs. (27) and (28) hold, where $\kappa_\cdot$ is some constant. After that, we shall conclude that π_p and c_p must also converge to zero as $\delta f_{m,k}$ converges to zero, which completes the global convergence proof. The relationship of π_p, c_p and π_m, c_m is due to A7.

$$\delta f_{m,k} \geq \kappa_1 \delta f_{m,k}^N \sim O(c_m) \sim O(c_p) \tag{27}$$

$$\delta f_{m,k} \geq \kappa_2 \delta f_{m,k}^T \sim O(\pi_m^2) \sim O(\pi_p^2) \tag{28}$$

The framework of the convergence proof comes from Section 15.4 of [10]. Nevertheless, there are two important differences. (1) The problem considered in [10] has equality constraints but does not involve inequality constraints. As a result, we need to substitute the projected gradient with a criticality measure suitable for inequality-constrained problems. (2) The proof in [10] used a quadratic model, whereas the RTO algorithm relies on more flexible and possibly nonconvex models. In this proof, we establish quadratic convex upper bound problems for Steps 2 and 3 to avoid analyzing the general nonlinear subproblems directly.

Constants used in the proof are summarized in the following list:

β_m	Assumption A3, bounds on n_k with respect to c_m
κ_c	Assumption A4, plant infeasibility reduction
β_c	Remark 1, Lipschitz constant of related functions
β^N	Lemma 3, normal step problem objective function curvature
β^T	Lemma 5, tangential step problem objective function curvature
κ_n	Lemma 6, bound on n_k with respect to $\delta f^N_{m,k}$

4.1 | Proof structure

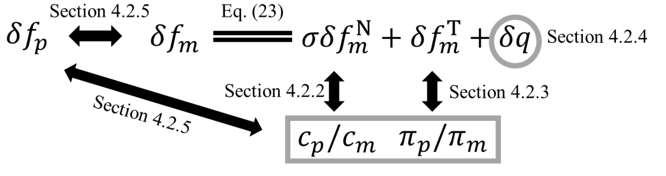

FIGURE 1 Proof Structure

The overall proof structure is shown in Fig. 1. Assumptions and their implications are presented in Section 4.2.1. The $\delta f^N_{m,k} \sim O(c_m)$ part in Eq. (27) is discussed in Section 4.2.2, while the $\delta f^T_{m,k} \sim O(\pi_m^2)$ part in Eq. (28) is discussed in Section 4.2.3. The requirement on the penalty coefficient σ and the relationship of $\delta f_{m,k}$, $\delta f^N_{m,k}$ and $\delta f^T_{m,k}$ are analyzed in Section 4.2.4. Section 4.2.5 completes the proof.

4.2 | Global convergence of composite-step method

4.2.1 | Assumptions

The following assumptions are needed for the convergence proof.

A1-Smoothness. For all iterations k, ϕ_p, $\phi_{m,k}$, g_p, and $g_{m,k}$ are twice continuously differentiable.

A2-Boundedness.

(a) All feasible inputs in the subproblems are contained in a convex compact set $\mathcal{U}$;

(b) $\phi_{m,k}$, $\nabla\phi_{m,k}$, $g_{m,k,i}$, $\nabla g_{m,k,i}$, and $\nabla^2 g_{m,k,i}$ are uniformly bounded on $\mathcal{U}$ over all k.

A3-Consistent normal steps. There exists a constant β_m such that $\|n_k\| \le \beta_m c_{m,k}(u_k)$ for all k.

A4-Plant constraints. For all feasible u, there exists a unit vector $d(u)$ such that $\nabla g^T_{p,i}(u)\, d(u) < 0$ for all constraints satisfying $g_{p,i}(u) = 0$. In addition, for all $u \in \mathcal{U}$, there exists a unit vector $d(u)$ and a small positive constant κ_c such that $\nabla g^T_{p,i}(u)\, d(u) < -\kappa_c$ for all constraints satisfying $g_{p,i}(u) > 0$.

A5-Subproblem optimality. All the optimization subproblems are solved to global optimality.

A6-Sufficiently large penalty. Penalty coefficient $\sigma \geq \sigma_{min}$, where σ_{min} is defined by Eq. (71) that will be discussed in Section 4.2.4.

A7-First-order matching. At each iteration, condition (5) holds.

Unless otherwise stated, all vector norms are L2-norms and all matrix norms are induced L2-norm in this paper. We make several remarks before the proof to explain the implications of the assumptions.

Remark 1: Lipschitz continuity and boundedness In RTO, the existence of $\mathcal{U}$ is usually because of input bounds. Due to A1, we have that ϕ_p, $\nabla\phi_p$, g_p, ∇g_p are bounded and Lipschitz continuous on the compact set $\mathcal{U}$. Due to A1 and A2, $\phi_{m,k}$, $\nabla\phi_{m,k}$, $g_{m,k}$, and $\nabla g_{m,k}$ are uniformly Lipschitz continuous on $\mathcal{U}$ for all k. Denote their Lipschitz constant as β_c for convenience.

The infeasibility measure c_p is the L2-norm of the maximum of Lipschitz continuous functions on $\mathcal{U}$, so it is Lipschitz continuous on $\mathcal{U}$. Due to the same reason as well as A1-A2, $c_{m,k}$ are uniformly Lipschitz continuous on $\mathcal{U}$ for all k. Similarly, f_p is Lipschitz continuous on $\mathcal{U}$ and $f_{m,k}$ are uniformly Lipschitz continuous on $\mathcal{U}$ for all k.

Remark 2: Consistent normal steps A3 prevents the normal step size from being too large when the infeasibility is small. In addition, it implies that the normal step size converges to zero if the infeasibility converges to zero.

Remark 3: Augmented constraint qualification A4 can be viewed as an augmentation of the Mangasarian-Fromowitz Constraint Qualification (MFCQ) condition. It has the following two consequences.

(1) A4 implies that $\forall i \in \mathcal{I} = \{i : g_{p,i}(u_k) > 0\}$, $\nabla g_{p,i} \neq 0$, so the algorithm cannot be trapped around an infeasible point.

(2) The following inequalities hold:

$$\begin{aligned}\left\|\nabla g_p\left(u_k\right)^T \cdot\max\left(g_p\left(u_k\right),0\right)\right\| &\geq \left|d(u_k)^T\nabla g_p\left(u_k\right)^T \cdot\max\left(g_p\left(u_k\right),0\right)\right| \\ &= \left|\sum_{i\in\mathcal{I}} d(u_k)^T\nabla g_{p,i}\left(u_k\right)g_{p,i}\left(u_k\right)\right| \\ &\geq \kappa_c\sum_{i\in\mathcal{I}} g_{p,i}\left(u_k\right) = \kappa_c\left\|\max\left(g_p\left(u_k\right),0\right)\right\|_1 \geq \kappa_c c_p\left(u_k\right).\end{aligned}$$

The first inequality is due to the Cauchy inequality $\|x\|\,\|d\| \geq |x^T d|$. The second inequality is due to A4. The last inequality follows that $\|x\|_1 \geq \|x\|_2$ for any vector x.

4.2.2 | Feasibility improvement

To derive a bound for the feasibility improvement $\delta f^N_{m,k}$ of a nonlinear problem, we first construct its quadratic upper-bound problem and then deal with the quadratic problem using Theorem 3.1.6 in [10].

Lemma 1 (quadratic upper bounding function) *Let $\mathcal{D}$ be an open convex subset of $\mathbb{R}^n$, and suppose $f : \mathcal{D} \to \mathbb{R}$ is continuously differentiable on $\mathcal{D}$. Suppose further that $\nabla f(x)$ is Lipschitz continuous on $\mathcal{D}$, with Lipschitz constant γ. Then, $\forall x, x+s \in \mathcal{D}$,*

$$f(x+s) \leq f(x) + \nabla f(x)^T s + \frac{1}{2}\gamma\|s\|^2 \tag{29}$$

Proof Since $\mathcal{D}$ is convex and $x, x+s \in \mathcal{D}$, the segment $x+\theta s \in \mathcal{D}$ for all $\theta \in [0,1]$. Then Theorem 3.1.6 in [10] gives that

$$\left| f(x+s) - [f(x) + \nabla f(x)^T s] \right| \leq \frac{1}{2}\gamma \|s\|^2 \tag{30}$$

Using the absolute value inequality $a \leq |a|$ and rearranging terms, we have Eq. (29). □

Lemma 2 (optimization progress for unconstrained nonlinear problem) *Let $\phi(x)$ be continuously differentiable, $\nabla\phi(x)$ Lipschitz continuous with a Lipschitz constant γ. Suppose s^* is the global minimizer of the following problem within the trust region.*

$$\begin{aligned} &\min_s \phi(x+s) \\ &\|s\| \leq \Delta \end{aligned} \tag{31}$$

Then we have that Eq. (32) *holds for all x, where $\beta \overset{def}{=} 1+\gamma$.*

$$\phi(x) - \phi\left(x+s^*\right) \geq \frac{1}{2}\|\nabla\phi(x)\| \min\left(\Delta, \frac{\|\nabla\phi(x)\|}{\beta}\right) \tag{32}$$

Proof According to Lemma 1, we can find an upper bounding function $\overline{\phi}(x+s) \geq \phi(x+s)$

$$\overline{\phi}(x+s) = \phi(x) + \nabla\phi(x)^T s + \frac{1}{2}\gamma\|s\|^2 = \phi(x) + \nabla\phi(x)^T s + \frac{1}{2}s^T(\gamma I)s \tag{33}$$

, where I is the identity matrix. Corollary 6.3.2 in [10] shows that for the quadratic trust-region problem $\min_s \overline{\phi}(x+s)$ $s.t.\ \|s\| \leq \Delta$, there exist a special feasible point s^c called Cauchy point such that improvement in Eq. (34) is guaranteed.

$$\overline{\phi}(x) - \overline{\phi}\left(x+s^c\right) \geq \frac{1}{2}\left\|\nabla\overline{\phi}(x)\right\| \min\left(\Delta, \frac{\left\|\nabla\overline{\phi}(x)\right\|}{1+\|\gamma I\|}\right) = \frac{1}{2}\left\|\nabla\overline{\phi}(x)\right\| \min\left(\Delta, \frac{\left\|\nabla\overline{\phi}(x)\right\|}{1+\gamma}\right) \tag{34}$$

Since $\overline{\phi}(x+s) \geq \phi(x+s)$ and $\overline{\phi}(x) = \phi(x)$,

$$\phi(x) - \phi\left(x+s^c\right) \geq \phi(x) - \overline{\phi}\left(x+s^c\right) = \overline{\phi}(x) - \overline{\phi}\left(x+s^c\right) \tag{35}$$

Since s^* is the global minimizer of problem (31),

$$\phi(x) - \phi\left(x+s^*\right) \geq \phi(x) - \phi\left(x+s^c\right) \tag{36}$$

Combining Eqs.(34)-(36), $\nabla\overline{\phi}(x) = \nabla\phi(x)$, we have Eq.(32). □

Based on Lemma 2, we establish a lower bound for the feasibility improvement in each iteration in the following theorem.

Theorem 3 (optimization progress due to normal step) *Suppose that A1, A2, A4 and A5 hold. For all k, the infeasibility* *reduction due to the normal step in Algorithm 4 is lower bounded as*

$$\delta f^N_{m,k} \geq \frac{\kappa_c}{2} \min\left(\xi\Delta_k, \frac{2\kappa_c}{\beta^N} c_{m,k}\left(u_k\right)\right), \tag{37}$$

where $\beta^N > 0$ is some constant.

Proof Since the tangential step does not increase the infeasibility, $\delta f^N_{m,k} \geq c_{m,k}\left(u_k\right) - c_{m,k}\left(u_k + n_k\right)$. It is enough to show

$$c_{m,k}\left(u_k\right) - c_{m,k}\left(u_k + n_k\right) \geq \frac{\kappa_c}{2} \min\left(\xi\Delta_k, \frac{2\kappa_c}{\beta^N} c_{m,k}\left(u_k\right)\right). \tag{38}$$

Consider the following smooth problem that is equivalent to (15) in Algorithm 4 Step 2:

$$\begin{aligned} n_k = \arg\min_n \quad & c_{m,k}(u_k + n)^2 \\ s.t. \quad & \|n\| \leq \xi\Delta_k. \end{aligned} \tag{39}$$

The objective function $c^2_{m,k}$ is the composition of $\max(\cdot, 0)^2$ and $g_{m,k}$ which are both differentiable, so it is differentiable. The gradient of $c^2_{m,k}$ is

$$\begin{aligned} \frac{d\left(c_{m,k}(u)^2\right)}{du} &= 2\sum_{i=1}^{n_g} \max\left(g_{m,k,i}\left(u\right), 0\right) \cdot \nabla g_{m,k,i}\left(u\right) \\ &= 2\nabla g_{m,k}\left(u\right) \cdot \max\left(g_{m,k}\left(u\right), 0\right). \end{aligned}$$

Since $\max\left(g_{m,k}\left(u\right), 0\right)$ and $\nabla g_{m,k}\left(u\right)$ are uniformly Lipschitz continuous on $\mathcal{U}$, the above gradient is uniformly Lipschitz continuous for all k. Then Lemma 2 applies to $c^2_{m,k}$ on $\mathcal{U}$, i.e., $\exists\, \beta^N > 0$ such that for all k,

$$\begin{aligned} & c_{m,k}(u_k)^2 - c_{m,k}(u_k + n_k)^2 \\ & \geq \left\|\nabla g_{m,k}\left(u_k\right) \max\left(g_{m,k}(u_k), 0\right)\right\| \min\left(\xi\Delta_k, \frac{2\left\|\nabla g_{m,k}\left(u_k\right) \max\left(g_{m,k}\left(u_k\right), 0\right)\right\|}{\beta^N}\right). \end{aligned} \tag{40}$$

Under A4 and A7, Remark 3 shows that

$$\left\|\nabla g_{m,k}\left(u_k\right) \max\left(g_{m,k}\left(u_k\right), 0\right)\right\| = \left\|\nabla g_p\left(u_k\right) \max\left(g_p\left(u_k\right), 0\right)\right\| \geq \kappa_c c_p(u_k) = \kappa_c c_{m,k}\left(u_k\right).$$

Therefore, Eq.(40) becomes

$$c_{m,k}(u_k)^2 - c_{m,k}(u_k + n_k)^2 \geq \kappa_c c_{m,k}\left(u_k\right) \min\left(\xi\Delta_k, \frac{2\kappa_c}{\beta^N} c_{m,k}\left(u_k\right)\right). \tag{41}$$

The left-hand side of Eq.(41) satisfies

$$
\begin{aligned}
& c_{m,k}(u_k)^2 - c_{m,k}(u_k+n_k)^2 \\
& \quad = \left(c_{m,k}(u_k) - c_{m,k}(u_k+n_k)\right)\left(c_{m,k}(u_k) + c_{m,k}(u_k+n_k)\right) \\
& \quad \leq 2c_{m,k}(u_k)\left(c_{m,k}(u_k) - c_{m,k}(u_k+n_k)\right).
\end{aligned}
\tag{42}
$$

Suppose that $c_{m,k}(u_k) > 0$. Combining Eq.(41) and Eq.(42) gives Eq.(43).

$$
c_{m,k}(u_k) - c_{m,k}(u_k+n_k) \geq \frac{\kappa_c}{2} \min\left(\xi\Delta_k, \frac{2\kappa_c}{\beta^N} c_{m,k}(u_k)\right). \tag{43}
$$

Otherwise, $c_{m,k}(u_k) = 0$ and $n_k = 0$, so Eq.(43) also holds. This completes the proof. □

4.2.3 | Objective function improvement

Another aspect of optimality is finding a stationary point of the Lagrange function, which can be characterized by criticality measures. A criticality measure is a nonnegative continuous function of the decision variable, which equals zero if and only if at a first-order critical point. For unconstrained optimization problems, the norm of the objective gradient is a criticality measure.

$$
\min_{x\in C} f(x) \tag{44}
$$

For the convex constrained optimization problem (44) where f is continuously differentiable and ∇f is Lipschitz continuous, [9] and Theorem 12.1.6 in [10] give two of its criticality measures $\chi(x)$ and $\pi(x)$. They equal to zero if an only if $\nabla f(x)^T d \geq 0$ for all feasible direction d at x (the first-order criticality condition at x).

Definition 1: Criticality measure $\chi(x)$. $\chi(x)$ defined by Eq. (45) is a criticality measure for problem (44).

$$
\chi(x) \overset{def}{=} -\min_{d} \nabla f(x)^T d, \quad s.t.\ x+d \in C, \|d\| \leq 1 \tag{45}
$$

Definition 2: Criticality measure $\pi(x)$. $\pi(x)$ defined by Eq. (46) is a criticality measure for problem (44).

$$
\pi(x) \overset{def}{=} \min(1, \chi(x)) \tag{46}
$$

In Lemma 4, we will derive a bound for the convex constrained nonlinear problem with trust region using these two criticality measures. Similar to the approach in Lemma 2, we once again construct a quadratic upper-bound constrained problem and examine the objective function value along the direction d^* determined by the criticality measure.

Lemma 4 (optimization progress for convex constrained problem) *Consider the convex-constrained problem*

$$
d^* = \arg\min_{d} f(x+d) \quad s.t.\ x+d \in C, \|d\| \leq \Delta \tag{47}
$$

, where C is a nonempty closed convex set, $x \in C$, and $\Delta > 0$. Let $x^* = x + d^*$. Suppose that $f(x)$ is continuously differentiable

and $\nabla f(x)$ is Lipschitz continuous with a Lipschitz constant γ. Then, we have

$$f(x) - f(x^*) \geq \frac{1}{2}\chi(x) \min\left[\frac{\chi(x)}{\beta}, \Delta, 1\right] \tag{48}$$

for $\beta \stackrel{def}{=} 1 + \gamma$ and a simpler form using $\pi(x)$.

$$f(x) - f(x^*) \geq \frac{1}{2}\pi(x) \min\left[\frac{\pi(x)}{\beta}, \Delta\right] \tag{49}$$

Proof Let the optimizer of Eq. (45) be $\bar{d}$.If $\bar{d} = 0$, then $\chi(x) = 0$ and Eq.(48) automatically holds. Otherwise, $\|\bar{d}\| > 0$ and $\nabla f(x)^T \bar{d} = -\chi(x)$. By Lemma 1 and $\beta > \gamma$, $\forall \bar{x} \in C$, we have an upper bound (50).

$$f(x) + \nabla f(x)^T (\bar{x} - x) + \frac{1}{2}\beta\|\bar{x} - x\|^2 \geq f(\bar{x}) \tag{50}$$

We shall focus on the segment that connects x and $x + \bar{d}$, which is included in C because of convexity. For $\bar{x} = x + \alpha\bar{d}$, $0 \leq \alpha \leq 1$, Eq.(50) is equivalent to Eq.(51).

$$f(x) + \alpha\nabla f(x)^T \bar{d} + \frac{1}{2}\alpha^2\beta\|\bar{d}\|^2 \geq f\left(x + \alpha\bar{d}\right) \tag{51}$$

The vertex of the left-hand quadratic function of α is $\alpha_v = -\frac{\nabla f(x)^T \bar{d}}{\beta\|\bar{d}\|^2} = \frac{\chi(x)}{\beta\|\bar{d}\|^2}$. If $0 \leq \alpha \leq \alpha_v$, we further have a linear bound Eq.(52) for the quadratic function in Eq.(51).

$$f(x) + \frac{1}{2}\alpha\nabla f(x)^T \bar{d} \geq f\left(x + \alpha\bar{d}\right) \tag{52}$$

There are three cases to be discussed. First, if $\|\bar{d}\| \leq \min\left(\Delta, \frac{\chi(x)}{\beta\|\bar{d}\|}\right)$, then $\alpha_v \geq 1$. Let $\alpha = 1 \leq \alpha_v$. Eq.(52) gives

$$f(x) - \frac{1}{2}\chi(x) = f(x) + \frac{1}{2}\nabla f(x)^T \bar{d} \geq f\left(x + \bar{d}\right)$$

Since $\bar{d} \leq \Delta$ and $x + \bar{d} \in C$, $x + \bar{d}$ is a feasible point of problem (47). Then,

$$f(x) - f(x^*) \geq f(x) - f\left(x + \bar{d}\right) \geq \frac{1}{2}\chi(x) \tag{53}$$

Second, if $\Delta < \min\left(\|\bar{d}\|, \frac{\chi(x)}{\beta\|\bar{d}\|}\right)$, then let $\alpha = \frac{\Delta}{\|\bar{d}\|} < \min(1, \alpha_v)$ and Eq.(52) gives

$$f(x) - \frac{\Delta}{2\|\bar{d}\|}\chi(x) = f(x) + \frac{\Delta}{2\|\bar{d}\|}\nabla f(x)^T \bar{d} \geq f\left(x + \frac{\Delta}{\|\bar{d}\|}\bar{d}\right)$$

Since $\Delta < \|\bar{d}\|$ and $x, x + \bar{d} \in C$, we have that $x + \frac{\Delta}{\|\bar{d}\|}\bar{d} \in C$. Moreover, $\left\|\frac{\Delta}{\|\bar{d}\|}\bar{d}\right\| = \Delta$, so $x + \frac{\Delta}{\|\bar{d}\|}\bar{d}$ also satisfies the trust region constraint. Therefore, $\frac{\Delta}{\|\bar{d}\|}\bar{d}$ is feasible point for problem (47), and inequality (54) holds, where the last inequality is due to $\|\bar{d}\| \leq 1$.

$$f(x) - f(x^*) \geq f(x) - f\left(x + \frac{\Delta}{\|\bar{d}\|}\bar{d}\right) \geq \frac{\Delta}{2\|\bar{d}\|}\chi(x) \geq \frac{1}{2}\chi(x)\Delta \tag{54}$$

Third, if $\frac{\chi(x)}{\beta\|\bar{d}\|} < \min(\Delta, \|\bar{d}\|)$, then let $\alpha = \alpha_v < 1$ and Eq.(52) gives

$$f(x) - \frac{1}{2\beta\|\bar{d}\|^2}\chi(x)^2 = f(x) + \frac{1}{2}\frac{\chi(x)}{\beta\|\bar{d}\|^2}\nabla f(x)^T\bar{d} \geq f(x + \alpha_v\bar{d})$$

Since $\|\alpha_v\bar{d}\| = \frac{\chi(x)}{\beta\|\bar{d}\|} < \min(\Delta, \|\bar{d}\|)$, by the same reasoning as the second case, we have that $x + \alpha_v\bar{d}$ is inside both C and the trust region. Therefore, $\alpha_v\bar{d}$ is a feasible point for problem (47) and

$$f(x) - f(x^*) \geq f(x) - f(x + \alpha_v\bar{d}) \geq \frac{1}{2\beta\|\bar{d}\|^2}\chi(x)^2 \geq \frac{1}{2\beta}\chi(x)^2 \tag{55}$$

The last inequality is due to $\|\bar{d}\| \leq 1$. Combining Eqs.(53)-(55) gives Eq.(48).

Because $\pi(x) \leq \chi(x)$, it follows Eq.(48) that

$$f(x) - f(x^*) \geq \frac{1}{2}\pi(x)\min\left[\frac{\pi(x)}{\beta}, \Delta, 1\right] \tag{56}$$

Since $\beta \geq 1$ and $\pi(x) \leq 1$ by their definition, the first term in the minimum is always less than 1, and Eq.(56) becomes Eq.(49). □

The tangential step aims to find a better point within the current infeasibility level. Consider an analogous tangential step problem to (16) in Algorithm 4.

$$\begin{aligned} \min_t \quad & \phi_{m,k}(u_k + n_k + t) \\ s.t. \quad & g_{m,k}(u_k + n_k + t) \leq \max\left(g_{m,k}(u_k + n_k), 0\right) \end{aligned} \tag{57}$$

Replacing its constraint with the quadratic upper bound function using Lemma 1, we get a more restrictive problem (58) that is convenient for analysis.

$$\begin{aligned} \min_t \quad & \phi_{m,k}(u_k + n_k + t) \\ s.t. \quad & g_{m,k,i}(u_k + n_k) + \nabla g_{m,k,i}(u_k + n_k)^T t + \frac{1}{2}\beta_c t^T t \leq \max\left(g_{m,k,i}(u_k + n_k), 0\right), i = 1, \cdots, n_g \end{aligned} \tag{58}$$

Problem (58) can be viewed as a parametric optimization problem that depends on two parameters u_k and n_k. Moreover, it depends on u_k in two ways. First, u_k appears in function arguments. Second, $\phi_{m,k}$ and $g_{m,k}$ are the approximated functions of the plant's at u_k. With this in mind, we denote the $\chi(t)$ and $\pi(t)$ criticality measures of problem (58) at $t = 0$ as $\chi_m(u_k, n_k)$ and $\pi_m(u_k, n_k)$, respectively.

Definition 3: Criticality measure $\chi_m(u_k, n_k)$. The $\chi(t)$ criticality measure of problem (58) at $t = 0$ is the value function of optimization problem (59).

$$
\begin{aligned}
\chi_m(u_k, n_k) &\overset{def}{=} -\min_d \nabla\phi_{m,k}(u_k+n_k)^T d \\
s.t. \quad g_{m,k,i}(u_k+n_k) + \nabla g_{m,k,i}(u_k+n_k)^T d + \frac{1}{2}\beta_c d^T d &\le \max\left(g_{m,k,i}(u_k+n_k), 0\right), i = 1, \cdots, n_g \\
d^T d &\le 1
\end{aligned}
\tag{59}
$$

Definition 4: Criticality measure $\pi_m(u_k, n_k)$. Criticality measure $\pi_m(u_k, n_k)$ is derived from $\chi_m(u_k, n_k)$.

$$
\pi_m(u_k, n_k) \overset{def}{=} \min\left(1, \chi_m(u_k, n_k)\right) \tag{60}
$$

In Theorem 5, we will derive a lower bound for the optimization progress due to the tangential step using $\pi_m(u_k, n_k)$.

Theorem 5 (optimization progress due to tangential step) *Suppose that A1, A2, and A5 hold. For all k, the lower bound for optimization progress due to the tangential step in Algorithm 4 is*

$$
\delta f_{m,k}^T \ge \frac{1}{2}\pi_m(u_k, n_k)\min\left(\frac{\pi_m(u_k, n_k)}{\beta^T}, (1-\xi)\,\Delta_k\right) \tag{61}
$$

, where $\beta^T > 0$ is some constant.

Proof Our basic idea is to use Lemma 4. For doing so, we need to find a feasible point for problem (16). The simplest choice is $t = 0$. We shall also adjust the trust region so that it is centered at this feasible point.

Consider problem (58) with $u = u_k + n_k + t$ and add a trust-region constraint centered at $t = 0$.

$$
\begin{aligned}
t_k' &= \arg\min_t \phi_{m,k}(u_k + n_k + t) \\
s.t. \quad & g_{m,k,i}\left(u_k+n_k\right) + \nabla g_{m,k,i}(u_k+n_k)^T t + \frac{1}{2}\beta_c t^T t \\
& \le \max\left(g_{m,k,i}\left(u_k+n_k\right), 0\right) \quad i = 1, \cdots, n_g \\
& \|t\| \le (1-\xi)\,\Delta_k
\end{aligned}
\tag{62}
$$

Since $t = 0$ is a feasible solution to problems (62) and $\nabla\phi_{m,k}$ is Lipschitz continuous on $\mathcal{U}$, Lemma 4 applies and guarantees that for some $\beta^T > 0$,

$$
\phi_{m,k}\left(u_k+n_k\right) - \phi_{m,k}\left(u_k+n_k+t_k'\right) \ge \frac{1}{2}\pi_m(u_k, n_k)\min\left(\frac{\pi_m(u_k, n_k)}{\beta^T}, (1-\xi)\,\Delta_k\right) \tag{63}
$$

Because problem (62) a restriction of problem (16) according to Lemma 1 and the definition of c_m, and because t_k is a global minimizer for problem (16), we have

$$
\delta f_{m,k}^T = \phi_{m,k}\left(u_k+n_k\right) - \phi_{m,k}\left(u_k+n_k+t_k\right) \ge \phi_{m,k}\left(u_k+n_k\right) - \phi_{m,k}\left(u_k+n_k+t_k'\right) \tag{64}
$$

Combining Eqs.(63) and (64) yields Eq.(61). □

4.2.4 | Sufficiently large penalty coefficient

To establish relation between $\delta f_{m,k}$ and $\delta f_{m,k}^N$, $\delta f_{m,k}^T$, we need A6 to ensure a large enough σ. When the penalty is not big enough, the improvement in terms of the normal and tangential step does not guarantee overall improvement because of the δq_k term.

Since both $\delta f_{m,k}^N$ and δq_k are related to $\|n_k\|$, we will use $\|n_k\|$ as an intermediate variable to establish a lower bound for $\delta f_{m,k}$. Our first result is that under A3, the length of the normal step is bounded in terms of the improvement of feasibility.

Lemma 6 (normal step size upper bound) *Suppose that A1- A5 and A7 hold. Then there is a constant $\kappa_n > 0$ such that for all k*

$$\kappa_n \|n_k\| \leq \delta f_{m,k}^N \leq c_{m,k}(u_k) \tag{65}$$

Proof By Theorem 3,

$$\delta f_{m,k}^N \geq \frac{\kappa_c}{2} \min\left(\xi \Delta_k, \frac{2\kappa_c}{\beta^N} c_{m,k}(u_k)\right)$$

If $\xi \Delta_k \leq \frac{2\kappa_c}{\beta^N} c_{m,k}(u_k)$,

$$\delta f_{m,k}^N \geq \frac{1}{2}\kappa_c \xi \Delta_k \geq \frac{1}{2}\kappa_c \|n_k\| \tag{66}$$

On the other hand, if $\xi \Delta_k > \frac{2\kappa_c}{\beta^N} c_{m,k}(u_k)$, then

$$\delta f_{m,k}^N \geq \frac{\kappa_c^2}{\beta^N} c_{m,k}(u_k) \tag{67}$$

Using A3,

$$\delta f_{m,k}^N \geq \frac{\kappa_c^2}{\beta^N \beta_m} \|n_k\| \tag{68}$$

By defining $\kappa_n = \min\left(\frac{\kappa_c}{2}, \frac{\kappa_c^2}{\beta^N \beta_m}\right)$ and combining Eqs. (66) and (68), we have in both cases that

$$\delta f_{m,k}^N \geq \kappa_n \|n_k\|$$

The second inequation in inequality (65) follows directly from the definition of $\delta f_{m,k}^N$ and the fact that $c_{m,k}(u_k + n_k + t_k) \geq 0$. The proof is completed. □

Now we are ready to determine the threshold for a large penalty coefficient, which makes δq_k unimportant.

Theorem 7 (sufficiently large penalty coefficient) *Suppose that A1- A5 and A7 hold. There exists a constant $\sigma_{min} > 0$, such that for all k and all $\sigma \geq \sigma_{min}$ (assumption A6) the following statement is true.*

$$\delta f_{m,k} \geq \frac{1}{4}\sigma\delta f^N_{m,k} + \delta f^T_{m,k} \tag{69}$$

Proof As Remark 1 mentioned, A1 and A2 leads to the uniformly Lipschitz continuity of $\phi_{m,k}$. Therefore, for some constant $\beta_c > 0$,

$$\delta q_k = \phi_{m,k}(u_k) - \phi_{m,k}(u_k + n_k) \geq -\beta_c \|n_k\| \tag{70}$$

Select σ_{min} according to Eq. (71), where κ_n is defined in Lemma 6.

$$\sigma_{min} = \frac{2\beta_c}{\kappa_n} \tag{71}$$

By Eqs. (23), (71) and $\forall\sigma \geq \sigma_{min}$,

$$\delta f_{m,k} - \frac{1}{4}\sigma\delta f^N_{m,k} - \delta f^T_{m,k} = \frac{3}{4}\sigma\delta f^N_{m,k} + \delta q_k \geq \frac{3\beta_c}{2\kappa_n}\delta f^N_{m,k} + \delta q_k \tag{72}$$

Using inequalities (65) and (70),

$$\frac{3\beta_c}{2\kappa_n}\delta f^N_{m,k} + \delta q_k \geq \frac{3\beta_c}{2}\|n_k\| - \beta_c\|n_k\| = \frac{\beta_c}{2}\|n_k\| \geq 0 \tag{73}$$

Combine Eqs. (72) and (73) yields Eq. (69). □

It is hard to know these constants $\kappa_\cdot$ and verify if σ is large enough before the RTO implementation. Therefore, a sufficiently large σ is selected empirically according to the knowledge about the nonlinearity of the plant. An alternative method is to adapt σ in each iteration so that condition (69) holds. In this case, A6 is not needed for global convergence. The composition-step trust-region method with adaptive σ is described as follows.

| Algorithm 5: Composition-Step Trust-Region Method with Adaptive Penalty Coefficient

Step 0: Initialization. Choose an initial point u_0, an initial trust-region radius $0 < \Delta_0 < \Delta_{\max}$, and an initial penalty coefficient $\sigma_0 > 0$. Choose constants $0 < \eta_1 \leq \eta_2 < 1$, $0 < \gamma_1 < 1 < \gamma_2$, $0 < \xi < 1$. $k \leftarrow 0$.

Step 4: Adapt Penalty Coefficient. Update σ_k according to Eq. (74).

$$\sigma_k \leftarrow \max\left(\sigma_{k-1}, \frac{-4\delta q_k}{3\delta f^N_{m,k}}\right) \tag{74}$$

Step 4: Acceptance of the trial point. The composite step is $s_k = n_k + t_k$. Compute the ratio

$$\rho_k = \frac{f_p(u_k, \sigma_k) - f_p(u_k + s_k, \sigma_k)}{f_{m,k}(u_k, \sigma_k) - f_{m,k}(u_k + s_k, \sigma_k)} \tag{75}$$

If $\rho_k > \eta_1$, then define $u_{k+1} = u_k + s_k$; otherwise define $u_{k+1} = u_k$.

Steps 1-3 of Algorithms 4 and 5 are the same. The main difference between Algorithm 5 and Algorithm 4 is that a new σ is calculated before evaluating ρ in Algorithm 5. Step 5 of Algorithm 4 then becomes Step 6 in Algorithm 5. Following the approach of Theorem 15.4.8 in [9], we can show that inequality (69) holds for all σ_k. Since σ is increasing, f_p is no longer decreasing. However, Lemma 15.4.5 in [9] shows that by defining a new function $\psi_p(u,\sigma)$

$$\psi_p(u,\sigma) = \frac{f_p(u,\sigma) - f_{p,min}}{\sigma} \tag{76}$$

, where $f_{p,min}$ is the lower bound of f_p, the sequence $\{\psi_p(u_k,\sigma_k)\}_k$ is decreasing for successful iterations. Moreover, the amount of decrease satisfies

$$\psi_p(u_{k_i},\sigma_{k_i}) - \psi_p(u_{k_j},\sigma_{k_j}) \geq \eta_1 \frac{\delta f_{m,k_i}\left(u_{k_i},\sigma_{k_i}\right)}{\sigma_{k_i}} \tag{77}$$

, where k_i and k_j are two consecutive successful iterations.

All the proofs in the paper assume f_p and $f_{m,k}$ use a sufficiently large constant penalty coefficient that satisfies assumption A6. However, by replacing f_p with ψ_p and slightly modifying the existing proof, we can prove the same global convergence results for Algorithm 5.

4.2.5 | First-order Optimality

Now we are ready to complete the convergence proof in this subsection. The remaining part resembles Section 15.4.2 [10], which relies on the continuity of $c(\cdot)$ and $\pi(\cdot)$. For equality-constrained problems, the criticality measure is the projected gradient. In our nonlinear inequality-constrained case, we rely on a more complicated quantity $\pi_m(u_k,n_k)$, whose continuity with respect to u_k and n_k is not obvious. Section 4.2.5 is divided into two parts. First, we show the continuity of $\pi_m(u_k,n_k)$ using parametric optimization results. Then, we summarize the current results and finish the global convergence proof.

Lemma 8 (continuity of the model criticality measure) *If A1, A2 and A7 hold, π_m is jointly continuous in u_k and n_k over $\mathcal{D} = \mathcal{U}\times\{0\}^{n_u}$.*

Proof Since the continuity of π_m follows the continuity of χ_m, it is enough to analyze the latter one. For clarity, we re-express the definition of χ_m is in the following form:

$$\begin{aligned} \chi_m(u_k,n_k) \overset{def}{=} &-\min_d F(d;u_k,n_k) \\ &s.t.\ G_i(d;u_k,n_k) \leq 0, \\ &d^T d \leq 1, \end{aligned} \tag{78}$$

where d is the decision variable, u_k and n_k are the parameters of the optimization problem, and the functions

$$\begin{aligned} F(d;u_k,n_k) =& \nabla\phi_{m,k}(u_k+n_k)^T d, \\ G_i(d;u_k,n_k) =& g_{m,k,i}(u_k+n_k) + \nabla g_{m,k,i}(u_k+n_k)^T d + \frac{1}{2}\beta_c d^T d - \max\left(g_{m,k,i}(u_k+n_k),0\right), i = 1,\cdots,n_g. \end{aligned}$$

According to the result in [18] (or Theorems 2.1 and 2.9 in [15]), χ_m is continuous at any $(u_k,n_k) \in \mathcal{D}$ if:

(1) The constraints that only involve d define a convex and compact set, which obviously holds for (78);

(2) G_i is strictly convex in d for any fixed (u_k, n_k) ($i = 1, \cdots, n_g$), which obviously holds;

(3) Functions F and G_i ($i = 1, \cdots, n_g$) are continuous in (u_k, n_k) for any point in $\mathcal{D}$.

So it remains to prove the last condition. Next, we prove that F is continuous in (u_k, n_k) for any point in $\mathcal{D}$. Note that F depends on u_k in two ways. First, the functional $\nabla\phi_{m,k}$ is updated from u_k and therefore dependent on u_k. Second, the value of $\nabla\phi_{m,k}$ at $u_k + n_k$ depends on u_k. When $d = 0$, the continuity of F is obvious. When $d \neq 0$, consider any $(u_k, n_k) \in \mathcal{D}$, $\forall \epsilon > 0$, $\exists \delta > 0$ such that $\forall (u_j, n_j) \in \{(u_j, n_j) \in \mathcal{D} \times \mathbb{R}^{n_u} : \|(u_j, n_j) - (u_k, 0)\| \leq \delta\}$, the following two inequalities hold:

$$
\begin{aligned}
|\nabla\phi_p(u_k) - \nabla\phi_p(u_j)| &\leq \frac{1}{2\|d\|}\epsilon, \\
|\nabla\phi_{m,j}(u_j + n_j) - \nabla\phi_{m,j}(u_j)| &\leq \frac{1}{2\|d\|}\epsilon.
\end{aligned}
$$

The first inequality comes from the continuity of ϕ_p and the second comes from the uniform continuity of $\phi_{m,j}$. Therefore,

$$
\begin{aligned}
|F(d; u_k, n_k) - F(d; u_j, n_j)| &\leq \|\nabla\phi_{m,j}(u_k) - \nabla\phi_{m,k}(u_j + n_j)\|\|d\| \\
&= \|\nabla\phi_{m,k}(u_k) - \nabla\phi_{m,j}(u_j) - (\nabla\phi_{m,j}(u_j + n_j) - \nabla\phi_{m,j}(u_j))\|\|d\| \\
&\leq (\|\nabla\phi_{m,k}(u_k) - \nabla\phi_{m,j}(u_j)\| + \|\nabla\phi_{m,j}(u_j + n_j) - \nabla\phi_{m,j}(u_j)\|)\|d\| \\
&= (\|\nabla\phi_p(u_k) - \nabla\phi_p(u_j)\| + \|\nabla\phi_{m,j}(u_j + n_j) - \nabla\phi_{m,j}(u_j)\|)\|d\| \\
&\leq (\frac{1}{2\|d\|}\epsilon + \frac{1}{2\|d\|}\epsilon)\|d\| = \epsilon.
\end{aligned}
$$

The second equality in the above derivation comes from the first-order matching in A7. This proves the continuity of F for any $(u_k, n_k) \in \mathcal{D}$.

Similarly, we can prove that G_i is continuous in (u_k, n_k) for any point in $\mathcal{D}$ ($\forall i \in \{1, \cdot, n_g\}$), based on the continuity of g_p, uniform continuity of $g_{m,k,i}$ and $\nabla g_{m,k,i}$, and the first-order matching in A7. □

Remark 4: Uniform continuity of π_m A continuous function is uniformly continuous on a compact set (Theorem 4.19 in [27]), so π_m is also uniformly continuous on $\mathcal{U}$.

Like in Section 4.2.3, we now define the criticality measure for the plant optimization problem. Consider the relaxed plant problem (79) of the original problem (2).

$$
\begin{aligned}
\min_s \quad & \phi_p(u_k + s) \\
\text{s.t.} \quad & g_p(u_k + s) \leq \max\left(g_p(u_k), 0\right)
\end{aligned}
\tag{79}
$$

Replacing its constraint using a quadratic upper bound function, problem (79) becomes problem (80).

$$
\begin{aligned}
\min_s \quad & \phi_p(u_k + s) \\
\text{s.t.} \quad & g_{p,i}(u_k) + \nabla g_{p,i}(u_k)^T s + \frac{1}{2}\beta_c s^T s \leq \max\left(g_{p,i}(u_k), 0\right), i = 1, \cdots, n_g
\end{aligned}
\tag{80}
$$

Problem (80) can be regarded as a parametric optimization problem with parameter u_k. Denote the $\chi(s)$ and $\pi(s)$ criticality measure of problem (80) at $s = 0$ as $\chi_p(u_k)$ and $\pi_p(u_k)$, respectively.

Definition 5: Criticality measure $\chi_p(u_k)$. $\chi_p(u_k)$ is the value function of optimization problem (81).

$$\begin{aligned} \chi_p(u_k) &\overset{def}{=} -\min_d \nabla\phi_p(u)^T d \\ \text{s.t.} \quad g_{p,i}(u_k) + \nabla g_{p,i}(u_k)^T d + \frac{1}{2}\beta_c d^T d &\le \max(g_{p,i}(u_k), 0), i = 1, \cdots, n_g \\ d^T d &\le 1 \end{aligned} \tag{81}$$

Definition 6: Criticality measure $\pi_p(u_k)$. Criticality measure $\pi_p(u_k)$ is derived from $\chi_p(u_k)$.

$$\pi_p(u_k) \overset{def}{=} \min(1, \chi_p(u_k)) \tag{82}$$

Theorem 9 (Algorithm 4 convergence) *Suppose that A1-A7 hold and Algorithm 4 is applied. Then u_k asymptotically satisfies the plant KKT condition when $k \to \infty$.*

Proof First, we shall show that $c_p(u_k)$ converges to zero when $k \to \infty$. This is identical to Theorem 15.4.6 in [10] despite different notations. Detailed proof using the notation consistent with this paper is available in the supplementary material for readers' convenience.

Second, we shall show that $\lim_{k\to\infty} \pi_p(u_k) = 0$, so that u_k asymptotically satisfies the first-order criticality condition (described in Definition 1) of problem (80).

Given the continuity of π_m analyzed in Lemma 8, with the same approach in Theorem 15.4.10 and Theorem 6.4.6 [10], we have $\lim_{k\to\infty} \pi_m(u_k, n_k) = 0$. Details are available in Lemma A.4 in the supplementary material. Because of A3, A7 and the convergence of $c_p(u_k)$, we have $\|n_k\| \to 0$. Combining Lemma 8, $\|n_k\| \to 0$, and $\lim_{k\to\infty} \pi_m(u_k, n_k) = 0$ gives $\lim_{k\to\infty} \pi_m(u_k, 0) = 0$. In addition, A7 assures that $\pi_p(u_k) = \pi_m(u_k, 0)$. Therefore, $\lim_{k\to\infty} \pi_p(u_k) = 0$ is true.

Last, we shall combine the above two results and complete the proof. Since u_k is a feasible solution to problem (80), $\lim_{k\to\infty} \pi_p(u_k) = 0$ together with the constraint qualification enforced by A4 gives that u_k asymptotically satisfies the KKT condition of problem (80) [29]. Moreover, the KKT conditions of problem (80) and problem (79) are the same at $u = u_k$ due to A7, so u_k also asymptotically satisfies the KKT condition of problem (79).

In addition, since $c_p(u_k)$ converges to zero, $\max(g_{p,i}(u_k), 0) \to 0$ as $k \to 0$ in problem (79), and problem (79) becomes problem (2). Therefore, u_k asymptotically satisfies the KKT condition for plant optimization problem (2). □

4.3 | Relationship with the penalty method

Both the penalty approach and the composite-step approach involve the merit function (11), and a sufficiently large penalty coefficient σ is required to guarantee convergence. However, there are three differences between them. First, σ does not appear in the optimization subproblems in the composite-step method, which avoids potential numerical difficulties due to large σ. Second, the optimization subproblem (16) in the composite-step method is constrained by c_m, which is consistent with most RTO algorithms for constrained problems. Third, by calculating the ratio of δq_k and $\delta f_{m,k}^N$, the update law in Algorithm 5 Step 4 guarantees a large enough penalty coefficient σ for the composite-step method.

5 | CASE STUDIES

The performance of the composite-step trust-region method is illustrated by two case studies. In the first quadratic example, we focus on the global convergence property and algorithm parameter tuning. In the second chemical reactor example, the proposed method is compared to the feasible-side convergence approach. In each iteration of the trust-region algorithms, Step 1 is in the same way as the modifier adaptation method. Trust-region parameters are selected according to [10]. Specifically, we choose $\eta_1 = 0.01$, $\eta_2 = 0.9$, $\gamma_1 = 0.5$, $\gamma_2 = 2$ throughout this section.

5.1 | Quadratic optimization problem

The proposed trust-region algorithm is compared with the standard modifier adaptation method (Algorithm 1) and penalty trust-region method (Algorithm 3). To make it comparable to the trust-region method, we replace the input filtering in Algorithm 1 by the trust-region constraint with trust radius Δ_{max} when solving problem (6). $\Delta_{max} = 2$ and $\Delta_0 = 1$. Global convergence of the proposed algorithm and the influence of σ and ξ are studied.

5.1.1 | Problem description

In the first example, we consider a quadratic plant problem (83).

$$\begin{aligned} \min_{u_1,u_2} \quad & u_1^2 + u_2^2 + u_1 u_2 \\ s.t. \quad & 1 - u_1 + u_2^2 + 2u_2 \leq 0 \end{aligned} \tag{83}$$

In RTO, oscillation is often due to model inadequacy, especially when the model has wrong curvature (second-order derivatives) in the objective function or the constraints. In this case study, three models with different structural mismatches are considered. The first model optimization problem (84) ignores the bilinear term in the objective function and the u_2 term in the constraint. In contrast, the other two problems (85) and (86) have the wrong curvature in the cost function and the constraint, respectively.

$$\begin{aligned} \min_{u_1,u_2} \quad & u_1^2 + u_2^2 \\ s.t. \quad & 1 - u_1 + u_2^2 \leq 0 \end{aligned} \tag{84}$$

$$\begin{aligned} \min_{u_1,u_2} \quad & -u_1^2 + u_2^2 \\ s.t. \quad & 1 - u_1 + u_2^2 \leq 0 \end{aligned} \tag{85}$$

$$\begin{aligned} \min_{u_1,u_2} \quad & u_1^2 + u_2^2 \\ s.t. \quad & 1 - u_1 - 4u_2^2 \leq 0 \end{aligned} \tag{86}$$

5.1.2 | Global convergence

In this subsection, we show that the proposed algorithm converges even when the objective and constraints curvatures of the model are wrong. The three model optimization problems (84)-(86) are investigated. Simulations begin at a feasible point $[2, -2]$. Algorithm 1 and 5 are studied. For the composite-step method, the composite-step parameter $\xi = 0.5$, the initial penalty coefficient $\sigma_0 = 1$.

As Figure 2 shows, the proposed composite-step algorithm converges to the plant optimum in all three scenarios, while the modifier adaptation method fails to find the optimum with the wrong curvature model. For both methods, the model's KKT condition matches the plant's. However, the second-order sufficient optimality condition may be violated for the modifier adaptation method due to the wrong curvature of the model. On the contrary, the trust-region framework lowers the requirement for model adequacy and converges to the plant optimum.

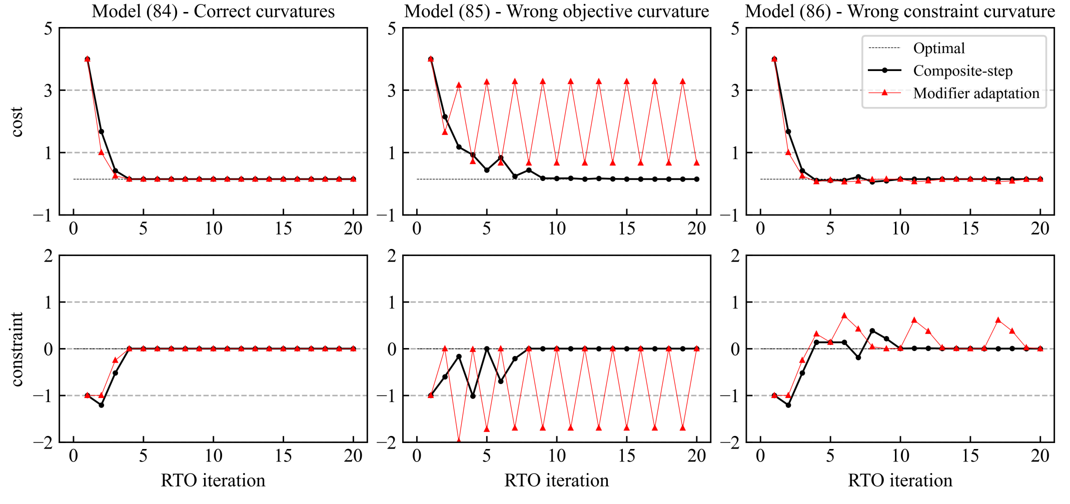

FIGURE 2 Iteration profiles under model mismatch

5.1.3 | Composite-step parameter

The composite-step parameter ξ determines the step size ratio of the normal step (improves feasibility) and the tangential step (improves cost function). In theory, if the iterations remain feasible for the plant, then the penalty method and Algorithm 5 with different ξ will produce the same input sequence if every subproblem has a unique global optimum. This subsection investigates how ξ affects performance starting from an infeasible point $[-1, 0]$. Other algorithm parameters are the same as in the previous subsection.

Figure 3 shows the input variable using Algorithm 5 with $\xi = 0.3, 0.6, 0.9$ and the penalty method. The infeasibility for the first iteration decreases when ξ increases. When the composite-step parameter is small, finding a feasible point usually takes more iteration, and the convergence could be slow.

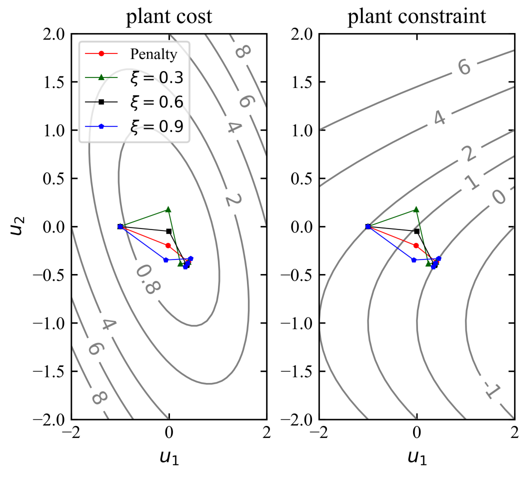

FIGURE 3 Influence of composite-step parameter ξ

5.1.4 | Penalty coefficient

In this subsection, we investigate the effect of a small σ on the penalty and the composite-step trust-region algorithms. RTO problem (86) from the starting point $[2, -2]$ is considered. Algorithm 3, 4, and 5 using different σ are studied. Other simulation settings are the same as the Section 5.1.2.

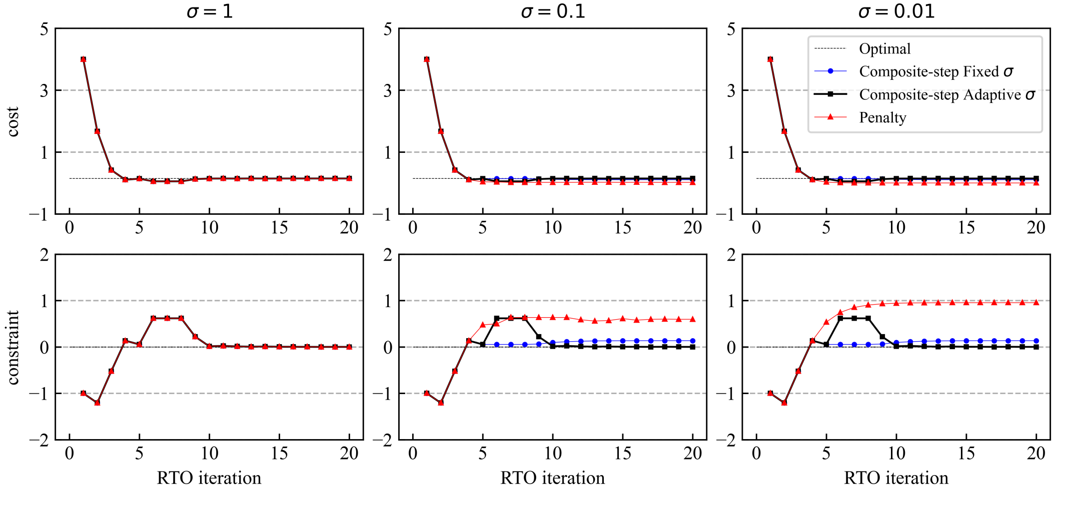

FIGURE 4 Influence of penalty coefficient

As Figure 4 shows, all methods converge to the optimum with $\sigma_0 = 1$. However, with smaller σ, the penalty method significantly violates the inequality constraints. The composite-step method with fixed σ violates the plant constraint to a lesser degree. The reason is that the composite-step method explicitly imposes the model constraint.

The composite-step method with adaptive σ converges to the plant optimum in all cases. In the last two scenarios, σ_k converges to 1.29 in the end. Algorithm 5 may yield large σ during the iteration. However, as σ only appears when evaluating the trial point in Eq. (75), not in solving optimization subproblems (15) or (16), it does not suffer from ill-conditioned optimization subproblems due to a large σ. If a very large σ is used in the penalty method, ill-conditioned problem could occur.

5.2 | William-Otto reactor

Trust-region optimization and feasible-side convergence (e.g., [21]) are two typical approaches to ensure global convergence in RTO. This subsection compares these two approaches using a chemical engineering example.

5.2.1 | Problem description

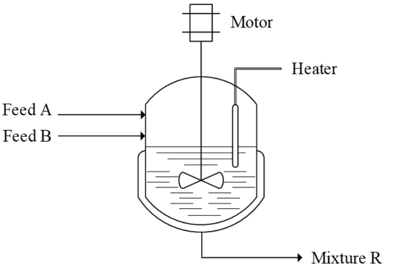

FIGURE 5 William-Otto Reactor

The case study is from [21]. It consists of an ideal continuous stirred tank reactor (CSTR) in which the following reactions occur:

$$\begin{aligned}
&A + B \xrightarrow{k_1} C && k_1 = 1.660\times10^6 exp(-666.4/T_R)\\
&B + C \xrightarrow{k_2} P + E && k_2 = 7.212\times10^8 exp(-8333.3/T_R)\\
&P + C \xrightarrow{k_3} G && k_3 = 2.675\times10^{12} exp(-11111/T_R)
\end{aligned}$$

Reactants A and B are fed with the mass flowrates F_A and F_B, respectively. The reactor mass holdup is fixed at 2105 kg. The manipulated variables are the flowrates of both reactants and the reactor temperature, $u = (F_A, F_B, T_R)$. Input bounds are $F_A \in [3, 4.5]$, $F_B \in [6, 11]$, and $T_R = [80, 105]$. The five output variables are the mass fraction $x_\cdot$ of components A, B, E, P, and G. The optimization problem is Eq. (87). The constraint on the concentration of G is active at the plant optimum.

$$\begin{aligned}
\min_{F_A, F_B, T_R} \ & \phi = -1143.38 x_P F_R - 25.92 x_E F_R + 76.23 F_A + 114.34 F_B \\
s.t. \quad & g = x_G - 0.08 \leq 0
\end{aligned} \tag{87}$$

It is assumed that the reaction scheme is not well understood, and plant-model mismatch is caused by neglecting the intermediate product C. The mismatched model has two reactions:

$$
\begin{aligned}
&A + 2B \xrightarrow{k_1'} P + E \qquad k_1' = 2.19 \times 10^8 exp(-8.08 \times 10^3 / T_R) \\
&A + B + P \xrightarrow{k_2'} G \qquad k_2' = 4.31 \times 10^{10} exp(-1.24 \times 10^4 / T_R)
\end{aligned}
$$

The measurements are assumed to be noise-free, and the plant gradients can be measured directly. RTO iteration begins from a plant-feasible point $u = [3.6, 10, 85]^T$, which is assumed to be the operating set point before RTO implementation. Input variables are normalized by their range. Output variables are scaled by $\overline{\phi} = \phi/10$, and $\overline{g} = g/0.1$.

Three algorithms are compared in the case study: standard modifier adaptation (Algorithm 1), feasible-side-convergent modifier adaptation [21], and the proposed method (Algorithm 5). For the standard adaptation method, the filter coefficient is $K = 0.5$. For the feasible-side-convergent modifier adaptation method, [21] shows that by adding suitable quadratic terms in the cost and constraint functions, the model optimization problem becomes convex, and the modifier adaptation method with filter coefficient $K = 1$ is globally convergent from the feasible side. The suggested convex problem is Eq. (88). For Algorithm 5, $\Delta_0 = 0.1$, $\Delta_{max} = 0.5$, $\xi = 0.5$, $\sigma_0 = 100$.

$$
\begin{aligned}
\min_{F_A, F_B, T_R} \ &\phi = -1143.38 x_P F_R - 25.92 x_E F_R + 76.23 F_A + 114.34 F_B + 74.38 \left[(F_A - F_{A,0})^2 + (F_B - F_{B,0})^2 + (T_R - T_{R,0})^2 \right] \\
s.t. \quad &x_G - 0.08 + 0.0563 \left[(F_A - F_{A,0})^2 + (F_B - F_{B,0})^2 + (T_R - T_{R,0})^2 \right] \leq 0
\end{aligned} \tag{88}
$$

5.2.2 | Simulation results

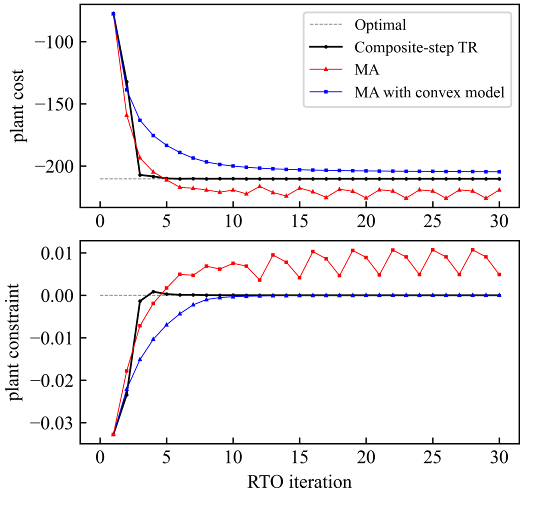

FIGURE 6 Iteration profile of the William-Otto reactor example

The profile of input and output variables are illustrated in Figure 6. The following remarks can be made.

- Convergence. The composite-step trust-region method converges to the plant optimum. Standard MA diverges due to an inadequate model. The oscillation can be reduced by decreasing the filter coefficient, but it can hardly be completely avoided. The feasible-side MA method converges to the plant optimum judged by the plant constraint. However, there is a bias in the plant cost due to its slow convergence rate near the optimum.

- Speed. The composite-step trust-region method is faster than the feasible-side MA method. The feasible-side MA method converge slowly because the model becomes very conservative with the additional quadratic terms.
- Constraint violation. As its name suggests, all iterates of feasible-side MA remain feasible for the plant. The reason is that the cost and constraint functions of the model are convex upper-bounding functions of the plant. The composite-step trust-region method slightly violates the purity constraint at iteration 4.
- Algorithm assumptions. The feasible-side MA method requires two assumptions that the trust-region method does not need. First, u_0 needs to be feasible. Second, at each RTO iteration, the model cost and constraint functions are strictly convex upper-bounding functions of the plant counterparts, which is fulfilled by carefully choosing the quadratic term based on the Hessian upper bound of the plant.

In conclusion, both the trust region and the feasible-side convergence approach are globally convergent regardless of an inadequate model. The trust-region approach is faster and needs less prior knowledge about the plant, but it may violate the plant constraints before convergence. The feasible-side convergence approach is better for dealing with hard constraints. However, it is usually slow and the additional quadratic term make the model less precise.

6 | CONCLUSION

This paper proposes a novel composite-step trust-region algorithm that handles plant-model mismatches for constrained RTO problems. The global convergence property is proved by establishing lower bounds on feasibility improvement and the cost function reduction in each iteration. The composite-step approach is free of numerical problems caused by a large penalty coefficient in the merit function. Adaptive penalty coefficient is discussed to ensure the equivalence of the first-order criticality condition of the plant and the merit function. Numerical simulations show the proposed method is globally convergent and reduces model adequacy requirements. It is faster than the feasible-side convergence approach at the cost of slightly violating the inequality constraints.

Data Availability and Reproducibility Statement

The numerical data from Figures 2, 3, 4, and 6 are tabulated in the Supplementary Material.

Supplementary Material

(1) Relevant lemmas in [10] used by Theorem 9. (2) Numerical data for case studies. The python codes implementing the numerical case studies are available on GitHub (https://github.com/WheatZhang/RTOdemo/tree/master/example/TR).

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