Computers and Chemical Engineering 72 (2015) 387–394

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Mixed integer polynomial programming

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ARTICLE INFO

Article history:
Received 16 January 2014
Received in revised form 15 July 2014
Accepted 20 July 2014
Available online 29 July 2014

Keywords:
Mixed integer programming
Polynomial programming
Nonlinear inversion
Multi-parametric programming

ABSTRACT

The mixed integer polynomial programming problem is reformulated as a multi-parametric programming problem by relaxing integer variables as continuous variables and then treating them as parameters. The optimality conditions for the resulting parametric programming problem are given by a set of simultaneous parametric polynomial equations which are solved analytically to give the parametric optimal solution as a function of the relaxed integer variables. Evaluation of the parametric optimal solution for integer variables fixed at their integer values followed by screening of the evaluated solutions gives the optimal solutions.

1. Introduction

Mathematical modelling and model-based optimization of chemical process systems have great potential for providing answers on how to optimally design and operate these systems. One key difficulty in not being able to fully exploit this potential is the presence of nonlinear terms in the mathematical models. This issue is further exacerbated when the model also includes integer variables, for incorporating structural choices. A generic formulation of such mathematical programming problems is given by mixed integer nonlinear programmes (MINLP) (Grossmann, 2002):

$$
\begin{aligned}
&\text{Problem P1}:\\
&z_1 = \min_{x,y} f(\mathbf{x}, \mathbf{y})\\
&\text{subject to}: \mathbf{h}(\mathbf{x}, \mathbf{y}) = 0\\
&\mathbf{g}(\mathbf{x}, \mathbf{y}) \le 0\\
&\mathbf{x} \in \Re^{n_x}\\
&\mathbf{y} \in \{0, 1\}^{n_y}
\end{aligned}
$$

where $\mathbf{x}$ is a vector of continuous variables, $\mathbf{y}$ is a vector of binary variables, $\mathbf{h}$ is an n_h dimensional vector of equality constraints, $\mathbf{g}$ is an n_g dimensional vector of inequality constraints and f is the scalar objective function. Synthesis of chemical process flowsheets and design of materials are two typical problems demonstrating the application of mathematical programmes simultaneously involving nonlinearities and integer variables (Dua and Pistikopoulos, 1998). For process synthesis problems, $\mathbf{x}$ represents continuously varying quantities such as temperature, pressure, flowrates etc., $\mathbf{y}$ is used to model structural decisions such as selection of appropriate processing units and inter-connections between the units etc., f represents an objective function such as cost or environmental impact to be optimized, $\mathbf{h}$ represents conservation equations i.e. mass and energy balances and $\mathbf{g}$ represents constraints on quantities such as lowest acceptable purity and highest allowable safe operating temperatures and pressures. For material design problems $\mathbf{x}$ represents material properties, $\mathbf{y}$ models selection of constituent molecular groups, f represents deviation from desired property values, $\mathbf{h}$ represents property prediction correlations and $\mathbf{g}$ represents lower and upper bounds on values of the material properties. Note that this approach for material design problems is based upon matching property targets but other formulations for such problems also exist in the literature.

Solving P1 is NP-hard and has created huge interest for developing computationally efficient algorithms for obtaining solution of P1. New theoretical developments for solving P1 have pushed the boundaries of application of P1 to many areas in engineering and science. Several software tools are available to solve these problems, DICOPT (Viswanathan and Grossmann, 1990), MINOPT (MINOPT, 1998), BARON (Sahinidis, 1996), GloMIQO (Misener and Floudas, 2013), Alpha-ECP (Westerlund and Lundqvist, 2005) – to name a few. The reader is referred to recent survey papers by Belotti et al. (2013) and D'Ambrosio and Lodi (2011) presenting an overview of advances for solving P1 and the books (Biegler et al.,

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http://dx.doi.org/10.1016/j.compchemeng.2014.07.020

1997; Floudas, 1995; Nemhauser and Wolsey, 1988) for an introduction to the topic.

Gueddar and Dua (2012) reformulated P1 as a multi-parametric nonlinear programme (mp-NLP) by first relaxing **y** as continuous variables and then treating **y** as parameters. An approximate solution of the mp-NLP is obtained and that solution is then used to estimate the solution at the terminal nodes of the Branch and Bound (B&B) tree and guide the search in the tree; integer variables are the branching variables in the tree. For details of multi-parametric programming the reader is referred to Dua and Pistikopoulos (1999), Pistikopoulos et al. (2007a,b), Pistikopoulos (2009) and Wittmann-Hohlbein and Pistikopoulos (2014).

In this work, the case when f, **h** and **g** are polynomial functions is considered, problem P1 therefore becomes a Mixed Integer Polynomial Optimization (MIPOPT) problem. Patil et al. (2012) presented a Bernstein polynomial approach for solving such problems. Teles et al. (2013) proposed a discretization approach using bilinear terms as the building block. In this work, the integer variables, **y**, are relaxed as continuous variables and then treated as parameters resulting in a multi-parametric polynomial programme (mp3). An exact solution of the resulting mp3 can be obtained by exact multi-parametric nonlinear inversion of the optimality conditions, see for example Fotiou et al. (2007). The proposed approach hence does not require approximate solution of the mp-NLP followed by a tree search as in Gueddar and Dua (2012).

In the next section polynomial programming is introduced and an example for exact solution of polynomial programmes is presented. An algorithm for solving MIPOPT based upon mp3 reformulation is proposed in Section 3 and in Section 4 illustrative examples are presented. A discussion of results and concluding remarks are provided in Section 5.

2. Polynomial programming

Consider the following nonlinear programming (NLP) problem:

Problem P2 :

$$z_2 = \min_x f(\mathbf{x})$$

$$\text{subject to : } \mathbf{h}(\mathbf{x}) = 0$$

$$\mathbf{g}(\mathbf{x}) \le 0$$

$$\mathbf{x} \in \Re^{n_x}$$

Descent or similar algorithms for computing solution of P2 are based upon an iterative strategy where the solution obtained at an iteration verifies Fritz–John (FJ) or Karush–Kuhn–Tucker (KKT) conditions (Bazaraa et al., 1993), in this work the KKT conditions are considered, as follows.

KKT conditions :

(a) Equality constraints :

$$\nabla_x L(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}) = 0$$

$$h(\mathbf{x}) = 0$$

$$\lambda_j g_j(\mathbf{x}) = 0, j = 1, \ldots, n_g$$

(b) Inequality constraints :

$$\mathbf{g}(\mathbf{x}) \le 0$$

$$\lambda_j \ge 0, j = 1, \ldots, n_g$$

where

$$L(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \sum_{i=1}^{n_h} \mu_i h_i(\mathbf{x}) + \sum_{j=1}^{n_g} \lambda_j g_j(\mathbf{x})$$

is the Lagrangian function.

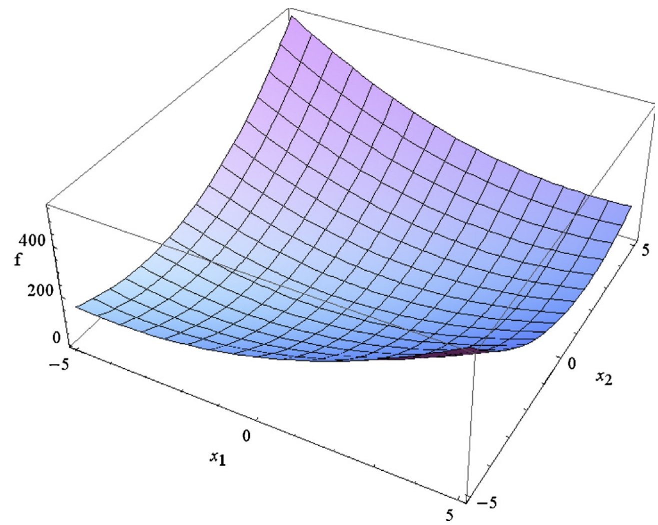

Fig. 1. Example 1, plot of the objective function, f, as a function of x_1 and x_2.

The equality constraints in the KKT conditions are $n_x + n_h + n_g$ dimensional and the vector of variables, $[\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}]$, is also $n_x + n_h + n_g$ dimensional. For generic nonlinear functions solution of equality constraints is usually obtained by employing a numerical technique, such as Newton's method. The solution of the equality constraints obtained is verified by checking whether it satisfies the inequality constraints in the KKT conditions. Considering a special case when f, **g** and **h** in the NLP are polynomial, a set of equations polynomial in $[\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}]$ is obtained. These polynomial equations can be solved analytically, at least in theory, to obtain a closed form solution which includes all the solutions (Hägglöf et al., 1995). This can be achieved by using the theory of Gröbner Bases where the Buchberger algorithm can be used to transform the set of polynomial equations into a triangular system of equations (Buchberger and Winkler, 1998). The triangular system is the nonlinear polynomial equivalent of the triangular system obtained by Gaussian elimination for a linear system of equations. The computational complexity of this method grows exponentially with the number of variables, but it is an active area of research with various developments including parallel computing to improve computational speed. There are softwares for symbolic manipulations such as Mathematica (Wolfram Research, 2013) that can analytically solve systems of polynomial equations, which in our case is given by the equality constraints in the KKT conditions. The set of solutions thus obtained can then be checked to see if they satisfy the inequality constraints in the KKT conditions. Further screening tests are also carried out, i.e., whether complementary slackness (CS) and constraints qualification (CQ) conditions are met is checked. In this paper linear independence constraint qualification (LICQ) was used for checking the CQ condition. Consider the following illustrative example for demonstrating the basic idea.

Example 1 : Polynomial programming

$$\min_{\mathbf{x}} f(\mathbf{x}) = 5x_1^2 + 9x_2^2 - 8x_1x_2$$

subject to :

$$g_1(\mathbf{x}) = 2 - x_1x_2 \le 0$$

$$g_2(\mathbf{x}) = -3 + x_1x_2 \le 0$$

$$g_3(\mathbf{x}) = -5 + x_1 \le 0$$

$$g_4(\mathbf{x}) = -5 - x_1 \le 0$$

The objective function is plotted as a function of x_1 and x_2 in Fig. 1 and the feasible region is given by the shaded area in Fig. 2. The two optimal solutions are also shown in Fig. 2.

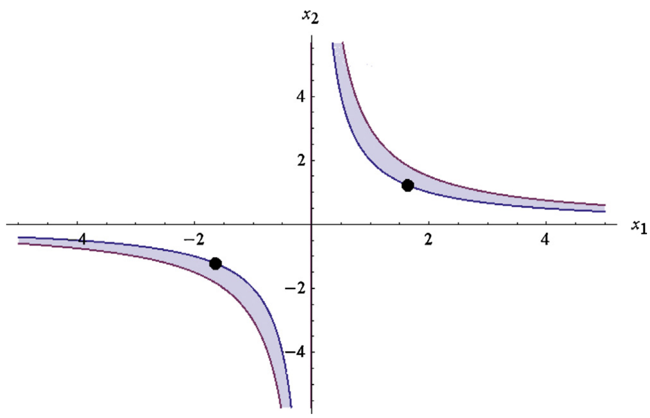

Fig. 2. Example 1, plots of $g_1=0$ and $g_2=0$ on x_1-x_2 axes. The feasible region is given by the shaded area. The optimal solutions are given by the two filled circles (●).

The Lagrangian function is given by:

$$L(\mathbf{x},\boldsymbol{\lambda}) = 5x_1^2+9x_2^2-8x_1x_2+\lambda_1(2-x_1x_2)+\lambda_2(-3+x_1x_2) + \lambda_3(-5+x_1)+\lambda_4(-5-x_1)$$

The KKT conditions are given by:

(a) Equality constraints:

$$\frac{\partial L}{\partial x_1} = 10x_1-8x_2+\lambda_1(-x_2)+\lambda_2(x_2)+\lambda_3-\lambda_4=0$$
$$\frac{\partial L}{\partial x_2} = 18x_2-8x_1+\lambda_1(-x_1)+\lambda_2(x_1)=0$$
$$\lambda_1(2-x_1x_2)=0$$
$$\lambda_2(-3+x_1x_2)=0$$
$$\lambda_3(-5+x_1)=0$$
$$\lambda_4(-5-x_1)=0$$

(b) Inequality constraints:

$$2-x_1x_2\le 0$$
$$-3+x_1x_2\le 0$$
$$-5+x_1\le 0$$
$$-5-x_1\le 0$$
$$\lambda_1,\lambda_2,\lambda_3,\lambda_4\ge 0$$

Table 1 shows all the fifteen solutions of the KKT equality constraints as obtained by using the Solve command in Mathematica. Solution numbers 1–3, 5–8, 11 and 13–14 are ignored because at least one Lagrange multiplier is negative, solution number 4 is ignored because the inequality constraint g_1 is violated, solution numbers 9 and 10 are ignored because they have imaginary parts and hence solution numbers 12 and 15 are the two candidate solutions. Note that considering both the positive and negative values of the square roots, the Lagrange multipliers of the 8th and 11th solutions could take positive values. These solutions however get rejected later because of the higher objective function values than the best identified. Solutions 12 and 15 were further tested and satisfied CS and CQ and hence are the two final solutions, as also shown in Fig. 2.

3. An algorithm for mixed integer polynomial optimization (MIPOPT) using multi-parametric polynomial programming (mp3)

Recall problem P1 and now consider the case that f, $\mathbf{h}$ and $\mathbf{g}$ are polynomial functions of $\mathbf{x}$ and that for simplicity the terms in $\mathbf{x}$ and $\mathbf{y}$ are separable, this results in a Mixed Integer Polynomial Optimization (MIPOPT) problem. Relaxing the integer variables as continuous variables and treating them as parameters results in the following multi-parametric polynomial programme (mp3):

Problem P3 :
$$z_3(\mathbf{y}) = \min_{\mathbf{x}} f(\mathbf{x},\mathbf{y})$$
$$\text{subject to}: \mathbf{h}(\mathbf{x},\mathbf{y})=0$$
$$\mathbf{g}(\mathbf{x},\mathbf{y})\le 0$$
$$\mathbf{x}\in\Re^{n_x}$$
$$\mathbf{y}\in[0,1]^{n_y}$$

The KKT conditions for the mp3 are as follows.
KKT conditions for Problem P3:

(a) Equality constraints:

$$\nabla_x L(\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\lambda})=0$$
$$\mathbf{h}(\mathbf{x},\mathbf{y})=0$$
$$\lambda_j g_j(\mathbf{x},\mathbf{y})=0, j=1,\ldots,n_g$$

(b) Inequality constraints:

$$\mathbf{g}(\mathbf{x},\mathbf{y})\le 0$$
$$\lambda_j\ge 0, j=1,\ldots,n_g$$

where

$$L(\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\lambda}) = f(\mathbf{x},\mathbf{y})+\sum_{i=1}^{n_h}\mu_i h_i(\mathbf{x},\mathbf{y})+\sum_{j=1}^{n_g}\lambda_j g_j(\mathbf{x},\mathbf{y})$$

is the Lagrangian function which is parametric in $\mathbf{y}$.

The equality constraints in the KKT conditions are $n_x+n_h+n_g$ dimensional, the vector of variables $[\mathbf{x},\boldsymbol{\mu},\boldsymbol{\lambda}]$ is also $n_x+n_h+n_g$ dimensional and the vector of parameters, $\mathbf{y}$, is n_y dimensional. These equality constraints which are parametric in $\mathbf{y}$ and polynomial in $[\mathbf{x},\boldsymbol{\mu},\boldsymbol{\lambda}]$ are solved analytically e.g. by using Mathematica. The parametric solution is given by $[\mathbf{x}(\mathbf{y}),\boldsymbol{\mu}(\mathbf{y}),\boldsymbol{\lambda}(\mathbf{y})]$. The parameters, $\mathbf{y}$, are then fixed at possible integer values and substituted into the parametric solution to evaluate $[\mathbf{x}(\mathbf{y}),\boldsymbol{\mu}(\mathbf{y}),\boldsymbol{\lambda}(\mathbf{y})]$. These values are then substituted into the inequality constraints in the KKT conditions. The solutions which satisfy these inequality constraints, CS and CQ are then substituted into the objective function, $f(\mathbf{x},\mathbf{y})$, and the solutions which give the lowest values are the final solutions. The algorithm is summarized in Table 2.

For some specific problems variations of the proposed algorithm can also be developed. For example, after step 4 the values of the continuous variables and the Lagrange multipliers are available. Therefore in step 5 the solutions which provide negative Lagrange multipliers for inequality constraints can be ignored from further analysis and satisfaction of other KKT inequality constraints, CS and CQ is not required to be carried out for those solutions. The solutions which give imaginary values for the continuous variables or Lagrange multipliers can also be removed. For the remaining candidate solutions two possible options are as follows.

Table 1
Example 1, solution of equality constraints in the KKT conditions. Note that i denotes the complex part of the solution.

(1)	$\lambda_1 = 0$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = -\frac{290}{9}$	$x_1 = -5$	$x_2 = -\frac{20}{9}$
(2)	$\lambda_1 = 0$	$\lambda_2 = \frac{146}{25}$	$\lambda_3 = 0$	$\lambda_4 = \frac{6088}{125}$	$x_1 = -5$	$x_2 = -\frac{3}{5}$
(3)	$\lambda_1 = -\frac{164}{25}$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = \frac{6178}{125}$	$x_1 = -5$	$x_2 = -\frac{2}{5}$
(4)	$\lambda_1 = 0$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = 0$	$x_2 = 0$
(5)	$\lambda_1 = 0$	$\lambda_2 = \frac{146}{25}$	$\lambda_3 = -\frac{6178}{125}$	$\lambda_4 = 0$	$x_1 = 5$	$x_2 = \frac{2}{5}$
(6)	$\lambda_1 = 0$	$\lambda_2 = \frac{146}{25}$	$\lambda_3 = \frac{6088}{125}$	$\lambda_4 = 0$	$x_1 = 5$	$x_2 = \frac{3}{5}$
(7)	$\lambda_1 = 0$	$\lambda_2 = 0$	$\lambda_3 = \frac{290}{9}$	$\lambda_4 = 0$	$x_1 = 5$	$x_2 = \frac{20}{9}$
(8)	$\lambda_1 = 0$	$\lambda_2 = 2(4-3\sqrt{5})$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = -\frac{3}{5^{1/4}}$	$x_2 = -5^{1/4}$
(9)	$\lambda_1 = 0$	$\lambda_2 = 2(4+3\sqrt{5})$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = -\frac{3i}{5^{1/4}}$	$x_2 = -i5^{1/4}$
(10)	$\lambda_1 = 0$	$\lambda_2 = 2(4+3\sqrt{5})$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = \frac{3i}{5^{1/4}}$	$x_2 = -i5^{1/4}$
(11)	$\lambda_1 = 0$	$\lambda_2 = 2(4-3\sqrt{5})$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = \frac{3}{5^{1/4}}$	$x_2 = 5^{1/4}$
(12)	$\lambda_1 = 2(-4+3\sqrt{5})$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = \frac{\sqrt{6}}{5^{1/4}}$	$x_2 = -\sqrt{\frac{2}{3}}5^{1/4}$
(13)	$\lambda_1 = 2(-4-3\sqrt{5})$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = -\frac{i\sqrt{6}}{5^{1/4}}$	$x_2 = i\sqrt{\frac{2}{3}}5^{1/4}$
(14)	$\lambda_1 = 2(-4-3\sqrt{5})$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = \frac{i\sqrt{6}}{5^{1/4}}$	$x_2 = -i\sqrt{\frac{2}{3}}5^{1/4}$
(15)	$\lambda_1 = 2(-4+3\sqrt{5})$	$\lambda_2 = 0$	$\lambda_3 = 0$	$\lambda_4 = 0$	$x_1 = \frac{\sqrt{6}}{5^{1/4}}$	$x_2 = \sqrt{\frac{2}{3}}5^{1/4}$

Table 2
MIPOPT algorithm.

Step 1.	Reformulate MIPOPT problem as a multi-parametric polynomial programme, by relaxing integer variables as continuous variables and treating them as parameters, as given in Problem P3.
Step 2.	Formulate first order KKT Conditions for Problem P3, given by Equality Constraints and Inequality Constraints.
Step 3.	Solve the Equality Constraints in the KKT Conditions parametrically to obtain continuous variables and Lagrange multipliers as function of relaxed integer variables.
Step 4.	Fix the integer variables at all the possible integer value combinations and evaluate the continuous variables and Lagrange multipliers obtained in the previous step.
Step 5.	Screen the solutions obtained in the previous step to obtain the best solution(s). This involves checking whether the Inequality Constraints in the KKT Conditions, Complementary Slackness (CS) and Constraint Qualification (CQ) and are satisfied and identifying the solutions which give the lowest value of the objective function.

- The first solution which satisfies all the conditions acts as an upper bound and the remaining solutions which have higher objective function value, even without checking whether they satisfy any conditions or constraints, are ignored. The upper bound is then updated as better optimal solutions are identified.
- The solutions which violate even one inequality constraint are removed. The remaining solutions are then tested for CS, CQ and lowest objective function value.

4. Numerical examples

This section presents four examples in detail. The first two examples are taken from Floudas et al. (1999) and have also been solved by Patil et al. (2012). The last two examples are taken from Floudas and Pardalos (1990) and also solved by Lasserre (2001), and have been modified for formulating MIPOPT problems.

4.1. Example 2: MIPOPT

Consider the following problem:

$$\min_{x,y} f = y_1 + y_2 + y_3 + 5x_1^2$$

subject to :

$$g_1 = 3x_1 - y_1 - y_2 \le 0$$

$$g_2 = -x_1 - 0.1y_2 + 0.25y_3 \le 0$$

$$g_3 = 0.2 - x_1 \le 0$$

where x_1 is the continuous variable and y_1, y_2, y_3 are the 0–1 binary variables. By relaxing the binary variables as continuous variables and then treating them as parameters an mp3 is obtained. For simplicity the lower and upper bounds on the binary variables are ignored at this stage. The Lagrangian function is given by:

$$L = y_1 + y_2 + y_3 + 5x_1^2 + \lambda_1(3x_1 - y_1 - y_2) + \lambda_2(-x_1 + 0.1y_2 + 0.25y_3) + \lambda_3(0.2 - x_1)$$

The KKT conditions are given by:

(a) Equality constraints:

$$\frac{\partial L}{\partial x_1} = 10x_1 + 3\lambda_1 - \lambda_2 - \lambda_3 = 0$$

$$\lambda_1(3x_1 - y_1 - y_2) = 0$$

$$\lambda_2(-x_1 + 0.1y_2 + 0.25y_3) = 0$$

$$\lambda_3(0.2 - x_1) = 0$$

(b) Inequality constraints:

$$3x_1 - y_1 - y_2 \le 0$$
$$-x_1 + 0.1y_2 + 0.25y_3 \le 0$$
$$0.2 - x_1 \le 0$$
$$\lambda_1, \lambda_2, \lambda_3 \ge 0$$

Solving the equality constraints in the KKT conditions by relaxing the integer variables as continuous variables and treating them as parameters, the following parametric solutions are obtained:

$$\left\{\begin{array}{ll} (1) & \{\lambda_1 = 0, \lambda_2 = 0, \lambda_3 = 2, x_1 = 0.2\} \\ (2) & \{\lambda_1 = 0, \lambda_2 = 0, \lambda_3 = 0, x_1 = 0\} \\ (3) & \{\lambda_1 = 0, \lambda_2 = y_2 + 2.5y_3, \lambda_3 = 0, x_1 = 0.1y_2 + 0.25y_3\} \\ (4) & \{\lambda_1 = -1.11(y_1 + y_2), \lambda_2 = 0, \lambda_3 = 0, x_1 = 0.33(y_1 + y_2)\} \end{array}\right\}$$

Remark 1. Note that these solutions are parametric in $[y_1,y_2,y_3]$ and no bounds were imposed on $[y_1,y_2,y_3]$ while obtaining these solutions. The solution thus obtained and the methodology proposed in this work is therefore also valid for the generic case where **y** can be any integer variable and not just limited to the 0–1 binary values. See Sections 4.3 and 4.4 for the generic mixed-integer case examples.

Now these solutions are screened by fixing the binary variables at the 0–1 values and substituting the values into these solutions and then checking the inequality constraints in the KKT conditions, CS and CQ conditions. The following two solutions pass the screening test and since the second solution gives the lowest objective function value, f = 2.20, it is the final solution.

λ_1	λ_2	λ_3	x_1	y_1	y_2	y_3	f
0	2.50	0	0.25	1.00	0	1.00	2.31
0	0	2.00	0.20	1.00	1.00	0	2.20

4.2. Example 3: MIPOPT

$$\min_{x,y} f = 2y_1 + 2y_2 + 4x_1 - x_1^2 - x_2^2 + 2x_2 + 2$$

subject to :

$$g_1 = -x_1 + 3x_2 - 5 \le 0$$
$$g_2 = 2x_1 - x_2 - 5 \le 0$$
$$g_3 = -2x_1 + x_2 \le 0$$
$$g_4 = x_1 - 3x_2 \le 0$$
$$g_5 = -6y_1 + x_1 \le 0$$
$$g_6 = -5y_2 + x_2 \le 0$$

where x_1 and x_2 are the continuous variable and y_1, y_2 are the 0–1 binary variables. The Lagrangian function, by relaxing the integer variables as continuous variables, treating them as parameters and by ignoring the lower and upper bounds on the binary variables, is given by:

$$\begin{aligned} L = {} & 2y_1 + 2y_2 + 4x_1 - x_1^2 - x_2^2 + 2x_2 + 2 + \lambda_1(-x_1 + 3x_2 - 5) \\ & + \lambda_2(2x_1 - x_2 - 5) + \lambda_3(-2x_1 + x_2) + \lambda_4(x_1 - 3x_2) \\ & + \lambda_5(-6y_1 + x_1) + \lambda_6(-5y_2 + x_2) \end{aligned}$$

The KKT conditions are given by:

(a) Equality constraints:

$$\frac{\partial L}{\partial x_1} = -2x_1 - \lambda_1 + 2\lambda_2 - 2\lambda_3 + \lambda_4 + \lambda_5 + 4 = 0$$
$$\frac{\partial L}{\partial x_2} = -2x_2 + 3\lambda_1 - \lambda_2 + \lambda_3 - 3\lambda_4 + \lambda_6 + 2 = 0$$
$$\lambda_1(-x_1 + 3x_2 - 5) = 0$$
$$\lambda_2(2x_1 - x_2 - 5) = 0$$
$$\lambda_3(-2x_1 + x_2) = 0$$
$$\lambda_4(x_1 - 3x_2) = 0$$
$$\lambda_5(-6y_1 + x_1) = 0$$
$$\lambda_6(-5y_2 + x_2) = 0$$

(b) Inequality constraints:

$$-x_1 + 3x_2 - 5 \le 0$$
$$2x_1 - x_2 - 5 \le 0$$
$$-2x_1 + x_2 \le 0$$
$$x_1 - 3x_2 \le 0$$
$$-6y_1 + x_1 \le 0$$
$$-5y_2 + x_2 \le 0$$
$$\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6 \ge 0$$

By solving the equality constraints in the KKT conditions the solutions obtained are given in Table 3. The solutions obtained after the screening test for values of **y** fixed at integer values are given in Table 4. The first solution gives the lowest possible value of f and hence is the final solution.

4.3. Example 4: MIPOPT

$$\begin{aligned} \min_{x,y} f = {} & -25(x_1 - 2)^2 - (x_2 - 2)^2 - (x_3 - 1)^2 - (y_1 - 4)^2 \\ & -(y_2 - 1)^2 - (y_3 - 4)^2 \end{aligned}$$

subject to :

$$g_1 = -(x_3 - 3)^2 - y_1 + 4 \le 0$$
$$g_2 = -(y_2 - 3)^2 - y_3 + 4 \le 0$$
$$g_3 = x_1 - 3x_2 - 2 \le 0$$
$$g_4 = -x_1 + x_2 - 2 \le 0$$
$$g_5 = x_1 + x_2 - 6 \le 0$$
$$g_6 = -x_1 - x_2 + 2 \le 0$$
$$x_1, x_2 \ge 0;\ 1 \le x_3 \le 5;\ 0 \le y_1 \le 6;\ 1 \le y_2 \le 5;\ 0 \le y_3 \le 10$$

where x_1, x_2, x_3 are the continuous variables and y_1, y_2, y_3 are the integer variables. For simplicity, ignoring the simple lower and upper bounds on the variables, the Lagrangian function is given by:

$$\begin{aligned} L = {} & -25(x_1 - 2)^2 - (x_2 - 2)^2 - (x_3 - 1)^2 - (y_1 - 4)^2 - (y_2 - 1)^2 \\ & -(y_3 - 4)^2 + \lambda_1(-(x_3 - 3)^2 - y_1 + 4) + \lambda_2(-(y_2 - 3)^2 - y_3 + 4) \\ & + \lambda_3(x_1 - 3x_2 - 2) + \lambda_4(-x_1 + x_2 - 2) + \lambda_5(x_1 + x_2 - 6) \\ & + \lambda_6(-x_1 - x_2 + 2) \end{aligned}$$

Table 3
Example 3, parametric solution of equality constraints in KKT conditions for integer variables relaxed as continuous variables and treated as parameters.

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	x_1	x_2
1	0	0	0	0	0	0	2	1
2	0	0	0	0	0	$2(-1+5y_2)$	2	$5y_2$
3	0	0	0	0	$4(-1+3y_1)$	0	$6y_1$	1
4	0	0	0	0	$4(-1+3y_1)$	$2(-1+5y_2)$	$6y_1$	$5y_2$
5	0	0	0	1/5	0	0	21/10	7/10
6	0	0	0	$(-2/3)(-1+2y_1)$	$(2/3)(-7+20y_1)$	0	$6y_1$	$2y_1$
7	0	0	0	$2(-2+15y_2)$	0	$2(-7+50y_2)$	$15y_2$	$5y_2$
8	0	0	6/5	0	0	0	4/5	8/5
9	0	0	14/5	8/5	0	0	0	0
10	0	0	$2(-1+12y_1)$	0	$4(-2+15y_1)$	0	$6y_1$	$12y_1$
11	0	0	$(1/2)(4-5y_2)$	0	0	$(1/2)(-8+25y_2)$	$5y_2/2$	$5y_2$
12	0	4/5	0	0	0	0	14/5	3/5
13	0	6/5	0	−2/5	0	0	3	1
14	0	$-12(-1+2y_1)$	0	0	$4(-7+15y_1)$	0	$6y_1$	$-5+12y_1$
15	0	$(1/2)(1+5yy_2)$	0	0	0	$(1/2)(-3+25y_2)$	$(5(1+y_2))/2$	$5y_2$
16	2/5	0	4/5	0	0	0	1	2
17	4/5	0	0	0	0	0	8/5	11/5
18	12/5	16/5	0	0	0	0	4	3
19	$(4/9)(1+3y_1)$	0	0	0	$(8/9)(-4+15y_1)$	0	$6y_1$	$(1/3)(5+6y_1)$
20	$-2(-7+15y_2)$	0	0	0	0	$4(-11+25y_2)$	$5(-1+3y_2)$	$5y_2$

where the integer variables are relaxed as continuous variables and treated as parameters. The KKT conditions are given by:

(a) Equality constraints:

$$\frac{\partial L}{\partial x_1} = -50(x_1-2)+\lambda_3-\lambda_4+\lambda_5-\lambda_6 = 0$$
$$\frac{\partial L}{\partial x_2} = -2(x_2-2)-3\lambda_3+\lambda_4+\lambda_5-\lambda_6 = 0$$
$$\frac{\partial L}{\partial x_3} = -2(x_3-1)-2\lambda_1(x_3-3) = 0$$
$$\lambda_1(-(x_3-3)^2-y_1+4) = 0$$
$$\lambda_2(-(y_2-3)^2-y_3+4) = 0$$
$$\lambda_3(x_1-3x_2-2) = 0$$
$$\lambda_4(-x_1+x_2-2) = 0$$
$$\lambda_5(x_1+x_2-6) = 0$$
$$\lambda_6(-x_1-x_2+2) = 0$$

(b) Inequality constraints:

$$-(x_3-3)^2-y_1+4 \le 0$$
$$-(y_2-3)^2-y_3+4 \le 0$$
$$x_1-3x_2-2 \le 0$$
$$-x_1+x_2-2 \le 0$$
$$x_1+x_2-6 \le 0$$
$$-x_1-x_2+2 \le 0$$
$$\lambda_1,\lambda_2,\lambda_3,\lambda_4,\lambda_5,\lambda_6 \ge 0$$

Solving the equality constraints in the KKT conditions the solutions obtained are given in Table 5. Evaluating these solutions for **y** fixed at integer values and screening these solutions the optimal solution is given by **x** = [5,1, 5], **y** = [0,5, 10], $f = -310$. Note that when evaluating the solutions in Table 5 both positive and negative signs of the square root values must be considered. g_2 is a pure integer/parametric constraint and can be taken out of the initial KKT analysis and be then used later in the screening test.

4.4. Example 5: MIPOPT

$$\min_{x,y} f = -12x_1 - 7y_1 + y_1^2$$
$$\text{subject to :}$$
$$h_1 = -2x_1^4 - y_1 + 2 = 0$$
$$0 \le x_1 \le 2;\ 0 \le y_1 \le 3$$

where x_1 is the continuous variable and y_1 is the integer variable. For simplicity, ignoring the simple lower and upper bounds on the variables, the Lagrangian function is given by:

$$L = -12x_1 - 7y_1 + y_1^2 + \mu_1(-2x_1^4 - y_1 + 2)$$

where the integer variable is relaxed as a continuous variable and treated as a parameter. The KKT conditions are given by:

$$\frac{\partial L}{\partial x_1} = -8\mu_1 x_1^3 - 12 = 0$$
$$h_1 = -2x_1^4 - y_1 + 2 = 0$$

Solving the equality constraints in the KKT conditions the solutions obtained are given by:

	μ_1	x_1
1	$\frac{3}{2^{1/4}(2-y_1)^{3/4}}$	$-\frac{(2-y_1)^{1/4}}{2^{1/4}}$
2	$\frac{3i}{2^{1/4}(2-y_1)^{3/4}}$	$-\frac{i(2-y_1)^{1/4}}{2^{1/4}}$
3	$-\frac{3i}{2^{1/4}(2-y_1)^{3/4}}$	$\frac{i(2-y_1)^{1/4}}{2^{1/4}}$
4	$-\frac{3}{2^{1/4}(2-y_1)^{3/4}}$	$\frac{(2-y_1)^{1/4}}{2^{1/4}}$

where i in the 2nd and 3rd solution is the complex part of the solution, the 2nd and 3rd solutions are thus ignored. Evaluating 1st and 4th solutions for **y** fixed at integer values and screening these solutions the optimal solution is given by $x_1 = 0.84$, $y_1 = 1$, $\mu_1 = -2.52$, $f = -16.09$.

Table 4
Example 3, set of candidate solutions satisfying the inequality constraints in the KKT conditions.

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	x_1	x_2	y_1	y_2	f
1	0.0	0.0	2.8	1.6	0.0	0.0	0.0	0.0	0.0	0.0	2.0
2	0.0	0.0	2.8	1.6	0.0	0.0	0.0	0.0	0.0	1.0	4.0
3	0.0	0.0	2.8	1.6	0.0	0.0	0.0	0.0	1.0	0.0	4.0
4	0.0	0.0	0.0	0.0	0.0	0.0	2.0	1.0	1.0	1.0	11.0
5	0.0	0.0	0.0	0.2	0.0	0.0	2.1	0.7	1.0	1.0	10.9
6	0.0	0.0	1.2	0.0	0.0	0.0	0.8	1.6	1.0	1.0	9.2
7	0.0	0.0	2.8	1.6	0.0	0.0	0.0	0.0	1.0	1.0	6.0
8	0.4	0.0	0.8	0.0	0.0	0.0	1.0	2.0	1.0	1.0	9.0
9	0.8	0.0	0.0	0.0	0.0	0.0	1.6	2.2	1.0	1.0	9.4
10	2.4	3.2	0.0	0.0	0.0	0.0	4.0	3.0	1.0	1.0	3.0

Table 5
Example 4, parametric solution of equality constraints in KKT conditions for integer variables relaxed as continuous variables and treated as parameters.

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	x_1	x_2	x_3
1	0	0	0	0	0	0	2	2	1
2	0	0	0	0	0	50/13	25/13	1/13	1
3	0	0	0	0	50/13	0	27/13	51/13	1
4	0	0	0	50/13	0	0	25/13	51/13	1
5	0	0	0	50	0	50	0	2	1
6	0	0	0	2	2	0	2	4	1
7	0	0	150/113	0	0	0	229/113	1/113	1
8	0	0	1	0	0	1	2	0	1
9	0	0	38	0	112	0	5	1	1
10	0	0	154	454	0	0	−4	−2	1
11	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	0	0	2	2	$3-\sqrt{4-y_1}$
12	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	0	50/13	25/13	1/13	$3-\sqrt{4-y_1}$
13	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	50/13	0	27/13	51/13	$3-\sqrt{4-y_1}$
14	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	50/13	0	0	25/13	51/13	$3-\sqrt{4-y_1}$
15	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	50	0	50	0	2	$3-\sqrt{4-y_1}$
16	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	2	2	0	2	4	$3-\sqrt{4-y_1}$
17	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	150/113	0	0	0	229/113	1/113	$3-\sqrt{4-y_1}$
18	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	1	0	0	1	2	0	$3-\sqrt{4-y_1}$
19	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	38	0	112	0	5	1	$3-\sqrt{4-y_1}$
20	$(4-2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	154	454	0	0	−4	−2	$3-\sqrt{4-y_1}$
21	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	0	0	2	2	$3+\sqrt{4-y_1}$
22	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	0	50/13	25/13	1/13	$3+\sqrt{4-y_1}$
23	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	0	50/13	0	27/13	51/13	$3+\sqrt{4-y_1}$
24	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	50/13	0	0	25/13	51/13	$3+\sqrt{4-y_1}$
25	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	50	0	50	0	2	$3+\sqrt{4-y_1}$
26	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	0	2	2	0	2	4	$3+\sqrt{4-y_1}$
27	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	150/113	0	0	0	229/113	1/113	$3+\sqrt{4-y_1}$
28	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	1	0	0	1	2	0	$3+\sqrt{4-y_1}$
29	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	38	0	112	0	5	1	$3+\sqrt{4-y_1}$
30	$(4+2\sqrt{4-y_1}-y_1)/(-4+y_1)$	0	154	454	0	0	−4	−2	$3+\sqrt{4-y_1}$

5. Discussion of results and concluding remarks

The proposed MIPOPT to mp3 reformulation followed by exact solution of the mp3 provides all the possible candidate solutions and does not use an iterative numerical method in the traditional sense to identify the global optimal solutions. In this work Mathematica was used for obtaining the parametric solution of the parametric polynomial equations, obtained from the KKT conditions of mp3, however other tools are also available for carrying out the same analysis. It may be mentioned that developments to improve the time required to solve the parametric polynomial equations will help increase the computational efficiency of the proposed algorithm. Although the focus here was on the nonlinearities arising only from the polynomial terms, theoretical research work on obtaining analytical solution of equations incorporating other types of nonlinearities will further expand the applicability of the proposed approach where mixed integer programmes were to be reformulated as multi-parametric programmes. Additionally, many nonlinear functions can be approximated as polynomials and in those cases the proposed approach can be explored for obtaining approximate global optimal solutions.

Acknowledgments

This paper is dedicated to Professor Ignacio Grossmann in celebration of his 65th birthday and in acknowledgement of his contributions to the field of Process Systems Engineering.

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