Math. Program., Ser. A
DOI 10.1007/s10107-012-0618-8

FULL LENGTH PAPER

Relaxations of factorable functions with convex-transformable intermediates

Aida Khajavirad · Jeremy J. Michalek · Nikolaos V. Sahinidis

Received: 30 June 2010 / Accepted: 25 November 2012

Abstract We propose to strengthen standard factorable relaxations of global optimization problems through the use of functional transformations of intermediate expressions. In particular, we exploit convex transformability of the component functions of factorable programs as a tool in the generation of bounds. We define suitable forms of transforming functions and assess, theoretically and computationally, the sharpness of the resulting relaxations in comparison to existing schemes.

Keywords Convexification · Generalized convexity · Factorable programming · G-convex functions · Global optimization

Mathematics Subject Classification 65K05 · 90C30 · 90C26

This research was supported in part by National Science Foundation award CMII-1030168.

A. Khajavirad
Mathematical Sciences, IBM T. J. Watson Research Center, Yorktown Heights, NY, USA
e-mail: aidakhajavi@us.ibm.com

J. J. Michalek
Department of Mechanical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA
e-mail: jmichalek@cmu.edu

J. J. Michalek
Department of Engineering and Public Policy, Carnegie Mellon University, Pittsburgh, PA, USA

N. V. Sahinidis (✉)
Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, USA
e-mail: sahinidis@cmu.edu

Published online: 19 December 2012

1 Introduction

Factorable programming techniques are used widely in global optimization for bounding nonconvex functions [16,28,32]. These techniques iteratively decompose a nonconvex factorable function, optionally through the introduction of variables and constraints for intermediate functional expressions, until each intermediate expression can be outer-approximated by a convex feasible set, typically a convex hull. This decomposition is invoked only to the extent that all intermediates in the hierarchy of functions thus generated can be convexified via known techniques. With the exception of univariate functions, at the time of this writing, there exists a small number of nonconvex functions for which convex and concave envelopes are known and lend themselves to practical implementations. This includes various functional types with polyhedral convex envelopes [1,3,17,18,27,29], fractional term [30,31], $(n-1)$ convex functions with indefinite Hessians [7], and products of convex and component-wise concave functions [9,10].

In this paper, we examine whether nested functional decompositions of factorable programs can be replaced by, or enhanced via, the use of functional transformations. In essence, in addition to convexifying simple intermediate expressions, we exploit *convex transformability* of more complex component functions of factorable programs as a tool in the generation of bounding functions for global optimization algorithms. Transformation techniques have been proposed in the global optimization literature to convexify signomial functions [11–15]. In particular, one can underestimate a signomial by applying term-wise power and exponential transformations to all or a subset of variables, followed by a relaxation of the inverse transformations. Our transformation scheme differs from existing methods in that it is applicable to general nonconvex mathematical programs and exploits pseudoconvexity of component functions to generate relaxations that are provably tighter than existing relaxations.

Convex-transformable functions have been studied extensively in the generalized convexity literature [2,26]. This literature has focused mostly on deriving necessary and sufficient conditions under which a certain nonconvex optimization problem can be transformed to a convex one. Furthermore, in the economics literature, there has been a line of research to identify whether a given convex preference ordering can be represented in terms of the upper level sets of a concave utility function [4,8]. This latter question can be restated in terms of whether a quasiconcave function can be converted to a concave one via a one-to-one transformation. While quite rich and interesting, the theory of convex-transformable functions has found limited applications in nonconvex optimization because the vast majority of nonconvex optimization problems are not convex transformable. However, the family of convex-transformable functions subsumes many functional forms, such as products and ratios of convex and/or concave functions, that appear frequently as building blocks of nonconvex expressions. Therefore, exploiting convex-transformability of component functions to construct outer approximations for the intermediate expressions of factorable programs can lead to relaxations that are tighter than those obtained by existing approaches.

The mere incorporation of functional transformations in global optimization of factorable programs may be viewed as obvious. However, the use of these transformations gives rise to interesting questions regarding suitable forms of transforming functions as well as the sharpness of the resulting relaxations, especially in comparison to existing relaxations for factorable programs. This paper addresses several questions of this nature. First, in Sect. 2, we review preliminary material from the generalized convexity literature and obtain some properties of convex-transformable functions. We introduce a new relaxation method for convex-transformable functions in Sect. 3. In Sect. 4, we derive the tightest, in a well-defined sense, transforming functions for signomial terms, propose a new method for overestimating signomials, and present theoretical comparisons of the proposed relaxation versus a conventional one. In Sect. 5, we generalize the results of Sect. 4 to a large class of composite functions involving products and ratios of convex and/or concave functions. As another important application of the proposed convexification method, in Sect. 6, we consider the class of log-concave functions. Finally, in Sect. 7, we use simple examples to illustrate the integration of the proposed relaxation within the factorable programming framework and examine its impact on the convergence rate of a branch-and-bound based global solver.

2 Convex-transformable functions

In this section, we derive some elementary properties of convex-transformable (G-convex) functions. The proofs are direct and not based on the equivalence of different classes of generalized convex functions. Analogous results for concave-transformable (G-concave) functions can be established in a similar manner. Throughout the paper, ϕ represents a nonconvex continuous function defined over a convex set $\mathcal{C} \subseteq \mathbb{R}^n$. The set of extreme points of $\mathcal{C}$ will be denoted by vert($\mathcal{C}$), while the relative interior of $\mathcal{C}$ will be denoted by ri($\mathcal{C}$). By G, we will denote a continuous univariate function that is increasing on $I_\phi(\mathcal{C})$, where $I_\phi(\mathcal{C})$ is the image of $\mathcal{C}$ under ϕ. The convex envelope of ϕ over $\mathcal{C}$, denoted by $\mathrm{conv}_{\mathcal{C}}\phi$, is defined as the tightest convex underestimator of ϕ over $\mathcal{C}$. Similarly, $\mathrm{conc}_{\mathcal{C}}\phi$ stands for the concave envelope of ϕ over $\mathcal{C}$ and is equal to the negative of the convex envelope of $-\phi$ over $\mathcal{C}$. When the domain is clear from the context, we may drop the subscript $\mathcal{C}$ from $\mathrm{conv}_{\mathcal{C}}\phi$ (or $\mathrm{conc}_{\mathcal{C}}\phi$). We begin by recalling the definition of G-convex functions.

Definition 1 ([2]) A continuous function $\phi : \mathcal{C} \to \mathbb{R}$ is said to be convex-transformable or G-convex if there exists a continuous increasing function G defined on $I_\phi(\mathcal{C})$ such that $G(\phi)$ is convex over $\mathcal{C}$.

Throughout the paper, we exclude the trivial case where $G(t) = t$, for all $t \in I_\phi(\mathcal{C})$. Namely, we assume that the G-convex function ϕ is not convex. We now derive sufficient conditions for G-convexity of composite functions. We will consider scalar composition, vector composition and composition with an affine mapping in turn.

Proposition 1 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex and let f be an increasing function on $\mathcal{D} \subseteq \mathbb{R}$, where $\mathcal{D} \supseteq I_\phi(\mathcal{C})$. Then, the composite function $h(x) = f(\phi(x))$ is $\tilde{G}$-convex on $\mathcal{C}$, where $\tilde{G} = G(f^{-1})$.*

Proof By assumption, f and G are both increasing over $I_\phi(\mathcal{C})$. Thus, the inverse function of f, denoted by f^{-1} exists and the function $\tilde{G} = G(f^{-1})$ is increasing over the range of h. By G-convexity of ϕ, $\tilde{G}(h)$ is convex on $\mathcal{C}$. □

Proposition 2 *Let $f : \mathcal{D} \to \mathbb{R}^n$ be a vector of functions $f_j,\ j \in J = \{1, \ldots, n\}$, where $\mathcal{D} \subseteq \mathbb{R}^m$ is a convex set. Let $\bar{J}$ contain the elements of J for which f_j is not affine. Assume that f_j is convex for $j \in J_1 \subseteq \bar{J}$ and concave for $j \in J_2 = \bar{J} \backslash J_1$. Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex, where $\mathcal{C}$ is a convex set in $\mathbb{R}^n$ such that $\mathcal{C} \supseteq I_f(\mathcal{D})$. Assume that $\phi(y_1, \ldots, y_n)$ is nondecreasing in $y_j,\ j \in J_1$ and is nonincreasing in $y_j,\ j \in J_2$. Then, $h(x) = \phi(f(x))$ is G-convex on $\mathcal{D}$.*

Proof We prove the case where $J = J_1$. The proof for the general case is similar. Let $x^1 \in \mathcal{D},\ x^2 \in \mathcal{D}$. By assumption, all components of f are convex, ϕ is nondecreasing over $I_f(\mathcal{D})$ and G is increasing over $I_\phi(\mathcal{C})$. Thus, the following holds for every $\lambda \in [0, 1]$:

$$G(\phi(f(\lambda x^1 + (1-\lambda)x^2))) \leq G(\phi(\lambda f(x^1) + (1-\lambda) f(x^2))). \tag{1}$$

From G-convexity of ϕ over $I_f(\mathcal{D})$, it follows that:

$$G(\phi(\lambda f(x^1) + (1-\lambda) f(x^2))) \leq \lambda G(\phi(f(x^1))) + (1-\lambda) G(\phi(f(x^2))). \tag{2}$$

Combining (1) and (2), we obtain:

$$G(\phi(f(\lambda x^1 + (1-\lambda)x^2))) \leq \lambda G(\phi(f(x^1))) + (1-\lambda) G(\phi(f(x^2))),$$

which is the definition of G-convexity for the composite function $h(x)$ over $\mathcal{D}$. □

Proposition 3 *Consider the function ϕ over a convex set $\mathcal{C} \subseteq \mathbb{R}^n$. Let $T : x \to Ax + b$ denote an affine transformation, where $A \in \mathbb{R}^{n\times m},\ x \in \mathcal{D} \subseteq \mathbb{R}^m$ and $b \in \mathbb{R}^n$. Assume $\mathcal{D}$ is a convex set and $Ax + b \in \mathcal{C}$ for all $x \in \mathcal{D}$. Then, $\phi(Ax + b)$ is G-convex on $\mathcal{D}$, if ϕ is G-convex on $\mathcal{C}$.*

Proof Follows directly from Proposition 2 by letting $f = Ax + b$. Since all components of f are affine functions, no monotonicity assumption on ϕ is required. □

Next, we present the concept of *least convexifying transformation*, which was first introduced by Debreu [4] in the economics literature to define least concave utility functions. In Sect. 3, we will show that least convexifying transformations are of crucial importance for convexifying nonconvex problems.

Definition 2 ([4]) If ϕ is G^*-convex and, for every G for which ϕ is G-convex, GG^{*-1} is convex on the image of the range of ϕ under G^*, then G^* will be referred to as a least convexifying transformation for ϕ.

Remark 1 Least convexifying transformations are unique up to an increasing affine transformation, i.e., if G_1 and G_2 are both least convexifying for ϕ, then $G_2 = \alpha G_1 + \beta$, for some $\alpha > 0$ and $\beta \in \mathbb{R}$.

Next, we make use of Propositions 1 and 2 to derive least convexifying transformations for composite functions.

Proposition 4 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex with a least convexifying transformation denoted by G^*. Consider an increasing function f defined on $\mathcal{D} \supseteq I_\phi(\mathcal{C})$. Then, a least convexifying transformation for $h(x) = f(\phi(x))$ is given by $G^*(f^{-1})$.*

Proof By Proposition 1, h is $\hat{G}$-convex with $\hat{G} = G^*(f^{-1})$. We claim that $\hat{G}$ is least convexifying for h. Assume the contrary and denote by $\tilde{G}$ a least convexifying transformation for h. By Definition 2, $\hat{G}\tilde{G}^{-1}$ is convex. Let $\bar{G} = \tilde{G}(f)$. It follows that $\bar{G}(\phi)$ is convex. It is easy to show that $\bar{G}G^{*-1} = (\hat{G}\tilde{G}^{-1})^{-1}$ and therefore is concave; contradicting the least convexifying assumption on G^*. Consequently, $G^*(f^{-1})$ is least convexifying for h. ☐

Corollary 1 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex with a least convexifying transformation denoted by G^*. Let $\mathcal{D}$ be a convex set in $\mathbb{R}^m$ such that $Ax + b \in \mathcal{C}$ for all $x \in \mathcal{D}$, where A is a real $n \times m$ matrix. Then, G^* is least convexifying for $\phi(Ax + b)$.*

Proof Follows directly from Proposition 3 by noting that the inverse image of a convex set under an affine transformation is convex (cf. Theorem 3.4 in [20]). ☐

In the sequel, we only consider the case where both ϕ and G are twice continuously differentiable (C^2) functions on open convex subsets of $\mathbb{R}^n$ and $\mathbb{R}$, respectively. Necessary and sufficient conditions for convex transformability of C^2 functions were first derived by Fenchel [5]. We summarize the main results in Propositions 5 and 6.

Proposition 5 *([2]) Let $\phi : \mathcal{C} \to \mathbb{R}$ be a differentiable G-convex function and let G be differentiable over $I_\phi(\mathcal{C})$. Then, ϕ is pseudoconvex on $\mathcal{C}$.*

Proposition 6 *([2]) Let $\phi : \mathcal{C} \to \mathbb{R}$ and G be C^2 functions. Then, ϕ is G-convex if and only if the Hessian of $G(\phi)$ is positive semidefinite for every $x \in \mathcal{C}$.*

Since G is increasing and ϕ is G-convex, we have $G'(t) > 0$ over $\mathrm{ri}(I_\phi(\mathcal{C}))$. Letting $\rho(x) = G''(\phi(x))/G'(\phi(x))$, and defining the augmented Hessian of ϕ as:

$$H(x; \rho) = \nabla^2\phi(x) + \rho(x)\nabla\phi(x)\nabla\phi(x)^T, \tag{3}$$

the condition of Proposition 6 implies that, for a G-convex function, there exists a function $\rho(x)$ defined on $\mathcal{C}$ such that $H(x; \rho)$ is positive semidefinite for all $x \in \mathcal{C}$. Furthermore, if the function $\rho_0(x)$ defined by

$$\rho_0(x) = \sup_{z \in \mathbb{R}^n} \left\{ -\frac{z^T\nabla^2\phi(x)z}{\left(z^T\nabla\phi(x)\right)^2} : \|z\| = 1,\ z^T\nabla\phi(x) \neq 0 \right\} \tag{4}$$

is bounded from above for every $x \in \mathcal{C}$, then $H(x; \rho)$ is positive semidefinite for every $\rho(x) \geq \rho_0(x)$ over $\mathcal{C}$. By Proposition 5, points where $\nabla\phi(x) = 0$ are minimizers of ϕ. Thus, the Hessian of ϕ is positive-semidefinite at these points and, as a result, $\rho(x)$ can take any nonnegative value. Moreover, it can be shown that (cf. Proposition 3.16 in [2]), for a C^2 pseudoconvex function ϕ, the restriction of its Hessian to the subspace orthogonal to $\nabla\phi$ is positive semidefinite. Hence, the nonzero assumption on $z^T\nabla\phi(x)$ in (4) is without loss of generality. From the definition of ρ_0, we can compute $G^*(t)$ as:

$$\frac{\mathrm{d}}{\mathrm{d}t} \ln\left(\frac{\mathrm{d}G^*(t)}{\mathrm{d}t}\right) = g(t), \tag{5}$$

where $g(t) = \sup_{x \in \mathcal{C}}\{\rho_0(x) : \phi(x) = t\}$.

As corollaries of the above results, we next derive several properties of the transforming function G that we will use in subsequent sections.

Corollary 2 *Let the G-convex function $\phi : \mathcal{C} \to \mathbb{R}$ be nonconvex. Then, G is nonconcave over $I_\phi(\mathcal{C})$. In particular, $G(t)$ is locally strictly convex at any $\hat{t} = \phi(\hat{x})$ for which ϕ is not locally convex at some $\hat{x} \in \mathcal{C}$.*

Proof From (4) it follows that, if $\nabla^2\phi(\hat{x})$ is not positive semidefinite at $\hat{x} \in \mathcal{C}$, then $\rho_0(\hat{x}) > 0$. Thus, $g(t)$ and $\mathrm{d}^2G^*(t)/\mathrm{d}t^2$ are both positive at $t = \hat{t} = \phi(\hat{x})$. By Definition 2, every G which convexifies ϕ is strictly convex at $\hat{t}$. □

The above result can be further refined for the class of merely pseudoconvex functions, defined as follows.

Definition 3 Let $\phi : \mathcal{C} \to \mathbb{R}$ be pseudoconvex. If ϕ is not locally convex at any $x \in \mathcal{C}$, then ϕ will be referred to as a *merely pseudoconvex* function.

Corollary 3 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex with a least convexifying function denoted by G^*. If ϕ is merely pseudoconvex over $\mathcal{C}$, then G^* is strictly convex over $I_\phi(\mathcal{C})$.*

Proof Follows directly from Corollary 2. □

The converse of the above corollary does not hold, in general, due to taking the supremum in the computation of $g(t)$ in (5).

3 Convexification via transformation

In this section, we consider the problem of outer-approximating the set

$$\Phi := \{(x, t) \in \mathcal{C} \times \mathcal{I} : \phi(x) \le t\}, \tag{6}$$

where the nonconvex function $\phi : \mathcal{C} \to \mathbb{R}$ is G-convex and $\mathcal{I} \supseteq I_\phi(\mathcal{C})$ denotes a closed interval over which $G(t)$ is increasing. This is the typical form of an intermediate constraint introduced within the factorable decomposition in the construction of relaxations of nonconvex optimization problems [32,33]. More specifically, $\phi(x)$ is assumed to be part of the initial nonconvex expression and t denotes an auxiliary variable introduced for the purpose of separable reformulation.

Proposition 7 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex with $\bar{G}(t)$ denoting a concave overestimator for $G(t)$ over $\mathcal{I}$. Then, the following is a convex relaxation of the set Φ:*

$$\tilde{\Phi} := \left\{(x, t) \in \mathcal{C} \times \mathcal{I} : G(\phi(x)) \le \bar{G}(t)\right\} \tag{7}$$

Proof Since G is increasing over $\mathcal{I}$, the set Φ can be equivalently written as $\Phi = \{(x, t) \in \mathcal{C}\times\mathcal{I} : G(\phi(x)) \le G(t)\}$. By Corollary 2, $G(t)$ is nonconcave. Therefore, to obtain a convex outer approximation of Φ, $G(t)$ should be replaced by a concave overestimator. Denoting such a relaxation by $\bar{G}(t)$, it follows that $\tilde{\Phi}$ is a convex relaxation for Φ. □

From (7), it follows that the quality of the proposed relaxation depends on the form of G and the tightness of $\bar{G}$. For a given transforming function G, by definition, $\mathrm{conc}_{\mathcal{I}}G(t) \le \bar{G}(t)$ for all $t \in \mathcal{I}$. Thus, setting $\bar{G}(t) = \mathrm{conc}_{\mathcal{I}}G(t)$ provides the tightest relaxation in (7). Next, we investigate the criteria for choosing the transforming function G.

Proposition 8 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G_1-convex and G_2-convex. Consider the following convex outer approximations of the set Φ defined by (6):*

1. $\tilde{\Phi}_1 = \{(x,t) \in \mathcal{C} \times \mathcal{I} : G_1(\phi(x)) \leq \mathrm{conc}_{\mathcal{I}} G_1(t)\}$,
2. $\tilde{\Phi}_2 = \{(x,t) \in \mathcal{C} \times \mathcal{I} : G_2(\phi(x)) \leq \mathrm{conc}_{\mathcal{I}} G_2(t)\}$.

Let $F(u) = G_2(G_1^{-1}(u))$ be defined over the image of $\mathcal{I}$ under G_1. Then,

(i) *If F is concave, $\tilde{\Phi}_2 \subseteq \tilde{\Phi}_1$;*
(ii) *If F is convex, $\tilde{\Phi}_1 \subseteq \tilde{\Phi}_2$;*
(iii) *Otherwise, neither $\tilde{\Phi}_1$ nor $\tilde{\Phi}_2$ globally dominates the other.*

Proof By definition, $G_2(t) = F(G_1(t))$. Since G_1 and G_2 are both increasing over $\mathcal{I}$, F is also increasing over the range of G_1. Hence, $\tilde{\Phi}_1 = \{(x,t) \in \mathcal{C} \times \mathcal{I} : F(G_1(\phi(x))) \leq F(\mathrm{conc}\, G_1(t))\}$ or, equivalently, $\tilde{\Phi}_1 = \{(x,t) \in \mathcal{C} \times \mathcal{I} : G_2(\phi(x)) \leq F(\mathrm{conc}\, G_1(t))\}$. Further, $\tilde{\Phi}_2 = \{(x,t) \in \mathcal{C} \times \mathcal{I} : G_2(\phi(x)) \leq \mathrm{conc}\, F(G_1(t))\}$. Since F is increasing, $F(G_1) \leq F(\mathrm{conc}\, G_1)$. When F is concave, $F(\mathrm{conc}\, G_1)$ is a concave function. By definition, $\mathrm{conc}_{\mathcal{I}} F(G_1)$ is the tightest concave function that majorizes $F(G_1)$ over $\mathcal{I}$. It follows that $\mathrm{conc}\, F(G_1) \leq F(\mathrm{conc}\, G_1)$ and, as a result, $\tilde{\Phi}_2 \subseteq \tilde{\Phi}_1$. Similarly, for Part (ii), $G_1(t) = F^{-1}(G_2(t))$ and, since F^{-1} is a concave increasing function over the range of G_2, it can be shown that $\tilde{\Phi}_1 \subseteq \tilde{\Phi}_2$. Finally, it follows from the first two parts that, if F is neither convex nor concave, then neither of the two relaxations is globally dominant. □

Remark 2 In Parts (i) and (ii) of Proposition 8, the set inclusion relations are often strict. For example, if G_1 and G_2 are both convex, and F is concave, then $\mathrm{conc}_{\mathcal{I}} F(G_1)$ is the affine underestimator of the concave function $F(\mathrm{conc} G_1)$. This implies that $\tilde{\Phi}_2 \subset \tilde{\Phi}_1$.

Remark 3 Employing a similar line of arguments, for a G-concave function ϕ, the conditions of Proposition 8 can be stated as: (i) if F is concave, $\tilde{\Phi}_1 \subseteq \tilde{\Phi}_2$, (ii) if F is convex, $\tilde{\Phi}_2 \subseteq \tilde{\Phi}_1$, (iii) otherwise, neither $\tilde{\Phi}_1$ nor $\tilde{\Phi}_2$ globally dominates the other.

Using the result of Proposition 8 and the concept of least convexifying transformations introduced in Sect. 2, we now show that the tightest relaxation of the form (7) has a well-defined mathematical description as given by the following corollary.

Corollary 4 *For a G-convex function $\phi : \mathcal{C} \to \mathbb{R}$, the tightest relaxation of the form (7) is obtained using $G = G^*$ and $\bar{G} = \mathrm{conc}_{\mathcal{I}} G^*$.*

Proof Assume the contrary and denote by $\tilde{G}$ the transforming function that yields the tightest relaxation of the set Φ defined by (7). Let $F = \tilde{G}(G^{*-1})$. By Part (i) of Proposition 8, it follows that F is concave. However, by Definition 2, if G^* is least convexifying for ϕ, then F is a convex function. Hence, G^* provides the tightest convex outer approximation of Φ. □

By Proposition 1, if $\phi : \mathcal{C} \to \mathbb{R}$ is G-convex and f is increasing over the range of ϕ, then $h(x) = f(\phi(x))$ is $\tilde{G}$-convex on $\mathcal{C}$, where $\tilde{G} = G(f^{-1})$. Next, we show that, under certain assumptions, a recursive outer approximation of $h(x)$ defined by $\phi(x) \le u$ and $f(u) \le t$ is equivalent to the direct convexification of $h(x) \le t$. Therefore, in such cases, detecting $\tilde{G}$-convexity of the composite function $h(x)$ is not necessary for bounding, as this property is automatically exploited within the factorable decomposition. In the following, we denote by $\mathrm{Proj}_{(x,t)}\tilde{\Phi}$ the projection of the set $\tilde{\Phi}$ onto the space of the variables (x, t).

Proposition 9 *Let $\phi : \mathcal{C} \to \mathbb{R}$ be G-convex and let f be increasing over $\mathcal{D} \supseteq I_\phi(\mathcal{C})$. Define $h(x) = f(\phi(x))$ and $\Phi = \{(x, t) \in \mathcal{C}\times\mathcal{I}_h(\mathcal{C}) : h(x) \le t\}$. Consider the following relaxations of the set Φ:*

1. $\tilde{\Phi}_1 = \left\{(x, t) \in \mathcal{C}\times\mathcal{I}_h(\mathcal{C}) : \tilde{G}(h(x)) \le \mathrm{conc}\ \tilde{G}(t)\right\}$,
2. $\tilde{\Phi}_2 = \left\{(x, u, t) \in \mathcal{C}\times\mathcal{I}_\phi(\mathcal{C})\times I_h(\mathcal{C}) : G(\phi(x)) \le \mathrm{conc}\ G(u),\ \mathrm{conv} f(u) \le t\right\}$,

where $\tilde{G} = G(f^{-1})$. Then, $\tilde{\Phi}_1 = \mathrm{Proj}_{(x,t)}\tilde{\Phi}_2$ if one of the following conditions holds:

(i) *f is convex on $\mathcal{D}$;*
(ii) *f is concave on $\mathcal{D}$ and G is convex on $\mathcal{D}$.*

Otherwise, $\tilde{\Phi}_1 \subseteq \mathrm{Proj}_{(x,t)}\tilde{\Phi}_2$.

Proof Since f and G are both increasing over the range of ϕ, and $G(u) = \tilde{G}(f(u))$, the set $\tilde{\Phi}_1$ can be equivalently written as:

$$\tilde{\Phi}_1 = \left\{(x, t) \in \mathcal{C}\times\mathcal{I}_h(\mathcal{C}) : G(\phi(x)) \le \mathrm{conc}\ G(f^{-1}(t))\right\}.$$

Furthermore, since f is univariate and increasing over $\mathcal{D}$, we have $(\mathrm{conv} f)^{-1} = \mathrm{conc}(f^{-1})$. Thus, we can project out u from $\tilde{\Phi}_2$ to obtain

$$\mathrm{Proj}_{(x,t)}\tilde{\Phi}_2 = \left\{(x, t) \in \mathcal{C}\times\mathcal{I}_h(\mathcal{C}) : G(\phi(x)) \le \mathrm{conc}(G(\mathrm{conc} f^{-1}(t)))\right\}.$$

Now, we consider three cases:

- If $f^{-1} = \mathrm{conc}(f^{-1})$, then $\tilde{\Phi}_1 = \tilde{\Phi}_2$. This condition holds if and only if f is convex on the range of ϕ.
- If f is concave on $\mathcal{D}$ and G is convex on $\mathcal{D}$, then both f^{-1} and $G(f^{-1})$ are convex on $\mathcal{I}_h(\mathcal{C})$. As a result, all corresponding concave envelopes are affine functions. It is simple to show that $\mathrm{aff}(G(f^{-1})) = \mathrm{aff}(G(\mathrm{aff}(f^{-1})))$, where $\mathrm{aff}(\cdot)$ denotes the corresponding affine overestimator. This implies that $\tilde{\Phi}_1 = \mathrm{Proj}_{(x,t)}\tilde{\Phi}_2$.
- Suppose that neither (i) nor (ii) holds. By assumption, f is nonconvex. It follows that $G(f^{-1}) \le G(\mathrm{conc}(f^{-1}))$. By Corollary 2, G is a nonconcave function. Thus, $G(\mathrm{conc}(f^{-1})) \le \mathrm{conc}(G(\mathrm{conc}(f^{-1})))$. Clearly, $\hat{G} = \mathrm{conc}(G(\mathrm{conc}(f^{-1})))$ is a concave function. By definition of the concave envelope, $\mathrm{conc}(G(f)^{-1}) \le \hat{G}$. Hence, $\tilde{\Phi}_1 \subseteq \mathrm{Proj}_{(x,t)}\tilde{\Phi}_2$. □

Remark 4 For a G-concave function ϕ, conditions of Proposition 9 can be equivalently stated as: if (i) f is concave on $\mathcal{D}$ or (ii) f is convex on $\mathcal{D}$ and G is concave on $\mathcal{D}$, then $\tilde{\Phi}_1 = \mathrm{Proj}_{(x,t)}\tilde{\Phi}_2$.

From (7), it follows that the function $\tilde{\phi}^G(x) := \inf\{t : (x,t) \in \tilde{\Phi}\}$ is a convex underestimator for ϕ over $\mathcal{C}$. Suppose that $\bar{G}(t)$ is increasing over $\mathcal{I}$. Then, $\tilde{\phi}^G(x)$ can be equivalently written as $\tilde{\phi}^G(x) = \inf\{t : (x,t) \in \mathcal{C}\times\mathcal{I},\ \bar{G}^{-1}(G(\phi(x))) \leq t\}$. Consequently,

$$\tilde{\phi}^G(x) = \bar{G}^{-1}(G(\phi(x))). \tag{8}$$

Let $\delta^G : \mathcal{C} \to \mathbb{R}$ denote the gap between $\phi(x)$ and $\tilde{\phi}^G(x)$, i.e.,

$$\delta^G(x) = \phi(x) - \tilde{\phi}^G(x). \tag{9}$$

Substituting for $\tilde{\phi}^G(x)$, we obtain $\delta^G(x) = \{t - \bar{G}^{-1}(G(t)) : t = \phi(x),\ x \in \mathcal{C}\}$. If $G(t)$ is convex over $\mathcal{I} = [\underline{t},\ \bar{t}]$ and $\bar{G}(t) = \mathrm{conc}_{\mathcal{I}} G$, then (8) simplifies to:

$$\tilde{\phi}^G(x) = \big(G(\phi(x)) - G(\underline{t})\big)\left(\frac{\bar{t} - \underline{t}}{G(\bar{t}) - G(\underline{t})}\right) + G(\underline{t}). \tag{10}$$

Moreover, in this case δ^G is a concave function of t and is given by:

$$\delta^G(t) = t - \left(\frac{\bar{t} - \underline{t}}{G(\bar{t}) - G(\underline{t})}\right) G(t) + \left(\frac{G(\underline{t})\bar{t} - G(\bar{t})\underline{t}}{G(\bar{t}) - G(\underline{t})}\right). \tag{11}$$

In the following sections, we employ the proposed relaxation scheme to convexify several classes of generalized convex functions and characterize their gap functions. For generalized concave functions, $\phi(x)$, we will construct concave overestimators, denoted by $\tilde{\phi}^G$, with corresponding gap functions defined as:

$$\delta^G(x) = \tilde{\phi}^G(x) - \phi(x). \tag{12}$$

The gap functions in (9) and (12) will be compared against similarly defined gap functions $\delta^M(x)$ between $\phi(x)$ and under- and over-estimators obtained by an alternative method M. We denote by δ^G_{tot} the total relaxation gap introduced by $\tilde{\phi}^G$:

$$\delta^G_{\mathrm{tot}} = \int_{\mathcal{C}} \delta^G(x).$$

Similarly, for a given method M, the total relaxation gap is defined as $\delta^M_{\mathrm{tot}} = \int_{\mathcal{C}} \delta^M(x)$. Furthermore, we will characterize the points at which these gap functions assume their maximal values $\delta^G_{\max}$ and $\delta^M_{\max}$. Finally, for a quantitative comparison of two alternative convexification techniques M_1 and M_2, we compute the percentage gap reduction when employing M_2 instead of M_1 as:

$$\gamma^{M_2/M_1}(x) = \left(\delta^{M_1}(x) - \delta^{M_2}(x)\right) \Big/ \delta^{M_1}(x) \times 100\,\%, \tag{13}$$

for all $x \in \mathcal{C}$. Similarly, the percentage reduction in maximum gap is defined as:

$$\gamma_{\max}^{M_2/M_1} = \left(\delta_{\max}^{M_1} - \delta_{\max}^{M_2}\right) \Big/ \delta_{\max}^{M_1} \times 100\,\%, \tag{14}$$

and the percentage reduction in total gap is as follows:

$$\gamma_{\text{tot}}^{M_2/M_1} = \left(\delta_{\text{tot}}^{M_1} - \delta_{\text{tot}}^{M_2}\right) \Big/ \delta_{\text{tot}}^{M_1} \times 100\,\%. \tag{15}$$

Remark 5 By relation (6), to construct a transformation relaxation $\tilde{\Phi}$, lower and upper bounds on the function ϕ should be provided. Clearly, the quality of these bounds affects the sharpness of the resulting relaxation. Since, by assumption, $G(\phi)$ is a convex function over $\mathcal{C} \subset \mathbb{R}^n$, a sharp lower bound on ϕ can be readily obtained by solving a convex optimization problem. It is known that the maximum of a convex function over a compact convex set $\mathcal{C}$ is attained over an extreme point of $\mathcal{C}$ (cf. Theorem I.1. in [6]). In this paper, and in the context of spacial branch-and-bound in general, we are interested in the case where the set $\mathcal{C}$ is a hyper-rectangle. It then follows that, to compute a sharp upper bound on ϕ, it will suffice to evaluate this function at all vertices of this rectangle. The latter operation can be carried out highly efficiently in practice, where these intermediate functions rarely involve more than ten variables, even when they appear in very large-scale high-dimensional global optimization problems.

4 Signomials

Throughout this section, we consider the signomial term $\phi = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R}\backslash\{0\}$, for all $i \in I = \{1, \ldots, n\}$. Define the subsets $I_1 = \{i \in I : 0 < a_i < 1\}$, $I_2 = \{i \in I : a_i \geq 1\}$, and $I_3 = \{i \in I : a_i < 0\}$. We consider the function ϕ over the domain

$$\mathcal{C} = \left\{x \in \mathbb{R}^n : x_i > 0,\ \forall i \in I_3,\ x_i \geq 0, \forall i \in I\backslash I_3\right\}. \tag{16}$$

First, we identify conditions under which ϕ is convex (resp. concave) transformable and derive its least convexifying (resp. concavifying) transformation. Subsequently, we employ the method described in Sect. 3 to construct a concave overestimator for ϕ and compare its tightness with a widely used conventional approach.

4.1 G-convexity and least convexifying transformations

First, we consider the case where the signomial term ϕ is convex transformable.

Proposition 10 *Consider $\phi = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R}\backslash\{0\}$ over the set $\mathcal{C}$ defined by (16). The function ϕ is G-convex if and only if $a_i < 0$ for all $i \in I\backslash\{j\}$ and $\sum_{i \in I\backslash\{j\}} |a_i| < a_j < \sum_{i \in I\backslash\{j\}} |a_i| + 1$. Moreover, a least convexifying transformation for ϕ is given by*

$$G^*(t) = t^{\frac{1}{\sum_{i \in I} a_i}}. \tag{17}$$

Proof By Proposition 6, if ϕ is G-convex, its augmented Hessian given by:

$$H_{(i,j)} = \begin{cases} a_i(a_i - 1 + \rho a_i \phi)\phi/x_i^2, & \text{if } i = j \\ a_i a_j(1 + \rho\phi)\phi/(x_i x_j), & \text{otherwise} \end{cases}, \ \forall i, j \in \{1, \ldots, n\}, \tag{18}$$

is positive semidefinite for every $\rho(x) \geq \rho_0(x)$ for all $x \in \mathrm{ri}(\mathcal{C})$. Let K_{kl} denote the index set of rows (columns) of H present in its lth principal minor of order k, where $l \in L = \{1, \ldots, \binom{n}{k}\}$. By definition, H is positive semidefinite if and only if all of its principal minors given by:

$$D_{kl} = (-1)^{k+1} \prod_{i \in K_{kl}} \frac{a_i}{x_i^2} \left((\rho\phi + 1) \sum_{i \in K_{kl}} a_i - 1 \right) \phi^k, \ \forall k \in I, \ l \in L \tag{19}$$

are nonnegative for all $\rho \geq \rho_0$. We have the following cases:

(i) $a_i < 0$ for all $i \in I$. By (19), H is positive semidefinite when $(\rho\phi + 1)\sum_{i \in K_{kl}} a_i \leq 1$ for all K_{kl}. By assumption, $\sum_{i \in K_{kl}} a_i < 0$ and $\phi > 0$. Thus, this condition holds for all $\rho \geq 0$, implying that ϕ is convex.

(ii) $a_i > 0$ for all $i \in \mathcal{S} \subseteq I$. First, consider the case where $|\mathcal{S}| \geq 2$. Consider any two principal minors D_{kl} and $D_{k'l'}$ of H, with k and k' denoting even and odd numbers, respectively, such that $K_{k'l'} \subset K_{kl} \subseteq \mathcal{S}$. By (19), D_{kl} is nonnegative if $\rho \leq \frac{1}{\phi}(1/\sum_i a_i - 1)$ for all $i \in K_{kl}$, whereas $D_{k'l'}$ is nonnegative if $\rho \geq \frac{1}{\phi}(1/\sum_i a_i - 1)$ for all $i \in K_{k'l'}$. Since, by construction $\sum_{i \in K_{kl}} a_i > \sum_{i \in K_{k'l'}} a_i$, it follows that no ρ meets these requirements. Next, consider the case where $|\mathcal{S}| = 1$. Let a_j denote the positive exponent. By Part (i), if $j \notin K_{kl}$, then D_{kl} is nonnegative. Thus, consider any D_{kl} such that $j \in K_{kl}$. By (19), D_{kl} is nonnegative when $(\rho\phi + 1)\sum_i a_i \geq 1$, for all $i \in K_{kl}$. Obviously, this condition holds only if $\sum_{i \in K_{kl}} a_i > 0$. Hence, H is positive semidefinite for all ρ such that:

$$\rho \geq \frac{1}{\phi}\left(\frac{1}{\sum_{i \in I} a_i} - 1\right). \tag{20}$$

If $\sum_{i \in I} a_i \geq 1$, then (20) holds for every $\rho \geq 0$, and ϕ is convex. Hence, ϕ is G-convex for $0 < \sum_{i \in I} a_i < 1$ with $\rho_0 = 1/\phi\left(\frac{1}{\sum_{i \in I} a_i} - 1\right)$. From (5), it follows that:

$$\frac{\mathrm{d}}{\mathrm{d}t} \ln\left(\frac{\mathrm{d}G^*(t)}{\mathrm{d}t}\right) = \left(\frac{1}{\sum_{i \in I} a_i} - 1\right)\frac{1}{t},$$

It is then simple to verify that G^* is given by (17). □

We now address the cases where the signomial term ϕ is concave transformable.

Proposition 11 *Consider* $\phi = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R}\backslash\{0\}$ *over the set* $\mathcal{C}$ *defined by* (16). *The function* ϕ *is* G*-concave if and only if one of the following holds:*

(i) $a_i > 0$ *for all* $i \in I$ *and* $\sum_{i \in I} a_i > 1$,
(ii) $a_j < 0$ *for some* $j \in I$ *such that* $\sum_{i \in I \setminus \{j\}} a_i < |a_j|$.

Moreover, a least concavifying transformation for ϕ *is given by* (17) *when condition (i) is met and by*

$$G^*(t) = -t^{\frac{1}{\sum_{i \in I} a_i}}, \tag{21}$$

when condition (ii) is met.

Proof By Proposition 6, if ϕ is G-concave, then all kth order principal minors of its augmented Hessian given by:

$$D_{kl} = (-1)^k \prod_{i \in K_{kl}} \frac{a_i}{x_i^2} \left((\rho\phi - 1) \sum_{i \in K_{kl}} a_i + 1 \right) \phi^k, \quad \forall k \in I, \ l \in L = \left\{ 1, \ldots, \binom{n}{k} \right\} \tag{22}$$

are nonnegative if k is even, and are nonpositive otherwise, where the index set K_{kl} is defined in the proof of Proposition 10. The following cases arise:

(i) $a_i > 0$ for all $i \in I$. Then, H is negative semidefinite if and only if:

$$\rho \geq \frac{1}{\phi} \left(1 - \frac{1}{\sum_{i \in K_{kl}} a_i} \right), \quad \forall K_{kl}. \tag{23}$$

If $\sum_{i \in I} a_i \leq 1$, then the above condition is satisfied for all $\rho \geq 0$, implying ϕ is concave. Let $\sum_{i \in I} a_i > 1$. It follows that (23) holds for all $\rho \geq \rho_0$ with:

$$\rho_0 = \frac{1}{\phi} \left(1 - \frac{1}{\sum_{i \in I} a_i} \right). \tag{24}$$

Substituting (24) in Eq. (5) and solving for G^*, we obtain (17).

(ii) $a_i < 0$ for all $i \in \mathcal{S} \subset I$. Using a similar argument as in part (ii) of Proposition 10, it can be shown that, if $|\mathcal{S}| \geq 2$, then ϕ is not G-concave. Thus, suppose that $|\mathcal{S}| = 1$. Let a_j denote the negative exponent. For any principal minor D_{kl} such that $j \notin K_{kl}$, by part (i), we conclude that condition (23) should hold. Thus, let $j \in K_{kl}$. In this case, the product $\prod_{i \in K_{kl}} a_i$ in (22) is negative. It follows that $\sum_{i \in K_{kl}} a_i < 0$ for all K_{kl} containing the index j, which in turn implies $\sum_{i \in I \setminus \{j\}} a_i < |a_j|$. Imposing this condition, it can be shown that the expressions for ρ_0 and G^* are given by (24) and (21), respectively. Note that the minus sign in (21) follows from the negativity of $\sum_{i \in I} a_i$. $\square$

Necessary and sufficient conditions for pseudo-convexity (-concavity) of signomials were derived by Schaible [24] using the basic definition of pseudoconvexity. Since pseudoconvexity is a necessary condition for G-convexity, we could have examined only instances satisfying those conditions. However, our proofs do not require knowledge of these conditions and the characterization of G^* follows naturally.

4.2 Exploiting G-concavity for upper bounding signomials

Next, we employ Proposition 11 to develop a new relaxation scheme for upper bounding signomials over a hyper-rectangle $\mathcal{H}^n$ in the nonnegative orthant. The factorable scheme overestimates signomials by first introducing a new variable for each univariate term $x_i^{a_i}$, $i \in I$. Next, convex univariates are overestimated by their affine envelopes. Finally, the resulting multilinear expression is outer-linearized using a recursive interval arithmetic scheme (rAI) [32]. It is known that (see [21,29]), when restricted to a box in the nonnegative orthant, the rAI scheme provides the *concave envelope* of a multilinear term. Consequently, the choice of a particular ordering in the recursive relaxation does not affect the quality of the overestimator; e.g., the following factorable decompositions of $w = x_1x_2x_3$ are equivalent: (i) $t = x_1x_2$, $w = tx_3$, (ii) $t = x_2x_3$, $w = x_1t$, and (iii) $w = x_1x_3$, $t = wx_2$. Nonetheless, it is important to note that this result follows from the supermodularity of a multilinear term over the vertices of a box in the nonnegative orthant [29]. Hence, a similar conclusion for the convex envelope of a multilinear term is not valid unless lower bounds on all variables are zero [21].

Denote by $\underline{x}_i$ and $\bar{x}_i$ the lower and upper bounds on x_i, $i \in I$, respectively. Introduce auxiliary variables $\eta_i \in [\underline{\eta}_i, \bar{\eta}_i]$, where $\underline{\eta}_i = \underline{x}_i^{a_i}$, $\bar{\eta}_i = \bar{x}_i^{a_i}$ for all $i \in I \backslash I_3$ and $\underline{\eta}_i = \bar{x}_i^{a_i}$, $\bar{\eta}_i = \underline{x}_i^{a_i}$ for all $i \in I_3$. A standard factorable relaxation $\tilde{\phi}^S$ is as follows:

$$\left.\begin{aligned}
\tilde{\phi}^S &= t_n \\
t_i &= \min\left\{\begin{array}{l} t_{i-1}\underline{\eta}_i + \bar{t}_{i-1}\eta_i - \bar{t}_{i-1}\underline{\eta}_i \\ \bar{\eta}_i t_{i-1} + \eta_i \underline{t}_{i-1} - \bar{\eta}_i \underline{t}_{i-1} \end{array}\right\}, \ \forall i \in I\backslash\{1\} \\
\eta_i &= x_i^{a_i}, \ \forall i \in I_1 \\
\eta_i &= \frac{\bar{x}_i^{a_i} - \underline{x}_i^{a_i}}{\bar{x}_i - \underline{x}_i}(x_i - \underline{x}_i) + \underline{x}_i^{a_i}, \quad \forall i \in I\backslash I_1,
\end{aligned}\right\} \tag{25}$$

where $t_1 = \eta_1$, $\underline{t}_i = \prod_{j=1}^{i} \underline{\eta}_j$ and $\bar{t}_i = \prod_{j=1}^{i} \bar{\eta}_j$ for all $i \in I$. If the signomial term is component-wise convex over a box, i.e., $I_1 = \emptyset$, then it has a polyhedral concave envelope. In [29], the authors show that a component-wise convex signomial can be converted to a supermodular function by an invertible linear transformation (see Example 3.22 in [29]). It is then simple to verify that the factorable scheme defined by (25), provides the concave envelope of ϕ in this case. We will henceforth assume that $I_1 \neq \emptyset$.

Now, suppose that ϕ is G-concave. Let $\xi = \sum_{i \in I} a_i$ and $\mathcal{I} = [\underline{\phi}, \bar{\phi}]$, where $\underline{\phi} = \prod_{i \in I} \underline{\eta}_i$ and $\bar{\phi} = \prod_{i \in I} \bar{\eta}_i$. By Propositions 7 and 11, and relation (10), the following is a concave overestimator for ϕ:

$$\tilde{\phi}^G = \left(\phi^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}\right)\left(\frac{\bar{\phi} - \underline{\phi}}{\bar{\phi}^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}}\right) + \underline{\phi}. \tag{26}$$

By Proposition 11, $G^*(\phi)$ is concave over the range of ϕ. Thus, by (12), the gap between $\tilde{\phi}^G$ and ϕ is a concave function of ϕ and its maximum value is given by:

$$\delta_{\max}^{G} = \frac{(\xi - 1)}{\xi^{\frac{\xi}{\xi-1}}} \left(\frac{\bar{\phi} - \underline{\phi}}{\bar{\phi}^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}} \right)^{\frac{\xi}{\xi-1}} - \left(\bar{\phi}\underline{\phi}\right)^{\frac{1}{\xi}} \left(\frac{\bar{\phi}^{1-\frac{1}{\xi}} - \underline{\phi}^{1-\frac{1}{\xi}}}{\bar{\phi}^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}} \right). \tag{27}$$

Next, we compare the relative tightness of the relaxations obtained by the factorable and transformation approaches.

Proposition 12 *Consider the G-concave signomial $\phi = \prod_{i \in I} x_i^{a_i}$ with $I_1 \neq \emptyset$ over a box $\mathcal{H}^n \subset \mathcal{C}$, where $\mathcal{C}$ is defined by (16). Then, $\tilde{\phi}^S$ globally dominates $\tilde{\phi}^G$, if Part (ii) of Proposition 11 is satisfied.*

Proof To prove this result, we will show that the optimal value of the following problem

$$\max_{x \in \mathcal{H}^n} \left(\tilde{\phi}^S - \tilde{\phi}^G\right) \tag{28}$$

is zero, if Part (ii) of Proposition 11 is valid. Consider an optimal solution (x, η, t) of the above problem. By (25), at this point we have

$$t_{i-1}\underline{\eta}_i + \bar{t}_{i-1}\eta_i - \bar{t}_{i-1}\underline{\eta}_i = \bar{\eta}_i t_{i-1} + \eta_i \underline{t}_{i-1} - \bar{\eta}_i \underline{t}_{i-1}, \quad \forall i \in I \backslash \{1\}. \tag{29}$$

Define $\tilde{t}_i = (t_i - \underline{t}_i)/(\bar{t}_i - \underline{t}_i)$ for all $i \in I$, $\tilde{x}_i = (x_i^{a_i} - \underline{x}_i^{a_i})/(\bar{x}_i^{a_i} - \underline{x}_i^{a_i})$ for all $i \in I_1$, $\tilde{x}_i = (x_i - \underline{x}_i)/(\bar{x}_i - \underline{x}_i)$ for all $i \in I_2$, and $\tilde{x}_i = (\bar{x}_i - x_i)/(\bar{x}_i - \underline{x}_i)$ for all $i \in I_3$. From (29) it follows that $\tilde{t}_{i-1} = \tilde{x}_i$ and $\tilde{t}_i = \tilde{t}_{i-1}$, for all $i \in I \backslash \{1\}$. Letting $\lambda = \tilde{x}_i$ for some $i \in I$, yields $\tilde{\phi}^S = (\bar{\phi} - \underline{\phi})\lambda + \underline{\phi}$. Let a_j denote the negative exponent. Substituting for λ into $\tilde{\phi}^G$, we obtain $\tilde{\phi}^G = (\bar{\phi} - \underline{\phi})\tilde{f}(\lambda) + \underline{\phi}$, where $\tilde{f}(\lambda) = (f(\lambda) - \underline{\phi}^{1/\xi})/(\bar{\phi}^{1/\xi} - \underline{\phi}^{1/\xi})$, and

$$f(\lambda) = \left\{ \left(\bar{x}_j - \lambda \Delta x_j\right)^{a_j} \prod_{i \in I_1} \left(\underline{\eta}_i + \lambda \Delta \eta_i\right) \prod_{i \in I_2} \left(\underline{x}_i + \lambda \Delta x_i\right)^{a_i} \right\}^{1/\xi},$$

where $\Delta\eta_i = \bar{\eta}_i - \underline{\eta}_i$ and $\Delta x_i = \bar{x}_i - \underline{x}_i$, for all $i \in I$. Now, we show that $f(\lambda)$ is convex in λ. It is simple to check that the second derivative of $f(\lambda)$ can be written as:

$$f''(\lambda) = \frac{f(\lambda)}{\xi^2} \left\{ \left(\sum_{I_1} \frac{\Delta\eta_i}{\underline{\eta}_i + \lambda\Delta\eta_i} + \sum_{I_2} \frac{a_i \Delta x_i}{\underline{x}_i + \lambda\Delta x_i} - \frac{a_j \Delta x_j}{\bar{x}_j - \lambda\Delta x_j} \right)^2 \right.$$
$$\left. -\xi \left(\sum_{I_1} \frac{\Delta\eta_i^2}{(\underline{\eta}_i + \lambda\Delta\eta_i)^2} + \sum_{I_2} \frac{a_i \Delta x_i^2}{(\underline{x}_i + \lambda\Delta x_i)^2} + \frac{a_j \Delta x_j^2}{(\bar{x}_j - \lambda\Delta x_j)^2} \right) \right\}. \tag{30}$$

The only negative expression in (30) is $g = -\xi a_j \Delta x_j^2/(\bar{x}_j - \Delta x_j \lambda)^2$. Since $\xi < 0$ and $|\xi| < |a_j|$, if we replace g by $\tilde{g} = -(a_j \Delta x_j/(\bar{x}_j - \Delta x_j \lambda))^2$, we obtain a lower bound for $f''(\lambda)$. However, $\tilde{g}$ cancels out when expanding (30), which implies that $f''(\lambda) \geq 0$. Since $\xi < 0$, we have $\bar{\phi}^{1/\xi} \leq f(\lambda) \leq \underline{\phi}^{1/\xi}$. It follows that $\tilde{f}(\lambda)$, $\lambda \in [0, 1]$, is a nonnegative concave function with $\tilde{f}(\lambda) = \lambda$ at $\lambda = 0$ and $\lambda = 1$. It follows that the optimal value of (28) is zero. Hence, we have $\tilde{\phi}^S \leq \tilde{\phi}^G$ for all $x \in \mathcal{H}^n$. □

We will henceforth assume that $a_i > 0$ for all $i \in I$ and $I_1 \neq \emptyset$. Next, we analyze the maximum gap between $\tilde{\phi}^S$ and ϕ; i.e., the optimal value of the following problem:

$$\max_{x \in \mathcal{H}^n} \left(\tilde{\phi}^S - \phi\right). \tag{31}$$

By (25), at any optimal point of the above problem, the equalities given by (29) are valid. First, consider $x_k = \bar{x}_k$ for $k \in K \subset I$. It follows that $t_k = t_{k-1}\bar{\eta}_k$ for all $k \in K$. Substitute the latter expression for t_k in (25) to compute t_n and factor out the constant term $\alpha = \prod_{k \in K} \bar{\eta}_k$. Define $I' = I \setminus K$, and $n' = |I'|$. The maximum gap in this case is equal to the maximum of the following problem:

$$\max_{x \in \mathcal{H}^{n'}} \alpha \left(\tilde{\varphi}^S - \varphi\right), \tag{32}$$

where $\varphi = \prod_{i \in I'} x_i^{a_i}$, and $\tilde{\varphi}^S$ denotes the corresponding factorable overestimator. As we argue later, for our cases of interest, any optimal solution of this problem is a local maximum of (31). Similarly, if $x_k = \underline{x}_k$ for $k \in K \subset I$, then the maximum gap is equal to the maximum of (32) with $\alpha = \prod_{k \in K} \underline{\eta}_k$, and φ and $\tilde{\varphi}^S$ as defined before. For now, suppose that the maximum of (31) is attained at an interior point. Using a similar argument as in the proof of Proposition 12, it follows that, at a point of maximum gap, $\tilde{x}_i = \lambda$ for all $i \in I$, where $\tilde{x}_i$ is defined in the proof of Proposition 12. Let $\beta_i = \underline{x}_i / \bar{x}_i$ for all $i \in I$. It follows that the maximum of (31) is attained at the optimal solution of the following univariate concave maximization problem:

$$\max_{0 \leq \lambda \leq 1} \left(1 - \prod_{i \in I} \beta_i^{a_i}\right)\lambda + \prod_{i \in I} \beta_i^{a_i} - \prod_{i \in I_1} \left(\left(1 - \beta_i^{a_i}\right)\lambda + \beta_i^{a_i}\right) \prod_{i \in I_2} \left((1 - \beta_i)\lambda + \beta_i\right)^{a_i}. \tag{33}$$

Proposition 13 *Consider the G-concave signomial $\phi = \prod_{i \in I} x_i^{a_i}$ over a box $\mathcal{H}^n \subset \mathcal{C}$, where $\mathcal{C}$ is defined by (16). Suppose that $a_i > 0$ for all $i \in I$, $\sum_{i \in I} a_i > 1$, and $I_1 \neq \emptyset$. Then, $\delta^G_{\max} < \delta^S_{\max}$ if one of the following conditions is met:*

(i) $\underline{x}_i = 0$ *for all* $i \in I$;
(ii) $\left(\frac{\underline{x}_i}{\bar{x}_i}\right)^{a_i} = \frac{\underline{x}_j}{\bar{x}_j} = \beta$ *for all* $i \in I_1$ *and for all* $j \in I_2$.

Proof Case (i). Define $\xi' = |I_1| + \sum_{I_2} a_i$. Letting $\beta_i = 0$ for all $i \in I$ in (33), we obtain:

$$\delta^S_{\max} = \frac{\xi' - 1}{\xi'^{\frac{\xi'}{\xi' - 1}}} \bar{\phi}. \tag{34}$$

Consider again the case where $x_k = \bar{x}_k$ for some $k \in K \subset I$. As argued earlier, the maximum gap in this case is given by (34) provided that ξ' is computed over $I' = I \backslash K$. Since $\delta^S_{\max}$ is an increasing function of ξ', the maximum gap for this case is strictly less than the value given by (34) and therefore corresponds to a local maximum of (31). Furthermore, if $x_k = 0$ for some $k \in I$, then α in (32) as well as the maximum gap go to zero. Letting $\underline{\phi} = 0$ in (26), we obtain:

$$\delta^G_{\max} = \frac{(\xi - 1)}{\xi^{\frac{\xi}{\xi - 1}}} \bar{\phi}. \tag{35}$$

By (34) and (35), $\delta^G_{\max} < \delta^S_{\max}$ when $\xi < \xi'$ or, equivalently, $\sum_{i \in I_1} a_i < |I_1|$. Since $a_i < 1$ for all $i \in I_1$, this condition holds if $I_1 \neq \emptyset$.

Case (ii). Substituting $\beta_i^{a_i} = \beta_j = \beta$ for all $i \in I_1$ and $j \in I_2$ in (33) yields:

$$\max_{0 \leq \lambda \leq 1} \quad \left(1 - \beta^{\xi'}\right) \lambda + \beta^{\xi'} - ((1 - \beta)\lambda + \beta)^{\xi'}.$$

It is then simple to verify that, the maximum gap in this case is equal to

$$\delta^S_{\max} = \bar{\phi} \left\{ \frac{(\xi' - 1)}{\xi'^{\frac{\xi'}{\xi' - 1}}} \left(\frac{1 - \beta^{\xi'}}{1 - \beta} \right)^{\frac{\xi'}{\xi' - 1}} - \beta \left(\frac{1 - \beta^{\xi' - 1}}{1 - \beta} \right) \right\}. \tag{36}$$

Now, assume $x_k = \bar{x}_k$ for $k \in K \subset I$. It can be shown that $\delta^S_{\max}$ in (36) is an increasing function of ξ'. Thus, the point x under consideration is a local maximum. A similar conclusion is immediate when $x_k = \underline{x}_k$, $k \in K \subset I$. It is simple to check that (36) can be equivalently written as:

$$\delta^S_{\max} = \frac{(\xi' - 1)}{\xi'^{\frac{\xi'}{\xi' - 1}}} \left(\frac{\bar{\phi} - \underline{\phi}}{\bar{\phi}^{\frac{1}{\xi'}} - \underline{\phi}^{\frac{1}{\xi'}}} \right)^{\frac{\xi'}{\xi' - 1}} - \left(\bar{\phi}\underline{\phi}\right)^{\frac{1}{\xi'}} \left(\frac{\bar{\phi}^{1 - \frac{1}{\xi'}} - \underline{\phi}^{1 - \frac{1}{\xi'}}}{\bar{\phi}^{\frac{1}{\xi'}} - \underline{\phi}^{\frac{1}{\xi'}}} \right). \tag{37}$$

From (27) and (37), it follows that, if $I_1 \neq \emptyset$, then $\delta^G_{\max} < \delta^S_{\max}$. $\square$

We conclude that the transformation method exploits the concavity of the univariate terms $x_i^{a_i}$, $i \in I_1$ to provide a tighter overestimator of ϕ, whereas, in the standard method, only the cardinality of the set of concave terms is accounted for. As an example, consider $\phi = x_1^{0.5} x_2^{0.7}$ over $[0, 1]^2$. The transformation and factorable overestimators are compared in Fig. 1 at various cross sections. As can be seen, the transformation overestimator does not globally dominate the factorable overestimator. Namely, $\tilde{\phi}^G$ is tighter in the interior, especially around the normalized center of the domain (i.e., $\tilde{x}_1 = \tilde{x}_2 = \cdots = \tilde{x}_n = 0.5$), while $\tilde{\phi}^S$ is tighter near the boundaries and is exact at the boundaries. Thus, it is mostly advantageous to include both relaxations in computational implementations.

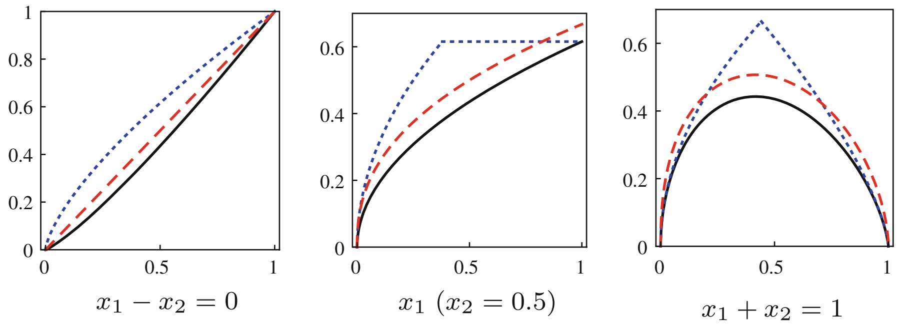

Fig. 1 Comparison of factorable and transformation overestimators for $\phi(x) = x_1^{0.5}x_2^{0.7}$ over $[0, 1]^2$ at various cross sections. The nonconcave function ϕ is shown in *solid black*, its factorable relaxation $\tilde{\phi}^S$ in *dotted blue*, and the proposed relaxation $\tilde{\phi}^G$ in *dashed red* (color figure online)

In the following, we denote by $\tilde{\phi}^B$ the point-wise minimum of the transformation and factorable overestimators; i.e., $\tilde{\phi}^B = \min\{\tilde{\phi}^G, \ \tilde{\phi}^S\}$. Maximum gap reductions, $\gamma_{\max}^{B/S}$, and total gap reductions, $\gamma_{\text{tot}}^{B/S}$, as defined by (14) and (15), respectively, are listed in Table 1 for a number of G-concave signomials with $n = 2, 3$ over different domains. We have chosen different domain configurations to show that, while the result of Proposition 13 is valid under certain restrictive assumptions on lower and upper bounds, the proposed overestimator leads to similar gap reductions for the general case, in practice. On average, combining the transformation and factorable relaxations, reduces the maximum and total gaps of the factorable overestimator by 55 and 29 %, respectively. In all these examples, it turned out that $\delta_{\max}^B = \delta_{\max}^G < \delta_{\max}^S$, and $\delta_{\text{tot}}^B < \min\{\delta_{\text{tot}}^G, \ \delta_{\text{tot}}^S\}$. The empirical results show that, while for signomials with $\xi/n \ll 1$, we often have $\delta_{\text{tot}}^G \ll \delta_{\text{tot}}^S$, for signomials with larger exponents, the total gap of the transformation method may become larger than the total gap of the factorable method. We will revisit this issue later in this section. We should also remark that the

Table 1 Maximum gap reduction, $\gamma_{\max}^{B/S}$ (%), and total gap reduction, $\gamma_{\text{tot}}^{B/S}$ (%), due to adding G-concavity transformations to factorable relaxations for overestimating G-concave signomials

Exponents	Domain of definition				
	$[0, 1]^2$	$[0.5, 4]^2$	$[0.1, 2]\times[1, 2]$	$[0.1, 5]^2$	$[0, 2]\times[1, 5]$
{0.4, 0.7}	86, 70	72, 63	79, 58	83, 66	79, 58
{0.3, 1.0}	62, 30	40, 14	54, 25	48, 19	52, 21
{0.6, 0.8}	51, 23	44, 17	25, 5	47, 20	32, 9
Exponents	Domain of definition				
	$[0, 1]^3$	$[0.5, 4]^3$	$[1, 5]^2\times[0, 2]$	$[0, 5]\times[1, 4]^2$	$[0, 4]\times[1, 2]\times[0, 3]$
{0.3, 0.4, 0.5}	83, 65	76, 52	65, 38	67, 35	76, 54
{0.2, 0.6, 0.7}	62, 27	48, 16	27, 5	42, 6	50, 17
{0.4, 0.5, 0.7}	55, 23	45, 13	24, 3	29, 3	40, 12

maximum gap of the transformation method is not always smaller than the maximum gap of the factorable method. For example, consider $\phi = (x_1 x_2)^{0.9}$ over $[1, 2]\times[3, 4]$. Then, we have $\delta^S_{\max} = 0.172 < \delta^G_{\max} = 0.184$.

Now, consider the G-concave signomial $\phi = x_1^{0.5} x_2^{0.6} x_3^{0.7}$ over the unit hypercube. The factorable overestimator of ϕ is given by

$$\tilde{\phi}^S = \min \left\{ x_1^{0.5},\ x_2^{0.6},\ x_3^{0.7} \right\},$$

with $\delta^S_{\max} = 0.385$ and $\delta^S_{\text{tot}} = 0.155$. Employing the transformation method, we obtain the following overestimator for ϕ:

$$\tilde{\phi}^G = \left(x_1^{0.5} x_2^{0.6} x_3^{0.7} \right)^{1/1.8},$$

with $\delta^G_{\max} = 0.213$, and $\delta^G_{\text{tot}} = 0.178$. As can be seen, while the transformation method results in a 45 % reduction in the maximum relaxation gap, the total gap increases by 15 %, as the factorable overestimator is much tighter near the boundaries. This undesirable volume increase becomes more significant for signomials in higher dimensions and/or with larger exponents. Next, consider an alternative relaxation scheme which is a combination of factorable and transformation approaches. Denote by t_1 the concave overestimator of $x_1^{0.5} x_2^{0.6}$, obtained by the transformation method, and let $t_2 = x_3^{0.7}$. It follows that the concave envelope of $t_1 t_2$ provides the following overestimator for ϕ:

$$\tilde{\phi}^{RT} = \min \left\{ \left(x_1^{0.5} x_2^{0.6} \right)^{1/1.1},\ x_3^{0.7} \right\},$$

with $\delta^{RT}_{\max} = 0.267$, and $\delta^{RT}_{\text{tot}} = 0.116$. Thus, $\tilde{\phi}^{RT}$ reduces the maximum and total gaps of the factorable relaxation $\tilde{\phi}^S$ by 31 and 25 %, respectively. Finally, letting $\tilde{\phi}^B = \min\{\tilde{\phi}^{RT},\ \tilde{\phi}^S\}$, i.e.,

$$\tilde{\phi}^B = \min \left\{ \left(x_1^{0.5} x_2^{0.6} \right)^{1/1.1},\ x_1^{0.5},\ x_2^{0.6},\ x_3^{0.7} \right\},$$

yields $\delta^B_{\max} = \delta^{RT}_{\max} = 0.267$, and $\delta^B_{\text{tot}} = 0.995\ \delta^{RT}_{\text{tot}}$. With the goal of reducing both maximum and total relaxation gaps, and benefiting from the transformation method to overestimate signomials that are not concave transformable, we propose a *recursive transformation and relaxation* (RT) scheme. Define the sets of subsets

$$\mathcal{S} := \left\{ \mathcal{S}_k \subseteq I_1 : \sum_{i \in \mathcal{S}_k} a_i \leq 1,\ \mathcal{S}_k \cap \mathcal{S}_j = \emptyset,\ \forall k,\ j \right\}, \tag{38}$$

and

$$\mathcal{T} := \left\{ \mathcal{T}_j \subseteq I_1 : \sum_{i \in \mathcal{T}_j} a_i > 1,\ \mathcal{T}_j \cap \mathcal{T}_k = \emptyset,\ \forall k,\ j \right\}. \tag{39}$$

In addition, assume that $\mathcal{S} \cup \mathcal{T}$ forms a partition of I_1. Let $\xi_j = \sum_{i \in \mathcal{T}_j} a_i$ for all $\mathcal{T}_j \in \mathcal{T}$, and let $K = |\mathcal{S}|,\ J = |\mathcal{T}|,\ N = K + J + |I \backslash I_1|$. Introduce $t_m \in [\prod_{\mathcal{S}_k} \underline{\eta}_i, \prod_{\mathcal{S}_k} \bar{\eta}_i]$ for all $\mathcal{S}_k \in \mathcal{S}$, $m = 1, \ldots, K$, $t_m \in \left[\prod_{\mathcal{T}_j} \underline{\eta}_i, \prod_{\mathcal{T}_j} \bar{\eta}_i\right]$ for all $\mathcal{T}_j \in \mathcal{T}$, $m = K + 1, \ldots, K + J$, and $t_m \in [\underline{\eta}_i, \bar{\eta}_i]$ for all $i \in I \backslash I_1$, $m = K + J + 1, \ldots, N$. We define the RT overestimator of ϕ as follows:

$$\left.\begin{array}{l}
\tilde{\phi}^{RT} = r_N \\
r_m = \min \left\{ \begin{array}{l} \bar{r}_{m-1} t_m + \underline{t}_m r_{m-1} - \bar{r}_{m-1} \underline{t}_m \\ \underline{r}_{m-1} t_m + \bar{t}_m r_{m-1} - \underline{r}_{m-1} \bar{t}_m \end{array} \right\}, \quad m = 2, \ldots, N \\
t_m = \prod_{i \in \mathcal{S}_k} x_i^{a_i}, \quad \forall \mathcal{S}_k \in \mathcal{S}, \quad m = 1, \ldots, K \\
t_m = \left(\prod_{i \in \mathcal{T}_j} x_i^{\frac{a_i}{\xi_j}} - \underline{t}_m^{\frac{1}{\xi_j}} \right) \left(\frac{\bar{t}_m - \underline{t}_m}{\bar{t}_m^{\frac{1}{\xi_j}} - \underline{t}_m^{\frac{1}{\xi_j}}} \right) + \underline{t}_m, \quad \forall \mathcal{T}_j \in \mathcal{T}, \quad m = K+1, \ldots, K+J \\
t_m = \frac{\bar{x}_i^{a_i} - \underline{x}_i^{a_i}}{\bar{x}_i - \underline{x}_i} (x_i - \underline{x}_i) + \underline{x}_i^{a_i}, \quad \forall i \in I \backslash I_1, \quad m = K + J + 1, \ldots, N,
\end{array}\right\} \tag{40}$$

where $r_1 = t_1$, $\underline{r}_m = \prod_{j=1}^m \underline{t}_j$ and $\bar{r}_m = \prod_{j=1}^m \bar{t}_j$ for all $m \in \{1, \ldots, N\}$. Each G-concave signomial associated with a subset $\mathcal{T}_j$ is overestimated via transformation as defined by (26). Convex terms are relaxed by affine envelopes, and the resulting multilinear is overestimated by its concave envelope. Obviously, for a given signomial ϕ, there are various ways of defining subsets $\mathcal{S}$ and $\mathcal{T}$. If $\sum_{i \in I_1} a_i \leq 1$, then $\mathcal{T} = \emptyset$, and we set $\mathcal{S} = \{\mathcal{S}_1\}$, where $\mathcal{S}_1 = I_1$. We will henceforth suppose that $\sum_{i \in I_1} a_i > 1$. Next, we demonstrate the effect of this partitioning on the maximum gap between $\tilde{\phi}^{RT}$ and ϕ, and define a variable grouping to obtain the least maximum gap.

Proposition 14 *Let $\phi = \prod_{i \in I} x_i^{a_i}$, where $a_i > 0$, $x_i \in [0, \bar{x}_i]$ for all $i \in I$, and $\sum_{i \in I_1} a_i > 1$. Consider an RT relaxation of ϕ as defined in (40). Let $\hat{\xi} = K + \sum_{\mathcal{T}_j \in \mathcal{T}} \xi_j + \sum_{i \in I_2} a_i$. Then, the maximum gap between $\tilde{\phi}^{RT}$ and ϕ is given by:*

$$\delta_{\max}^{RT} = \frac{\hat{\xi} - 1}{\hat{\xi}^{\frac{\hat{\xi}}{\hat{\xi}-1}}} \bar{\phi}. \tag{41}$$

Proof Let $\underline{x}_i = 0$ for all $i \in I$ in (40). By the second equation of (40), at any point of maximum gap between $\tilde{\phi}^{RT}$ and ϕ, we have $\tilde{r}_{m-1} = t_m / \bar{t}_m$ and $\tilde{r}_m = \tilde{r}_{m-1}$, for all $m = 2, \ldots, N$, where $\tilde{r}_m = r_m / \bar{r}_m$. Using the last three of (40), t_m can all be eliminated and the above relations can be rewritten in terms of $\tilde{x}_i = x_i / \bar{x}_i$ for all $i \in I$ to yield

$$\prod_{m\in\mathcal{S}_k}\tilde{x}_m^{a_m}=\left(\prod_{m\in\mathcal{T}_j}\tilde{x}_m^{a_m}\right)^{1/\hat{\xi}_j}=\tilde{x}_i,\quad\forall\mathcal{S}_k\in\mathcal{S},\ \mathcal{T}_j\in\mathcal{T},\ i\in I_2.$$

Letting $\tilde{r}_N=\lambda$, it follows that $\prod_{i\in\mathcal{S}_k}\tilde{x}_i^{a_i}=\lambda$, for all $\mathcal{S}_k\in\mathcal{S}$, $\prod_{i\in\mathcal{T}_j}\tilde{x}_i^{a_i}=\lambda^{\hat{\xi}_j}$, for all $\mathcal{T}_j\in\mathcal{T}$, and $\prod_{i\in\mathcal{I}_2}\tilde{x}_i^{a_i}=\lambda^{\sum_{i\in I_2}a_i}$. Hence, at any point of maximum gap $\phi=\lambda^{\hat{\xi}}\bar{\phi}$, where $\hat{\xi}$ is defined in the statement of the proposition. As a result, the maximum gap between $\tilde{\phi}^{RT}$ and ϕ can be found by solving the following univariate concave maximization problem

$$\max_{\lambda\in[0,1]}\bar{\phi}\left(\lambda-\lambda^{\hat{\xi}}\right),$$

It is then simple to check that $\delta_{\max}^{RT}$ is given by (41). □

Under the conditions of Proposition 14, the least maximum gap is attained when $\hat{\xi}$ is minimum. The value of $\hat{\xi}$ depends on the form of the sets $\mathcal{S}$ and $\mathcal{T}$. Next, we characterize a partitioning of the set $\mathcal{A}:=\{a_i : i\in I_1\}$ that minimizes $\hat{\xi}$. We assume $|\mathcal{S}_k|\leq 2$ for all $\mathcal{S}_k\in\mathcal{S}$ and $|\mathcal{T}_j|\leq 2$ for all $\mathcal{T}_j\in\mathcal{T}$. We denote by Π a partitioning of the set $\mathcal{A}$ with its corresponding $\hat{\xi}$ denoted by $\hat{\xi}(\Pi)$.

Proposition 15 *Let $\mathcal{A}=\{a_i : i\in I_1\}$ and $\sum_{i\in I_1}a_i>1$. Without loss of generality, suppose that the elements of $\mathcal{A}$ are in ascending order. Consider a partition of $I_1=\mathcal{S}\cup\mathcal{T}$ as defined by (38) and (39), with $|\mathcal{S}_k|\leq 2$, $\forall\,\mathcal{S}_k\in\mathcal{S}$ and $|\mathcal{T}_j|\leq 2$, $\forall\,\mathcal{T}_j\in\mathcal{T}$. Then, a partition of $\mathcal{A}$ that minimizes $\hat{\xi}$ is given by:*

$$\Pi^*=\{\{a_1,a_{2m}\},\{a_2,a_{2m-1}\},\ldots,\{a_m,a_{m+1}\}\},\tag{42}$$

if $|\mathcal{A}|=2m$ (even), and by $\Pi^*\cup\{a_{2m+1}\}$, if $|\mathcal{A}|=2m+1$ (odd).

Proof First, we address the case where $|\mathcal{A}|=2m$. Consider a partition $\Pi=\{d_1,\ldots,d_m\}$ of the set $\mathcal{A}$, where $d_i=\{a_j,\ a_k\}$ for some $j,k\in I_1$ and $i=1,\ldots,m$. We are interested in finding partition improving strategies, i.e., given $d_{i_1}=\{a_{j_1},a_{k_1}\}$ and $d_{i_2}=\{a_{j_2},a_{k_2}\}$ in Π, we are looking for exchanges that result in new subsets $d'_{i_1}=\{a_{j_1},a_{k_2}\}$ and $d'_{i_2}=\{a_{j_2},a_{k_1}\}$ that provide a partition Π' of $\mathcal{A}$ such that $\hat{\xi}(\Pi')\leq\hat{\xi}(\Pi)$. It is simple to show that, if $d_{i_1},d_{i_2}\in\mathcal{S}$ or $d_{i_1},d_{i_2}\in\mathcal{T}$, then $\hat{\xi}(\Pi')\geq\hat{\xi}(\Pi)$. Let $d_{i_1},d_{i_2}\in\mathcal{S}$. Two cases arise: (i) if $d'_{i_1},d'_{i_2}\in\mathcal{S}$, then $\hat{\xi}(\Pi)=\hat{\xi}(\Pi')$; (ii) if $d'_{i_1}\in\mathcal{T}$ and $d'_{i_2}\in\mathcal{S}$, then $\hat{\xi}(\Pi')>\hat{\xi}(\Pi)$. A similar conclusion is immediate, if $d_{i_1},d_{i_2}\in\mathcal{T}$. Thus, without loss of generality, suppose that $d_{i_1}\in\mathcal{S}$ and $d_{i_2}\in\mathcal{T}$. It can be shown that an exchange is improving, if and only if one of the following holds:

1. $d'_{i_1},d'_{i_2}\in\mathcal{S}$;
2. $d'_{i_1}\in\mathcal{S}$, $d'_{i_2}\in\mathcal{T}$ such that $a_{k_1}\leq a_{k_2}$;
3. $d'_{i_1},d'_{i_2}\in\mathcal{T}$.

We claim that, given any partition Π of $\mathcal{A}$ and $\Pi \neq \Pi^*$, it is possible to construct Π^* from Π, through a series of improving exchanges. By (42), the partition Π^* can be uniquely characterized by the following *inclusion* property: given any $d_{i_1}, d_{i_2} \in \Pi^*$, if $a_{j_1} \leq a_{j_2}$, then $a_{k_2} \leq a_{k_1}$. It follows that for any partition $\Pi \neq \Pi^*$, there exists some $d_{i_1}, d_{i_2} \in \Pi$ such that $a_{j_1} \leq a_{j_2}$ and $a_{k_1} < a_{k_2}$. Now apply the exchange $d'_{i_1} = \{a_{j_1}, a_{k_2}\}$ and $d'_{i_2} = \{a_{j_2}, a_{k_1}\}$, which satisfies the inclusion property. We show that such an exchange is always improving. First, suppose that $d_{i_1}, d_{i_2} \in \mathcal{S}$ (resp. $d_{i_1}, d_{i_2} \in \mathcal{T}$); it follows that $d'_{i_1}, d'_{i_2} \in \mathcal{S}$ (resp. $d'_{i_1}, d'_{i_2} \in \mathcal{T}$), i.e., the value of $\hat{\xi}(\Pi)$ remains unchanged. Without loss of generality, let $d_{i_1} \in \mathcal{S}$ and $d_{i_2} \in \mathcal{T}$. The following cases arise:

(i) $d'_{i_1}, d'_{i_2} \in \mathcal{S}$ (resp. $d'_{i_1}, d'_{i_2} \in \mathcal{T}$). By Case 1 (resp. Case 3) above, this exchange is always improving.
(ii) $d'_{i_1} \in \mathcal{S}$, $d'_{i_2} \in \mathcal{T}$. By Case 2 above, this exchange is improving provided that $a_{k_1} \leq a_{k_2}$, which is satisfied by assumption.

After updating Π by replacing d_{i_1}, d_{i_2} with d'_{i_1}, d'_{i_2}, we apply a similar exchange to any $d_{i_1}, d_{i_2} \in \Pi$ that does not satisfy the inclusion property. By employing this procedure recursively, we construct the partition Π^* from any partition $\Pi \neq \Pi^*$, through a set of exchanges all of which are improving. Consequently, Π^* is optimal.

Now, we prove the result for the case where $|\mathcal{A}| = 2m + 1$. We claim that $\tilde{\Pi} = \Pi^* \cup \{a_{2m+1}\}$ is optimal. Let $\Pi' = \hat{\Pi} \cup \{a_k\}$, where $\hat{\Pi}$ is obtained by replacing $d_i = \{a_j, a_k\} \in \Pi^*$ with $d'_i = \{a_j, a_{2m+1}\}$ such that $a_k < a_{2m+1}$, for some $k \in \{1, \ldots, m\}$. We show that $\hat{\xi}(\tilde{\Pi}) \leq \hat{\xi}(\Pi')$. To calculate $\hat{\xi}(\Pi')$, consider the following cases:

(i) $d_i \in \mathcal{S}$. If $d'_i \in \mathcal{S}$, then $\hat{\xi}(\tilde{\Pi}) = \hat{\xi}(\Pi')$. Otherwise, $\hat{\xi}(\Pi') = \hat{\xi}(\tilde{\Pi}) + a_j + a_{2m+1} - 1$. It follows that $\hat{\xi}(\tilde{\Pi}) < \hat{\xi}(\Pi')$.
(ii) $d_i \in \mathcal{T}$. In this case we have $\hat{\xi}(\Pi') = \hat{\xi}(\tilde{\Pi}) - a_k + a_{2m+1}$, which implies $\hat{\xi}(\tilde{\Pi}) < \hat{\xi}(\Pi')$.

Thus, $\tilde{\Pi} = \Pi^* \cup \{a_{2m+1}\}$ is optimal. □

Proposition 14 requires nonnegative exponents and zero lower bounds for all variables. Via numerical examples, we now demonstrate that similar gap reductions are observed for the general case. Let $\tilde{\phi}^B = \min\{\tilde{\phi}^S,\ \tilde{\phi}^{RT}\}$. Again, as defined in (15) (resp. (14)), denote by $\gamma_{\text{tot}}^{RT/S}$ (resp. $\gamma_{\max}^{RT/S}$) and $\gamma_{\text{tot}}^{B/S}$ (resp. $\gamma_{\max}^{B/S}$), the percentage reduction of the total gap (resp. maximum gap) when employing $\tilde{\phi}^{RT}$ and $\tilde{\phi}^B$ instead of $\tilde{\phi}^S$, respectively. The maximum and total gap reductions for a number of signomials with $n \in \{3, 4, 5\}$ are provided in Table 2. Since, for all cases it turned out that $\gamma_{\max}^{RT/S} = \gamma_{\max}^{B/S}$, we have listed this number as $\gamma_{\max}$ in Table 2. As can be seen, replacing the factorable relaxation by the RT method based on the partitioning outlined in Proposition 15 results in average reductions of 28 and 18 % of the maximum andtotal

Table 2 Maximum ($\gamma_{\max}$) and total ($\gamma_{\text{tot}}^{M/S}$) gap reductions for overestimating signomials. Two cases are presented. In the first case ($M = RT$), a factorable relaxation scheme is replaced by the proposed relaxations. In the second case ($M = B$), the two relaxations are combined

Exponents	Domain	$\gamma_{\max}$ (%)	$\gamma_{\text{tot}}^{RT/S}$ (%)	$\gamma_{\text{tot}}^{B/S}$ (%)
$\{-0.5,\ 0.5,\ 0.6\}$	$[0.1, 1]\times[0, 1]^2$	24	21	22
	$[1, 2]\times[0.5, 3]^2$	31	24	27
	$[0.5, 4]^3$	11	9	11
	$[1, 5]\times[0, 2]^2$	27	28	29
	$[0.5, 3]\times[0, 2]\times[1, 4]$	37	9	11
$\{0.4,\ 0.7,\ 0.8\}$	$[0, 1]^3$	31	23	24
	$[0.5, 4]^3$	30	13	15
	$[0.1, 5]^2\times[0, 2]$	24	16	18
	$[0, 5]\times[1, 4]^2$	31	13	18
	$[0, 4]\times[0.5, 3]\times[1, 2]$	47	25	30
$\{0.6,\ 0.6,\ 1.2\}$	$[0, 1]^3$	23	12	15
	$[0.5, 4]^2\times[2, 3]$	37	11	20
	$[0, 4]^2\times[1, 3]$	34	18	23
	$[0.1, 5]^2\times[0, 1]$	19	7	11
	$[0, 2]\times[0.1, 4]\times[0.5, 1]$	38	15	23
$\{0.3,\ 0.4,\ 0.4,\ 0.8\}$	$[0, 1]^4$	44	33	34
	$[0.5, 4]^4$	31	16	24
	$[0, 4]^2\times[0.1, 3]^2$	40	23	28
	$[0, 1]^3\times[0.5, 2]$	40	19	29
	$[0, 5]\times[0, 2]^2\times[0, 5]$	44	33	34
$\{0.4,\ 0.5,\ 0.6,\ 0.7\}$	$[0, 1]^4$	40	30	31
	$[0.5, 4]^4$	30	11	22
	$[0, 4]^2\times[0.1, 3]^2$	37	20	26
	$[0, 1]^3\times[0.5, 2]$	35	15	24
	$[0, 5]\times[0, 2]^2\times[0, 5]$	40	30	32
$\{-0.5,\ 0.4,\ 0.7,\ 1.0\}$	$[1, 2]\times[0, 4]^2\times[0.5, 2]$	31	21	22
	$[1, 2]\times[0, 3]^2\times[1, 2]$	39	26	27
	$[0.5, 1]\times[0, 1]^3$	25	16	17
	$[0.1, 1]\times[0, 1]^2\times[0.5, 1]$	17	14	15
	$[0.1, 2]\times[0, 4]^2\times[0, 2]$	9	9	10
$\{0.3,\ 0.6,\ 0.6,\ 0.7, 1.5\}$	$[0, 1]^5$	20	16	18
	$[0, 3]^4\times[1, 2]$	29	21	23
	$[0, 5]\times[0.5, 3]^2\times[0, 5]\times[0, 1]$	18	17	19
	$[0, 2]^2\times[0.1, 3]^2\times[0.5, 1.5]$	17	13	17
	$[0.5, 1]\times[0, 2]^3\times[0.5, 1]$	7	12	15

Table 2 continued

Exponents	Domain	$\gamma_{\max}$ (%)	$\gamma_{\text{tot}}^{RT/S}$ (%)	$\gamma_{\text{tot}}^{B/S}$ (%)
$\{-1.0,\ 0.4,\ 0.5,\ 0.6, 0.8\}$	$[0.5, 1]\times[0, 1]^4$	27	17	21
	$[1, 2]\times[0, 4]^3\times[0.1, 2]$	26	15	20
	$[1, 3]\times[0, 3]\times[0.5, 5]^2\times[0, 3]$	18	22	31
	$[1, 4]\times[0, 5]^4$	18	14	17
	$[0.1, 2]\times[0, 2]^2\times[0.5, 4]^2$	3	10	12

relaxation gaps, respectively. An additional 4 % reduction of the average total gap is obtained by combining both factorable and RT relaxations.

5 Products and ratios of convex and/or concave functions

In this section, we generalize the results of Propositions 10 and 11 using the composition rules developed in Sect. 2. This generalization will enable us to provide tight relaxations for a large class of convex-transformable functions, including products and ratios of convex and/or concave functions. Such functional forms appear frequently as component functions of nonconvex factorable expressions. To demonstrate the benefits of the new relaxation over the factorable scheme, we provide numerical examples consisting of univariate and bivariate G-convex functions with the following form:

$$\phi(x) = (f(x))^a (g(x))^b, \quad x \in \mathcal{H}, \quad a, b \in \mathbb{R},$$

where $\mathcal{H}$ denotes a box and $f(x)$ and $g(x)$ are convex and/or concave functions over $\mathcal{H}$. In all examples, the lower and upper bounds on $f(x)$ and $g(x)$ utilized in the factorable scheme, as well as the lower and upper bounds on $\phi(x)$ utilized in the transformation scheme are sharp (see Remark 5). Clearly, a factorable decomposition of a nonconvex function can be obtained in various ways, and the quality of resulting relaxation is affected by the decomposition scheme, in general. In the sequel, we compare the G-convexity relaxation against the tightest possible factorable relaxation. The following lemma provides a simple criterion for determining the tightest factorable relaxation for a function of the form $\phi = f(x)/g(x)$ (see [31] for details).

Lemma 1 *Consider $\phi = f(x)/g(x)$, $x \in \mathcal{H} \subset \mathbb{R}^n$, $g(x) > 0$. Let $f^l(x)$ (resp. $g^l(x)$) and $f^u(x)$ (resp. $g^u(x)$) denote a convex underestimator and a concave overestimator of $f(x)$ (resp. $g(x)$) over $\mathcal{H}$, and denote by $\underline{f}$ and $\bar{f}$ (resp. $\underline{g}$ and $\bar{g}$) a lower and an upper bound on $f(x)$ (resp. $g(x)$) over $\mathcal{H}$. Define $\underline{\phi} = \min\{\underline{f}/\underline{g},\ \underline{f}/\bar{g}\}$, $\bar{\phi} = \max\{\bar{f}/\underline{g},\ \bar{f}/\bar{g}\}$. Introduce the intermediate constraints $t_1 = f(x)$, $t_2 = g(x)$, $t_3 = 1/t_2$, and denote by $h(\cdot)$ the affine overestimator of the convex term $1/t_2$ over the range of t_2. Consider the following convex outer approximations of these intermediates:*

(i) $f^l(x) - t_1 \leq 0,\ t_1 - f^u(x) \leq 0,\ x \in \mathcal{H},\ \underline{f} \leq t_1 \leq \bar{f}$;
(ii) $g^l(x) - t_2 \leq 0,\ t_2 - g^u(x) \leq 0,\ x \in \mathcal{H},\ \underline{g} \leq t_2 \leq \bar{g}$;
(iii) $1/t_2 - t_3 \leq 0,\ t_3 - h(t_2) \leq 0,\ \underline{g} \leq t_2 \leq \bar{g},\ 1/\bar{g} \leq t_3 \leq 1/\underline{g}$.

We have the following cases:

I. *Consider the following convex underestimators of* ϕ*:*
   1. $\tilde{\phi}_1(x) = \inf_y\{(x, y) : \mathrm{conv}(t_1/t_2) \le y, \ \text{inequalities } (i), \ (ii)\}$*;*
   2. $\tilde{\phi}_2(x) = \inf_y\{(x, y) : t_1 \le \mathrm{conc}(t_2 y), \ \underline{\phi} \le y \le \bar{\phi}, \ \text{inequalities } (i), \ (ii)\}$*;*
   3. $\tilde{\phi}_3(x) = \inf_y\{(x, y) : \mathrm{conv}(t_1 t_3) \le y, \ \text{inequalities } (i), \ (iii)\}$.

   If $f(x) \le 0$ *for all* $x \in \mathcal{H}$*, then the above underestimators are equivalent. Otherwise,* $\tilde{\phi}_1(x)$ *provides the tightest relaxation.*

II. *Consider the following concave overestimators of* ϕ*:*
   1. $\tilde{\phi}_1(x) = \sup_y\{(x, y) : y \le \mathrm{conc}(t_1/t_2), \ \text{inequalities } (i), \ (ii)\}$*;*
   2. $\tilde{\phi}_2(x) = \sup_y\{(x, y) : \mathrm{conv}(y\, t_2) \le t_1, \ \underline{\phi} \le y \le \bar{\phi}, \ \text{inequalities } (i), \ (ii)\}$*;*
   3. $\tilde{\phi}_3(x) = \sup_y\{(x, y) : y \le \mathrm{conc}(t_1 t_3), \ \text{inequalities } (i), \ (iii)\}$.

   If $f(x) \ge 0$ *for all* $x \in \mathcal{H}$*, then the above overestimators are equivalent. Otherwise,* $\tilde{\phi}_1$ *provides the tightest relaxation.*

We now present the main results of this section. In Propositions 16 and 17, we present new overestimators for concave transformable products and ratios. Subsequently, we consider convex-transformable products in Proposition 18.

Proposition 16 *Consider* $\phi = \prod_{i\in I} \phi_i^{a_i}$ *over a box, where* $a_i > 0$ *for all* $i \in I$ *and* $\sum_{i\in I} a_i > 1$*. Let* ϕ_i *be concave and nonnegative for all* $i \in I$*. Then,* ϕ *is G-concave with* $G(t) = t^{1/\xi}$*, where* $\xi = \sum_{i\in I} a_i$*. Furthermore,* $\tilde{\phi}^G$ *is given by:*

$$\tilde{\phi}^G = \left(\phi^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}\right)\left(\frac{\bar{\phi} - \underline{\phi}}{\bar{\phi}^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}}\right) + \underline{\phi}, \tag{43}$$

where $\underline{\phi}$ *and* $\bar{\phi}$ *denote a lower bound and an upper bound on* ϕ*, respectively.*

Proof Follows directly from Propositions 2 and 11. □

Remark 6 For a given function ϕ and cardinality of I in Proposition 16, there are infinitely many possible representations in terms of ϕ_i and a_i. However, by Proposition 8, the tightness of the transformation relaxation is determined by the value of ξ alone. To obtain the tightest relaxation, each a_i should be as small as possible, provided that the concavity of the corresponding ϕ_i is preserved. For example, consider the function $\psi = \left(\sum_{i\in I} x_i^{1/p}\right)^p, \ p > 1, \ x_i \ge 0$ for all $i \in I$. Let $\phi_k^{a_k} = \psi$ for some $k \in I$. Then, the condition of Proposition 16 holds for any $a_k \in [1, p]$. However, letting $a_k = 1$ and $\phi_k = \psi$ provides the tightest relaxation.

Example 1 Consider $\phi(x) = (x^2 - 1)\left(\log(x+2)\right)^2, \ x \in [-1, 1]$. To construct a factorable relaxation, let $t_1 = x^2 - 1$ and $t_2 = \log(x+2)$. Denote by t_3 the affine overestimator of t_2^2 over the range of t_2. After convexifying $t_1 t_3$ using bilinear envelopes [1], we obtain the following underestimator for ϕ:

$$\tilde{\phi}^S = \max\left\{(\log 3)^2(x^2 - 1), \ -\log 3 \log(x+2)\right\}.$$

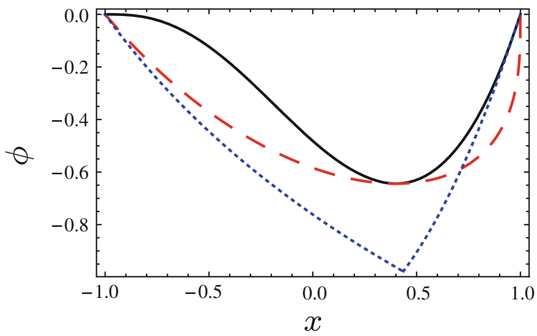

Fig. 2 Comparison of the factorable and transformation relaxations for $\phi = (x^2 - 1)(\log(x+2))^2$, $x \in [-1, 1]$ in Example 1. The nonconvex function ϕ is shown in *solid black*, its factorable underestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed underestimator $\tilde{\phi}^G$ in *dashed red* (color figure online)

By Proposition 16, the function $-\phi$ is G-concave with $G(t) = t^{1/3}$. Thus, an alternative underestimator of ϕ is given by:

$$\tilde{\phi}^G = -0.746\left((1 - x^2)(\log(x+2))^2\right)^{1/3}.$$

The factorable and transformation relaxations are compared in Fig. 2. While neither of the underestimators is globally dominant, $\tilde{\phi}^G$ reduces the total relaxation gap of $\tilde{\phi}^S$ by 43 %. Clearly, a tighter relaxation will be obtained by letting $\tilde{\phi}^B = \max\{\tilde{\phi}^S, \tilde{\phi}^G\}$.

Example 2 Consider $\phi = \sqrt{1 - x_1^2}(x_1 + x_2)^4,\ x_1 \in [-0.2, 0.9],\ x_2 \in [0.5, 1.5]$. We would like to construct a concave overestimator for ϕ. Let $t_1 = \sqrt{1 - x_1^2},\ t_2 = x_1 + x_2$ and denote by t_3 the affine overestimator of t_2^4 over the range of t_2. Relaxing the bilinear term $t_1 t_3$ using its concave envelope [1], we obtain:

$$\tilde{\phi}^S = \min\Big\{0.0081\sqrt{1 - x_1^2} + 15.80(x_1 + x_2) - 4.74,$$
$$33.18\sqrt{1 - x_1^2} + 6.89(x_1 + x_2) - 16.52\Big\}.$$

By Proposition 16, ϕ is G-concave with $G(t) = t^{2/9}$. Hence, a transformation overestimator of ϕ is given by:

$$\tilde{\phi}^G = 11.04\left(\sqrt{1 - x_1^2}(x_1 + x_2)^4\right)^{2/9} - 3.76.$$

The two relaxation are compared in Fig. 3b at $x_2 = 1.0$, and the percentage gap reduction when using $\tilde{\phi}^G$ instead of $\tilde{\phi}^S$, as defined in (13), is depicted in Fig. 3a. In this example, $\tilde{\phi}^G$ reduces the total gap of the factorable relaxation by 46 %.

Proposition 17 *Consider $\phi = \prod_{i \in I} \phi_i^{a_i}$ over a box, where $a_j < 0$ for some $j \in I$ and $\sum_{i \in I \setminus \{j\}} a_i < |a_j|$. Let ϕ_i be positive and concave for all $i \in I \setminus \{j\}$, and let ϕ_j be positive and convex. Then, ϕ is G-concave with $G(t) = -t^{1/\xi}$, $\xi = \sum_{i \in I} a_i$, and its associated overestimator $\tilde{\phi}^G$ is given by* (43).

Proof Follows directly from Propositions 2 and 11. □

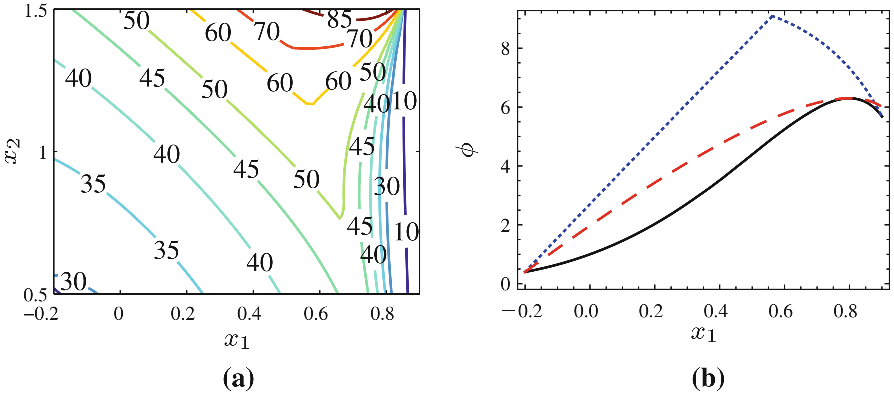

Fig. 3 Comparison of the factorable and transformation relaxations for $\phi = \sqrt{1-x_1^2}(x_1+x_2)^4$ $x_1 \in [-0.2, 0.9]$, $x_2 \in [0.5, 1.5]$ in Example 2. In **b**, the nonconcave function ϕ is shown in *solid black*, its factorable overestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed overestimator $\tilde{\phi}^G$ in *dashed red*. **a** $\gamma^{G/S}(\%)$. **b** $x_2 = 1.0$ (color figure online)

Remark 7 As a special case of Proposition 17, namely, when ϕ is a ratio of a nonnegative concave function over a positive convex function, the above transformation has been applied to convert a class of fractional programs to concave programs [25].

Remark 8 Proposition 17 requires the value of the negative exponent a_j to be finite. For example, consider the G-concave function $\phi = \sqrt{x}\exp(-x)$. Since $\exp(ax)$ is convex for all $a < 0$, Proposition 17 cannot be used for overestimating ϕ. However, as we detail in the next section, setting $G(t) = \log t$ provides a tight overestimator for ϕ in this case.

Proposition 18 *Consider $\phi = \prod_{i \in I} \phi_i^{a_i}$ over a box, where $a_i < 0$ for all $i \in I \backslash \{j\}$ and $\sum_{i \in I\backslash\{j\}} |a_i| < a_j < \sum_{i \in I\backslash\{j\}} |a_i| + 1$. Let ϕ_i be positive and concave for all $i \in I\backslash\{j\}$, and let ϕ_j be nonnegative and convex. Then, ϕ is G-convex with $G(t) = t^{1/\xi}$, $\xi = \sum_{i \in I} a_i$, and (43) provides an underestimator for it.*

Proof Follows directly from Propositions 2 and 10. □

Remark 9 Using a similar argument as in Remark 6, it is simple to show that, for a given function ϕ and cardinality of I, the tightest relaxation in Proposition 17 (resp. Proposition 18) is obtained by setting a_j and a_i, $i \in I\backslash\{j\}$ to the smallest (resp. largest) possible values while preserving convexity of ϕ_j and concavity of ϕ_i, $i \in I\backslash\{j\}$.

Example 3 Consider $\phi(x) = \log(x+1)/(x^4+x^2+1)$, $x \in [0.1, 4]$. To construct a concave overestimator of ϕ using a standard factorable method, let $t_1 = \log(x+1)$ and $t_2 = (x^4+x^2+1)$. Employing the concave envelope of the fractional term [30,31] to overestimate t_1/t_2, we obtain:

$$\tilde{\phi}^S = 10^{-2} \min \Big\{ 0.37\log(x+1) - 0.58(x^4+x^2) + 158.75, \\ 100\log(x+1) - 0.035(x^4+x^2) \Big\}.$$

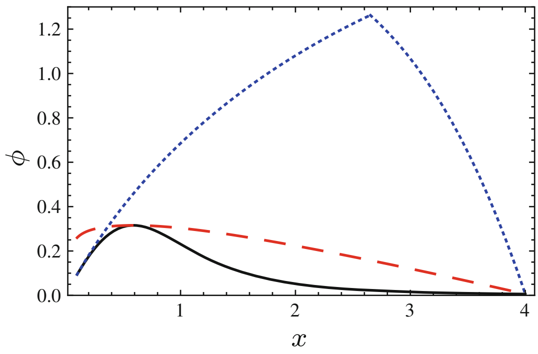

Fig. 4 Comparison of the factorable and transformation relaxations for $\phi = \log(x+1)/(x^4+x^2+1),\ x \in [0.1, 4]$ in Example 3. The nonconcave function ϕ is shown in *solid black*, its factorable overestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed overestimator $\tilde{\phi}^G$ in *dashed red* (color figure online)

By Proposition 17, ϕ is G-concave with $G(t) = -t^{-1/3}$. Thus, we have the following transformation overestimator for ϕ:

$$\tilde{\phi}^G = 0.427 - 0.076\left(\log(x+1)/(x^4+x^2+1)\right)^{-1/3}$$

The two relaxations are depicted in Fig. 4. Clearly, the transformation method provides a significantly tighter relaxation and results in a 86 % reduction in the total gap in comparison to the factorable overestimator.

Example 4 Consider $\phi = 1/(1+x_1^2+3x_2^2)$, over $[-4, 4]^2$. Letting $t_1 = 1+x_1^2+3x_2^2$ and overestimating the convex term $t_2 = 1/t_1$ using its affine envelope, we obtain the following concave relaxation of ϕ:

$$\tilde{\phi}^S = 1 - 0.015\left(x_1^2 + 3x_2^2\right).$$

By Proposition 17, ϕ is G-concave with $G(t) = -t^{-1/2}$. Hence, $\tilde{\phi}^G$ is given by:

$$\tilde{\phi}^G = 1.14 - 0.14\sqrt{1+x_1^2+3x_2^2}.$$

The two relaxations are compared in Fig. 5. The transformation relaxation dominates the factorable approach with $\delta_{\text{tot}}^{G/S} = 27\,\%$.

6 Log-concave functions

Another important class of concave-transformable functions are log-concave functions [19]. A function $\phi : \mathcal{C} \to \mathbb{R}_+$ is logarithmically concave (log-concave) if $\log\phi$ is concave over $\mathcal{C}$. It is simple to check that $\phi = \prod_{i\in I}\phi_i^{a_i}$, where $a_i > 0$ and ϕ_i is positive and concave for all $i \in I$ is log-concave and can be overestimated after a logarithmic transformation. However, by Proposition 8, the transforming function defined in Proposition 16 dominates the log function. Thus, in this section, we are considering classes of log-concave functions that are not concave transformable by means of the transformations of the previous section.

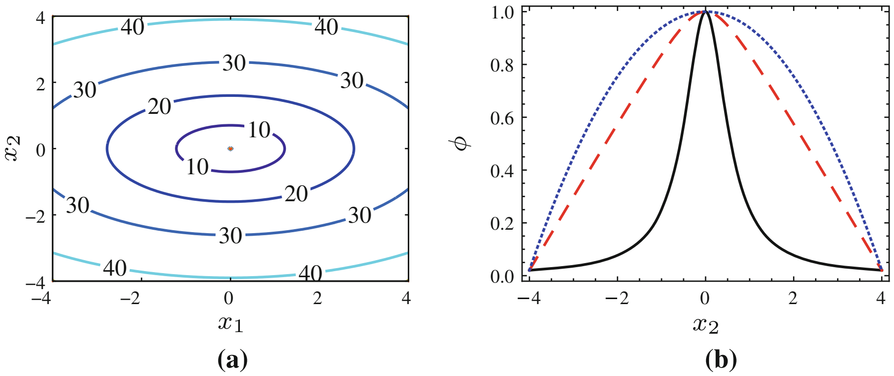

Fig. 5 Comparison of the factorable and transformation relaxations for $\phi = 1/(1 + x_1^2 + 3x_2^2)$, over $[-4, 4]^2$ in Example 4. In **b**, the nonconcave function ϕ is shown in *solid black*, its factorable overestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed overestimator $\tilde{\phi}^G$ in *dashed red*. **a** $\gamma^{G/S}(\%)$, **b** $x_1 = 0$ (color figure online)

Proposition 19 *Consider the function*

$$\phi = \frac{f(x)^a \exp g_0(x)}{1 + \sum_{i \in I} \exp g_i(x)}, \quad a > 0$$

over a convex set $\mathcal{C} \subset \mathbb{R}^n$. Let $f(x)$ be concave and positive, $g_0(x)$ be concave, and $g_i(x)$, $i \in I$ be convex over $\mathcal{C}$. Then, ϕ is log-concave. Further, let $[\underline{\phi}, \bar{\phi}] \supseteq I_\phi(\mathcal{C})$. Then, a concave overestimator of ϕ over $\mathcal{C}$ is given by:

$$\tilde{\phi}^G = \frac{(\log \phi - \log \underline{\phi})\left(\bar{\phi} - \underline{\phi}\right)}{\log\left(\bar{\phi}/\underline{\phi}\right)} + \underline{\phi}. \tag{44}$$

Proof Taking the log of ϕ, we obtain $\log \phi = a \log f(x) + g_0(x) - \log(1 + \sum_{i \in I} \exp g_i(x))$. The log-sum-exp function is convex and increasing. Thus, its composition with convex functions g_i, $i \in I$ is convex as well. It follows that $\log \phi$ is concave. Letting $G(t) = \log t$ in (8), yields (44). □

Several important instances of log-concave functions are derived from the function ϕ introduced in Proposition 19. As an example, consider $I = \emptyset$, for which $\phi = f(x)^a \exp g(x)$. As another example, consider $f(x) = 1$, $g_0(x) = 1$, and $g(x) = x$, which yields $\phi = 1/(1+\exp x)$. Next, we examine some of these functional forms and compare the relaxation given by Proposition 19 with a standard factorable approach. As in Sect. 5, the lower and upper bounds on convex/concave functions employed in the factorable relaxation, as well as the bounds on log-concave functions employed in the transformation relaxation are sharp.

Example 5 Consider the sigmoidal function $\phi = 1/(1 + \exp(-x))$, $x \in [-6, 6]$. Letting $t = \exp(-x)$ and overestimating the convex term $1/(1 + t)$ using its affine envelope, we obtain the following factorable overestimator of ϕ:

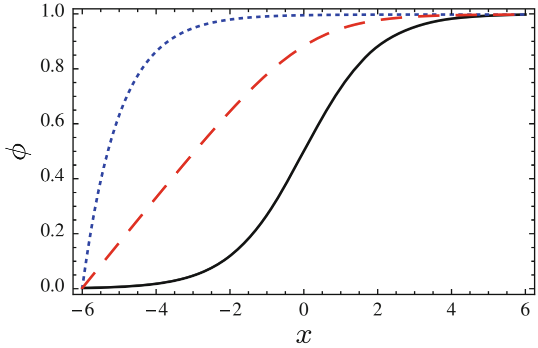

Fig. 6 Comparison of the factorable and transformation overestimators for $\phi = 1/(1+\exp(-x)),\ x \in [-6, 6]$ in Example 5. The nonconcave function ϕ is shown in *solid black*, its factorable overestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed overestimator $\tilde{\phi}^G$ in *dashed red* (color figure online)

$$\tilde{\phi}^S = 0.9975 - 0.0025\exp(-x).$$

Clearly, the sigmoidal function is log-concave. Thus, an alternative overestimator for ϕ can be obtained from (44):

$$\tilde{\phi}^G = 0.98 - 0.166\log\left(1+\exp(-x)\right).$$

The two overestimators are compared in Fig. 6. The transformation overestimator is strongly dominant and results in a 50 % reduction in the total relaxation gap in comparison to the factorable overestimator.

Example 6 Consider $\phi(x) = x_1^2\exp(x_2 - x_1),\ x_1 \in [0.1, 5],\ x_2 \in [-1, 1]$. Let $t_1 = x_2 - x_1$ and denote by t_2 and t_3 the affine overestimators of x_1^2 and $\exp(t_1)$, respectively. Utilizing bilinear envelopes [1] to overestimate $t_2 t_3$, yields:

$$\tilde{\phi}^S = \min\{12.54x_1 + 0.0036x_2 - 1.23,\ -8.89x_1 + 8.90x_2 + 53.41\}.$$

Exploiting the log-concavity of ϕ, we obtain the following overestimator for ϕ:

$$\tilde{\phi}^G = 0.62 + 0.13(2\log x_1 - x_1 + x_2).$$

The two overestimators are depicted in Fig. 7. The proposed overestimator is significantly tighter than the factorable relaxation, and results in 99.72 % reduction in the total gap.

7 Integration within the factorable framework and effect on branch-and-bound

In this section, we utilize convex transformability in the construction of a convex relaxation for a general nonconvex factorable function defined over a convex set. As in the standard factorable approach, a convex relaxation is constructed by recursively decomposing the nonconvex function up to the level that all intermediate expressions can be bounded. We depart from the standard approach in that we also outer-approximate

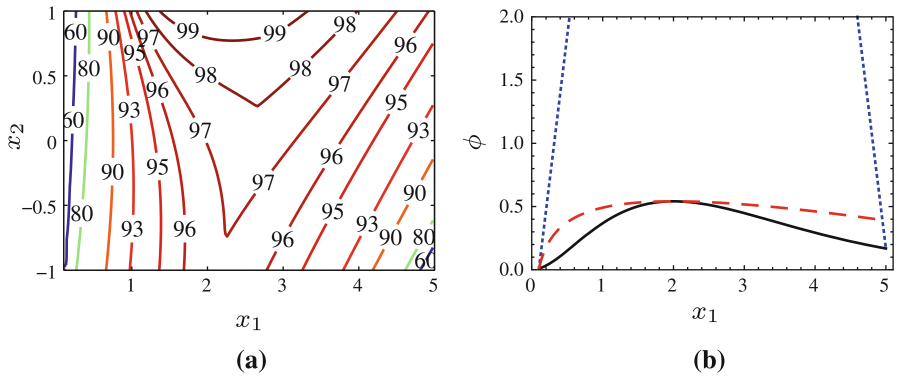

Fig. 7 Comparison of the factorable and transformation overestimators for $\phi(x) = x_1^2 \exp(x_2 - x_1)$, $x_1 \in [0.1, 5]$, $x_2 \in [-1, 1]$ in Example 6. In **b**, the nonconcave function ϕ is shown in *solid black*, its factorable overestimator $\tilde{\phi}^S$ in *dotted blue*, and the proposed overestimator $\tilde{\phi}^G$ in *dashed red*. **a** $\gamma^{G/S}(\%)$. **b** $x_2 = 0$ (color figure online)

some intermediate expressions after a convex or concave transformation. Via examples, we demonstrate that incorporation of the functional transformations introduced in previous sections into the standard factorable framework leads to stronger relaxations and enhances the performance of a global solver.

Example 7 Consider

$$\phi(x) = \frac{(x+3)}{(x^2+x+1)^2} - \sqrt{6-x-x^2}(0.4x+1)^{3/2}, \quad x \in [-2, 1.8].$$

This function has two local minima at $x = -1.676$ and $x = 1.456$, and one local maximum at $x = -0.481$ (see Fig. 8). A standard factorable decomposition of ϕ is as follows:

$$\begin{aligned}
&t_1 = x + 3,\ \ t_2 = (x^2 + x + 1)^2, \quad t_3 = t_1/t_2,\\
&t_4 = \sqrt{6 - x^2 - x},\ \ t_5 = (0.4x + 1)^{3/2}, \quad t_6 = t_4 t_5,\\
&\phi = t_3 - t_6.
\end{aligned}$$

All convex and concave univariate terms are over- and under-estimated, respectively, by their affine envelopes. Bilinear and fractional terms are replaced by their convex and concave envelopes [1,30,31]. We denote the resulting convex set by $\tilde{\phi}^S$. By Propositions 16 and 17, ϕ is the difference of two G-concave functions. Thus, we have the following alternative decomposition:

$$\begin{aligned}
&t'_1 = (x + 3) \Big/ (x^2 + x + 1)^2,\\
&t'_2 = \sqrt{6 - x^2 - x}(0.4x + 1)^{3/2},\\
&\phi = t'_1 - t'_2.
\end{aligned}$$

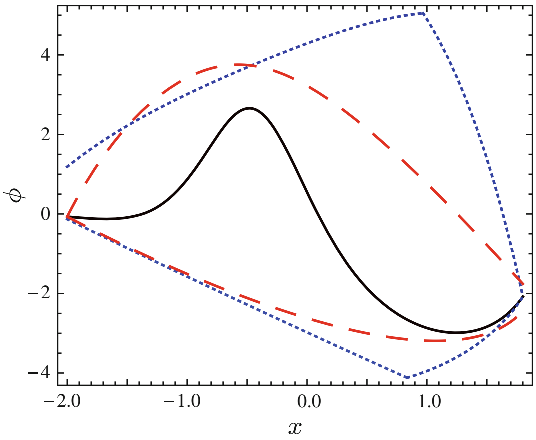

Fig. 8 Comparison of the standard and integrated factorable relaxations of $\phi = (x+3)/(x^2+x+1)^2 - \sqrt{6-x-x^2}(0.4x+1)^{1.5}$, $x \in [-2, 1.8]$ in Example 7. The nonconvex function ϕ is shown in *solid black*, a standard relaxation $\tilde{\phi}^S$ in *dotted blue*, and the proposed relaxation $\tilde{\phi}^G$ in *dashed red* (color figure online)

Propositions 16 and 17 provide overestimators for t_1' and t_2'. We replace the overestimators of t_3 and t_6 in the standard relaxation by the overestimators of t_1' and t_2', respectively, and denote the resulting integrated relaxation by $\tilde{\phi}^G$. The standard and integrated relaxations of ϕ are compared in Fig. 8. As can be seen, exploiting convex transformability of the component functions leads to a tighter relaxation of the overall nonconvex expression. An even tighter outer approximation is obtained by combining both relaxations.

Example 8 Consider the following optimization problem:

$$\begin{aligned} (\mathrm{P}) \quad \max \quad & \frac{0.6\exp(-5x_1)(x_1+1.5)}{(1+\exp(-5x_1)+\exp(-4x_2))} + \frac{0.4\exp(-4x_2)(x_2+2)}{(1+\exp(-3x_1)+\exp(-4x_2))} \\ \text{s.t.} \quad & -1 \le x_1 \le 2 \\ & -1 \le x_2 \le 2 \end{aligned}$$

The objective function of P, denoted by ϕ, has a local maximum at $(x_1, x_2) = (2.0, -0.419)$ with $\phi = 0.5325$, and attains its global maximum at $(x_1, x_2) = (-0.4, -0.329)$ with $\phi = 0.7124$. The following shows the factorable decomposition of P that is constructed by BARON [22,33]:

$$\left.\begin{aligned} & t_1 = \exp(-5x_1),\ t_2 = x_1 + 1.5,\ t_3 = t_1 t_2,\ t_4 = \exp(-4x_2), \\ & t_5 = 1 + t_1 + t_4,\ t_6 = t_3/t_5,\ t_7 = x_2 + 2,\ t_8 = t_4 t_7, \\ & t_9 = \exp(-3x_1),\ t_{10} = 1 + t_4 + t_9,\ t_{11} = t_8/t_{10}, \\ & \phi = 0.6\, t_6 + 0.4\, t_{11}. \end{aligned}\right\} \quad (\mathrm{SR})$$

By Proposition 19, the objective function of P is the sum of two log-concave functions. Thus, we have the following alternative decomposition for P:

$$\left.\begin{aligned} & t_1 = \exp(-5x_1)(x_1+1.5)/\,(1+\exp(-5x_1)+\exp(-4x_2)), \\ & t_2 = \exp(-4x_2)(x_2+2)/\,(1+\exp(-3x_1)+\exp(-4x_2)), \\ & \phi = 0.6\, t_1 + 0.4\, t_2. \end{aligned}\right\} \quad (\mathrm{GR})$$

Table 3 Reduction in the number of nodes and relative gap by using G-convexity relaxations in Example 8

Standard relaxation (SR)			New relaxation (SR + GR)		
N_t	UB	δ_{rel} (%)	N_t	UB	δ_{rel} (%)
1	199.3300	99.64	1	1.0537	32.39
10	26.9659	97.36	3	1.0423	31.66
20	6.4919	89.03	7	0.8979	20.66
30	4.2242	83.14	9	0.8617	17.33
40	3.1605	77.46	11	0.7915	10.00
50	2.0880	65.88			
60	1.7490	59.27			
70	1.4626	51.29			
80	1.2236	41.78			
90	1.0543	32.43			
99	0.7915	10.00			

In this table, the progress of the branch-and-bound search is shown as N_t, the number of nodes solved by the algorithm, increases. UB is an upper bound on the global maximum, and δ_{rel} denotes the relative gap between lower (LB) and upper bounds and is given by δ_{rel} = (UB-LB)/UB $\times 100$

In all following `BARON 9.3` runs, we used the default algorithmic options of the `GAMS/BARON` distribution [23], including a relative optimality tolerance of 10 % as the termination criterion. Employing the conventional decomposition strategy SR, `BARON` enumerates 99 nodes. The sequence of upper bounds as well as the percentage relative relaxation gaps are listed in Table 3. We should remark that, one can obtain a slightly different relaxation of P by defining:

$$\left.\begin{array}{l} t_1 = \exp(-5x_1),\ t_2 = \exp(-4x_2),\ t_3 = 1 + t_1 + t_2,\ t_4 = t_1/t_3, \\ t_5 = x_1 + 1.5,\ t_6 = t_4 t_5,\ t_7 = \exp(-3x_1),\ t_8 = 1 + t_2 + t_7, \\ t_9 = t_7/t_8,\ t_{10} = x_2 + 2,\ t_{11} = t_9 t_{10}, \\ \phi = 0.6\, t_6 + 0.4\, t_{11}. \end{array}\right\} \qquad (\text{SR}')$$

If we employ decomposition SR′, `BARON` enumerates 101 nodes, and the branch-and-tree looks quite similar to the one when using SR. Thus, we do not include the details here. Finally, we employ the new decomposition scheme GR to generate tighter relaxations for P. As can be seen in Table 3, due to adding G-convexity cuts to the factorable relaxation, `BARON` is now able to terminate after exploring only 11 nodes. The new cutting planes lead to a 99.83 % reduction in the root node relaxation gap and a decrease of 90 % in the total number of nodes. Similar improvements are observed when employing tighter optimality tolerances. For instance, with relative/absolute optimality tolerance of 0.001 %, incorporating the proposed cuts in `BARON` results in a 85 % reduction in the total number of nodes enumerated. Clearly, these are preliminary results and we do not attempt to make any conclusion about the computational benefits of the proposed relaxation in general. The purpose of this example is to demonstrate that the sharpness of G-convexity relaxations has the potential to significantly improve the performance of global solvers. A comprehensive study of the computational implications of the proposed relaxation is the subject of future research.

We conclude this section by remarking that, for certain functional types, G-convexity relaxations have a more complex structure than the widely used factorable relaxations. This may be viewed as a disadvantage for global solvers that solve nonlinear convex relaxations in the lower bounding step. However, for global solvers that construct polyhedral relaxations and employ robust LP solvers to obtain bounds, the functional form of a convex relaxation is not an issue. For instance, at each node of the branch-and-bound tree, `BARON` first constructs and solves a crude LP relaxation of the nonconvex problem (see [33] for details). Next, cutting planes corresponding to the supporting hyperplanes of convex functions and/or convex underestimators of nonconvex intermediates at the LP optimal solution are generated and added to the current relaxation only if they reduce the size of the feasible region of the relaxation. Hence, once a G-convex expression ϕ is recognized, the coefficients of the associated hyperplane given by the gradient of $\tilde{\phi}^G$ are computed, and the resulting cut can serve as a valid inequality to enhance the tightness of the relaxation.

8 Conclusions

This paper demonstrates the potential benefits from exploiting generalized convexity in the global optimization of nonconvex factorable programs. We studied convex-transformable functions, an important class of generalized convex functions. We proposed a new method to outer-approximate such functions and applied it to a number of important functional forms including signomials, products and ratios of convex and/or concave functions, and log-concave functions. In all instances, the transformation relaxations were shown to be considerably tighter than a widely used factorable scheme. Via an integrated factorable framework, we showed that exploiting the convex transformability of sub-expressions of a nonconvex function leads to factorable decompositions that often provide stronger relaxations than a standard approach. This work can be considered as a step towards bridging the gap between generalized convexity and global optimization. Future research will integrate the proposed relaxations into a global solver and study their effect on the convergence rate of branch-and-bound algorithms.

Acknowledgments The authors would like to thank two anonymous referees for comments and suggestions that improved the quality of this manuscript.

References

1. Al-Khayyal, F.A., Falk, J.E.: Jointly constrained biconvex programming. Math. Oper. Res. **8**, 273–286 (1983)
2. Avriel, M., Diewert, W.E., Schaible, S., Zang, I.: Generalized Concavity. Plenum Press, New York (1988)
3. Bao, X., Sahinidis, N.V., Tawarmalani, M.: Multiterm polyhedral relaxations for nonconvex, quadratically-constrained quadratic programs. Optim. Methods Softw. **24**, 485–504 (2009)
4. Debreu, G.: Least concave utility functions. J. Math. Econ. **3**, 121–129 (1976)

5. Fenchel, W.: Convex Cones, Sets, and Functions (Mimeographed Lecture Notes). Princeton University Press (1953)
6. Horst, R., Tuy, H.: Global Optimization: Deterministic Approaches, 3rd edn. Springer, Berlin (1996)
7. Jach, M., Michaels, D., Weismantel, R.: The convex envelope of $(n-1)$-convex functions. SIAM J. Optim. **19**, 1451–1466 (2008)
8. Kannai, Y.: Concavifiability and construction of concave utility functions. J. Math. Econ. **4**, 1–56 (1977)
9. Khajavirad, A., Sahinidis, N.V.: Convex envelopes generated from finitely many compact convex sets. Math. Program. (2011). doi:10.1007/s10107-011-0496-5
10. Khajavirad, A., Sahinidis, N.V.: Convex envelopes of products of convex and component-wise concave functions. J. Glob. Optim. **52**, 391–409 (2012)
11. Li, H., Tsai, J., Floudas, C.A.: Convex underestimation for posynomial functions of positive variables. Optim. Lett. **2**, 333–340 (2008)
12. Lu, H., Li, H., Gounaris, C.E., Floudas, C.A.: Convex relaxation for solving posynomial programs. J. Glob. Optim. **46**, 147–154 (2010)
13. Lundell, A., Westerlund, J., Westerlund, T.: Some transformation techniques with applications in global optimization. J. Glob. Optim. **43**, 391–405 (2009)
14. Lundell, A., Westerlund, T.: Convex underestimation strategies for signomial functions. Optim. Methods Softw. **24**, 505–522 (2009)
15. Maranas, C.D., Floudas, C.A.: Global optimization in generalized geometric programming. Comput. Chem. Eng. **21**, 351–369 (1997)
16. McCormick, G.P.: Computability of global solutions to factorable nonconvex programs: part I-convex underestimating problems. Math. Program. **10**, 147–175 (1976)
17. Meyer, C.A., Floudas, C.A.: Trilinear monomials with mixed sign domains: facets of the convex and concave envelopes. J. Glob. Optim. **29**, 125–155 (2004)
18. Meyer, C.A., Floudas, C.A.: Convex envelopes for edge-concave functions. Math. Program. **103**, 207–224 (2005)
19. Prékopa, A.: On logarithmic concave measures and functions. Acta Sci. Math. **34**, 335–343 (1973)
20. Rockafellar, R.T.: Convex Analysis. Princeton Mathematical Series. Princeton University Press, Princeton (1970)
21. Ryoo, H.S., Sahinidis, N.V.: Analysis of bounds for multilinear functions. J. Glob. Optim. **19**, 403–424 (2001)
22. Sahinidis, N.V.: BARON: a general purpose global optimization software package. J. Glob. Optim. **8**, 201–205 (1996)
23. Sahinidis, N.V., Tawarmalani, M.: BARON 9.3: Global Optimization of Mixed-Integer Nonlinear Programs. User's Manual (2011)
24. Schaible, S.: Quasiconvex optimization in general real linear spaces. Zeitschrift fur Operations Research **16**, 205–213 (1972)
25. Schaible, S.: Maximization of quasiconcave quotients and products of finitely many functional. Cahiers du Centre d'Etudes de Recherche Opérationelle **16**, 45–53 (1974)
26. Schaible, S., Ziemba, W.T.: Generalized Concavity in Optimization and Economics. Academic Press, London (1981)
27. Sherali, H.D.: Convex envelopes of multilinear functions over a unit hypercube and over special discrete sets. Acta Math. Vietnam. **22**, 245–270 (1997)
28. Sherali, H.D., Wang, H.: Global optimization of nonconvex factorable programming problems. Math. Program. **89**, 459–478 (2001)
29. Tawarmalani, M., Richard, J.-P., Xiong, C.: Explicit convex and concave envelopes through polyhedral subdivisions. Math. Program. (2012). doi:10.1007/s10107-012-0581-4
30. Tawarmalani, M., Sahinidis, N.V.: Semidefinite relaxations of fractional programs via novel techniques for constructing convex envelopes of nonlinear functions. J. Glob. Optim. **20**, 137–158 (2001)
31. Tawarmalani, M., Sahinidis, N.V.: Convex extensions and convex envelopes of l.s.c. functions. Math. Program. **93**, 247–263 (2002)
32. Tawarmalani, M., Sahinidis, N.V.: Global optimization of mixed-integer nonlinear programs: a theoretical and computational study. Math. Program. **99**, 563–591 (2004)
33. Tawarmalani, M., Sahinidis, N.V.: A polyhedral branch-and-cut approach to global optimization. Math. Program. **103**, 225–249 (2005)