

Global optimization of signomial mixed-integer nonlinear programming problems with free variables

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Abstract Mixed-integer nonlinear programming (MINLP) problems involving general constraints and objective functions with continuous and integer variables occur frequently in engineering design, chemical process industry and management. Although many optimization approaches have been developed for MINLP problems, these methods can only handle signomial terms with positive variables or find a local solution. Therefore, this study proposes a novel method for solving a signomial MINLP problem with free variables to obtain a global optimal solution. The signomial MINLP problem is first transformed into another one containing only positive variables. Then the transformed problem is reformulated as a convex mixed-integer program by the convexification strategies and piecewise linearization techniques. A global optimum of the signomial MINLP problem can finally be found within the tolerable error. Numerical examples are also presented to demonstrate the effectiveness of the proposed method.

Keywords Global optimization · Mixed-integer nonlinear programming · Free variable · Convexification

1 Introduction

Mixed-integer nonlinear programming (MINLP) problems involving both continuous and discrete variables arise in many applications of engineering design, chemical engineering, process operations research and management. These applications are extensively surveyed in [12, 14, 26], for example, synthesis and design of separations [1–4], nonisothermal complex

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reactor networks [20], phase equilibrium [28] and mass-exchange networks [29]. Biegler and Grossmann [7] provided a retrospective on optimization techniques that have been applied in process systems engineering. They indicated that design and synthesis problems have been dominated by nonlinear programming (NLP) and MINLP models. Floudas et al. [13] presented an overview of the research process in global optimization during 1998–2003, including the deterministic global optimization advances in MINLPs and related applications. With the increasing reliance on modeling optimization problems in practical problems, a number of theoretical and algorithmic contributions of MINLP have been proposed. However, these problems often include nonconvex functions that can not be dealt with by the standard local optimization techniques to guarantee global optimality. For treating the nonconvexities in MINLP problems, the methods developed can be divided into two approaches:

- (i) Stochastic methods: The stochastic methods involve random elements in their search and rely on a statistical argument to prove their convergence. For instance, Salcedo et al. [32] proposed an improved random search algorithm for solving nonlinear optimization problems. Hussain and Al-Sultan [19] proposed a hybrid algorithm for nonconvex function minimization by utilizing the genetic technique to generate search directions. Yiu et al. [39] developed a hybrid descent approach based on a simulated annealing algorithm and a gradient-based method to solve multidimensional nonconvex continuous optimization problems. The heuristic technique is a variant of stochastic methods, for instance, the tabu search technique [16]. The set of all candidate solutions that can be generated in a given iteration should not only depend on the current iteration point but should also be modified by excluding a subset of candidate solutions called tabu. The definition of which candidate solutions are tabu depends on the moves that have been made between recent iteration points. Although the tabu search has been found to be more effective than simulated annealing or genetic algorithm, these stochastic methods mentioned above can not guarantee to find the global optimum. Therefore, the quality of the solution is not ensured. Moreover, the probability of finding the global solution decreases when the problem size increases.
- (ii) Deterministic methods: In a general survey of optimization techniques [7, 17, 18], many deterministic methods for convex MINLP problems have been reviewed. The methods include branch and bound (BB) [9, 22, 33], generalized benders decomposition (GBD) [15], outer-approximation (OA) [10, 11, 31], extended cutting plane method (ECP) [37], and generalized disjunctive programming (GDP) [21]. The BB method can find the global solution only when each subproblem can be solved to global optimality. The GBD method, the OA method and the ECP method can not solve MINLP problems with nonconvex constraints or nonconvex objective functions because the subproblems may not have a unique optimum in the solution process. Lee and Grossmann [21] proposed a solution algorithm for the GDP models which correspond to discrete/continuous optimization problems that involve disjunctions with nonlinear inequalities and logic propositions. The objective functions and the constraints in the GDP problem are assumed to be convex and bounded. Maranas and Floudas [25] provided a method to generate convex underestimators for generalized geometric programming problems via the exponential transformation and linear underestimation of the concave terms. Adjiman et al. [1, 2] proposed two global optimization approaches, SMIN- α BB and GMIN- α BB for nonconvex MINLP based on the concept of branch-and-bound and rely on optimization or interval-based variable-bound updates to enhance efficiency. Although one possible approach to circumvent nonconvexities in MINLP models is reformulation, for instance, using the exponential transformation to treat the generalized geometric programming problems

in which a signomial term $x_1^\alpha x_2^\beta$ is transferred into an exponential term $e^{\alpha \ln x_1 + \beta \ln x_2}$ [12, 14, 26], the exponential transformation technique can only be applied to strictly positive variables and is thus unable to deal with nonconvex MINLP problems with free variables. Pörn et al. [30] introduced different convexification strategies for transforming a nonconvex MINLP problem into a convex problem and solving it by an MINLP solver. They suggested a simple translation, $x + \bar{\tau} = e^X$, to treat a free discrete variable x . Nevertheless, inserting the transformed result into the original signomial terms will bring additional signomial terms and thereby increasing computational complexity.

Although positive variables are adopted frequently to represent engineering and scientific systems, it is also common to introduce free variables to model the system behavior, such as stresses, temperatures, electrical currents, velocities and accelerations, etc. Consequently, deriving a global optimum for the nonconvex MINLP problem with free variables is essential for real applications. Li and Tsai [23] proposed a technique for treating free variables in generalized geometric programming problems. Their method necessitates more additional 0–1 variables and constraints, therefore causing heavy computational burden. This paper presents a generalized method to solve signomial MINLP problems with free variables efficiently. The advantages of the proposed method over the current signomial MINLP methods mentioned above are summarized as follows:

- (i) *Guaranteeing a global optimum*: compared with the stochastic methods, the proposed method is capable of transforming a nonconvex signomial MINLP problem into a convex MINLP program by the convexification strategies and is thus guaranteed to reach a global optimum.
- (ii) *Increasing the efficiency*: the proposed method utilizes a straightforward substitution for free variables to cause less additional signomial terms than the Pörn et al. [30] method and less additional 0–1 variables and constraints than the Li and Tsai [23] method, thereby significantly decreasing the computational complexity.

The rest of this paper is organized as follows. Section 2 introduces some propositions for treating free variables. The convexification strategies for signomial terms are analyzed in Sect. 3. Subsequently, Sect. 4 presents some examples for illustration. After that, conclusion remarks are made in Sect. 5.

2 Transformation of free variables

The mathematical formulation of a signomial MINLP problem with free variables considered in this study is expressed as follows:

$$\begin{aligned} &\text{Minimize } f(\mathbf{x}, \mathbf{y}) \\ &\text{subject to } g_t(\mathbf{x}, \mathbf{y}) \leq 0, \quad t = 1, \dots, T, \end{aligned} \quad (1)$$

$$\mathbf{x} = (x_1, \dots, x_p, x_{p+1}, \dots, x_n), \quad \underline{x}_i \leq x_i \leq \bar{x}_i, \quad (2)$$

$$\mathbf{y} = (y_1, \dots, y_q, y_{q+1}, \dots, y_m), \quad \underline{y}_j \leq y_j \leq \bar{y}_j, \quad (3)$$

where $x_i \in \mathbb{R}^+$ for $1 \leq i \leq p$, x_i are bounded free variables for $p+1 \leq i \leq n$, y_j are positive integer/discrete variables for $1 \leq j \leq q$, y_j are bounded integer/discrete variables for $q+1 \leq j \leq m$, $f(\mathbf{x}, \mathbf{y})$ and $g_t(\mathbf{x}, \mathbf{y})$ are mixed-integer signomial functions, \underline{x}_i and \bar{x}_i are lower and upper bounds of the continuous variable x_i , and \underline{y}_j and \bar{y}_j are lower and upper bounds of the integer/discrete variable y_j , respectively.

For dealing with the free variables, we first use a standard substitution that expresses the free variable as a function of two non-negative variables as below.

$$\text{Let : } x_i = x_i^+ - x_i^-, x_i^+, x_i^- \geq 0, \quad \text{for } i = p+1, \dots, n, \quad (4)$$

$$y_j = y_j^+ - y_j^-, y_j^+, y_j^- \geq 0, \quad \text{for } j = q+1, \dots, m. \quad (5)$$

And nonlinear terms $x_i^{\alpha_i}$ and $y_j^{\beta_j}$ are expressed as

$$x_i^{\alpha_i} = (x_i^+)^{\alpha_i} + (-1)^{\alpha_i} (x_i^-)^{\alpha_i}, \quad \alpha_i \in \text{integer}, \quad \text{for } i = p+1, \dots, n, \quad (6)$$

$$y_j^{\beta_j} = (y_j^+)^{\beta_j} + (-1)^{\beta_j} (y_j^-)^{\beta_j}, \quad \beta_j \in \text{integer}, \quad \text{for } j = q+1, \dots, m. \quad (7)$$

If $x_i^+ > 0$ and $x_i^- = 0$, then x_i is positive. Otherwise, if $x_i^- > 0$ and $x_i^+ = 0$, then x_i is negative. To prohibit from yielding positive values for x_i^+ and x_i^- simultaneously, we have the following remark.

Remark 1 A free variable x_i can be expressed as $x_i = x_i^+ - x_i^-$, $x_i^+, x_i^- \geq 0$, and x_i^+ and x_i^- will not be positive concurrently by the following inequalities.

- (i) $x_i^+ \leq \bar{x}_i \theta_i$,
- (ii) $x_i^- \leq \bar{x}_i (\theta_i - 1)$.

where $\theta_i \in \{0, 1\}$.

Similarly, integer/discrete free variables y_j have the same result.

By means of changing variables, the MINLP problem with free variables can be equivalently solved with another one having non-negative variables. To deal with variables containing zero, herein we introduce a strictly positive variable \tilde{x}_i^+ . For computer implementation, $\tilde{x}_i^+ \geq \varepsilon_0$ where ε_0 is a zero tolerance. A value below ε_0 is considered to be zero. We also set the feasibility tolerance as ε_1 . All the constraints are feasible when they are satisfied to within a prespecified tolerance ε_1 . For instance, a constraint $g(\mathbf{x}, \mathbf{y}) \leq 0$ is commonly considered to be feasible if $g(\mathbf{x}, \mathbf{y}) \leq \varepsilon_1$. In most cases, $\varepsilon_0 \leq \varepsilon_1$. Consider the following propositions:

Proposition 1 [23] Let $\bar{x}_i \in \mathbb{R}^+$, $0 \leq x_i^+ \leq \bar{x}_i$, $\lambda_i \in \{0, 1\}$, $\varepsilon_0 \leq \tilde{x}_i^+ \leq \bar{x}_i$, $\varepsilon_0 > 0$, then:

$$x_i^+ = \tilde{x}_i^+ \lambda_i \Leftrightarrow \begin{cases} \text{(i)} & 0 \leq x_i^+ \leq \bar{x}_i \lambda_i, \\ \text{(ii)} & \bar{x}_i (\lambda_i - 1) + \tilde{x}_i^+ \leq x_i^+ \leq \tilde{x}_i^+. \end{cases}$$

Proof

If $x_i^+ = 0$, then (i) is activated and $\lambda_i = 0$, therefore $\tilde{x}_i^+ \lambda_i = 0$ and $x_i^+ = \tilde{x}_i^+ \lambda_i$.

If $x_i^+ > 0$, then (ii) is activated and $\lambda_i = 1$, therefore $x_i^+ = \tilde{x}_i^+$ and $x_i^+ = \tilde{x}_i^+ \lambda_i$.

The reverse can be proved below.

If $\tilde{x}_i^+ \lambda_i = 0$, then $\lambda_i = 0$ and (i) is activated, therefore $x_i^+ = 0$ and $x_i^+ = \tilde{x}_i^+ \lambda_i$.

If $\tilde{x}_i^+ \lambda_i > 0$, then $\lambda_i = 1$ and (ii) is activated, therefore $x_i^+ = \tilde{x}_i^+$ and $x_i^+ = \tilde{x}_i^+ \lambda_i$.

The above demonstrates that the equivalence of $x_i^+ = \tilde{x}_i^+ \lambda_i$ is established.

Now denote z^+ and \tilde{z}^+ as below:

$$z^+ = x_1^{\alpha_1} \cdots x_p^{\alpha_p} (x_{p+1}^+)^{\alpha_{p+1}} \cdots (x_n^+)^{\alpha_n} \quad \text{and} \quad \tilde{z}^+ = x_1^{\alpha_1} \cdots x_p^{\alpha_p} (\tilde{x}_{p+1}^+)^{\alpha_{p+1}} \cdots (\tilde{x}_n^+)^{\alpha_n},$$

where \tilde{x}_i^+ are positive variables.

From Proposition 1, $z^+ = x_1^{\alpha_1} \cdots x_p^{\alpha_p} (\tilde{x}_{p+1}^+ \lambda_{p+1})^{\alpha_{p+1}} \cdots (\tilde{x}_n^+ \lambda_n)^{\alpha_n}$ and it is clear that

$$z^+ = \tilde{z}^+ \lambda_{p+1} \cdots \lambda_n, \quad \lambda_i \in \{0, 1\}. \quad (8)$$

Remark 2 [23] Let $\lambda, \lambda_i \in \{0, 1\}$ for $i = p + 1, \dots, n$, then:

$$\lambda = \lambda_{p+1}\lambda_{p+2}\cdots\lambda_n \Leftrightarrow \begin{cases} \text{(i)} & \lambda \leq \lambda_i \text{ for } i = p + 1, \dots, n, \\ \text{(ii)} & \lambda \geq \sum_{i=p+1}^n \lambda_i - n + p + 1. \end{cases}$$

By referring to Remark 2, Eq. (8) becomes

$$z^+ = \bar{z}^+\lambda, \quad \lambda \in \{0, 1\}. \quad (9)$$

From Proposition 1, Eq. (9) is equivalent to the following two linear inequalities.

- (i) $0 \leq z^+ \leq \bar{z}\lambda$,
- (ii) $\bar{z}^+ + \bar{z}(\lambda - 1) \leq z^+ \leq \bar{z}^+$.

$\lambda \in \{0, 1\}$, \bar{z} is the upper bound of z^+ .

According to the above discussions, an MINLP problem with free variables can be totally transformed into another one containing only strictly positive variables. For finding a global optimum of the transformed program, next section proposes convexification strategies to convert the program into a convex MINLP program.

3 Identification of convex terms and convex relaxation strategies

Convexification strategies for signomial terms are important techniques for global optimization problems. Sun et al. [34] proposed a convexification method for a class of global optimization problems with monotone functions under some restrictive conditions. Wu et al. [38] developed a more general convexification and concavification transformation for solving a general global optimization problem with certain monotone properties. With different convexification approaches, an MINLP problem can be reformulated into another convex mixed-integer program solvable to obtain an approximately global optimum. Björk et al. [8] proposed a global optimization technique based on convexifying signomial terms. They discussed that the right choice of transformation for convexifying nonconvex signomial terms has a clear impact on the efficiency of the optimization approach. Tsai et al. [36] also suggested convexification techniques for the signomial terms with three variables. This study presents generalized convexification techniques and rules to transform an MINLP problem into a convex mixed-integer program. Consider the following propositions:

Proposition 2 A twice-differentiable function $f(\mathbf{x}) = c \prod_{i=1}^n x_i^{\alpha_i}$, $\mathbf{x} = (x_1, x_2, \dots, x_n)$, $c, x_i, \alpha_i \in \mathbb{R}$, $\forall i$, is convex if $c \leq 0$, $x_i \geq 0$, $\alpha_i \geq 0$ (for $i = 1, 2, \dots, n$), and $1 - \sum_{i=1}^n \alpha_i \geq 0$.

Proof Let $H_i(\mathbf{x})$ be the i th principal minor of a Hessian matrix $H(\mathbf{x})$ of $f(\mathbf{x})$. The determinant of $H_i(\mathbf{x})$ can be expressed as $\det H_i(\mathbf{x}) = (-1)^i (\prod_{j \in J_i} c \alpha_j x_j^{i \alpha_j - 2}) (\prod_{\substack{j \notin J_i \\ J_i \neq \Phi}}^n x_j^{i \alpha_j}) (1 - \sum_{j \in J_i} \alpha_j)$.

Since $\det H_i(\mathbf{x}) \geq 0$ when $c \leq 0$, $x_i \geq 0$, $\alpha_i \geq 0$, $\forall i$, and $1 - \sum_{i=1}^n \alpha_i \geq 0$, $H_i(\mathbf{x})$, $i = 1, 2, \dots, n$, are positive semi-definite and $f(\mathbf{x})$ is convex.

Corollary 1 A twice-differentiable function $f(\mathbf{x}) = c \prod_{i=1}^n x_i^{\alpha_i}$, $\mathbf{x} = (x_1, x_2, \dots, x_n)$, $c, x_i, \alpha_i \in \mathbb{R}$, $\forall i$, is convex if $c \geq 0$, $x_i \geq 0$ and $\alpha_i \leq 0$ for $i = 1, 2, \dots, n$.

For a given signomial term s , if s satisfies Propositions 2 or Corollary 1, then s is a convex term without any transformation. For instance, $s = -x_1^{0.2}x_2^{0.7}$ with $x_1, x_2 \geq 0$ is a convex term requiring no transformation by Proposition 2, and $s = x_1^{-1}x_2^{-2}x_3^{-1}$ with $x_1, x_2, x_3 \geq 0$ is also a convex term by Corollary 1. Denote $\dot{=}$ as a notation of linear approximation, consider the following propositions.

Proposition 3 A nonlinear term $s = x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}$, where $x_1, x_2, \dots, x_n > 0$, $\alpha_i < 0$ (for $i = 1, 2, \dots, k$), and $\alpha_i \geq 0$ (for $i = k+1, k+2, \dots, n$), can be transformed as follows.

- (i) $s = \prod_{i=1}^k x_i^{\alpha_i} \prod_{i=k+1}^n z_i^{-\alpha_i}$,
- (ii) $z_i + L(-x_i^{-1}) \leq 0$ for $i = k+1, k+2, \dots, n$,
- (iii) $x_i^{-1} - z_i \leq 0$ for $i = k+1, k+2, \dots, n$,

where $L(-x_i^{-1})$ is a piecewise linearization function of a concave term $-x_i^{-1}$.

Proof $L(-x_i^{-1}) \dot{=} -x_i^{-1}$, $z_i = x_i^{-1}$ for $i = k+1, k+2, \dots, n$, following (ii) and (iii).

Since $z_i > 0$ and $-\alpha_i \leq 0$ for $i = k+1, k+2, \dots, n$, s is then a convex term referring to Corollary 1.

Herein the concept of special ordered set of type 2 (SOS-2) constraints can be utilized to generate the piecewise linear function $L(f(x))$ for approximating the concave function $f(x)$ [27, 35]. Since extensive enough relaxation can be tight to the original nonlinear problem within any predefined accuracy, branching should be performed to close the gap. Branching schemes for classical SOS Type 2 case can be found for instance in [5, 6].

The accuracy of the linear approximation significantly depends on the selection of break points. More break points can be selected to increase the accuracy of the linear approximation of $f(x)$. In this study, $\left| \frac{f(x) - L(f(x))}{f(x)} \right|$ is used to estimate the error in linear approximation. If $f(x)$ is an objective function and x^* is the solution derived from the transformed program, then the linearization does not require to be refined until $\left| \frac{f(x^*) - L(f(x^*))}{f(x^*)} \right| \leq \varepsilon_2$, where ε_2 is the optimality tolerance. If $g(x) < 0$ is a constraint and x^* is the solution, then x^* is feasible if $\left| \frac{g(x^*) - L(g(x^*))}{g(x^*)} \right| \leq \varepsilon_1$ and $L(g(x^*)) \leq \varepsilon_1$, where ε_1 is the feasibility tolerance.

Proposition 4 A nonlinear term $s = -x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n}$, where $x_1, x_2, \dots, x_n > 0$, $0 \leq \alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_k$, $0 \geq \alpha_{k+1} \geq \alpha_{k+2} \geq \dots \geq \alpha_n$ and $\sum_{i=1}^r \alpha_i < 1$ for some largest integer r , such that $r \leq k$, can be convexified as follows.

- (i) $s = -\prod_{i=1}^r x_i^{\alpha_i} \prod_{i=r+1}^n z_i^{\beta}$, $\beta = \frac{1 - \sum_{i=1}^r \alpha_i}{n-r}$,
- (ii) $z_i + L(-x_i^{\frac{\alpha_i}{\beta}}) \leq 0$ for $i = r+1, r+2, \dots, n$,
- (iii) $x_i^{\frac{\alpha_i}{\beta}} - z_i \leq 0$ for $i = r+1, r+2, \dots, n$,

where $L(-x_i^{\frac{\alpha_i}{\beta}})$ is a piecewise linearization function of a concave term $-x_i^{\frac{\alpha_i}{\beta}}$.

Proof

$L(-x_i^{\frac{\alpha_i}{\beta}}) \dot{=} -x_i^{\frac{\alpha_i}{\beta}}$, $z_i = x_i^{\frac{\alpha_i}{\beta}}$ for $i = r+1, r+2, \dots, n$, following (ii) and (iii).

Since $\alpha_i > 0$ for $i = 1, 2, \dots, r$, $z_i > 0$ for $i = k+1, k+2, \dots, n$, $\beta > 0$ and $\sum_{i=1}^r \alpha_i + (n-r)\beta = 1$, s is then a convex term referring to Proposition 2.

Remark 3 A function $f(x) = x^\alpha$ for $x > 0$ is convex when $\alpha \leq 0$ or $\alpha \geq 1$. $f(x)$ is concave when $0 \leq \alpha \leq 1$.

Remark 4 For a discrete variable $y \in \{d_1, d_2, \dots, d_m\}$, $d_{j+1} > d_j > 0$ for $j = 1, 2, \dots, m-1$, the nonlinear term y^α where α is a real constant can be represented as follows by the concept of special ordered set type 1 (SOS-1)[35]:

$$y^\alpha = \sum_{j=1}^m d_j^\alpha u_j, \quad \text{where } \sum_{j=1}^m u_j = 1, u_j \in \{0, 1\}.$$

Remark 5 A product term $s = uf(x)$ where $f(x)$ is a linear function is equivalent to the following linear inequalities:

- (i) $\overline{f(x)}(u-1) + f(x) \leq s \leq \overline{f(x)}(1-u) + f(x)$,
- (ii) $-\overline{f(x)}u \leq s \leq \overline{f(x)}u$,

where $u \in \{0, 1\}$, s is an unrestricted in sign variable, and $\overline{f(x)}$ is the upper bound of $f(x)$.

4 Examples

Example 1 Consider the following nonconvex minimization problem:

$$\begin{aligned} &\text{Minimize } x_1^2 x_2^{-2} x_3 - 2x_2^{0.7} x_3^{0.2} + x_4 x_5^{-2} - 2x_1 - 4x_3 \\ &\text{subject to } x_1 + 6x_2 - x_3 - 5x_4 \leq 2, \end{aligned} \quad (10)$$

$$x_3^{1.5} x_4 + 0.5x_2 + 3x_1 \leq -10, \quad (11)$$

$$-x_1 - 0.5x_4 + x_5 \leq 6, \quad (12)$$

$$-7 \leq x_1 \leq 5, 1 \leq x_2 \leq 10, 1 \leq x_3 \leq 5, 2 \leq x_4 \leq 8, 2 \leq x_5 \leq 9,$$

$$x_1, x_2, x_4, x_5 \in \mathbb{R}, \quad x_3 \in \mathbb{Z}.$$

This program is a nonconvex mixed-integer program containing a bounded free variable. Current exponential transformation methods developed for MINLP problems can not be adopted to solve this kind of problem. By adopting the proposed method, we can solve this problem to reach an approximately global optimum. First, we utilize variable substitution to transform the nonconvex MINLP problem with free variables into another one having non-negative variables. By Remark 1, $x_1 = x_1^+ - x_1^-$, $x_1^+, x_1^- \geq 0$. The original problem becomes as follows:

$$\begin{aligned} &\text{Minimize } (x_1^+)^2 x_2^{-2} x_3 + (x_1^-)^2 x_2^{-2} x_3 - 2x_2^{0.7} x_3^{0.2} + x_4 x_5^{-2} - 2x_1 - 4x_3 \\ &\text{subject to } x_1 = x_1^+ - x_1^-, \end{aligned} \quad (13)$$

$$x_1^+ \leq 5\theta_1, \quad (14)$$

$$x_1^- \leq 7(\theta_1 - 1), \quad (15)$$

$$x_1^+ - x_1^- + 6x_2 - x_3 - 5x_4 \leq 2, \quad (16)$$

$$x_3^{1.5} x_4 + 0.5x_2 + 3x_1^+ - 3x_1^- \leq -10, \quad (17)$$

$$-x_1^+ + x_1^- - 0.5x_4 + x_5 \leq 6, \quad (18)$$

$$0 \leq x_1^+ \leq 5, 0 \leq x_1^- \leq 7, 1 \leq x_2 \leq 10, 1 \leq x_3 \leq 5, 2 \leq x_4 \leq 8,$$

$$2 \leq x_5 \leq 9, \theta_1 \in \{0, 1\}, \quad x_2, x_4, x_5 \in \mathbb{R}, \quad x_3 \in \mathbb{Z}.$$

By changing variables, the problem with non-negative variables can be equivalently transformed into another one having positive variables. Herein we introduce two strictly positive variables \tilde{x}_1^+ and \tilde{x}_1^- as follows:

$$0 \leq x_1^+ \leq 5\lambda_1, \quad (19)$$

$$\tilde{x}_1^+ + 5(\lambda_1 - 1) \leq x_1^+ \leq \tilde{x}_1^+, \quad (20)$$

$$0 \leq x_1^- \leq 7\lambda_2, \quad (21)$$

$$\tilde{x}_1^- + 7(\lambda_2 - 1) \leq x_1^- \leq \tilde{x}_1^-. \quad (22)$$

For computer implementation, $\tilde{x}_1^+, \tilde{x}_1^- \geq \varepsilon_0$ where $\varepsilon_0 = 10^{-7}$ is a zero tolerance. The signomial terms $z_1^+ = (x_1^+)^2 x_2^{-2} x_3$ and $z_1^- = (x_1^-)^2 x_2^{-2} x_3$ in the objective function can be replaced by $\bar{z}_1^+ = (\tilde{x}_1^+)^2 x_2^{-2} x_3$ and $\bar{z}_1^- = (\tilde{x}_1^-)^2 x_2^{-2} x_3$, respectively, where

$$\begin{aligned} 0 \leq z_1^+ \leq \bar{z}_1^+, \quad \bar{z}_1^+ + \bar{z}(\lambda_1 - 1) \leq z_1^+ \leq \tilde{z}_1^+, \\ 0 \leq z_1^- \leq \bar{z}_1^-, \quad \bar{z}_1^- + \bar{z}(\lambda_2 - 1) \leq z_1^- \leq \tilde{z}_1^-. \end{aligned}$$

Then this program is a nonconvex MINLP program with six positive variables. From Proposition 2, the nonlinear term $-2x_2^{0.7}x_3^{0.2}$ is convex. The nonconvex terms can be transformed as follows:

- (i) The nonconvex terms $x_3^{1.5}x_4$ and $x_4x_5^{-2}$ can be converted into convex terms $z_3^{-1.5}z_4^{-1}$ and $z_4^{-1}x_5^{-2}$, respectively, where $z_3 = x_3^{-1}$ and $z_4 = x_4^{-1}$ by Proposition 3. According to Remark 4, $z_3 = x_3^{-1}$ can be linearized as $z_3 = u_1 + \frac{1}{2}u_2 + \frac{1}{3}u_3 + \frac{1}{4}u_4 + \frac{1}{5}u_5$ where $x_3 = u_1 + 2u_2 + 3u_3 + 4u_4 + 5u_5$.
- (ii) The nonconvex terms $(\tilde{x}_1^+)^2 x_2^{-2} x_3$ and $(\tilde{x}_1^-)^2 x_2^{-2} x_3$ can be transferred into convex terms $e^{2y_1^+ - 2y_2 + y_3}$ and $e^{2y_1^- - 2y_2 + y_3}$, respectively, where $y_1^+ = \ln \tilde{x}_1^+$, $y_1^- = \ln \tilde{x}_1^-$, $y_2 = \ln x_2$ and $y_3 = \ln x_3$.

Subsequently, the transformed program is presented as below:

Minimize $z_1^+ + z_1^- - 2x_2^{0.7}x_3^{0.2} + z_4^{-1}x_5^{-2} - 2x_1 - 4x_3$

subject to (13), (15)–(22),

$$\begin{aligned} z_3^{-1.5}z_4^{-1} + 0.5x_2 + 3x_1^+ - 3x_1^- &\leq -10, \\ y_1^+ &= L(\ln \tilde{x}_1^+), y_1^- = L(\ln \tilde{x}_1^-), y_2 = L(\ln x_2), \\ y_3 &= u_1 \ln 1 + u_2 \ln 2 + u_3 \ln 3 + u_4 \ln 4 + u_5 \ln 5, \\ 0 \leq z_1^+ \leq \bar{z}_1^+, e^{2y_1^+ - 2y_2 + y_3} + \bar{z}(\lambda_1 - 1) &\leq z_1^+ \leq L(e^{2y_1^+ - 2y_2 + y_3}), \\ 0 \leq z_1^- \leq \bar{z}_1^-, e^{2y_1^- - 2y_2 + y_3} + \bar{z}(\lambda_2 - 1) &\leq z_1^- \leq L(e^{2y_1^- - 2y_2 + y_3}), \\ x_3 &= u_1 + 2u_2 + 3u_3 + 4u_4 + 5u_5, \\ z_3 &= u_1 + \frac{1}{2}u_2 + \frac{1}{3}u_3 + \frac{1}{4}u_4 + \frac{1}{5}u_5, \\ u_1 + u_2 + u_3 + u_4 + u_5 &= 1, \\ x_4^{-1} - z_4 &\leq 0, z_4 + L(-x_4^{-1}) \leq 0, \\ \varepsilon_0 \leq \tilde{x}_1^+ \leq 5, \varepsilon_0 \leq \tilde{x}_1^- \leq 7, 1 \leq x_2 \leq 10, 1 \leq x_3 \leq 5, 2 \leq x_4 \leq 8, 2 \leq x_5 \leq 9, \\ \theta_1, \lambda_1, \lambda_2 \in \{0, 1\}, u_1, u_2, u_3, u_4, u_5 \in \{0, 1\}, \tilde{x}_1^+, \tilde{x}_1^-, x_2, x_4, x_5 \in \mathbb{R}^+, x_3 \in \mathbb{Z}. \end{aligned}$$

The transformed program above is a convex MINLP program solvable by conventional MINLP methods. The error evaluation of the piecewise linear approximation of the concave functions significantly decreases as the number of break points increases. Using 33 break points to solve this problem by LINGO [24], both the optimality tolerance and the feasibility tolerance are within the prespecified error 0.001. The globally optimal solution obtained is $(x_1, x_2, x_3, x_4, x_5) = (-5.353, 4.548, 1, 3.787, 2.541)$ and the objective value is 2.904. Table 1

Table 1 Number of variables in the reformulated model of each example

	Number of original variables	Number of additional continuous variables in reformulated model	Number of additional binary variables in reformulated model	Number of original variables eliminated from formulation
Example 1	5	206	206	1
Example 2	2	4	4	1
Example 3	4	202	202	1

lists the number of the original variables in Example 1, the number of the additional continuous variables and binary variables in the reformulated model, and the number of the original variables completely eliminated from formulation.

Example 2

$$\begin{aligned}
 &\text{Minimize } x_1^{0.5} x_2 + 3 \ln x_1 \\
 &\text{subject to } -x_1 + x_2 \leq 5, \\
 &\quad x_1^{0.5} - x_2 \leq 6, \\
 &\quad x_1 \in \{0.1, 0.5, 0.7, 1.2\}, -6 \leq x_2 \leq 4.
 \end{aligned}$$

This example contains a discrete variable and a free variable which cannot be treated by the exponential-based methods. The nonlinear terms $x_1^{0.5} x_2$, $3 \ln x_1$ and $x_1^{0.5}$ are nonconvex functions. By Remarks 4 and 5, the problem can be equivalently transformed into a linear mixed-integer programming problem as follows.

$$\begin{aligned}
 &\text{Minimize } 0.1^{0.5} s_1 + 0.5^{0.5} s_2 + 0.7^{0.5} s_3 + 1.2^{0.5} s_4 + 3(u_1 \ln 0.1 + u_2 \ln 0.5 + u_3 \ln 0.7 \\
 &\quad + u_4 \ln 1.2) \\
 &\text{subject to } -0.1u_1 - 0.5u_2 - 0.7u_3 - 1.2u_4 + x_2 \leq 5, \\
 &\quad u_1 + u_2 + u_3 + u_4 = 1, \\
 &\quad 0.1^{0.5} u_1 + 0.5^{0.5} u_2 + 0.7^{0.5} u_3 + 1.2^{0.5} u_4 - x_2 \leq 6, \\
 &\quad -6u_i \leq s_i \leq 6u_i, \quad 6(u_i - 1) + x_2 \leq s_i \leq 6(1 - u_i) + x_2, \quad i = 1, 2, 3, 4, \\
 &\quad s_1, s_2, s_3, s_4 \text{ are unrestricted in sign variables, } u_1, u_2, u_3, u_4 \in \{0, 1\}, \\
 &\quad -6 \leq x_2 \leq 4.
 \end{aligned}$$

The transformed program can be solved by LINGO [24] to obtain the globally optimal solution $(x_1, x_2) = (0.1, -5.864)$ and the objective value -8.705 within the optimality tolerance 0.001 and the feasibility tolerance 0.001. Table 1 lists the number of variables used in the transformed model of Example 2.

Example 3

$$\begin{aligned}
 &\text{Minimize } x_1 x_4^3 - x_3 - 0.5 x_1^2 x_2^4 \\
 &\text{subject to } x_1 x_4^{1.5} - x_2 - x_2^{0.5} x_3^{0.4} \leq 4, \\
 &\quad -x_1 - 2x_2 + x_3 \leq -2, \\
 &\quad 0 \leq x_1 \leq 6, 1 \leq x_2 \leq 10, 1 \leq x_3 \leq 6, 20 \leq x_4 \leq 30, \quad x_1, x_2, x_3, x_4 \in \mathbb{R}^+.
 \end{aligned}$$

Example 3 is a nonconvex problem with zero-value lower bound variables that cannot be treated by current exponential-based methods. The nonlinear terms $x_1 x_4^3$, $x_1^2 x_2^4$ and $x_1 x_4^{1.5}$

where x_1 has a zero-value lower bound can be transformed into another ones with only strictly positive variables by the proposed method in Sect. 2. Then the transformed terms can be relaxed by the proposed technique in Sect. 3. Table 1 lists the number of variables used in the transformed model of Example 3. Although the proposed method requires the addition of new variables, binary variables and constraints, it can avoid some inaccuracy introduced by just specifying a small $\varepsilon > 0$ lower bound for x_1 . Solving this program by the proposed method with LINGO [24], the globally optimal solution obtained is $(x_1, x_2, x_3, x_4) = (0, 4, 6, 20)$ and the objective value is -6 . However, solving this program by just specifying $x_1 \geq 0.001$, the globally optimal solution obtained is $(x_1, x_2, x_3, x_4) = (0.001, 10, 6, 20)$ and the objective value is 1.995. This example demonstrates that the importance of the proposed transformation for treating the issue of lower bound being zero.

5 Conclusions

This study proposes an optimization method for treating a signomial MINLP problem with free variables to find a global optimum. The techniques of dealing with free variables aim to change variables and to convert the logical relationship among the variables in a product term into a set of linear inequalities, which can be merged conveniently into the MINLP models. Some useful rules to effectively convexify more general signomial terms in MINLP programs are also presented. Numerical examples are illustrated to support the contributions of the proposed method.

References

1. Adjiman, C.S., Androulakis, I.P., Floudas, C.A.: Global optimization of MINLP problems in process synthesis and design. *Comput. Chem. Eng.* **21**, S445–S450 Suppl. S (1997)
2. Adjiman, C.S., Androulakis, I.P., Floudas, C.A.: Global optimization of mixed-integer nonlinear problems. *AIChE J.* **46**(9), 1769–1797 (2000)
3. Adjiman, C.S., Androulakis, I.P., Maranas, C.D., Floudas, C.A.: A global optimization method α BB for process design. *Comput. Chem. Eng.* **20**, S419–S424 Suppl. A (1996)
4. Aggarwal, A., Floudas, C.A.: Synthesis of general separation sequences-nonsharp separations. *Comput. Chem. Eng.* **14**(6), 631–653 (1990)
5. Beale, E.M.L., Forrest, J.J.H.: Global optimization using special ordered sets. *Math. Prog.* **10**, 52–69 (1976)
6. Beale, E.L.M., Tomlin, J.A.: Special facilities in a general mathematical programming system for nonconvex problems using ordered sets of variables. In: Lawrence, J. (ed.) *Proceedings of the Fifth International Conference on Operations Research*, pp. 447–454. Tavistock Publications, London (1970)
7. Biegler, L.T., Grossmann, I.E.: Retrospective on optimization. *Comput. Chem. Eng.* **28**, 1169–1192 (2004)
8. Björk, K.M., Lindberg, P.O., Westerlund, T.: Some convexifications in global optimization of problems containing signomial terms. *Comput. Chem. Eng.* **27**, 669–679 (2003)
9. Borchers, B., Mitchell, J.E.: An improved branch and bound algorithm for mixed integer nonlinear programs. *Comput. Oper. Res.* **21**(4), 359–367 (1994)
10. Duran, M., Grossmann, I.E.: An outer-approximation algorithm for a class of mixed integer nonlinear programs. *Math. Prog.* **36**, 307–339 (1986)
11. Fletcher, R., Leyffer, S.: Solving mixed integer nonlinear programs by outer approximation. *Math. Prog.* **66**, 327–349 (1994)
12. Floudas, C.A.: *Deterministic Global Optimization: Theory, Methods and Application*. Kluwer Academic Publishers, Boston (2000)
13. Floudas, C.A., Akrotirianakis, I.G., Caratzoulas, S., Meyer, C.A., Kallrath, J.: Global optimization in the 21st century: advances and challenges. *Comput. Chem. Eng.* **29**, 1185–1202 (2005)

14. Floudas, C.A., Pardalos, P.M.: State of the Art in Global Optimization: Computational Methods and Applications. Kluwer Academic Publishers, Boston (1996)
15. Geoffrion, A.M.: Generalized benders decomposition. *J. Opt. Theory Appl.* **10**, 237–260 (1972)
16. Glover, F., Laguna, M.: Tabu Search. Kluwer Academic Publishers, Boston (1997)
17. Grossmann, I.E.: Review of nonlinear mixed-integer and disjunctive programming techniques. *Opt. Eng.* **3**, 227–252 (2002)
18. Grossmann, I.E., Biegler, L.T.: Part II. Future perspective on optimization. *Comput. Chem. Eng.* **28**, 1193–1218 (2004)
19. Hussain, M.F., Al-Sultan, K.S.: A hybrid genetic algorithm for nonconvex function minimization. *J. Global Opt.* **11**, 313–324 (1997)
20. Kokossis, A.C., Floudas, C.A.: Optimization of complex reactor networks-II: nonisothermal operation. *Chem. Eng. Sci.* **49**(7), 1037–1051 (1994)
21. Lee, S., Grossmann, I.E.: New algorithms for nonlinear generalized disjunctive programming. *Comput. Chem. Eng.* **24**, 2125–2142 (2000)
22. Leyffer, S.: Integrating sqp and branch-and-bound for mixed integer nonlinear programming. *Computat. Opt. Appl.* **18**, 295–309 (2001)
23. Li, H.L., Tsai, J.F.: Treating free variables in generalized geometric global optimization programs. *J. Global Opt.* **33**, 1–13 (2005)
24. LINGO Release 9.0. LINDO System Inc., Chicago (2004)
25. Maranas, C.D., Floudas, C.A.: Finding all solutions of nonlinearly constrained systems of equations. *J. Global Opt.* **7**(2), 143–182 (1995)
26. Maranas, C.D., Floudas, C.A.: Global optimization in generalized geometric programming. *Comput. Chem. Eng.* **21**(4), 351–369 (1997)
27. Martin, A., Möller, M., Moritz, S.: Mixed integer models for the stationary case of gas network optimization. *Math. Prog.* **105**, 563–582 (2006)
28. McDonald, C.M., Floudas, C.A.: Global optimization for the phase and chemical equilibrium problem: application to the NRTL equation. *Comput. Chem. Eng.* **19**(11), 1111–1141 (1995)
29. Papalexandri, K.P., Pistikopoulos, E.N., Floudas, C.A.: Mass-exchange networks for waste minimization – a simultaneous approach. *Chem. Eng. Res. Design* **72**(A3), 279–294 (1994)
30. Pörn, R., Harjunkoski, I., Westerlund, T.: Convexification of different classes of nonconvex MINLP problems. *Comput. Chem. Eng.* **23**, 439–448 (1999)
31. Quesada, I., Grossmann, I.E.: An LP/NLP based branch and bound algorithm for convex MINLP optimization problems. *Comput. Chem. Eng.* **16**, 937–947 (1992)
32. Salcedo, R.L., Goncalves, M.J., Feyo de Azevedo, S.: An improved random-search algorithm for nonlinear optimization. *Comput. Chem. Eng.* **14**, 1111–1126 (1990)
33. Stubbs, R.A., Mehrotra, S.: A branch-and-cut method for 0–1 mixed convex programming. *Math. Prog.* **86**, 515–532 (1999)
34. Sun, X.L., McKinnon, K.I.M., Li, D.: A convexification method for a class of global optimization problems with applications to reliability optimization. *J. Global Opt.* **21**, 185–199 (2001)
35. Tomlin, J.A.: A suggested extension of special ordered sets to non-separable non-convex programming. Problems. In: Hansen, P. (ed.) *Studies on Graphs and Discrete Programming*, pp. 359–370. North-Holland Publishing Company, Amsterdam (1981)
36. Tsai, J.F., Li, H.L., Hu, N.Z.: Global optimization for signomial discrete programming problems in engineering design. *Eng. Opt.* **34**, 613–622 (2002)
37. Westerlund, T., Pettersson, F.: An Extended cutting plane method for solving convex MINLP problems. *Comput. Chem. Eng.* **19**, S131–S136 Suppl. (1995)
38. Wu, Z.Y., Bai, F.S., Zhang, L.S.: Convexification and concavification for a general class of global optimization problems. *J. Global Opt.* **31**, 45–60 (2005)
39. Yiu, K.F.C., Liu, Y., Teo, K.L.: A hybrid descent method for global optimization. *J. Global Opt.* **28**, 229–238 (2004)