A Quadratic Approximation-Based Algorithm for the Solution of Multiparametric Mixed-Integer Nonlinear Programming Problems

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An algorithm for the solution of convex multiparametric mixed-integer nonlinear programming problems arising in process engineering problems under uncertainty is introduced. The proposed algorithm iterates between a multiparametric nonlinear programming subproblem and a mixed-integer nonlinear programming subproblem to provide a series of parametric upper and lower bounds. The primal subproblem is formulated by fixing the integer variables and solved through a series of multiparametric quadratic programming (mp-QP) problems based on quadratic approximations of the objective function, while the deterministic master subproblem is formulated so as to provide feasible integer solutions for the next primal subproblem. To reduce the computational effort when infeasibilities are encountered at the vertices of the critical regions (CRs) generated by the primal subproblem, a simplicial approximation approach is used to obtain CRs that are feasible at each of their vertices. The algorithm terminates when there does not exist an integer solution that is better than the one previously used by the primal problem. Through a series of examples, the proposed algorithm is compared with a multiparametric mixed-integer outer approximation (mp-MIOA) algorithm to demonstrate its computational advantages.
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Introduction

Many process engineering problems, and in particular those encountered in the field of chemical engineering, are complex and often non-linear. They involve two types of decisions: (1) discrete decisions — those which define a specific (optimal) structure of the underlying system and (2) continuous decisions — those which optimize its operation. Typical examples include synthesis problems in chemical process design, and production planning and scheduling of multiproduct batch plants among others. These types of problems can be approached very efficiently via mathematical programming techniques such as mixed-Integer nonlinear programming (MINLP).[1] On the other hand, the inevitable presence of fluctuations in some process variables such as demand, prices, or quality in raw materials, and the lack of exact knowledge of certain parameters such as kinetic data or physical properties require that uncertainty be taken into account in MINLP process models. As a result, various approaches which address the uncertainty in MINLP models have been proposed[2]: stochastic programming,[3] fuzzy programming,[4] and robust optimization.[5]

Recently, Pistikopoulos and coworkers[6–8] have shown that process engineering problems under uncertainty can also be addressed via multiparametric mixed-integer nonlinear programming (mp-MINLP). Acevedo and Pistikopoulos[6] proposed a mp-MINLP algorithm based on the Outer Approximation/equality relaxation algorithm of Kocis and Grossmann.[9] Dua and Pistikopoulos[7] proposed three mp-MINLP algorithms based on the reformulation of a master problem using (1) deterministic, (2) outer-approximation (OA), and (3) generalized benders decomposition (GBD) principles. Nevertheless, while these algorithms proved to be successful they remained computationally intensive.

In this work, we present a novel mp-MINLP algorithm for the solution of process engineering problems under uncertainty. The algorithm is based on a decomposition strategy where a sequence of multiparametric nonlinear programming (mp-NLP) (primal) subproblems and deterministic MINLP (master) subproblems are solved. Since the solution of primal subproblems is the most expensive step of mp-MINLP algorithms, we propose a multiparametric quadratic approximation (mp-QA) algorithm for the solution of primal subproblems. To reduce the computational effort involved when infeasible vertices are encountered in the critical regions (CRs) found by the primal subproblem, a simplicial approximation approach is used to explicitly characterize sections of the constrained and parameter space that are feasible. This article is organized as follows. We first present the motivation for this work and point out some of the limitations of current mp-MINLP algorithms. Then, we introduce a novel multiparametric mixed-integer quadratic approximation algorithm (mp-MIQA) for the solution of mp-MINLP problems. A series of example problems are then presented to illustrate the proposed algorithm. Finally, we conclude with some final remarks.

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mp-MINLP Algorithms—Earlier Developments

Consider the following mp-MINLP problem

$$\begin{aligned} z(\theta) = \quad & \min_{x,y} d^T y + f(x) \\ \text{s.t.} \quad & Ey + g(x) \leq b + F\theta \\ & \mathbf{x} \in X \subseteq R^n \\ & y \in Y \subseteq \{0,1\}^m \\ & \theta \in \Theta \subseteq R^p \end{aligned} \tag{1}$$

where y is a vector of 0-1 binary variables, x is a vector of continuous variables, and θ is a vector of parameters. f is a scalar objective function and g is a vector of constraints, both continuously differentiable and convex in x. b and d are constant vectors and E and F are constant matrices.

For mp-MINLP problems of the form of Eq. 1, Dua and Pistikopoulos[7] proposed a multiparametric mixed-integer outer approximation (mp-MIOA) algorithm. The algorithm followed a decomposition procedure where the mp-MINLP problem was decomposed into two subproblems: a "primal" and a "master." The primal subproblem was obtained by fixing the integer variables (e.g., $y = \bar{y}$) and solving the resulting multiparametric nonlinear programming (mp-NLP) problem via OA.[9] The solution procedure for the primal subproblem was then reduced to solving a series of relaxed multiparametric linear programming (mp-LP) problems

$$\begin{aligned} \check{z}(\theta) = \quad & \min_{x} d^T \bar{y} + f(x^*) + \nabla_x f(x^*)(x - x^*) \\ \text{s.t.} \quad & g(x^*) + \nabla_x g(x^*)(x - x^*) \leq b + F\theta - E\bar{y} \\ & x \in X \subseteq R^n \\ & \theta \in \Theta \subseteq R^p \end{aligned} \tag{2}$$

The solution of Eq. 2 provided parametric upper bounds for the solution of Eq. 1. Subsequently, parametric solutions were compared and the greatest of the solutions was retained. As a result of these comparisons, the parameter space was partitioned into multiple regions (these regions are commonly called CRs in the multiparametric programming literature[8]) where each of the linear parametric solutions are valid. The procedure then continued until a prespecified approximation tolerance for the optimal value function was satisfied.

For the solution of the master subproblem, three formulations were proposed (Table 1) based on (1) deterministic, (2) OA, (3) and GBD principles. While the deterministic formulation led to a standard MINLP problem, the OA and GBD formulations corresponded to multiparametric mixed-integer linear programming (mp-MILP) problems.[10] In all cases, the solution of the master subproblem produced the next integer vector for the primal subproblem. For the cases where a different integer vector was identified inside a given CR, linear parametric profiles corresponding to two different integer vectors were, again, compared and the CR further partitioned.

One of the drawbacks of the algorithm proposed by Dua and Pistikopoulos[7] is that it may require many iterations to converge to a solution, mainly due to expensive comparisons between parametric solutions derived at various linearization points. Moreover, comparison procedures performed in the primal subproblem causes the original parameter space to be partitioned and, thus, increase the number of CRs produced by the primal subproblem. This is, of course, not desirable since the CRs produced by the primal subproblem have to be examined later during the solution of the master subproblem. This implies that a large number of MINLP/mp-MILP problems may need to be solved. Similarly, comparison procedures between parametric profiles with different integer solutions (master subproblem) contribute to the exponential growth (due to linearizations) in the number of the CRs that need to be examined. As in the primal case, this results in an increase on the overall number of MINLP/mp-MILP subproblems that need to be solved. The following sections illustrate these issues.

Table 1. Mathematical Formulations for Master Subproblem Presented in the work of Dua and Pistikopoulos[7]

Deterministic

$$\begin{aligned} \check{z}(\theta) = & \min_{x,y,\theta} d^T y + f(\mathbf{x}) \\ \text{s.t.} \quad & Ey + g(x) \leq b + F\theta \\ & d^T y + f(x) \leq \check{z}_i(\theta) \\ & \sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \leq |J^{ik}| - 1, \quad k = 1, \ldots K^i \\ & x \in X \subseteq R^n \\ & y \in Y \subseteq \{0,1\}^m \\ & \theta \in CR_i \end{aligned}$$

OA

$$\begin{aligned} \check{z}(\theta) = & \min_{x,y,\mu} d^T y + \mu \\ \text{s.t.} \quad & \mu \geq f(x^v) + \nabla_x f(x^v)(x - x^v) \\ & g(x^v) + \nabla_x g(x^v)(x - x^v) \leq b + F\theta - Ey \\ & \sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \leq |J^{ik}| - 1, \quad k = 1, \ldots K^i \\ & x \in X \subseteq R^n \\ & y \in Y \subseteq \{0,1\}^m \\ & \theta \in CR_i \end{aligned}$$

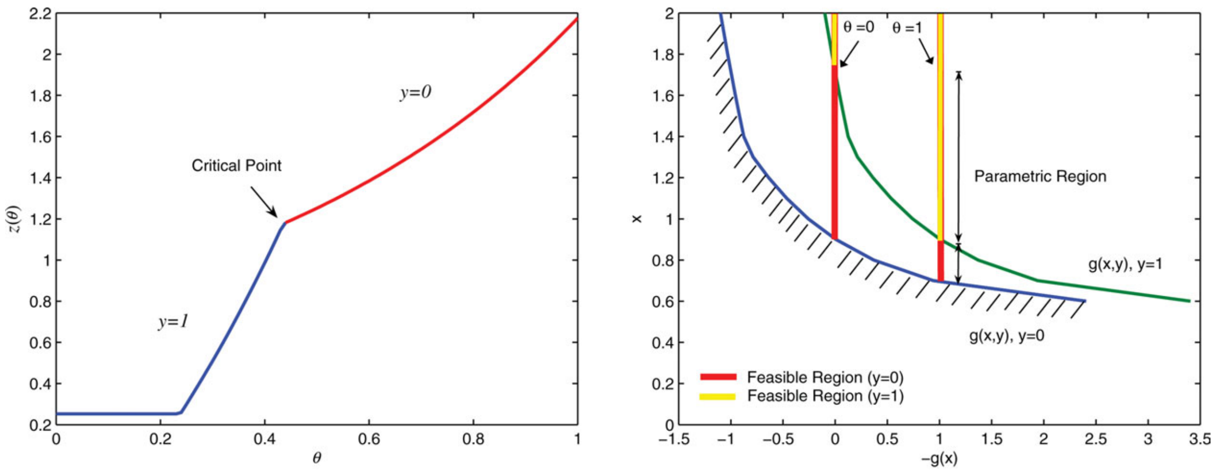
GBD

$$\begin{aligned} \check{z}(\theta) = & \min_{y,\mu} \mu \\ \text{s.t.} \quad & \mu \geq d^T y + f(x^v) + \lambda^T [Ey + g(x^v) - b - F\theta] \\ & 0 \geq \lambda^T [Ey + g(x^v_{feas}) - b - F\theta \\ & \sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \leq |J^{ik}| - 1, \quad k = 1, \ldots K^i \\ & x \in X \subseteq R^n \\ & y \in Y \subseteq \{0,1\}^m \\ & \theta \in CR_i \end{aligned}$$

Motivating example

Example 1*. The following example illustrates how the mp-MIOA algorithm of Dua and Pistikopoulos[7] can become computationally expensive even for small problems. The problem is given by*

$$\begin{aligned} z(\theta) = \min_{x,y} \quad & -2.7y + x^2 \\ \text{s.t.} \quad & g_1(x) = \log(1 + x) - y \geq 0 \\ & g_2(x) = \log(x - 0.57) - y + 1.1 \geq \theta \\ & 0 \leq x \leq 2 \\ & 0 \leq \theta \leq 1 \\ & y \in \{0,1\} \end{aligned} \tag{3}$$



(a) (b)

Figure 1. Optimal value function (a) and feasible and parametric regions (b) for Example 1.

Note that $g(x)$ is taken as $\min(g_1(x), g_2(x))$. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where the parameter is present in the right hand side of one of the constraints. The optimal value function, $z(\theta)$, and the feasible and parametric regions are shown in Figure 1. It can be observed that the feasible region is discontinuous and that the optimal integer solution changes at the critical point, $\theta^* \approx 0.45$.

Consider an approximation tolerance of $\epsilon = 0.02$. To initialize the mp-OA algorithm, the MINLP problem in Eq. 3 is solved considering θ as an additional optimization variable. The optimal solution is obtained at $(x^*, y^*, \theta^*) = (1.7183, 1, 0)$ with an optimal value function $\bar{z} = 0.252$. At this point, the integer value is fixed with $\bar{y} = 1$ and the objective function and constraints are linearized. The following relaxed primal subproblem is then formulated at the first iteration

$$
\begin{aligned}
\check{z}(\theta) = \min_x \quad & 3.436x - 5.647 && \text{(linearization at } x^* = 1.718\text{)} \\
\text{s.t.} \quad & 0.367x \geq 0.637 && \text{(linearization of } g_1 \text{ at } x^* = 1.718\text{)} \\
& 0.870\,x \geq 1.263 + \theta && \text{(linearization of } g_2 \text{ at } x^* = 1.718\text{)} \\
& 0 \leq x \leq 2 \\
& 0 \leq \theta \leq 1
\end{aligned}
\tag{4}
$$

As Eq. 4 is a relaxation to the original primal subproblem, the solution of Eq. 4 provides a parametric solution that underestimates the value function and overestimates the parametric region of Eq. 3 for fixed $\bar{y} = 1$, as shown in Figure 2. The optimal solution of Eq. 4 is given by the parametric linear functions: $\check{z}_1(\theta) = 0.252$ $\forall \theta \in [0, 0.245]$ and $\check{z}_2(\theta) = 3.946\,\theta - 0.687$ $\forall \theta \in [0.245, 0.478]$.

To verify the accuracy of the linear approximations, all vertices of the CRs generated are checked where it is identified that the vertex point $\theta = 0.478$ is infeasible. A feasibility problem[7] is formulated and solved. The solution of the feasibility problem provides the feasible point $(x^*, \theta^*) = (2, 0.457)$ for the next iteration. At iteration 2, the objective function and constraints are linearized at the point obtained and the following mp-LP problem is formulated

$$
\begin{aligned}
\check{z}(\theta) = \min_x \quad & 4x - 6.7 && \text{(linearization at } x^* = 2\text{)} \\
\text{s.t.} \quad & 0.333\,x \geq 0.568 && \text{(linearization of } g \text{ at } x^* = 2\text{)} \\
& 0.699\,x \geq 0.940 + \theta && \text{(linearization of } g_2 \text{ at } x^* = 2\text{)} \\
& 0 \leq x \leq 2 \\
& 0 \leq \theta \leq 1
\end{aligned}
\tag{5}
$$

The solution of Eq. 5 provides the second set of parametric solutions for Eq. 3: $\check{z}_1(\theta) = 0.116$ $\forall \theta \in [0, 0.250]$ and $\check{z}_2(\theta) = 5.72\,\theta - 1.317$ $\forall \theta \in [0.250, 0.457]$ (Figure 3a). Following the steps of the mp-OA algorithm, parametric solutions $\check{z}_1(\theta)$ and $\check{z}_2(\theta)$ are then compared and the tightest lower bound is retained. As a result of this comparison, the parameter space of Eq. 3 is partitioned into Eq. 4 CRs (Figure 3b) and the parametric solution is updated as follows

$$
y = 1 \begin{cases}
\check{z}_1(\theta) = 0.252 & \forall \theta \in [0.000, 0.238] (\mathrm{CR}_1) \\
\check{z}_2(\theta) = 3.946\theta - 0.687 & \forall \theta \in [0.238, 0.351] (\mathrm{CR}_2) \\
\check{z}_3(\theta) = 4.914\theta - 1.028 & \forall \theta \in [0.351, 0.359] (\mathrm{CR}_3) \\
\check{z}_4(\theta) = 5.720\theta - 1.317 & \forall \theta \in [0.359, 0.457] (\mathrm{CR}_4)
\end{cases}
$$

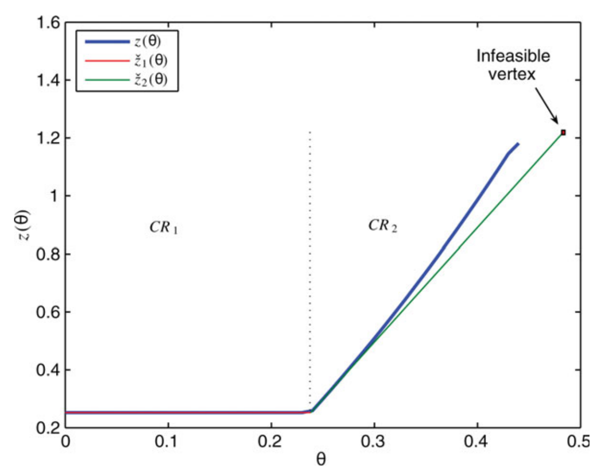


Figure 2. Parametric solution for Example 1 at the first iteration.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

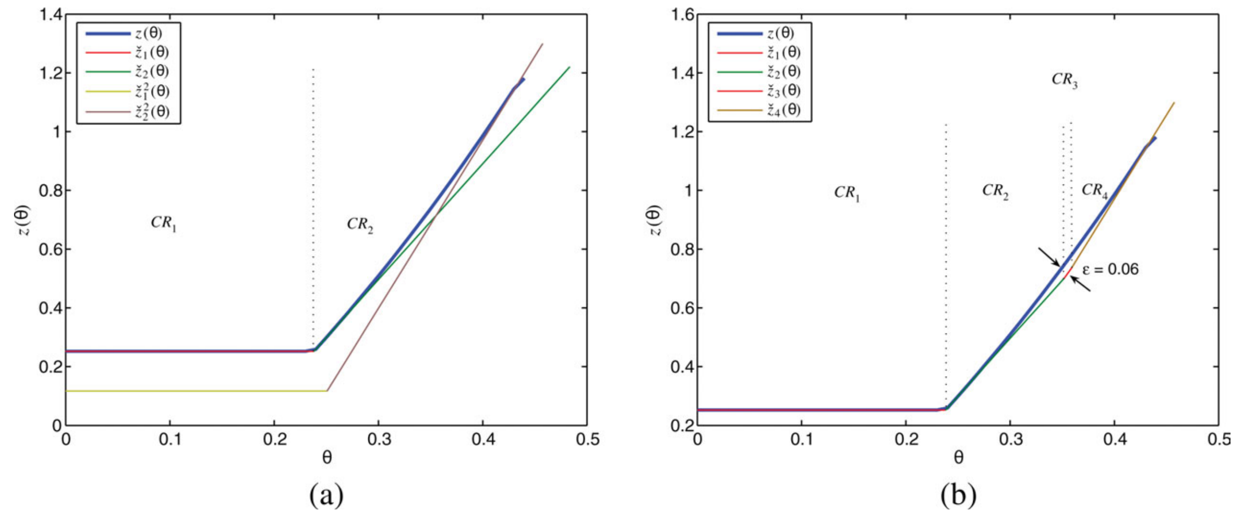


Figure 3. Partition of the parameter space before (a) and after (b) comparison procedure.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Again, the accuracy of the approximations are verified by evaluating the value function and its linear approximation at each vertex of the CRs generated. For the updated parametric solution, the maximum error of approximation is found to be $\epsilon = 0.06$ in CR_3. Since the approximation error is greater than the approximation tolerance imposed, the algorithm continues further partitioning the parameter space. The parametric solution for the first identified integer solution, ($\bar{y} = 1$), is given by the following parametric profiles (Figure 4a)

$$y = 1 \begin{cases} \check{z}_1(\theta) = 0.252 & \forall\theta \in [0.000, 0.238](CR_1) \\ \check{z}_2(\theta) = 3.946\theta - 0.687 & \forall\theta \in [0.238, 0.244](CR_2) \\ \check{z}_3(\theta) = 3.995\theta - 0.700 & \forall\theta \in [0.244, 0.245](CR_3) \\ \check{z}_4(\theta) = 4.029\theta - 0.708 & \forall\theta \in [0.245, 0.305](CR_4) \\ \check{z}_5(\theta) = 4.484\theta - 0.847 & \forall\theta \in [0.305, 0.307](CR_5) \\ \check{z}_6(\theta) = 4.824\theta - 0.951 & \forall\theta \in [0.307, 0.361](CR_6) \\ \check{z}_7(\theta) = 4.877\theta - 0.970 & \forall\theta \in [0.361, 0.411](CR_7) \\ \check{z}_8(\theta) = 5.355\theta - 1.167 & \forall\theta \in [0.411, 0.413](CR_8) \\ \check{z}_9(\theta) = 5.720\theta - 1.317 & \forall\theta \in [0.413, 0.457](CR_9) \\ z_{\inf}(\theta) = \infty & \forall\theta \in [0.457, 1.000](CR_{\inf}) \end{cases} \tag{6}$$

For each of the CRs generated in Eq. 6 (the solution of the primal subproblem), a MINLP/mp-MILP is formulated as indicated in Eq. 1. A feasible solution $y = 0$ is found in CR_9 and the infeasible region, $CR_{\inf}$. For CR_9 a new primal subproblem is then solved to give the parametric solution $\check{z}_{10}(\theta) = 1.117\theta + 0.6896$. Since two parametric solutions are valid in the same region, $\check{z}_9(\theta)$ and $\check{z}_{10}(\theta)$ are compared to retain the tightest bound. As a result of the comparison, CR_9 is split into two further regions (Figure 4b)

$$\begin{array}{ll} y = 1 & \{\check{z}_9(\theta) = 5.720\theta - 1.317 \quad \forall\theta \in [0.413, 0.436](CR_9) \\ y = 0 & \{\check{z}_{10}(\theta) = 1.117\theta + 0.6896 \quad \forall\theta \in [0.436, 0.457](CR_{10}) \end{array} \tag{7}$$

Using the integer solution $y = 0$, another primal subproblem is formulated and solved in the infeasible region, $CR_{\inf} = \forall\theta \in [0.457, 1.000]$. The following parametric profiles are obtained by applying the mp-OA algorithm to the primal subproblem

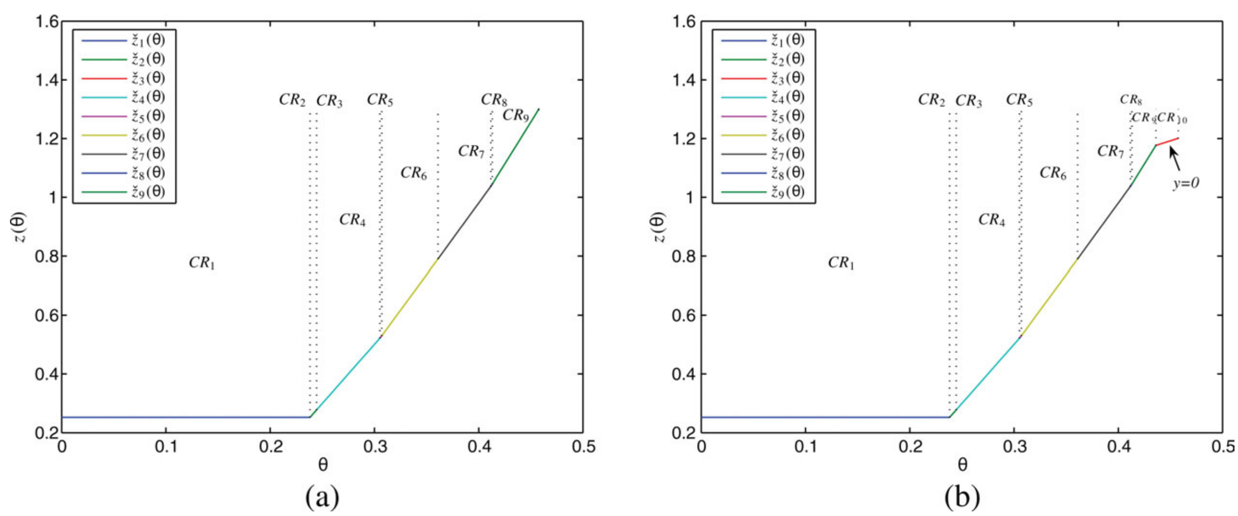


Figure 4. Parametric solution for Example 1 for $\bar{y} = 1$ and $\epsilon = 0.02$.

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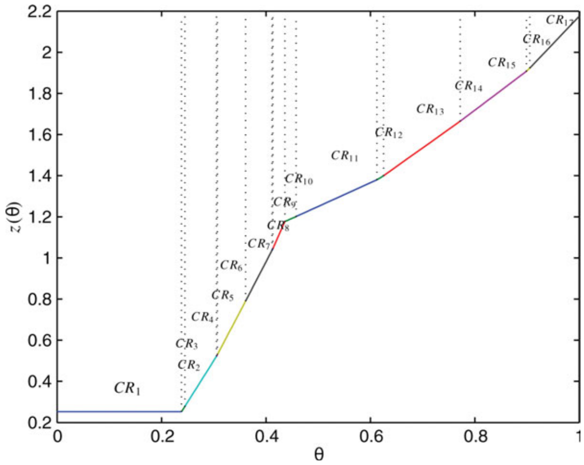


Figure 5. Final partition of parameter space in Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

$$y = 0 \begin{cases} \check{z}_{11}(\theta) = 1.153\theta + 0.672 & \forall\theta \in [0.457, 0.612](\mathrm{CR}_{11}) \\ \check{z}_{12}(\theta) = 1.154\theta + 0.430 & \forall\theta \in [0.612, 0.625](\mathrm{CR}_{12}) \\ \check{z}_{13}(\theta) = 1.180\theta + 0.270 & \forall\theta \in [0.625, 0.772](\mathrm{CR}_{13}) \\ \check{z}_{14}(\theta) = 1.874\theta + 0.217 & \forall\theta \in [0.772, 0.773](\mathrm{CR}_{14}) \\ \check{z}_{15}(\theta) = 1.914\theta + 0.186 & \forall\theta \in [0.773, 0.898](\mathrm{CR}_{15}) \\ \check{z}_{16}(\theta) = 2.359\theta - 0.213 & \forall\theta \in [0.898, 0.905](\mathrm{CR}_{16}) \\ \check{z}_{17}(\theta) = 2.668\theta - 0.493 & \forall\theta \in [0.905, 1.000](\mathrm{CR}_{17}) \end{cases} \tag{8}$$

The final partition of the parameter space is shown in Figure 5 with parametric solutions given by Eqs. 6–8.

For this example, the mp-MIOA algorithm requires the solution of 20 MINLPs, 39 NLPs, and nine mp-LPs. Table 2 shows the computational burden of the mp-MIOA algorithm for various approximation tolerances imposed. Clearly, the amount of computation increases as tighter approximations are imposed.

A Novel mp-MINLP Algorithm—Recent Developments

Consider the mp-MINLP problem in Eq. 1.

Primal subproblem

An initial feasible point (x^*, y^*, θ^*) can be obtained by solving Eq. 1 considering θ as additional optimization variables. A second-order approximation of the objective function and an outer approximation of the constraints in Eq. 1 can then be constructed in the continuous space by fixing the integer variables at the integer solution obtained (i.e., $\bar{y} = y^*$). A multiparametric quadratic programming (mp-QP) problem can then be formulated as follows

$$\begin{aligned} z_Q(\theta) = \quad & \min_x d^T\bar{y} + f(x^*) + \nabla_x f(x^*)(x - x^*) + \tfrac{1}{2}\nabla_x^2 f(x^*)(x - x^*)^2 \\ \text{s.t.} \quad & g(x^*) + \nabla_x g(x^*)(x - x^*) \le b + F\theta - E\bar{y} \\ & x \in X \subseteq R^n \\ & \theta \in \Theta \subseteq R^p \end{aligned} \tag{9}$$

where $\nabla_x f$ and $\nabla_x^2 f$ represent the Jacobian and Hessian with respect to the objective function, respectively, and $\nabla_x g$ represent the Jacobian of the constraints.

The solution of Eq. 9 can be obtained using, for instance, the algorithm of Dua et al.[11] However, because Eq. 9 is a relaxation of Eq. 1 for a fixed y, its approximation will be only valid in the neighborhood of x^*. As a result, some parametric solutions and their corresponding CRs obtained by solving Eq. 9 with a single point of approximation, may result in ‘‘poor’’ solutions in some parts of the parameter space.

In our previous work,[12] we proposed a partitioning procedure that tried to reduce the approximation error produced by the quadratic approximation in Eq. 9. The procedure was based on the partitioning of those CRs that did not meet the approximation tolerance imposed. For a given region in which the quadratic approximation produced large errors, the approximation was updated by performing another QA at the centre of the CR and then solving the corresponding mp-QP problem in that region. As a result of the new approximation, some CRs were split into sub-regions and the QA was improved. In this work, we propose an alternative strategy for the solution of the primal subproblem.

Successive Quadratic Approximation. The idea of this strategy is to successively construct quadratic approximations (QA) of the original problem while exploring the parameter space. The solution set of the mp-NLP problem is then characterized by a collection of parametric solutions derived by solving mp-QP subproblems at various points of the parameter space. We denote mp-QA as the algorithm resulting from this strategy.

Consider a local second-order approximation to Eq. 1 for fixed y

$$\begin{aligned} z_Q(\theta) = \quad & \min_x \quad \tfrac{1}{2}x^TQx + c^Tx + e \\ & \text{s.t.} \quad Ax \le b' + F\theta \\ & \qquad x \in X \\ & \qquad \theta \in \Theta \end{aligned} \tag{10}$$

where $Q_{n\times n}$, $c_{n\times 1}$, $e_{1\times 1}$, are defined as follows

$$\begin{aligned} Q &= \nabla_x^2 f(x^*) \\ c &= \nabla_x^T f(x^*) - \nabla_x^2 f(x^*)x^* \\ e &= f(x^*) - \nabla_x f(x^*)x^* + \frac{1}{2}x^{*T}\nabla_x^2 f(x^*)x^* + d^T\bar{y} \\ A &= \nabla_x g(x^*) \\ b' &= b - g(x^*) + \nabla_x g(x^*)x^* - E\bar{y} \end{aligned}$$

Dua et al.[11] and Bemporad et al.[13] showed that, under certain conditions, a continuous optimizer can be obtained from the Karush–Kuhn–Tucker (KKT) optimality conditions of 10

$$\left.\begin{aligned} Qx + A^T\lambda = 0 \\ \lambda_i(A_ix - b'_i - F_i\theta) = 0 \\ Ax - b' - F\theta \le 0 \\ \lambda_i \ge 0 \end{aligned}\right\} \quad \forall i = 1, .., q \tag{11}$$

where λ are the Lagrange multipliers.

Table 2. Computational Bourden of mp-MIOA Algorithm on the Motivating Example for Various ϵ Values

Subproblems	$\epsilon \le 0.5$	$\epsilon \le 0.1$	$\epsilon \le 0.05$	$\epsilon \le 0.02$	$\epsilon \le 1e^{-3}$
MINLPs	10	13	18	20	60
NLPs	17	23	38	39	132
mp-LPs	5	7	9	9	15
CPU(s)	3.6	4.22	6.10	6.47	20.71

Let $\mathcal{A}$ be an optimal active set for some $\theta \in \Theta$. If the constraint gradients of A are linearly independent (i.e., linear independence constraint qualification is satisfied), then the conditions in Eq. 11 can be manipulated so as to give the following affine functions

$$\begin{aligned} x(\theta) &= -Q^{-1}A_{\mathcal{A}}^T\lambda_{\mathcal{A}} \\ \lambda(\theta) &= -(A_{\mathcal{A}}Q^{-1}A_{\mathcal{A}}^T)^{-1}(b'_{\mathcal{A}} + F_{\mathcal{A}}\theta) \end{aligned} \tag{12}$$

It can be shown[11,13] that the above affine functions remain optimal in a CR of the parameter space which is polyhedral. Such a region can be derived by imposing feasibility and optimality restrictions as follows

$$\mathrm{CR} = \Delta\left\{\theta \in \theta \;\middle|\; \begin{array}{l} A_{\mathcal{I}}x^{\mathcal{A}}(\theta) \le b'_{\mathcal{I}} + F_{\mathcal{I}}\theta \\ \lambda_{\mathcal{A}}(\theta) \ge 0 \end{array}\right\} \tag{13}$$

where $\mathcal{I}$ is the index set of inactive inequalities and Δ is an operator which removes redundant constraints.[14]

The approximation in Eq. 10 is valid, however, only in the neighborhood of x^* and in approximate region of the parameter space defined by Eq. 13. On the other hand, because the CR obtained with the local approximation is polyhedral, this polyhedral property allows us to explore the rest of the parameter space by following an exploration procedure similar to the one presented in our previous work.[15]

The strategy can be briefly summarized as follows: Choose a parameter $\theta \in \Theta$. Solve an NLP to find an initial point of approximation. At the solution point obtained, perform a QA and solve the corresponding mp-QP problem. The solution of this problem will provide a parametric solution, $z(\theta)$, and a corresponding CR where it is valid. With the CR obtained proceed to divide the rest of the parameter reversing one by one each of the inequalities which characterize the newly found CR. Finally, successively subdivide the rest of parameter space in a similar way.

Handling Infeasibility in CRs. Because of the nonlinearity of the constraints some parts of the CRs generated by the mp-QA algorithm may result infeasible. In this section, we propose two strategies to alleviate this situation.

Removal of Infeasible Regions by Minimization of Constraint Violations (Vertex-based mpQA). As shown in the work of Dua and Pistikopoulos,[7] sections of the CRs that are infeasible can be eliminated by identifying feasible points that minimize the constraint violations of a multiparametric program. Such points can be obtained by solving the following NLP problem at each infeasible vertex of the CRs obtained

$$\begin{aligned} \min_{x,\theta} \quad & \sum \delta^2 \\ \text{s.t.} \quad & g(x) \le b + F\theta - E\bar{y} \\ & \delta = \theta - \theta_{\inf}^v \\ & x \in X \\ & \theta \in \mathrm{CR}_i \end{aligned} \tag{14}$$

where $\theta_{\inf}^v$ corresponds to an infeasible vertex and δ is a vector of free variables.

Points of maximal discrepancies where $|z(\theta^v) - z_Q^i(\theta^v)| > \epsilon$, that is, points where the difference between the value function and its QA is maximal, can also be identified and recorded. The above points can then be used in a new QA subproblem to improve the quality of the solution as follows

$$\begin{aligned} z_Q(\theta) = \min_{x,\mu} \quad & \tfrac{1}{2}x^TQx + \mu \\ \text{s.t.} \quad & Ax \le b' + F\theta \\ & g(x^l) + \nabla_x g(x^l)(x - x^l) \le b + F\theta - E\bar{y} \quad \forall l \in L \\ & f(x^w) + \nabla_x f(x^w)(x - x^w) \le \mu \quad \forall w \in W \\ & x \in X \\ & \theta \in \Theta \end{aligned} \tag{15}$$

where $l \in L$ are the index set of the feasible points found in Eq. 14 and $w \in W$ are the index set of points in X with maximum discrepancy.

Explicit Representation of Feasible space via Simplicial Approximation (Simplicial based mpQA). On the other hand, due to the nonlinearity of the constraints, a large number of feasibility NLP subproblems may need to be solved, which may increase the computational burden of the of the proposed algorithm. To alleviate this limitation, we propose to explicitly characterize the sections of the constrained and parametric spaces that are feasible before applying the mp-QA algorithm. The simplicial approximation approach (see Goyal and Ierapetritou[16,17] and Appendix A) allows one to obtain such feasible representation of both the constrained and parametric regions within a tolerance imposed, δr. By obtaining an explicit feasible representation of both the constrained and parametric regions a priori, computational savings can be made since the repetitive solution of NLP feasibility subproblems at infeasible vertices can be avoided.

The following mp-QP can then be formulated

$$\begin{aligned} z_Q(\theta) = \min_{x} \quad & \tfrac{1}{2}x^TQx + c^Tx + e \\ \text{s.t.} \quad & Ax \le b' + F\theta \\ & Ch(x, y, \theta, \epsilon) \le 0 \\ & x \in X \\ & \theta \in \Theta \end{aligned} \tag{16}$$

where $Ch(x,\ y,\ \theta,\ \epsilon)$ is a reduced set of convex hull outer approximating constraints which are linearizations of the active constraints at simplicial points.

As the simplicial approximation approach is used to derive the parametric solutions for the mp-NLP subproblem, we will hereto refer to the Simplical mp-QA as the implementation derived from this strategy.

Remark 1. *Note that the solution obtained with both strategies results in a collection of convex piecewise quadratic (PWQ) functions of the parameters θ. This set of PWQ functions, although continuous inside each CR, may, however, be discontinuous between neighboring regions as a result of quadratic approximations.*

Master subproblem

In this section, two deterministic MINLPs formulations are proposed for obtaining new integer vectors for subsequent iterations of the algorithm.

Master Subproblem—Deterministic Formulation. The following master problem can be derived following the arguments established in the work of Dua and Pistikopoulos[7]

$$\begin{aligned} \bar{z}(\theta) = \min_{x,y,\theta} \quad & d^Ty + f(x) \\ \text{s.t.} \quad & Ey + g(x) \le b + F\theta \\ & d^Ty + f(x) - z_Q^{ik}(\theta) \le 0, \quad k = 1, \ldots K^i \\ & \textstyle\sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \le |J^{ik}| - 1, \quad k = 1, \ldots K^i \\ & x \in X \subseteq R^n \\ & y \in Y \subseteq \{0,1\}^m \\ & \theta \in \mathrm{CR}_i \end{aligned} \tag{17}$$

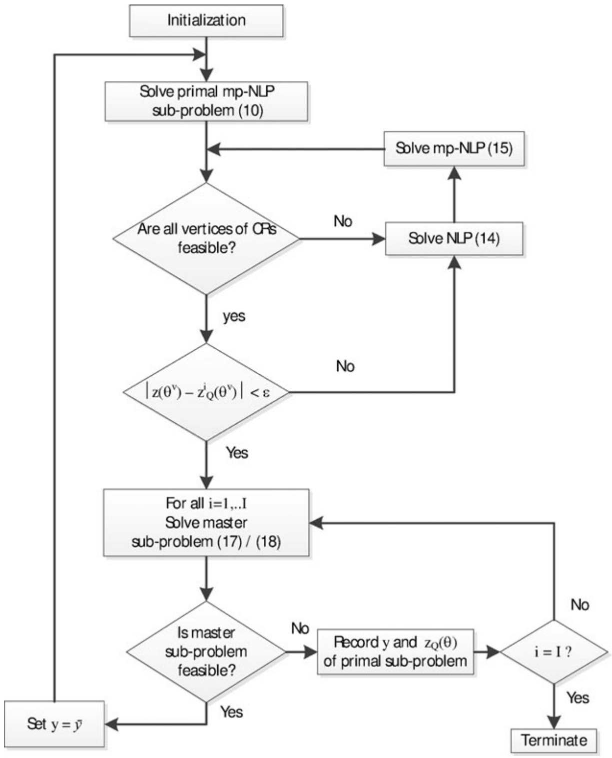


Figure 6. Vertex-based mpMIQA algorithm.

where $J^{ik} = (j|y_j^{ik} = 1)$ and $L^{ik} = (j|y_j^{ik} = 0)$, $|J^{ik}|$ is the cardinality of J^{ik} and K^i is the number of integer solutions that have been analyzed in CR_i. The inequalities $f(x,y) - z_Q^{ik}(\theta) \leq 0$ and $\sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \leq |J^{ik}| - 1$ correspond to parametric and integer cuts respectively. While the former constraint restricts the solution of Eq. 17 from taking on values which are higher than the current upper bound, $z_Q^{ik}(\theta)$, the latter, restricts Eq. 17 from taking on integer values that have already been analyzed.

Master Subproblem—Deterministic Formulation 2. The following master subproblem can also be derived by directly using the explicit solution obtained in the QA algorithm

$$\begin{aligned}
\bar{z}(\theta) = \min_{x,y,\theta} \quad & d^T y + f(x) \\
\text{s.t} \quad & Ey + g(x) \leq b + F\theta \\
& d^T y + f(x) - f(x(\theta), y)^{ik} \leq 0, \\
& \textstyle\sum_{j \in J^{ik}} y_j^{ik} - \sum_{j \in L^{ik}} y_j^{ik} \leq |J^{ik}| - 1, \quad k = 1, \ldots K^i \\
& x \in X \subseteq R^n \\
& y \in Y \subseteq \{0,1\}^m \\
& \theta \in \mathrm{CR}_i
\end{aligned} \tag{18}$$

Note that in the above formulations, the master subproblem is solved for each CR_i and θ is treated as a decision variable bounded by the constraints that define CR_i. The solution of Eq. 18 will provide the next integer solution for which to solve the next primal subproblem. If the solution of Eq. 18 results in an infeasible solution, the proposed algorithm then continues with the rest of the regions. The algorithms stops until the master subproblem is infeasible in all of the CRs generated by the primal subproblem.

Remark 2. *The formulations in* 17 *and* 18 *are non-convex mixed-integer nonlinear optimization problems, with the source of non-convexity being the term $z_Q^{ik}(\theta)$. Accordingly, their solution requires a global optimization procedure, e.g., Baron*[18] *or α-BB.*[19] *Alternatively, a presolve test*[11] *can be used to determine the next integer solution and, therefore, to avoid the issue of global optimization.*

The mp-MIQA Algorithm

Based on the above results, the main steps of the proposed algorithm can be summarized as follows (see the corresponding flowcharts in Figures 6 and 7):

Step 0 (Initialization). *Set the parametric upper bound $z(\theta)$, to a large value (i.e., $z(\theta) = \infty$), the integer variable to an initial value (i.e, $y = \bar{y}$) and define an initial CR CR_I and an approximation tolerance ϵ for which to solve the mp-MINLP problem.*

Successive quadratic approximation (vertex based)

Step 1 (Primal Subproblem). *Solve the mp-NLP problem* 10 *and proceed to explore the parameter space using the strategy described in the previous section. For each of vertices of the CRs, compute the optimal value function, $z(\theta)$, and its QA, $z_Q(\theta)$. If for some θ, $|z(\theta^v) - z_Q^i(\theta^v)| > \epsilon$ or the NLP for fixed θ is infeasible, take the corresponding values in X and solve Eq.* 15. *The repetitive solution of Eq.* 15 *over the parameter space will provide a set of parametric expressions, $z_Q(\theta)$ and the regions, CR_i $\forall i \in I$ where they are valid.*

Successive quadratic approximation (simplicial based)

Step 1 (Primal Subproblem). *Using a simplicial approximation approach, obtain an explicit representation of the feasible constrained and parametric spaces. Substitute the inequalities in Eq.* 1 *by the polytopical convex hull outer approximations and proceed to solve the mp-NLP problem* 16.

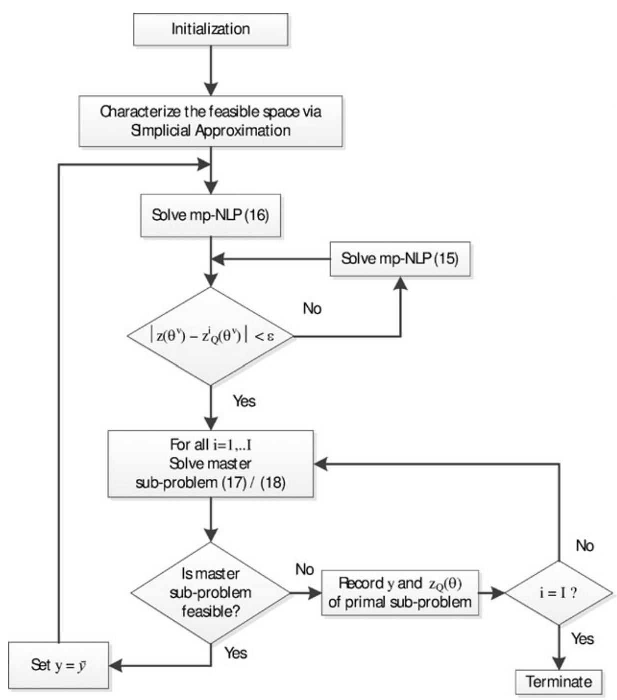


Figure 7. Simplicial-based mpMIQA algorithm.

Deterministic master subproblem 1 and 2

Step 2 (Master Subproblem). *For each of the CRs generated in the primal subproblem, formulate and solve the deterministic (MINLP) master subproblem* 17 *or* 18 *by (1) treating θ as optimization variable, (2) introducing integer and parametric cuts. Return to Step 1 with the new integer solution and the corresponding region.*

Step 3 (Convergence). *The algorithm terminates when master subproblems* 17 *or* 18 *result in infeasible solutions in all the CRs. The final solution is given by a collection of parametric, $z_Q(\theta)$, and integer solutions, y, obtained in each region.*

Remark 3. *Note that, at the moment, it is not possible to compare nonlinear (quadratic) parametric profiles. As a result, comparison procedures between parametric solutions of two integer vectors are not performed. Instead, parametric solutions corresponding to different integer vectors are retained to form an envelope of parametric expressions.*[11] *The optimal solution for a given point in the parameter space is obtained by evaluating the corresponding parametric expressions and taking the minimum of them on-line.*

With the steps of the algorithm formally introduced, in the next section the proposed algorithm is illustrated with a series of example problems.

Example Problems

Example 1

Consider the motivating example 3 for which an approximation tolerance of $\epsilon = 0.02$ was used.

Vertex-Based Implementation

Primal Subproblem. The mp-QA algorithm starts by computing an initial point of approximation. Again, the point $(x^*, y^*, \theta^*) = (1.718,\ 1{,}0)$ with optimal value function $z = 0.252$ is selected to initialize the algorithm. The integer variable is fixed to the solution point obtained, that is, $\bar{y} = 1$, the objective function is quadratically approximated and the constraints are linearized thus leading to the following mp-QP problem

$$\begin{aligned} z_Q(\theta) = \min_x \quad & x^2 - 2.7 && \text{(QA at } x^* = 1.718) \\ \text{s.t.} \quad & 0.367x \geq 0.637 && \text{(linearization of } g_1 \text{ at } x^* = 1.718) \\ & 0.870x \geq 1.263 + \theta && \text{(linearization of } g_2 \text{ at } x^* = 1.718) \\ & 0 \leq x \leq 2 \\ & 0 \leq \theta \leq 1 \end{aligned} \tag{19}$$

The optimal solution of Eq. 19 near $\theta = 0$ is given by $z_Q^1(\theta) = 0.252\ \forall\theta \in [0{,}0.238]$. The value function and its quadratic approximation are then checked at each vertex of the CRs and the maximum error is found to be $\epsilon = 1e^{-6}$. Since the maximum approximation error is less than the tolerance imposed, the algorithm continues exploring the rest of the parameter space. Note that QA provides and exact characterization of the CR as compared to the OA where it is over estimated at the first iteration.

Following the procedure described in Section 3.1.1, the parameter space is further divided. The rest of the parameter space is then defined as $CR_{Rest} = \theta \in [0.238{,}1]$. A second point in CR_{Rest}, $\theta = 0.3$, is chosen to perform the next QA. An NLP is solved at this point to give $x^* = 1.791$ as the point for the next approximation. Again, another mp-QP similar to Eq. 10 is formulated and solved to give $z_Q^2(\theta) = 1.491\ \theta^2 + 3.480\theta - 0.670\ \forall\theta \in [0.238{,}0.470]$ as the next parametric solution. All vertices are checked and the point $\theta = 0.470$ is found to be infeasible. A feasibility problem of the form of Eq. 14 is solved to give the point $(\theta^*, x^*) = (0.457{,}1.999)$ as feasible solution. The following mp-QP is then formulated

$$\begin{aligned} z_Q(\theta) = \min_x \quad & x^2 - 2.7 && \text{(QA at } x^* = 1.791) \\ \text{s.t.} \quad & 0.358x \geq 0.615 && \text{(linearization of } g_1 \text{ at } x^* = 1.791) \\ & 0.818x \geq 1.166 + \theta && \text{(linearization of } g_2 \text{ at } x^* = 1.791) \\ & 0.334x \geq 0.570 && \text{(linearization of } g_1 \text{ at } x^* = 1.999) \\ & 0.704x \geq 0.951 + \theta && \text{(linearization of } g_2 \text{ at } x^* = 1.999) \\ & 0 \leq x \leq 2 \\ & 0 \leq \theta \leq 1 \end{aligned} \tag{20}$$

The solution of Eq. 20 results in $z_Q^2(\theta) = 1.491\theta^2 + 3.480\theta - 0.670$ with an updated CR $\forall\theta \in [0.238{,}0.376]$. Each of the vertices are checked and the maximum error is found to be $\epsilon = 0.02$. Since the maximum error is less than the specified tolerance imposed, the parametric solution is recorded and the algorithm continues exploring the rest of parameter space. Using the solution obtained, the rest of the parameter space is then divided as $CR_{Rest} = \theta \in [0.376{,}1]$. Another mp-QP is then solved in the region $\theta \in [0.376{,}1]$, to give $z_Q^3(\theta) = 2.03\theta^2 + 3.831\ \theta - 0.876\ \forall\theta \in [0.376{,}0.457]$ respectively. Again, the accuracy of the QA is checked by computing the error at each of the vertices of the CRs generated. The maximum error is found in CR_3 with $\epsilon = 0.02$. The following parametric profile characterizes the solution of the primal subproblem at the first integer solution, $\bar{y} = 1$

$$y = 1 \quad \begin{cases} z_Q^1(\theta) = 0.252 & \forall\theta \in [0.000, 0.238](CR_1) \\ z_Q^2(\theta) = 1.491\theta^2 + 3.480\theta - 0.670 & \forall\theta \in [0.238, 0.376](CR_2) \\ z_Q^3(\theta) = 2.013\theta^2 + 3.831\theta - 0.876 & \forall\theta \in [0.376, 0.457](CR_3) \\ z_Q^{\inf}(\theta) = \infty & \forall\theta \in [0.457, 1.000](CR_{\inf}) \end{cases} \tag{18}$$

Master Subproblem. For each of the CRs generated in Eq. 21, deterministic master MINLP subproblems of the form of Eqs. 17–18 are formulated and solved. For instance, for CR_i, $i = 1,..,3$ the following deterministic MINLP problems are solved

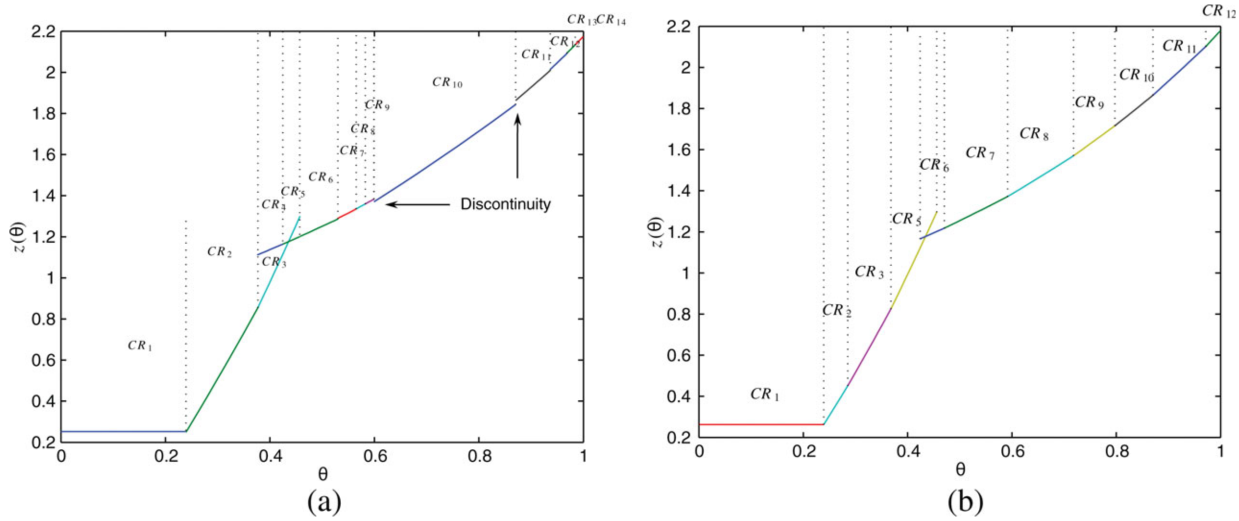


Figure 8. mp-MIQA Parametric solution for Example 1.

(a) Vertex based and (b) Simplicial-based implementations. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

$$
\begin{aligned}
\bar{z}(\theta) = \min_{x,y,\theta} \quad & -2.7y + x^2 \\
\text{s.t.} \quad & \log(1+x) - y \geq 0 \\
& \log(x-0.57) - y + 1.1 \geq \theta \\
& -2.7y + x^2 - z_Q^i(\theta) \leq 0, \quad \forall i = 1, ..3 \\
& y \leq 0 \\
& 0 \leq x \leq 2 \\
& \theta \in \mathrm{CR}_i \\
& y \in \{0,1\}
\end{aligned}
\tag{22}
$$

The solution of Eq. 22 is infeasible in CR_1 and CR_2. For regions, CR_3 and $\mathrm{CR}_{\mathrm{inf}}$, the solution of the master subproblem gives $y = 0$ as the next integer solution. At this point, a new primal subproblem is formulated and solved. The following parametric solutions are obtained in CR_3

$$
y = 0
$$
$$
\begin{cases}
z_Q^4(\theta) = 0.257\theta^2 + 0.876\theta + 0.745 & \forall\theta \in [0.376, 0.424](\mathrm{CR}_4) \\
z_Q^5(\theta) = 0.260\theta^2 + 0.879\theta + 0.743 & \forall\theta \in [0.424, 0.457](\mathrm{CR}_5)
\end{cases}
\tag{23}
$$

Similarly, the following parametric solutions are obtained in $\mathrm{CR}_{\mathrm{inf}}$

$$
y = 0
$$
$$
\begin{cases}
z_Q^6(\theta) = 0.277\theta^2 + 0.899\theta + 0.731 & \forall\theta \in [0.457, 0.530](\mathrm{CR}_6) \\
z_Q^7(\theta) = 0.319\theta^2 + 0.945\theta + 0.698 & \forall\theta \in [0.530, 0.565](\mathrm{CR}_7) \\
z_Q^8(\theta) = 0.343\theta^2 + 0.966\theta + 0.680 & \forall\theta \in [0.563, 0.582](\mathrm{CR}_8) \\
z_Q^9(\theta) = 0.355\theta^2 + 0.976\theta + 0.670 & \forall\theta \in [0.582, 0.599](\mathrm{CR}_9) \\
z_Q^{10}(\theta) = 0.476\theta^2 + 1.044\theta + 0.573 & \forall\theta \in [0.599, 0.870](\mathrm{CR}_10) \\
z_Q^{11}(\theta) = 0.631\theta^2 + 1.069\theta + 0.452 & \forall\theta \in [0.870, 0.936](\mathrm{CR}_{11}) \\
z_Q^{12}(\theta) = 0.721\theta^2 + 1.059\theta + 0.389 & \forall\theta \in [0.936, 0.968](\mathrm{CR}_{12}) \\
z_Q^{13}(\theta) = 0.769\theta^2 + 1.047\theta + 0.356 & \forall\theta \in [0.968, 0.984](\mathrm{CR}_{13}) \\
z_Q^{14}(\theta) = 0.798\theta^2 + 1.040\theta + 0.340 & \forall\theta \in [0.984, 1.000](\mathrm{CR}_{14})
\end{cases}
\tag{24}
$$

The application of the vertex-based mp-MIQA algorithm required the solution of 15 mp-QPs, 21 NLPs, and 13 MINLPs requiring a total solution time of 8.25 CPU s. From this, we can see that a lot of the computational effort involved in the mp-MIQA algorithm is due to the computation of NLP feasibility subproblems at the vertices of the CRs. In the next section, we show how the amount of computations can be reduced using a simplicial-based implementation.

Simplicial-Based Implementation. For the application of the simplicial-based mp-MIQA algorithm, we can take advantage of the fact that the integer variables appear linearly in the constraints. Accordingly, we can apply the simplicial approximation approach directly to the constraints in Example 1 before attempting to solve the problem.

Using a radius tolerance of $\delta r = 1e^{-3}$, the application of the simplicial approximation approach to Example 1 results in the following convex-hull outer approximating constraints

$$
\begin{array}{rcr}
-0.904x + 0.301y + 0.301\theta & \leq & -0.816 \\
-0.680x + 0.517y + 0.517\theta & \leq & -0.477 \\
-0.567x + 0.582y + 0.582\theta & \leq & -0.250 \\
-0.496x + 0.613y + 0.613\theta & \leq & -0.090 \\
-0.647x + 0.538y + 0.538\theta & \leq & -0.414 \\
-0.580x + 0.573y + 0.573\theta & \leq & -0.289 \\
-0.736x + 0.478y + 0.478\theta & \leq & -0.579 \\
-0.810x + 0.413y + 0.413\theta & \leq & -0.699 \\
-0.604x + 0.563y + 0.563\theta & \leq & -0.328 \\
-0.597x + 0.566y + 0.566\theta & \leq & -0.313 \\
-0.812x + 0.412y + 0.412\theta & \leq & -0.701 \\
-0.516x + 0.605y + 0.605\theta & \leq & -0.137 \\
-0.785x + 0.437y + 0.437\theta & \leq & -0.660 \\
-0.700x + 0.504y + 0.504\theta & \leq & -0.516 \\
-0.455x + 0.629y + 0.629\theta & \leq & 0.007 \\
-0.345x + 0.938y & \leq & 0.344
\end{array}
\tag{25}
$$

$$
\begin{aligned}
0 \leq x \leq 2 \\
0 \leq y \leq 1 \\
0 \leq \theta \leq 1
\end{aligned}
\tag{26}
$$

The characterization of feasible parameter space then requires 29 two-dimentional (2-D)-line searches and the solution six NLP subproblems. Note that the polytopical convex-hull approximations in 25–26 correspond to outer approximations of

Table 3. Parametric Solutions of Example 2

y	mp-MIOA $z(\theta)$	CR
$y = 0$	$0.821\ \theta + 2.467$	$\forall\ \theta \in [0.000, 0.167]$
	$1.129\ \theta + 2.416$	$\forall\ \theta \in [0.167, 0.184]$
	$1.279\ \theta + 2.388$	$\forall\ \theta \in [0.184, 0.344]$
	$1.347\ \theta + 2.364$	$\forall\ \theta \in [0.344, 0.345]$
	$1.380\ \theta + 2.353$	$\forall\ \theta \in [0.344, 0.479]$
	$1.705\ \theta + 2.197$	$\forall\ \theta \in [0.479, 0.487]$
	$1.910\ \theta + 2.097$	$\forall\ \theta \in [0.487, 0.648]$
	$2.179\ \theta + 1.923$	$\forall\ \theta \in [0.648, 0.652]$
	$2.370\ \theta + 1.798$	$\forall\ \theta \in [0.652, 0.863]$
	$3.156\ \theta + 1.120$	$\forall\ \theta \in [0.863, 0.879]$
	$3.954\ \theta + 0.418$	$\forall\ \theta \in [0.879, 1.000]$
y	Simplicial mp-MIQA $z_Q(\theta)$	CR
$y = 0$	$0.142\ \theta^2 + 0.825\ \theta + 2.480$	$\forall\ \theta \in [0.000, 0.184]$
	$0.237\ \theta^2 + 1.019\ \theta + 2.441$	$\forall\ \theta \in [0.184, 0.260]$
	$0.369\ \theta^2 + 1.118\ \theta + 2.388$	$\forall\ \theta \in [0.260, 0.464]$
	$0.477\ \theta^2 + 1.237\ \theta + 2.342$	$\forall\ \theta \in [0.464, 0.588]$
	$0.727\ \theta^2 + 1.238\ \theta + 2.255$	$\forall\ \theta \in [0.588, 0.714]$
	$0.932\ \theta^2 + 1.189\ \theta + 2.185$	$\forall\ \theta \in [0.714, 0.793]$
	$1.075\ \theta^2 + 1.120\ \theta + 2.150$	$\forall\ \theta \in [0.793, 0.866]$
	$1.435\ \theta^2 + 0.774\ \theta + 2.181$	$\forall\ \theta \in [0.866, 0.967]$
	$1.878\ \theta^2 + 0.341\ \theta + 2.184$	$\forall\ \theta \in [0.967, 1.000]$

the feasible space. Accordingly, to prevent infeasibilities of parametric solutions, we convert the convex-hull outer approximations into inner ones by substracting a small number $\epsilon_s = 1e^{-3}$ (see Dominguez and Pistikopoulos, in preparation).

With the explicit representation of the feasible space already obtained, we are now in the position to solve Example 1. First, we note that the objective function is quadratic; therefore, substituting the nonlinear constraints by their convex-hull outer approximations transforms Example 1 into a mp-MIQP problem, the solution of which can be obtained by applying the algorithm of Dua et al.[11] The solution of Example 1 using a simplicial-based approach then requires the solution of 1 mp-MIQP problem, including the execution of a Simplicial Approximation algorithm, with a total execution time of 0.172 s.

Figure 8 shows the final parametric solution obtained with both implementations of the mp-MIQA algorithm. We note that the parametric solution obtained with the vertex-based implementation in CR_9 is discontinuous. On the other hand, the Simplicial-based approach produces parametric solutions that are continuous over the entire parametric range. Indeed, this is expected since the objective function is quadratic in the continuous variable and linear in the integer variable. Replacing the nonlinear constraints by their polytopical approximations transforms the mp-MINLP problem into an mp-MIQP problem, the solution of which is continuous over the entire parameter space.

Comparing the performance of both the mp-MIQA and mp-MIOA algorithms, we note that both implementations of the mp-MIQA algorithm produced fewer CRs (14 and 12) than the mp-MIOA, which produced 17 CRs, using the same approximation tolerance imposed ($\epsilon = 0.02$).

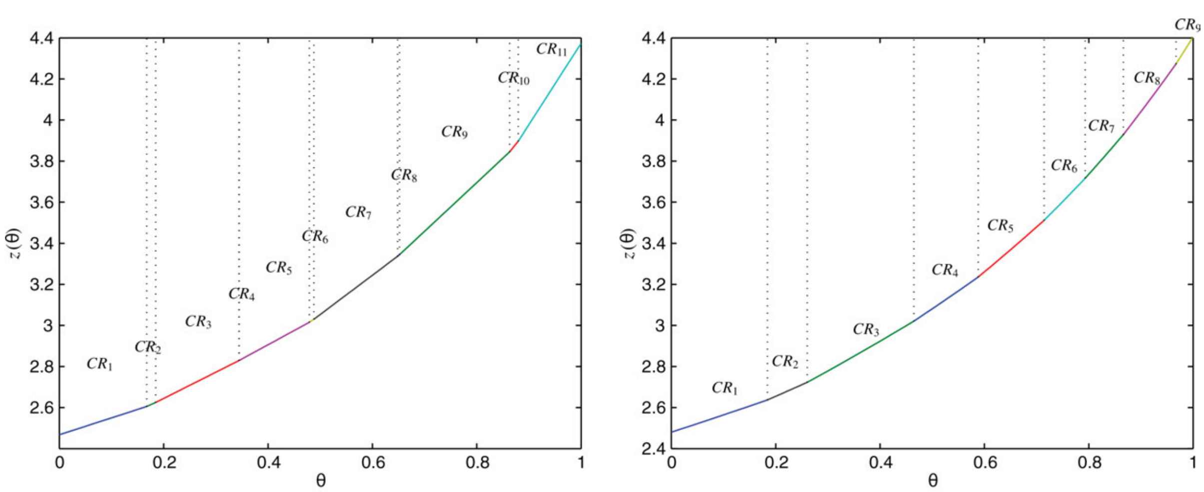
On the other hand, it may be argued that the reason for the simplicial-based implementation of the mp-MIQA algorithm to outperform the mp-MIOA is because the objective function was quadratic and the quadratic approximation is exact in this case. However, numerical tests demonstrate that the simplicial-based implementation of the mp-MIQA algorithm performs well even in the presence of additional nonlinearities in the objective function and constraints. The following example illustrates this case.

Example 2

Consider a modification of the motivating example introduced earlier where the nonlinearity in objective function has been replaced by an exponential function in the continuous variable.

$$\begin{aligned} z(\theta) = \min_{x,y} \quad & -2.7y + \exp(x) \\ \text{s.t.} \quad & \log(1+x) - y \geq 0 \\ & \log(x-0.57) - y + 1.1 \geq \theta \\ & 0 \leq x \leq 2 \\ & 0 \leq \theta \leq 1 \\ & y \in \{0,1\} \end{aligned} \tag{27}$$

Note that since the only the objective function is changed, the feasible and parametric regions of 27 remain exactly the same as those of 3. Accordingly, the inequalities in 25 and 26



(a) (b)

Figure 9. Parametric solutions for Example 2.

(a) mpMIOA and (b) Simplicial mpMIQA. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

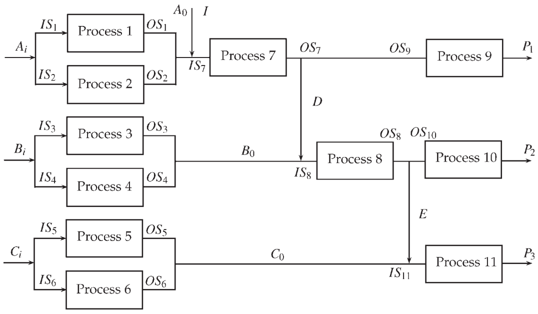


Figure 10. Process flow sheet for Example 3.

are utilized in the derivation of the parametric solutions for this problem.

Table 3 summarizes the results (all within a 2% tolerance), where only one integer solution is feasible. The Simplicial-based mp-MIQA algorithm requires the solution of 11 MINLPs, 15 NLPs, and 10 mp-QPs with a total execution time of 3.38 CPU s. In contrast, the mp-MIOA algorithm requires the solution of 12 MINLPs, 27 NLPs, five mp-LPs with a total execution time of 3.69 CPU s. Note that, in this case, the computational times between the two algorithms differ slightly. This is mainly because, while the mp-MIOA algorithm spends much of the computational effort solving NLP subproblems at the vertices of the CRs, the mp-MIQA algorithm spends much of the computational time solving mp-QP subproblems over the parameter space. This difference, however, becomes more profound as the size of the problem increases as shown in the next example.

Figure 9 depicts the parametric solutions obtained with both the mp-MIOA and Simplicial-based mp-MIQA algorithms. Note that the number of CRs obtained with the Simplicial-based mp-MIQA algorithm is smaller than that of the mp-MIOA algorithm. Clearly, this is an indication that the quadratic approximations closely approximate the optimal value function over larger areas of the parameter space than its counterpart, the linear approximation.

Example 3

The following example is taken from the work of Dua and Pistikopoulos.[7] It involves the design of a chemical plant that can process the optimal amounts of raw materials A, B, and C and an intermediate I despite uncertainty in the demand of three products: P_1, P_2, and P_3. An initial superstructure, including two alternatives for producing each product, is available and is shown in Figure 10. The design problem is mathematically formulated as the following mp-MINLP problem

$$
\begin{aligned}
z(\theta) = \quad & \min \sum_{i=1}^{6} FC_i y_i + \sum_{i=7}^{11} FC_i + \textstyle\sum_{i=1}^{11} OC_i IS_i^2 + 1.2A + 1.5B + 1.8C \\
& -50P_1 - 60P_2 - 68P_3 \\
\text{s.t.} \quad & -IS_i + KC_i \exp(OS_i/PC_i) \le KC_i \quad i=\{1,..,6\} \\
& -PC_i IS_i + OS_i = 0 \quad i=\{1,..,11\} \\
& -MI_i y_i + IS_i \le 0 \quad i=\{1,..,6\} \\
& -A_i + IS_1 + IS_2 = 0 \\
& -A_0 + OS_1 + OS_2 = 0 \\
& -B_i + IS_3 + IS_4 = 0 \\
& -B_0 + OS_3 + OS_4 = 0 \\
& -C_i + IS_5 + IS_6 = 0 \\
& -C_0 + OS_5 + OS_6 = 0 \\
& -IS_7 + A_0 + I = 0 \\
& -OS_7 + D + IS_9 = 0 \\
& -IS8 + D + B_0 = 0 \\
& -OS_8 + E + IS_10 = 0 \\
& -IS_1 + E + C_0 = 0 \\
& A_i \le 1.5, \ \ B_i \le 1.6, \ \ C_i \le 1.7, \\
& OS_9 = P_i = \theta_1, \ \ OS_{10} = P_2 = \theta_2, \ \ OS_{11} = P_3 = \theta_3 \\
& MI_i = \{4, 3, 3.5, 5.5, 7.5, 6, 8, 6, 5, 5, 5\} \\
& PC_i = \{1.8, 2.0, 2.5, 2.2, 2.8, 3.0, 0.65, 0.9, 0.72, 0.68, 0.71\} \\
& KC_i = \{2.0, 2.1, 2.6, 2.1, 2.5, 3.0\} \\
& FC_i = \{1.9, 2.0, 3.0, 3.2, 3.7, 3.9, 1.1, 1.0, 5.0, 5.3, 6.2\} \\
& OC_i = \{1.1, 1.3, 1.6, 1.5, 2.1, 1.9, 1.7, 1.0, 3.0, 3.7, 4.1\}
\end{aligned}
\tag{28}
$$

and involves 41 equations, 31 continuous variables, six binary variables, and three uncertain parameters.

Table 4 shows the parametric solutions obtained with both, the Simplicial-based mp-MIQA and mp-MIOA algorithms. As can be observed, the mp-MIOA algorithm requires two partitions and two integer configurations to characterize the parameter space. In contrast, the mp-MIQA algorithm requires one partition and one integer solution. The difference between the two solutions lies in the fact that the mp-MIOA algorithm requires two linearizations in to approximate the nonlinear value function of the problem. As a result, an additional error is introduced which over estimates the master problem and, thus, identifies an integer solution which is lower than the current one. Note that the objective function in this problem is quadratic and, thus, the quadratic approximation of the value function used by the mp-MIQA algorithm is exact in this case. In terms of the computational effort involved, the mp-MIQA algorithm requires the solution of 93 2-D line searches and 1 mp-MIQP with a total execution time of 4.2 CPU seconds. In contrast, the mp-MIOA requires the solution 4 MINLPs, 16 NLPs, and 2 mp-LPs with an execution time of 5.8 CPU seconds.

All algorithms were coded in MATLAB[20] with an interface to GAMS.[21,22] For the solution of NLP subproblems, the

Table 4. Parametric Solutions of Example 3

y	$z(\theta)$	CR
mpMIOA		
(0,0,1,1,1,1,1,1,1,1,1)	$-28.32\ \theta_1 - 37.91\ \theta_2 - 44.27\theta_3 + 1.23$	$\theta_2 \le 0.8$ $\theta_3 \le 1.1$ $0.8 \le \theta_1 \le 0.85$ $-0.128\ \theta_1 - 0.827\theta_2 - \theta_3 \le -1.838$
(0,0,0,1,1,0,1,1,1,1,1,)	$-26.43\ \theta_1 - 25.74\ \theta_2 - 29.56\ \theta_3 - 25.81$	$0.8 \le \theta_1 \le 0.85$ $0.75 \le \theta_2 \le 1.05$ $1.05 \le \theta_3 \le 1.1$ $0.128\ \theta_1 + 0.827\theta_2 + \theta_3 \le 1.838$
Simplicial mpMIQA		
(0,0,1,1,1,1,1,1,1,1,1)	$13.54\theta_1^2 + 21.41\ \theta_2^2 + 11.14\theta_3 + 9.13\ \theta_1\ \theta_2$ $-63.92\ \theta_1 - 76.38\ \theta_2 - 68.80\ \theta_3 + 39.54$	$0.8 \le \theta_1 \le 0.85$ $0.75 \le \theta_2 \le 1.05$ $1.05 \le \theta_3 \le 1.1$

fmincon solver was used whereas for the solution of MINLP subproblems the BARON solver Sahinidis[18] was used. For the characterization of the feasible constrained and parameter regions, a prototype version of the simplicial approximation algorithm of Goyal and Ierapetritou[17] was coded in MATLAB.

Concluding Remarks

We have presented a multiparametric mixed-integer quadratic approximation algorithm for the solution of mp-MINLP. The proposed algorithm tackles such problems by decomposing them into subproblems which are smaller in size—a primal subproblem which represents a parametric upper bound and a master subproblem which represents a lower bound. The primal subproblem is approached by fixing the binary variables and approximating the nonlinear solution by piecewise quadratic parametric profiles with corresponding regions of optimality obtained through the solution of mp-QP problems. These parametric solutions obtained in the primal subproblem are then utilized in the solution of the master subproblem to determine the next set of integer values for which to solve the primal subproblem. The algorithm terminates when there is no integer solution that is better than the current one in each region (i.e., the master subproblem is infeasible). To avoid the repetitive solution of feasibility subproblems and to improve the computational performance of proposed algorithm when infeasible vertices are encountered in the CRs generated by the solution of the primal subproblem, a simplicial approximation approach was used to generate CRs whose vertices are feasible. Computational studies and comparisons to an earlier algorithm, the mixed-integer outer approximation-based algorithm, were performed using three numerical example problems highlighting the potential of the proposed algorithm.

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Appendix A: Simplicial Approximation Algorithm

The simplicial approximation algorithm[16,17] characterizes the section of the constrained and parametric spaces that is feasible by successively performing polytopical approximations from inside and outside of the joint region using n-dimensional simplicies.

The algorithm proceeds as follows.

1. Perform $2(n+p)$ line searchers in the negative and positive directions to locate points, u_1, u_2,…u_{n+p}, on the boundary of the constrained and parametric regions, $\mathcal{G} \subset R^{n+p}$.

2. Using the points obtained in the previous step, obtain a polyhedral convex hull inner representation of the feasible space, $\mathcal{P}_{\text{inner}}$. The convex hull can be computed using the "Quick Hull Algorithm".[23] The following set of inequalities describing the inner polytope are obtained

$$l_k^T u \le c_k, \quad k = 1, 2, \ldots, K \tag{A1}$$

where l_k is a unit vector normal to the kth hyperplane pointing outwards and c_k is a measure of the distance of the kth hyperplane to the origin.

3. Determine the center of the inner polytope, $\check{u}^*$, by inscribing a hypersphere of maximum radius, $\check{r}$, inside the polytope. Such point can be obtained by solving the following LP[24]

$$\begin{aligned} \check{u}^*, \check{r} = \quad & arg\ \max r \\ \text{s.t.} \quad & l_k^T u + r\|l_i\|_2 \le c_k, \quad k = 1, 2, \ldots, K, \end{aligned} \tag{A2}$$

4. Identify the largest facet in inner polytope by solving K linear programs (LPs) (see Appendix B or a derivation of the procedure)

$$
\begin{aligned}
u_j^*, r = \quad & arg \ \max r \\
\text{s.t.} \quad & l_j^T u_j^* = c_j \\
& l_k^T u_j^* + r_j \sin \omega_{jk} \le c_k, \quad k = 1, 2, \ldots, K; k \ne j
\end{aligned} \tag{A3}
$$

where ω_{jk} is the angle between hyperplanes l_k and l_j.

5. Obtain a new boundary point by performing a one-dimensional search in the outward normal direction, starting from the center of the largest facet.

6. Add the new boundary point found in Step 5 to the set of points obtained in Step 1 and construct a new inner polytope.

7. At the points obtained in Step 1, generate a set of tangent hyperplanes by evaluating the gradients of the active constraints that describe the joint region as follows

$$[\nabla g(u_0)]^T u = [\nabla g(u_0)]^T u_0 \tag{A4}$$

where $g(u) \le 0$ is an active constraint at the simplicial point u_0 and $\bigtriangledown g(u)$ is the gradient of $g(u)$. Note that information on the active constraints is available from the solution of the line searches performed in Step 1. As a result, no additional computation is necessary.

The set of active constraints in Eq. A4 defines the outer polytope, $\mathcal{P}_{\text{outer}}$, which overestimates the feasible space boundary of the constrained and parametric regions. The outer polytope can be expressed in compact form as follows

$$\mathcal{P}_{\text{outer}} = \{u \mid Au \le b\}, \quad A \in R^{m\times(n+p)}; b \in R^m \tag{A5}$$

where m corresponds to the number of halfspaces in R^{n+p}.

8. Compute the center point, $\hat{u}^*$ by solving an LP similar to Eq. A2.

9. Check for radius convergence. If $|\hat{r} - \check{r}| \le \delta r$, where δr is a user-defined radius tolerance, then terminate. Otherwise, go to Step 5.

Proof of convergence

As shown in the works of Goyal and Ierapetritou[16,17] and Director and Hachtel,[25] the simplicial approximation algorithm will generate a sequence of polytopes, $\mathcal{P}^1_{\text{inner}} \subset \mathcal{P}^1_{\text{outer}}, \ldots, \mathcal{P}^i_{\text{inner}} \subset \mathcal{P}^i_{\text{outer}}$ that will approximate the feasible constrained and parametric regions from inside and outside as $i \to \infty$. Convergence is expected in the light of the following theorem[26]:

Theorem 1 *Let r^i be the radius of the largest hypersphere in the polytope $\mathcal{P}^i$ at iteration i formed by $2n + p + i$ points on the surface of the joint region and let r^{i+1} be the radius of the largest hypersphere (hyperellipsoid) inscribed in polytope $\mathcal{P}^{i+1}$ then*

$$r^{i+1} \le r^i \tag{A6}$$

Furthermore, when the facets of polytope $\mathcal{P}^{i+1}$ are not parallel to those of polytope $\mathcal{P}^i$, the strict inequality holds:

$$r^{i+1} < r^i \tag{A7}$$

Remark 4. *For cases in which the parametric and constrained regions are asymmetric in shape, it is advantageous to inscribe a hyperellipsoid instead of a hypersphere in Step 3 in order to obtain better approximation of the feasible region. This can be achieved by scaling the decision variables and the parameters as shown in Appendix C.*

Appendix B: Procedure for Determining the Largest Facet in the Inner Polytope

Step 4 is based on the fact that, to obtain an exact approximation of the feasible region, an infinite number of facets (boundary points) would be required. In theory, breaking the largest facet would produce a tighter inner approximation of the feasible constrained and parametric regions.

Let l_j be the jth facet belonging to the polyhedron $\mathcal{P}_{\text{inner}}$ and u_j^* the center of such facet. The surface of a hypersphere of radius r_j, lying on the jth hyperplane is described by

$$l_j^T u_j^* = c_j \tag{B1}$$

where $l_j^\perp$ is a unit vector perpendicular to l_j, that is

$$(l_j^\perp)^T l_j = 0 \tag{B2}$$

Therefore, $l_j^\perp$ lies in the jth hyperplane and the surface of the hypersphere with radius r_j and centered at u_j^* lies in the jth hyperplane described by $r_j \, l_j^{\,\perp} + u_j^*$.

The largest hypersphere, which can be inscribed, is that whose surface lies within the polyhedron described by the following inequalities

$$l_k^T (r_j l_j^\perp + u_j^*) \le c_k, \quad k = 1, 2, \ldots, K; k \ne j \tag{B3}$$

It can be shown[25] that the constraints in 38 are equivalent to the following constraints

$$r_j \sin \omega_{jk} + l_k^T u_j^* \le c_k, \quad k = 1, 2, \ldots, K \tag{B4}$$

where ω_{jk} is the angle between l_k and l_j.

Thus, the problem of determining the largest facet of a polyhedron reduces to maximizing r_j subject to the constraints in Eqs. B1 and B4 $\forall$ $k = 1,2,\ldots K$; $k \ne j$.

Appendix C: Scaling Procedure for Parameters and Decision Variables

Once the values of $u_i^{\max}$ and $u_i^{\min}$ have been obtained, a scale factor for the ith variable can be obtained as follows

$$\Gamma_i = u_i^{\max} - u_i^{\min}, \quad i = 1, 2, \ldots, n + p \tag{C1}$$

Defining a scaling matrix, Γ, as

$$\Gamma = \text{diag } \Gamma_1, \quad \Gamma_2, \ldots, \Gamma_{n+p} \tag{C2}$$

a scaled boundary point, $\bar{u}_k$, can be defined as

$$\bar{u}_k = \Gamma^{-1} u_k, \quad k = 1, 2, \ldots, n + p \tag{C3}$$

where k is the index set of the boundary points found.

The unscaled variable can be obtained by applying the reverse transformation

$$u_k = \Gamma \bar{u}_k, \quad k = 1, 2, \ldots, n + p \tag{C4}$$

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