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Convexification Techniques for Global Optimization of Nonconvex Nonlinear Optimization Problems

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Convexification Techniques for Global Optimization of Nonconvex Nonlinear Optimization Problems

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Abstract

Fueled by applications across science and engineering, general-purpose deterministic global optimization algorithms have been developed for nonconvex nonlinear optimization problems over the past two decades. Central to the efficiency of such methods is their ability to construct sharp convex relaxations. Current general-purpose global solvers rely on factorable programming techniques to iteratively decompose nonconvex factorable functions, through the introduction of variables and constraints for intermediate functional expressions, until each intermediate expression can be outer-approximated by a convex feasible set. While it is easy to automate, this factorable programming technique often leads to weak relaxations.

In this thesis, we develop the theory of several new classes of cutting planes based upon ideas from generalized convexity and convex analysis. Namely, we (i) introduce a new method to outer-approximate convex-transformable functions, an important class of generalized convex functions that subsumes many functional forms that frequently appear in nonconvex problems and, (ii) derive closed-form expressions for the convex envelopes of various types of functions that are the building blocks of nonconvex problems. We assess, theoretically and computationally, the sharpness of the new relaxations in comparison to existing schemes. Results show that the proposed convexification techniques significantly reduce the relaxation gaps of widely-used factorable relaxations.

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Chapter 1

Introduction

1.1 Motivation

Fundamental theoretical and algorithmic developments have transformed linear optimization (LP) and convex nonlinear optimization (NLP) into mature technologies. Robust general-purpose solvers are capable of solving problems with thousands or even millions of variables efficiently and accurately with little user effort. For nonconvex NLPs, however, the situation is completely different. As noted by one of the founders of convex analysis:

> "*In fact the great watershed in optimization is not between linearity and nonlinearity, but convexity and nonconvexity.*" –R. T. Rockafellar, SIAM Review, 1993.

Motivated by diverse applications across science and engineering, deterministic global solvers have been developed for nonconvex NLPs over the past two decades. While these new classes of algorithms have already had a significant impact in operations research, computer science and engineering, there exist a multitude of important applications that these methods are unable to address. Compared to the LP and convex NLP solvers, global solvers are very slow, cannot handle large-scale problems, and require a high level of user expertise. In fact, many optimization experts believe that in the case of nonconvex problems, one has to give up on either speed or the guarantee of solution quality. The key to bridge this gap is given by the following insightful observation of Rockafellar (SIAM Review, 1993):

> "*Even for problems that are not themselves of convex type, convexity may enter for instance in setting up subproblems as part of an iterative numerical scheme.*"

Central to the efficiency of global solvers is their ability to construct sharp convex relaxations. Current general-purpose global optimization codes rely on factorable programming techniques [36] to iteratively decompose nonconvex factorable functions, through the introduction of variables and constraints for intermediate functional expressions, until each intermediate expression can be outer-approximated by a convex feasible set, via known techniques [49, 63]. While it is easy to automate, this factorable programming technique often leads to weak relaxations.

This thesis is focused on developing new convexification techniques for noconvex NLPs by building upon ideas from generalized convexity and convex analysis. While convex analysis has been employed extensively to develop the theory of convex optimization, its crucial role in deterministic global optimization is not yet well-understood. Likewise, the extensive literature on generalized convexity has not found much practical use in nonconvex optimization, as almost all nonconvex problems are not generalized convex. In this thesis, we develop the theory of several new classes of cutting planes by exploring various implications of convexity in global optimization. Namely, we (i) introduce a new method to outer-approximate convex-transformable functions, an important class of generalized convex functions that subsumes many functional forms that frequently appear in nonconvex problems [23] and, (ii) derive closed-form expressions for the convex envelopes of various types of functions that are the building blocks of nonconvex problems [25, 26].

1.2 Outline and contributions

In the following, we summarize the main contributions of this thesis.

1.2.1 Generalized convexity and global optimization

Generalized convex functions have been studied extensively in both optimization and economics [2]. Hundreds of articles, several books, and scientific meetings are devoted to introduce and study various generalizations of convex functions. The main idea is that convexity is only a *sufficient* condition for the key properties needed in the context of *local optimization*. Indeed, there exists a vast class of nonconvex functions that possess these key properties. For the purpose of global optimization, however, the important question is whether the *generalized convexity* of sub-expressions of nonconvex functions can be exploited to generate tighter relaxations for nonconvex programs. In Chapter 2, we focus on convex transformable or G-convex functions, an important class of generalized convex functions. We develop a novel technique to outer-approximate G-convex functions and compare and contrast it with existing convexification techniques. The main contributions of this study can be summarized as follows [23].

- We develop a new method to outer-approximate convex-transformable functions and derive the tightest, in a well-defined sense, transforming function;
- We propose a new scheme to overestimate signomials which is provably tighter than a popular standard approach;
- We develop tighter relaxations for many classes of functions including products and ratios of convex and/or concave functions, and log-concave functions.

1.2.2 Convex analysis and global optimization

Consider an optimization problem of the form $P : \min_{x \in \mathcal{C}} \phi(x)$, where $\mathcal{C}$ is a compact convex set and $\phi(x)$ is a lower semi-continuous (lsc) function that is nonconvex over $\mathcal{C}$. It is well-known that this optimization problem is intractable in general. Now, consider the convex optimization problem $Q : \min_{x \in \mathcal{C}} \mathrm{conv}_{\mathcal{C}}\phi(x)$, where $\mathrm{conv}_{\mathcal{C}}\phi(x)$ denotes the convex envelope of $\phi(x)$ over $\mathcal{C}$. Recall that the convex envelope of $\phi(x)$ over $\mathcal{C}$ is defined as the greatest convex function majorized by $\phi(x)$ over $\mathcal{C}$. It follows that the optimal values of P and Q are equal and the set of optimal solutions of P is contained in that of Q (cf. [19]). In general, however, constructing the convex envelope of $\phi(x)$ over $\mathcal{C}$ is as hard as solving the nonconvex problem P. This difficulty is due to the fact that, even for computing the value of the convex envelope of a function at a given point, one needs to solve a highly nonconvex optimization problem [62, 25]. Now, suppose that $\phi(x) = \phi_1(x) + \phi_2(x)$. Let $\mathcal{X}$ denote a convex set such that $\mathcal{X} \supseteq \mathcal{C}$. Assume that, due to some special structure, it is simple to construct the convex envelopes of ϕ_1 and ϕ_2 over $\mathcal{X}$. It follows that $\tilde{\phi}(x) = \mathrm{conv}_{\mathcal{X}}\phi_1(x) + \mathrm{conv}_{\mathcal{X}}\phi_2(x)$ is a (possibly tight) convex underestimator for $\phi(x)$ over $\mathcal{C}$. Such a convex relaxation can then be incorporated in a deterministic global optimization algorithm to generate a lower bound for the nonconvex problem. For general-purpose global solvers and, in the context of factorable programming in particular [36, 49], it is highly advantageous to have closed-form expressions for the convex envelopes of primitive functions that frequently appear as sub-expressions in nonconvex functions. These envelopes significantly enhance the strength of the relaxations thus generated.

Motivated by the above discussion, in Chapters 3 and 4, we study the problem of constructing the convex envelope of a lsc function over a compact convex set. The main contributions of this work are as follows [25, 26]:

- We formulate, as a *convex* NLP, the problem of constructing the convex envelope of a lsc function whose generating set is representable as the union of a finite number of compact convex sets. This development unifies all prior results in the literature and extends to many additional classes of functions.

- We consider functions of the form $\phi = f(x)g(y)$, $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ over a box, where $f(x)$ is a nonnegative convex function and $g(y)$ is a component-wise concave function. We derive explicit characterizations for the convex envelope of a wide class of such functions. The proposed envelopes cover roughly 30% of nonconvex functions that appear in the widely used `GLOBALLib` and `MINLPLib` collections of global optimization test problems.

1.2.3 Deterministic global optimization in product design

Optimization problems in mechanical design applications are often highly nonconvex. Gradient-based local solvers and stochastic global solvers are used widely to solve these problems. However, since these methods do not guarantee global optimality, the modeler is left with the hope of having a *good enough* design (*i.e.* better than the starting point) in hand. Deterministic global optimization avoids this uncertainty by finding the solutions within a selected tolerance of the global optimum in finite time.

In chapter 5, we present a deterministic Lagrangian-based approach for global optimization of quasi-separable problems and apply it to two product design applications: (i) product family optimization with a fixed platform configuration and (ii) product design for maximum profit. Results show that the proposed method is quite scalable and outperforms the commercial solver `BARON` when increasing the size of the problem. Furthermore, we demonstrate that the global solutions are significantly better than those obtained by prior approaches in the literature.

Chapter 2

Relaxations of factorable functions with convex-transformable intermediates

Factorable programming techniques are used widely in global optimization for bounding nonconvex functions. 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. In this chapter, we examine whether these nested functional decompositions of factorable programs can be replaced by, or enhanced via, the use of functional transformations. In essence, instead of relying on convexity of simple intermediate expressions, we exploit *convex transformability* of the component functions of factorable programs as a tool in the generation of bounding functions for global optimization algorithms.

2.1 Introduction

Convex-transformable functions have been studied extensively in the generalized convexity literature [2, 52]. 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 [11, 21]. 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.

Transformation techniques have been proposed in the global optimization literature to convexify signomial functions [34, 35]. 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 the 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.

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 chapter addresses several questions of this nature. First, in Section 2.2, 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 Section 2.3. In Section 2.4, 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 Section 2.5, we generalize the results of Section 2.4 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 Section 2.6, we consider the class of log-concave functions. Finally, in Section 2.7, we demonstrate the integration of the proposed relaxation within the factorable programming framework through some examples and compare and contrast it with existing relaxations.

2.2 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 chapter, 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 $\text{vert}(\mathcal{C})$, while the relative interior of $\mathcal{C}$ will be denoted by $\text{ri}(\mathcal{C})$. 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 $\text{conv}_{\mathcal{C}}\phi$, is defined as the tightest convex underestimator of ϕ over $\mathcal{C}$. Similarly, $\text{conc}_{\mathcal{C}}\phi$ 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 $\text{conv}_{\mathcal{C}}\phi$ (or $\text{conc}_{\mathcal{C}}\phi$).

Definition 2.1. ([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 chapter, 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 2.1. 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 2.2. 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 $j \in J_2 = \bar{J} \setminus J_1$. 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 $\phi(y_1, \ldots, y_n)$ is nondecreasing in y_j, $j \in J_1$ and is nonincreasing in y_j, $j \in J_2$. Then, the composite function $h(x) = \phi(f(x))$ 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 $\lambda \in [0, 1]$:

$$G(\phi(f(\lambda x^1 + (1 - \lambda)x^2))) \leq G(\phi(\lambda f(x^1) + (1 - \lambda)f(x^2))). \tag{2.1}$$

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

$$G(\phi(\lambda f(x^1) + (1 - \lambda)f(x^2))) \leq \lambda G(\phi(f(x^1))) + (1 - \lambda)G(\phi(f(x^2))). \tag{2.2}$$

Combining (2.1) and (2.2), 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 2.3. 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 2.2 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 [11] in the economics literature to define least concave utility functions. In Section 2.3, we will show that least convexifying transformations are of crucial importance for convexifying nonconvex problems.

Definition 2.2. ([11]) 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 2.1. 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 2.1 and 2.2 to derive least convexifying transformations for composite functions.

Proposition 2.4. 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 2.1, 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 2.2, $\hat{G}\tilde{G}^{-1}$ 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 2.1. 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 2.3 by noting that the inverse image of a convex set under an affine transformation is convex (cf. Theorem 3.4 in [47]). □

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 [12]. We summarize the main results in Propositions 2.5 and 2.6.

Proposition 2.5. *([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 2.6. *([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:

$$H(x;\rho) = \nabla^2\phi(x) + \rho(x)\nabla\phi(x)\nabla\phi(x)^T, \tag{2.3}$$

the condition of Proposition 2.6 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

$$\rho_0(x) = \sup_{z\in\mathbb{R}^n} \Big\{ -\frac{z^T\nabla^2\phi(x)z}{(z^T\nabla\phi(x))^2} : \|z\| = 1, z^T\nabla\phi(x) \neq 0 \Big\} \tag{2.4}$$

is bounded above for every $x \in \mathcal{C}$, then $H(x;\rho)$ is positive semidefinite for every $\rho(x) \geq \rho_0(x)$ over $\mathcal{C}$. Note that, by Proposition 2.5, the set of points where $\nabla\phi(x) = 0$, correspond to the minimal points of ϕ. Thus, the Hessian of ϕ is positive-semidefinite at these points and, as a result, $\rho_0(x)$ can take any 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 (2.4) is without loss of generality. From the definition of ρ_0, we can compute $G^*(t)$ as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\ln\Big(\frac{\mathrm{d}G^*(t)}{\mathrm{d}t}\Big) = g(t), \tag{2.5}$$

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

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

Corollary 2.2. Let the G-convex function $\phi : \mathcal{C} \to \mathbb{R}$ be nonconvex. Then, G is nonconcave over $I_\phi(\mathcal{C})$. Namely, $G(t)$ 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 (2.4) 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, $g(\hat{t})$ and $G^{*\prime\prime}(\hat{t})$ are both positive, where $\hat{t} = \phi(\hat{x})$. By Definition 2.2, every G which convexifies ϕ is strictly convex at $\hat{t}$. $\square$

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

Definition 2.3. 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 2.3. 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 convex over $I_\phi(\mathcal{C})$.

Proof. Follows directly from Corollary 2.2. □

The converse of the above corollary does not hold, in general, due to taking the supremum in the computation of $g(t)$ in (2.5).

2.3 Convexification via transformation

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

$$\Phi := \{(x,t) \in \mathcal{C} \times \mathcal{I} : \phi(x) \le t\}, \tag{2.6}$$

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 [63, 64]. Namely, $\phi(x)$ is assumed to be part of the initial nonconvex expression and t denotes an auxiliary variable introduced for the purpose of separable reformulation.

Proposition 2.7. 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:

$$\tilde{\Phi} := \{(x,t) \in \mathcal{C} \times \mathcal{I} : G(\phi(x)) \le \bar{G}(t)\} \tag{2.7}$$

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 2.2, $G(t)$ 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 the set Φ. □

From (2.7), 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, $\mathrm{conc}_{\mathcal{I}}G(t) \leq \bar{G}(t)$ for all $t \in \mathcal{I}$. Thus, setting $\bar{G}(t) = \mathrm{conc}_{\mathcal{I}}G(t)$ provides the tightest relaxation in (2.7). Next, we investigate the criteria for choosing the transforming function G.

Proposition 2.8. 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 (2.6):

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. $\square$

Remark 2.2. In Parts (i) and (ii) of the above proposition, 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 $\tilde{\Phi}_2 \subset \tilde{\Phi}_1$.

Remark 2.3. Employing a similar line of arguments, for a G-concave function ϕ, the conditions of Proposition 2.8 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 2.8 and the concept of least convexifying transformations introduced in Section 2.2, we now show that the tightest relaxation of the form (2.7) has a well-defined mathematical description as given by the following corollary.

Corollary 2.4. For a G-convex function $\phi : \mathcal{C} \to \mathbb{R}$, the tightest relaxation of the form (2.7) is obtained using $G = G^*$ and $\bar{G} = \mathrm{conc}_{\mathcal{I}} G^*$.

Proof. Follows from Proposition 2.8 and Definition 2.2. □

From (2.7), 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,

$$\tilde{\phi}^G(x) = \bar{G}^{-1}(G(\phi(x))). \tag{2.8}$$

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

$$g^G(x) = \phi(x) - \tilde{\phi}^G(x). \tag{2.9}$$

Substituting for $\tilde{\phi}^G(x)$, we obtain $g^G(x) = \{t - \bar{G}^{-1}(G(t)) : t = \phi(x),\ x \in \mathcal{C}\}$. If $G(t)$ is convex over $\mathcal{I} = [\underline{t},\ \bar{t}]$ and $\bar{G}(t) = \mathrm{conc}_{\mathcal{I}} G$, then g^G is a concave function of t and is given by:

$$g^G(t) = t - \Big(\frac{\bar{t} - \underline{t}}{G(\bar{t}) - G(\underline{t})}\Big) G(t) + \Big(\frac{G(\underline{t})\bar{t} - G(\bar{t})\underline{t}}{G(\bar{t}) - G(\underline{t})}\Big). \tag{2.10}$$

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:

$$g^G(x) = \tilde{\phi}^G(x) - \phi(x). \tag{2.11}$$

The gap functions in (2.9) and (2.11) will be compared against similarly defined gap functions $g^S(x)$ between $\phi(x)$ and standard factorable programming under- and overestimators denoted by $\tilde{\phi}^S(x)$. In particular, we will characterize the points at which these gap functions assume their maximal values $g^G_{\max}$ and $g^S_{\max}$.

2.4 Signomials

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

$$\mathcal{C} = \{x \in \mathbb{R}^n : x_i > 0,\ \forall i \in I_3,\ x_i \geq 0, \forall i \in I \setminus I_3\}. \tag{2.12}$$

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 Section 2.3 to generate a concave overestimator of ϕ and compare its tightness with a widely used conventional approach.

2.4.1 G-convexity and least convexifying transformations

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

Proposition 2.9. Consider $\phi = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R}$ over the set $\mathcal{C}$ defined by (2.12). The function ϕ is G-convex if and only if $a_i < 0$ for all $i \in I \setminus \{j\}$ and $\sum_{i \in I \setminus \{j\}} |a_i| < a_j < \sum_{i \in I \setminus \{j\}} |a_i| + 1$. Moreover, a least convexifying transformation for ϕ is given by

$$G^*(t) = t^{\frac{1}{\sum_{i \in I} a_i}}. \tag{2.13}$$

Proof. By Proposition 2.6, if ϕ is G-convex, its augmented Hessian given by:

$$H_{(i,j)} = \begin{cases} a_i(a_i - 1 + \rho a_i \phi)\phi / x_i^2, & \text{if } i = j \\ a_i a_j (1 + \rho\phi)\phi/(x_i x_j), & \text{otherwise} \end{cases}, \ \forall i, j \in \{1, \ldots, n\}, \tag{2.14}$$

is positive semidefinite for every $\rho(x) \geq \rho_0(x)$ for all $x \in \text{ri}(\mathcal{C})$. 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:

$$D_{kl} = (-1)^{k+1} \prod_{i \in K_{kl}} \frac{a_i}{x_i^2} \Big(\sum_{i \in K_{kl}} a_i(\rho\phi + 1) - 1 \Big) \phi^k, \ \forall k \in I, \ l \in L \tag{2.15}$$

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

(i) $a_i < 0$ for all $i \in I$. By (2.15), H is positive semidefinite when $\sum_{i \in K_{kl}} a_i(\rho\phi+1) \leq 1$ 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 $|\mathcal{S}| \geq 2$. 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 (2.15), 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 $|\mathcal{S}| = 1$. 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 (2.15), D_{kl} is nonnegative when $\sum_{i \in K_{kl}} a_i(\rho\phi+1) \geq 1$. Obviously, this condition holds only if $\sum_{i \in K_{kl}} a_i > 0$. Hence, H is positive semidefinite for all ρ such that:

$$\rho \geq \frac{1}{\phi}\Big(\frac{1}{\sum_{i \in I} a_i} - 1\Big). \tag{2.16}$$

If $\sum_{i \in I} a_i \geq 1$, then (2.16) 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 $\rho_0 = 1/\phi(\frac{1}{\sum_{i \in I} a_i} - 1)$. From (2.5), it follows that:

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

It is then simple to verify that G^* is given by(2.13).

□

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

Proposition 2.10. Consider $\phi = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R}$ over the set $\mathcal{C}$ defined by (2.12). 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 (2.13) when condition (i) is met and by

$$G^*(t) = -t^{\frac{1}{\sum_{i \in I} a_i}}, \tag{2.17}$$

when condition (ii) is met.

Proof. By Proposition 2.6, if ϕ is G-concave, then all kth order principal minors of its augmented Hessian given by:

$$D_{kl} = (-1)^k \prod_{i \in K_{kl}} \frac{a_i}{x_i^2} \Big(\sum_{i \in K_{kl}} a_i(\rho\phi - 1) + 1 \Big) \phi^k, \ \forall k \in I, \ l \in L = \left\{ 1, \ldots, \binom{n}{k} \right\} \tag{2.18}$$

are nonnegative if k is even, and are nonpositive otherwise, where the index set K_{kl} is as defined in the proof of Proposition 2.9. The following cases arise:

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

$$\rho \geq \frac{1}{\phi}\Big(1 - \frac{1}{\sum_{i \in K_{kl}} a_i}\Big), \quad \forall K_{kl}. \tag{2.19}$$

First, consider $\sum_{i \in I} a_i \leq 1$. It follows that (2.19) is satisfied for all $\rho \geq 0$, implying ϕ is concave. Assuming $\sum_{i \in I} a_i > 1$, it follows that (2.19) holds for all $\rho \geq \rho_0$ with:

$$\rho_0 = \frac{1}{\phi}\Big(1 - \frac{1}{\sum_{i \in I} a_i}\Big). \tag{2.20}$$

Substituting (2.20) in equation (2.5) and solving for G^*, we obtain (2.13).

(ii) $a_i < 0$ for all $i \in \mathcal{S} \subset I$. Using a similar argument as in Part (ii) of Proposition 2.9, 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 (2.19) should hold. Thus, let $j \in K_{kl}$. In this case, the product $\prod_{i \in K_{kl}} a_i$ in (2.18) 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 $\sum_{i \in I \setminus \{j\}} a_i <$ vert$a_j$vert. Imposing this condition, it can be shown that the expressions for ρ_0 and G^* are given by (2.20) and (2.17), respectively. Note that the minus sign in (2.17) 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 [50] using the basic definition of pseudoconvexity. Since pseudo-convexity 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.

2.4.2 Exploiting G-concavity for upper bounding signomials

Next, we employ Proposition 2.10 to develop a new relaxation scheme for upper bounding signomials over a hyper-rectangle $\mathcal{H}^n$ in the nonengative orthant. The standard factorable scheme overestimates signomials by first replacing each convex univariate term by its affine envelope. Next, the resulting expression is outer-linearized using a recursive interval arithmetic scheme (rAI) [63]. 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 $i \in I \setminus I_3$ and $\underline{\eta}_i = \bar{x}_i^{a_i}$, $\bar{\eta}_i = \underline{x}_i^{a_i}$ for all $i \in I_3$. The standard relaxation $\tilde{\phi}^S$ is as follows:

$$\left.\begin{array}{rcl}
\tilde{\phi}^S & = & t_n \\
t_i & = & \min\left\{\begin{array}{l} t_{i-1}\underline{\eta}_i + \bar{t}_{i-1}\eta_i - \bar{t}_{i-1}\underline{\eta}_i \\ \bar{\eta}_i t_{i-1} + \eta_i \underline{t}_{i-1} - \bar{\eta}_i \underline{t}_{i-1} \end{array}\right\}, \ \forall i \in I \setminus \{1\} \\
\eta_i & = & x_i^{a_i}, \ \forall i \in I_1 \\
\eta_i & = & \frac{\bar{x}_i^{a_i} - \underline{x}_i^{a_i}}{\bar{x}_i - \underline{x}_i}(x_i - \underline{x}_i) + \underline{x}_i^{a_i}, \ \forall i \in I \setminus I_1,
\end{array}\right\} \tag{2.21}$$

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 $i \in I$.

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 2.7 and 2.10, the following is a concave overestimator for ϕ:

$$\tilde{\phi}^G = (\phi^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}})\Big(\frac{\bar{\phi} - \underline{\phi}}{\bar{\phi}^{\frac{1}{\xi}} - \underline{\phi}^{\frac{1}{\xi}}}\Big) + \underline{\phi}. \tag{2.22}$$

By Proposition 2.10, $G^*(\phi)$ is concave over the range of ϕ. Thus, by (2.11), the gap between $\tilde{\phi}^G$ and ϕ is a concave function of ϕ and its maximum value is given by:

$$g^G_{\max} = \frac{(\xi-1)}{\xi^{\frac{\xi}{\xi-1}}}\left(\frac{\bar{\phi}-\underline{\phi}}{\bar{\phi}^{\frac{1}{\xi}}-\underline{\phi}^{\frac{1}{\xi}}}\right)^{\frac{\xi}{\xi-1}} - (\bar{\phi}\underline{\phi})^{\frac{1}{\xi}}\left(\frac{\bar{\phi}^{1-\frac{1}{\xi}}-\underline{\phi}^{1-\frac{1}{\xi}}}{\bar{\phi}^{\frac{1}{\xi}}-\underline{\phi}^{\frac{1}{\xi}}}\right). \tag{2.23}$$

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

Proposition 2.11. Consider the G-concave signomial $\phi = \prod_{i\in I} x_i^{a_i}$ defined over a box $\mathcal{H}^n \subset \mathcal{C}$. Then, $\tilde{\phi}^S$ globally dominates $\tilde{\phi}^G$, if one of the following conditions is met:

(i) $I_1 = \emptyset$;

(ii) $a_j < 0$ for some $j \in I$ such that $\sum_{i\in I\setminus\{j\}} a_i < |a_j|$.

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

$$\max_{x\in\mathcal{H}^n} (\tilde{\phi}^S - \tilde{\phi}^G) \tag{2.24}$$

is zero under conditions (i) or (ii). Consider an optimal solution (x, η, t) of the above problem. By (2.21), at this point we have

$$t_{i-1}\underline{\eta}_i + \bar{t}_{i-1}\eta_i - \bar{t}_{i-1}\underline{\eta}_i = \bar{\eta}_i t_{i-1} + \eta_i \underline{t}_{i-1} - \bar{\eta}_i \underline{t}_{i-1}, \ \forall i \in I \setminus \{1\}. \tag{2.25}$$

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 (2.25) it follows that $\tilde{t}_{i-1} = \tilde{x}_i$ and $\tilde{t}_i = \tilde{t}_{i-1}$ for all $i \in I \setminus \{1\}$. Letting $\lambda = \tilde{x}_i$ for some $i \in I$, yields $\tilde{\phi}^S = (\bar{\phi} - \underline{\phi})\lambda + \underline{\phi}$. We now consider two cases:

Case (i). When $I_1 = \emptyset$, any optimal solution of (2.24) is attained over the line segment $\mathcal{L}$ given by $\tilde{x}_1 = \ldots = \tilde{x}_n$, $\tilde{x}_i \in [0, 1]$ for all $i \in I$. Furthermore, the restriction of $\tilde{\phi}^S$ to $\mathcal{L}$ is the line segment connecting the minimum and maximum of $\tilde{\phi}^G$, *i.e.* the points $\lambda = 0$, $\phi = \underline{\phi}$ and $\lambda = 1$, $\phi = \bar{\phi}$. Since $\tilde{\phi}^G$ is concave, we have $\tilde{\phi}^S \leq \tilde{\phi}^G$ for all $x \in \mathcal{H}^n$.

Case (ii). When $I_1 \neq \emptyset$, 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

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

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:

$$f''(\lambda) = \frac{f(\lambda)}{\xi^2}\Big\{\Big(\sum_{I_1} \frac{\Delta\eta_i}{\underline{\eta}_i + \lambda\Delta\eta_i} + \sum_{I_2} \frac{a_i\Delta x_i}{\underline{x}_i + \lambda\Delta x_i} - \frac{a_j\Delta x_j}{\bar{x}_j - \lambda\Delta x_j}\Big)^2 \\ - \xi\Big(\sum_{I_1} \frac{\Delta\eta_i^2}{(\underline{\eta}_i + \lambda\Delta\eta_i)^2} + \sum_{I_2} \frac{a_i\Delta x_i^2}{(\underline{x}_i + \lambda\Delta x_i)^2} + \frac{a_j\Delta x_j^2}{(\bar{x}_j - \lambda\Delta x_j)^2}\Big)\Big\}. \tag{2.26}$$

The only negative expression in (2.26) is $g = -\xi\frac{a_j\Delta x_j^2}{(\bar{x}_j - \Delta x_j\lambda)^2}$. Since $\xi < 0$ and $|\xi| < |a_j|$, if we replace g by $\tilde{g} = -(\frac{a_j\Delta x_j}{\bar{x}_j - \Delta x_j\lambda})^2$, we obtain a lower bound for $f''(\lambda)$. However, $\tilde{g}$ cancels out when expanding (2.26), 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 $\lambda = 1$. Hence, at any optimal solution of (2.24), we have $\tilde{\phi}^S \leq \tilde{\phi}^G$. $\square$

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

$$\max_{x \in \mathcal{H}^n} (\tilde{\phi}^S - \phi). \tag{2.27}$$

By (2.21), at an optimal solution of the above problem, the equalities given by (2.25) 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 (2.21) 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:

$$\max_{x \in \mathcal{H}^{n'}} \alpha(\tilde{\varphi}^S - \varphi), \tag{2.28}$$

where $\varphi = \prod_{i\in I'} x_i^{a_i}$, and $\tilde{\varphi}^S$ denotes the corresponding standard overestimator. As we argue later, for our cases of interest, any optimal solution of this problem is a local maximum of (2.27). Similarly, if $x_k = \underline{x}_k$ for $k \in K \subset I$, then the maximum gap is equal to the maximum of (2.28) 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 (2.27) is attained at an interior point. Using a similar argument as in the proof of Proposition 2.11, it follows that, at a point of maximum gap, $\tilde{x}_i = \lambda$ for all $i \in I$, where $\tilde{x}_i$ is as defined in the proof of Proposition 2.11. Let $\beta_i = \underline{x}_i/\bar{x}_i$

for all $i \in I$. It follows that, the maximum of (2.27) is attained at the optimal solution of the following univariate concave maximization problem:

$$\max_{0 \leq \lambda \leq 1} \ \Big(1 - \prod_{i \in I} \beta_i^{a_i}\Big)\lambda + \prod_{i \in I} \beta_i^{a_i} - \prod_{i \in I_1} \Big((1 - \beta_i^{a_i})\lambda + \beta_i^{a_i}\Big) \prod_{i \in I_2} \Big((1 - \beta_i)\lambda + \beta_i\Big)^{a_i}. \quad (2.29)$$

Proposition 2.12. Consider the G-concave signomial $\phi = \prod_{i \in I} x_i^{a_i}$ over a box $\mathcal{H}^n$, with $a_i > 0$ for all $i \in I$ and $\sum_{i \in I} a_i > 1$. Assume that $I_1 \neq \emptyset$. Then, $g^G_{\max} < g^S_{\max}$ 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 $j \in I_2$.

Proof. Case (i). Define $\xi' = |I_1| + \sum_{I_2} a_i$. Letting $\beta_i = 0$ for all $i \in I$ in (2.29), we obtain:

$$g^S_{\max} = \frac{\xi' - 1}{\xi'^{\frac{\xi'}{\xi'-1}}} \bar{\phi}. \quad (2.30)$$

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 (2.30) provided that ξ' is computed over $I' = I \setminus K$. Since $g^S_{\max}$ is an increasing function of ξ', the maximum gap for this case is strictly less than the value given by (2.30) and therefore corresponds to a local maximum of (2.27). Further, if $x_k = 0$ for some $k \in I$, then α in (2.28) as well as the maximum gap go to zero. Letting $\underline{\phi} = 0$ in (2.22), we obtain:

$$g^G_{\max} = \frac{(\xi - 1)}{\xi^{\frac{\xi}{\xi-1}}} \bar{\phi}. \quad (2.31)$$

By (2.30) and (2.31), $g^G_{\max} < g^S_{\max}$ 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 (2.29) yields:

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

The maximum gap in this case is equal to

$$g^S_{\max} = \bar{\phi}\left\{\frac{(\xi'-1)}{\xi'^{\frac{\xi'}{\xi'-1}}}\left(\frac{1-\beta^{\xi'}}{1-\beta}\right)^{\frac{\xi'}{\xi'-1}} - \beta\left(\frac{1-\beta^{\xi'-1}}{1-\beta}\right)\right\}. \tag{2.32}$$

Now, assume $x_k = \bar{x}_k$ for $k \in K \subset I$. It can be shown that $g^S_{\max}$ in (2.32) 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 (2.32) can be equivalently written as:

$$g^S_{\max} = \frac{(\xi'-1)}{\xi'^{\frac{\xi'}{\xi'-1}}}\left(\frac{\bar{\phi}-\underline{\phi}}{\bar{\phi}^{\frac{1}{\xi'}}-\underline{\phi}^{\frac{1}{\xi'}}}\right)^{\frac{\xi'}{\xi'-1}} - (\bar{\phi}\underline{\phi})^{\frac{1}{\xi'}}\left(\frac{\bar{\phi}^{1-\frac{1}{\xi'}}-\underline{\phi}^{1-\frac{1}{\xi'}}}{\bar{\phi}^{\frac{1}{\xi'}}-\underline{\phi}^{\frac{1}{\xi'}}}\right). \tag{2.33}$$

From (2.23) and (2.33), it follows that, if $I_1 \neq \emptyset$, then $g^G_{\max} < g^S_{\max}$. $\square$

Thus, we conclude that the transformation method exploits the concavity of the univariate terms $x_i^{a_i}$ to provide a tighter overestimator of ϕ, whereas, in the standard method, only the cardinality of the set of concave terms is accounted for. However, the transformation overestimator does not globally dominate the standard overestimator. Namely, $\tilde{\phi}^G$ is tighter in the interior, especially around the normalized center of the domain (*i.e.* $\tilde{x}_1 = \tilde{x}_2 = \ldots = \tilde{x}_n$), 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. As an example, consider $\phi = x_1^{0.5}x_2^{0.7}$ over $[0,1]^2$. The two overestimators are compared in Figure 2.1 at various cross sections.

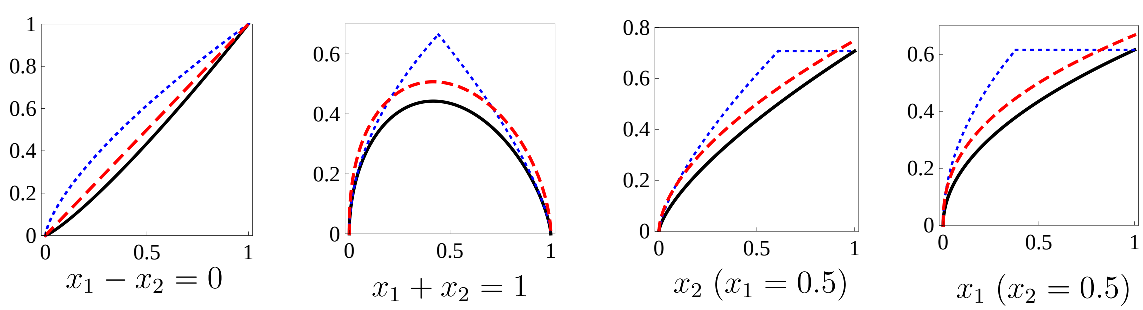


Figure 2.1: Comparison of the standard and transformation overestimators for $\phi(x) = x_1^{0.5}x_2^{0.7}$ over $[0,1]^2$ at various cross sections. The nonconcave function ϕ is shown in solid black, its standard relaxation $\tilde{\phi}^S$ in dotted blue, and the proposed relaxation $\tilde{\phi}^G$ in dashed red.

While Proposition 2.12 is valid under certain restrictive assumptions on the lower and upper bounds, similar gap reductions are observed for the general case in practice. Denote by γ the percentage reduction of the maximum gap when employing $\tilde{\phi}^G$ instead of $\tilde{\phi}^S$:

$$\gamma = (g^S_{\max} - g^G_{\max})/g^S_{\max} \times 100\%.$$

The maximum gap reduction values for a number of G-concave signomials are listed in Table 2.1. For each case, γ is the average value of maximum gap reductions computed over five randomly generated domains in $[0.1, 2.0]$ for each variable.

Table 2.1: Average maximum gap reduction (γ) due to G-concavity transformations for overestimating G-concave signomials

exponents	$\gamma(\%)$	exponents	$\gamma(\%)$	exponents	$\gamma(\%)$
{0.4, 0.7}	80.71	{0.3, 0.4, 0.5}	76.53	{0.2, 0.3, 0.4, 0.5}	65.67
{0.3, 1.0}	42.97	{0.5, 0.6, 0.7}	35.30	{0.3, 0.4, 0.5, 0.8}	37.57
{0.6, 0.8}	39.24	{0.4, 0.7, 1.0}	21.42	{0.4, 0.5, 0.6, 0.8}	28.98

By transforming a G-concave signomial in one step, we obtain an overestimator which is a function of n variables, while, in the standard approach, all intermediate constraints are functions of two variables. The latter feature is mostly advantageous for methods that rely on polyhedral outer-approximations in low-dimensional spaces [64]. To decompose the multivariate relaxation into low-dimensional subspaces and benefit from both methods to overestimate general nonconcave signomials, we propose a *recursive transformation and relaxation* (RT) scheme, which combines the standard relaxation and G-concavity transformations. Define the sets of subsets

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

and

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

Further, assume $\mathcal{S} \cup \mathcal{T}$ 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 $K = |\mathcal{S}|$, $J = |\mathcal{T}|$, $N = K + J + |I \setminus I_1|$. 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 $i \in I \setminus I_1$, $m = K+J+1, \dots, N$. We define the RT overestimator of ϕ as follows:

$$\left.\begin{array}{lcl} \tilde{\phi}^{RT} & = & r_N \\ r_m & = & \min\left\{\begin{array}{l} \bar{r}_{m-1}t_m + \underline{t}_m r_{m-1} - \bar{r}_{m-1}\underline{t}_m \\ \underline{r}_{m-1}t_m + \bar{t}_m r_{m-1} - \underline{r}_{m-1}\bar{t}_m \end{array}\right\}, m = 2, \dots, N \\ t_m & = & \prod_{i \in \mathcal{S}_k} x_i^{a_i},\ \forall \mathcal{S}_k \in \mathcal{S},\ m = 1, \dots, K \\ t_m & = & \left(\prod_{i \in \mathcal{T}_j} x_i^{\frac{a_i}{\xi_j}} - \underline{t}_m^{\frac{1}{\xi_j}}\right)\left(\frac{\bar{t}_m - \underline{t}_m}{\bar{t}_m^{\frac{1}{\xi_j}} - \underline{t}_m^{\frac{1}{\xi_j}}}\right) + \underline{t}_m,\ \forall \mathcal{T}_j \in \mathcal{T},\ m = K{+}1, \dots, K{+}J \\ t_m & = & \frac{\bar{x}_i^{a_i} - \underline{x}_i^{a_i}}{\bar{x}_i - \underline{x}_i}(x_i - \underline{x}_i) + \underline{x}_i^{a_i},\ \forall i \in I \setminus I_1,\ m = K+J+1, \dots, N, \end{array}\right\} \quad (2.34)$$

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 $m \in \{1, \dots, N\}$. Each G-concave signomial associated with a subset $\mathcal{T}_j$ is overestimated via transformation as defined by (2.22). Convex terms are relaxed by affine envelopes, and the resulting expression is outer-approximated using rAI. Obviously, for a given signomial ϕ, there are various ways of defining subsets $\mathcal{S}$ and $\mathcal{T}$. Next, we demonstrate the effect of this partitioning on the maximum relaxation gap between $\tilde{\phi}^{RT}$ and ϕ, and define an optimal variable grouping to obtain the least maximum gap.

Proposition 2.13. Consider $\phi = \prod_{i \in I} x_i^{a_i}$, with $a_i > 0$, $x_i \in [0, \bar{x}_i]$ for all $i \in I$ and $\sum_{i \in I} a_i > 1$. Consider an RT relaxation of ϕ as defined in (2.34). 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:

$$g_{\max}^{RT} = \frac{\hat{\xi} - 1}{\hat{\xi}^{\frac{\hat{\xi}}{\hat{\xi}-1}}}\bar{\phi}. \quad (2.35)$$

Proof. Let $\underline{x}_i = 0$ for all $i \in I$ in (2.34). By the second equation of (2.34), 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 $m = 2, \dots, N$, where $\tilde{r}_m = r_m/\bar{r}_m$. Using the last three of (2.34), 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

$$\prod_{m \in \mathcal{S}_k} \tilde{x}_m^{a_m} = \Big(\prod_{m \in \mathcal{T}_j} \tilde{x}_m^{a_m}\Big)^{1/\hat{\xi}_j} = \tilde{x}_i, \quad \forall \mathcal{S}_k \in \mathcal{S},\ \mathcal{T}_j \in \mathcal{T},\ i \in I \setminus I_1.$$

Letting $\tilde{r}_N = \lambda$, it can be shown that the maximum gap between $\tilde{\phi}^{RT}$ and ϕ can be found by solving the following univariate concave maximization problem

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

where $\hat{\xi}$ is defined in the statement of the proposition. It is then simple to check that $g_{\max}^{RT}$ is given by (2.35). $\square$

Under the conditions of Proposition 2.13, 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 2.14. Let $\mathcal{A} = \{a_i : i \in I_1\}$. Without loss of generality, assume that the elements of $\mathcal{A}$ are in ascending order. Then, a partition of $\mathcal{A}$ that minimizes $\hat{\xi}$ is given by:

$$\Pi^* := \{\{a_1, a_{2m}\}, \{a_2, a_{2m-1}\}, \ldots, \{a_m, a_{m+1}\}\}, \tag{2.36}$$

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

Proof. First, we address the case $|\mathcal{A}| = 2m$. 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 (2.36), 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 $|\mathcal{A}| = 2m+1$. We claim that $\Pi = \Pi^* \cup \{a_{2m+1}\}$ 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 $\hat{\xi}(\Pi) \leq \hat{\xi}(\Pi')$. To calculate $\hat{\xi}(\Pi')$, consider the following cases:

(i) $d_i \in \mathcal{S}$. If $d'_i \in \mathcal{S}$, then $\hat{\xi}(\Pi) = \hat{\xi}(\Pi')$. Otherwise, $\hat{\xi}(\Pi') = \hat{\xi}(\Pi) + a_j + a_{2m+1} - 1$. It follows that $\hat{\xi}(\Pi) < \hat{\xi}(\Pi')$.

(ii) $d_i \in \mathcal{T}$. In this case, we have $\hat{\xi}(\Pi') = \hat{\xi}(\Pi) - a_k + a_{2m+1}$, which implies $\hat{\xi}(\Pi) < \hat{\xi}(\Pi')$.

Thus, Π is optimal. $\square$

Proposition 2.13 requires nonnegative exponents and zero lower bounds for all variables. In practice, however, similar gap reductions are observed for the general case. The percentage reduction of the maximum gap when employing $\tilde{\phi}^{RT}$ instead of the standard relaxation $\tilde{\phi}^{S}$, *i.e.*

$$\gamma = (g^S_{\max} - g^{RT}_{\max})/g^S_{\max} \times 100\%$$

is provided in Table 2.2 for a number of nonconcave signomials. Note that, in all instances the signomial term is not concave transformable. As before, the values of γ in this table represent averages over five randomly generated domains in $[0.1, 2.0]$ for each variable. We conclude that G-concavity transformations and decompositions based on the partitioning outlined in Proposition 2.14 lead to considerable reductions of the maximum gap of factorable relaxations for nonconcave signomials.

Table 2.2: Average maximum gap reduction (γ) due to RT method for overestimating signomials

exponents	γ(%)	exponents	γ(%)	exponents	γ(%)
{-0.6, 0.4, 0.5}	44.37	{-0.5, 0.4, 0.6, 1.2}	25.66	{-0.5, 0.4, 0.5, 0.6, 0.7}	25.75
{-0.5, 0.4, 0.8}	35.67	{ 0.4, 0.5, 0.7, 1.5}	23.51	{-0.3, 0.4, 0.6, 0.8, 1.5}	20.56
{-1.5, 0.5, 0.6}	20.52	{-0.8,-0.5, 0.4, 0.7}	22.14	{-0.8,-0.5, 0.5, 0.6, 0.7}	20.01
{ 0.6, 0.7, 1.5}	13.15	{-1.5, 0.5, 0.6, 1.0}	14.03	{-1.5, 0.5, 0.6, 1.0, 1.2}	10.50

2.5 Products and ratios of convex and/or concave functions

In this section, we generalize the results of Propositions 2.9 and 2.10 using the composition rules developed in Section 2.2. 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. For numerical comparisons of the proposed relaxations with the conventional factorable scheme, we compute the percentage gap closed by transformation relaxation denoted by $\tilde{\phi}^G$, as follows:

$$(\tilde{\phi}^S - \tilde{\phi}^G)/(\tilde{\phi}^S - \phi) \times 100\%,$$

where $\tilde{\phi}^S$ denotes a factorable relaxation of ϕ.

Proposition 2.15. 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 (2.22).

Proof. Follows directly from Propositions 2.2 and 2.10. □

Remark 2.4. For a given function ϕ and cardinality of I in Proposition 2.15, there are infinitely many possible representations in terms of ϕ_i and a_i. However, by Proposition 2.8, 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 $\psi = \left(\sum_{i\in I} x_i^{1/p}\right)^p$, $p > 1$, $x_i \geq 0$ for all $i \in I$. Let $\phi_k^{a_k} = \psi$ for some $k \in I$. Then, the condition of Proposition 2.15 holds for any $a_k \in [1, p]$. However, letting $a_k = 1$ and $\phi_k = \psi$ provides the tightest relaxation.

Example 2.1. Consider $\phi(x) = (x^2 - 1)\big(\log(x+2)\big)^2$, $x \in [-1, 1]$. 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:

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

By Proposition 2.15, 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 standard and transformation relaxations are compared in Figure 2.2. While neither of the underestimators is globally dominant, $\tilde{\phi}^G$ leads to a much smaller gap integrated over the domain of interest.

Example 2.2. 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 are interested 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:

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

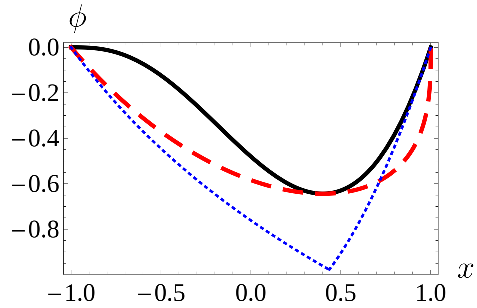
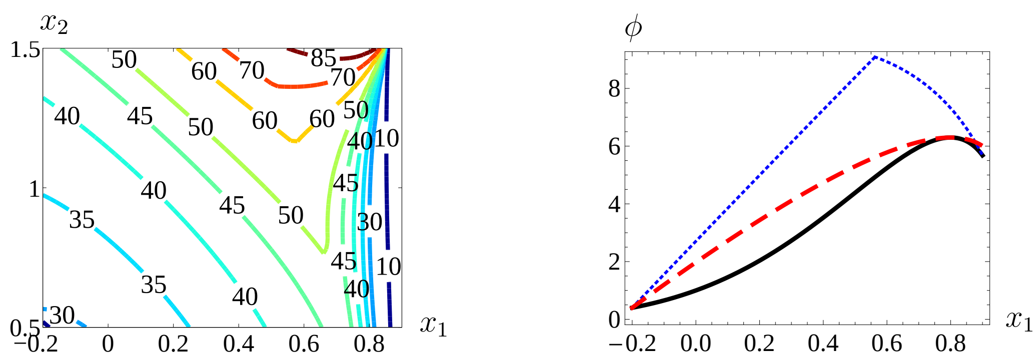


Figure 2.2: Comparison of the standard and transformation relaxations for $\phi = (x^2 - 1)(\log(x+2))^2$, $x \in [-1, 1]$ in Example 2.1. The nonconvex function ϕ is shown in solid black, its standard underestimator $\tilde{\phi}^S$ in dotted blue, and the proposed underestimator $\tilde{\phi}^G$ in dashed red.

By Proposition 2.15, 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 Figure 2.3(b) at $x_2 = 1.0$, and the gap closed by $\tilde{\phi}^G$, is depicted in Figure 2.3(a). Up to over 85% of the gap is closed by $\tilde{\phi}^G$.



(a) % Gap closed by $\tilde{\phi}^G$

(b) $x_2 = 1.0$

Figure 2.3: Comparison of the standard 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 2.2. In Fig 2.3(b), the nonconcave function ϕ is shown in solid black, its standard overestimator $\tilde{\phi}^S$ in dotted blue, and the proposed overestimator $\tilde{\phi}^G$ in dashed red.

Proposition 2.16. 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 (2.22).

Proof. Follows directly from Propositions 2.2 and 2.10. □

Remark 2.5. As a special case of Proposition 2.16, 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 [51].

Remark 2.6. Proposition 2.16 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 2.16 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 2.17. Consider $\phi = \prod_{i\in I} \phi_i^{a_i}$ over a box, where $a_i < 0$ for all $i \in I\setminus\{j\}$ and $\sum_{i\in I\setminus\{j\}} |a_i| < a_j < \sum_{i\in I\setminus\{j\}} |a_i| + 1$. Let ϕ_i be positive and concave for all $i \in I \setminus \{j\}$, 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 (2.22) provides an underestimator for it.

Proof. Follows directly from Propositions 2.2 and 2.9. □

Remark 2.7. Using a similar argument as in Remark 2.4, it is simple to show that, for a given function ϕ and cardinality of I, the tightest relaxation in Proposition 2.16 (resp. Proposition 2.17) is obtained by setting a_j and a_i, $i \in I\setminus\{j\}$ to the smallest (resp. largest) possible values while preserving convexity of ϕ_j and concavity of ϕ_i, $i \in I \setminus \{j\}$.

Example 2.3. Consider $\phi(x) = \log(x + 1)/(x^4 + x^2 + 1)$, $x \in [0.1, 4]$. To construct a concave overestimator of ϕ using the 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 [61, 62] to overestimate t_1/t_2, we obtain:

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

By Proposition 2.16, 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 Figure 2.4. Clearly, the transformation method provides a significantly tighter relaxation.

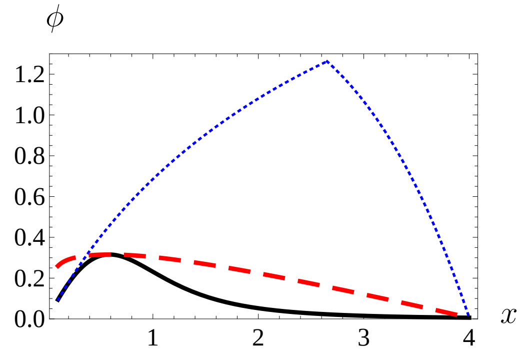


Figure 2.4: Comparison of the standard and transformation relaxations for $\phi = \log(x+1)/(x^4+x^2+1)$, $x \in [0.1, 4]$ in Example 2.3. The nonconcave function ϕ is shown in solid black, its standard overestimator $\tilde{\phi}^S$ in dotted blue, and the proposed overestimator $\tilde{\phi}^G$ in dashed red.

Example 2.4. 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:

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

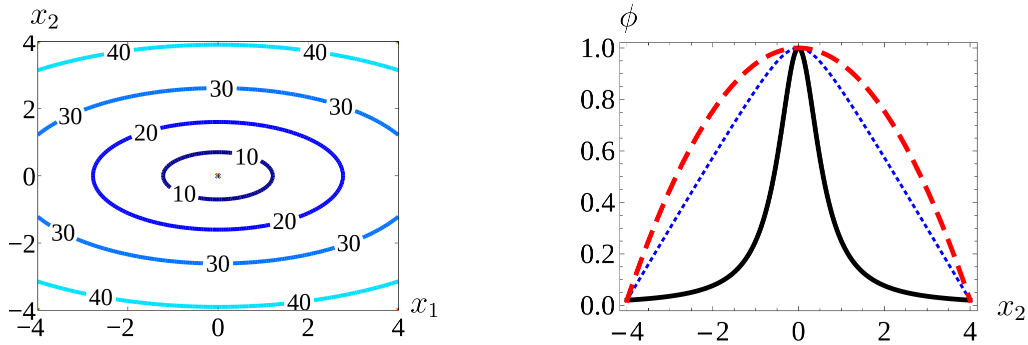
By Proposition 2.16, ϕ is G-concave with $G(t) = -t^{-1/2}$. Hence, $\tilde{\phi}^G$ is given by:

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

The two relaxations are compared in Figure 2.5. The transformation relaxation dominates the standard approach.

2.6 Log-concave functions

Another important class of concave-transformable functions are log-concave functions [45]. 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.



(a) % Gap closed by $\tilde{\phi}^G$ (b) $x_1 = 0$

Figure 2.5: Comparison of the standard and transformation relaxations for $\phi = 1/(1 + x_1^2 + 3x_2^2)$, over $[-4, 4]^2$ in Example 2.4. In Fig 2.5(b), the nonconcave function ϕ is shown in solid black, its standard overestimator $\tilde{\phi}^S$ in dotted blue, and the proposed overestimator $\tilde{\phi}^G$ in dashed red.

However, by Proposition 2.8, the transforming function defined in Proposition 2.15 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.

Proposition 2.18. 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:

$$\tilde{\phi}^G = \frac{(\log \phi - \log \underline{\phi})(\bar{\phi} - \underline{\phi})}{\log(\bar{\phi}/\underline{\phi})} + \underline{\phi}. \tag{2.37}$$

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 (2.8), yields (2.37). □

Several important instances of log-concave functions are derived from the function ϕ introduced in Proposition 2.18. 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 2.18 with a standard factorable approach.

Example 2.5. 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:

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

Clearly, the sigmoidal function is log-concave. Thus, an alternative overestimator for ϕ can be obtained from (2.37):

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

The two overestimators are compared in Figure 2.6. The transformation overestimator is strongly dominant.

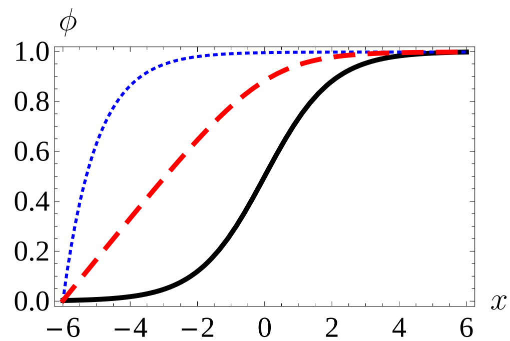


Figure 2.6: Comparison of the standard and transformation overestimators for $\phi = 1/(1+\exp(-x))$, $x \in [-6, 6]$ in Example 2.5. The nonconcave function ϕ is shown in solid black, its standard overestimator $\tilde{\phi}^S$ in dotted blue, and the proposed overestimator $\tilde{\phi}^G$ in dashed red.

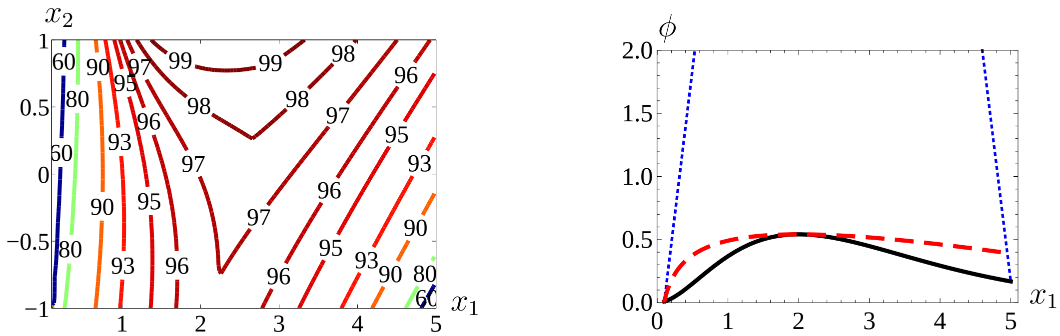
Example 2.6. Consider $\phi(x) = x_1^2 \exp(x_2 - x_1)$, $x_1 \in [0.1, 5]$, $x_2 \in [-1, 1]$. Let $t_1 = x_2 - x_1$ and denote by t_2 and t_3 the affine overestimators of x_1^2 and $\exp(t_1)$, respectively. Utilizing bilinear envelopes [1] to overestimate $t_2 t_3$, yields:

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

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 Figure 2.7. The proposed overestimator is significantly tighter than the standard relaxation, and results in gap reductions of up to 99%.



(a) % Gap closed by $\tilde{\phi}^G$ (b) $x_2 = 0$

Figure 2.7: Comparison of the standard 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 2.6. In Figure 2.7(b), the nonconcave function ϕ is shown in solid black, its standard overestimator $\tilde{\phi}^S$ in dotted blue, and the proposed overestimator $\tilde{\phi}^G$ in dashed red

2.7 Integration within the factorable framework

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, this 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 some intermediate expressions are not further decomposed but outer-approximated 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.

Example 2.7. Consider

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

This function has two local minima at $x_1^* = -1.676$ and $x_2^* = 1.456$, and one local maximum at $x_3^* = -0.481$ (see Figure 2.8). A standard factorable decomposition of ϕ is as follows:

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

All convex and concave univariate terms are over- and under-estimated, respectively, by their affine envelopes. The bilinear and fractional terms are replaced by their convex and concave envelopes [1, 61, 62]. We denote the resulting convex set by $\tilde{\phi}^S$. By Propositions 2.15 and 2.16, ϕ is the difference of two G-concave functions. Thus, we have the following alternative decomposition:

$$\begin{aligned}
&t_1' = (x+3)/\left(x^2+x+1\right)^2,\\
&t_2' = \sqrt{6-x^2-x}\left(0.4x+1\right)^{3/2},\\
&\phi = t_1' - t_2'.
\end{aligned}$$

Propositions 2.15 and 2.16 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 Figure 2.8. 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 including both relaxations.

Example 2.8. Consider

$$\phi(x) = x\frac{\sqrt{x+4}}{(1+x^2)^2} + 0.05x^3,\quad x \in [-1.5,\ 3.0].$$

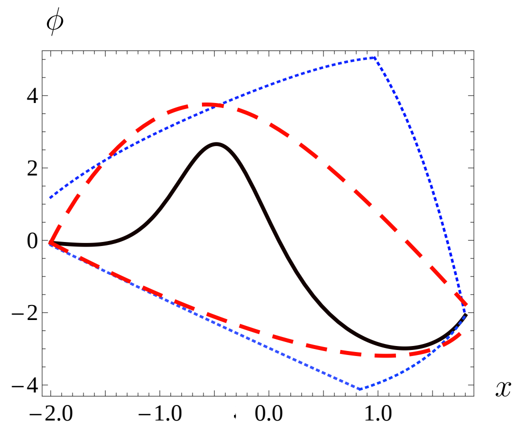


Figure 2.8: Comparison of the standard and integrated relaxations of $\phi = (x+3)/(x^2 + x + 1)^2 - \sqrt{6 - x - x^2}(0.4x+1)^{1.5}$, $x \in [-2, 1.8]$ in Example 2.7. The nonconvex function ϕ is shown in solid black, its standard relaxation $\tilde{\phi}^S$ in dotted blue, and the proposed relaxation $\tilde{\phi}^G$ in dashed red.

This function has two local minima at $x_1^* = -0.562$ and $x_2^* = 1.53$, and two local maxima at $x_3^* = -1.475$ and $x_4^* = 0.624$ (see Figure 2.9). A standard decomposition of ϕ is given by:

$$
\begin{aligned}
&t_1 = \sqrt{x+4},\ t_2 = (1+x^2)^2,\ t_3 = t_1/t_2, \\
&t_4 = x\, t_3,\ t_5 = x^3, \\
&\phi = t_4 + 0.05 t_5.
\end{aligned}
$$

By Proposition 2.15, the function $\sqrt{x+4}/(1+x^2)^2$ is G-concave. Thus, we have the following alternative decomposition for ϕ:

$$
\begin{aligned}
&t_1' = \sqrt{x+4}/(1+x^2)^2,\ t_2' = x\, t_1',\ t_3' = x^3, \\
&\phi = t_2' + 0.05 t_3'.
\end{aligned}
$$

The integrated relaxation exploits G-concavity of t_1'. The standard and integrated relaxations are compared in Figure 2.9. Clearly, the integrated relaxation is dominant.

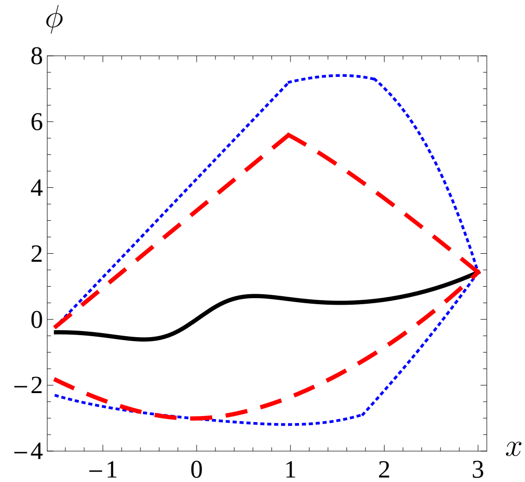


Figure 2.9: Comparison of the standard and integrated relaxations of $\phi = x\sqrt{x+4}/(1+x^2)^2 + 0.05x^3$, $x \in [-1.5, 3.0]$ in Example 2.8. The nonconvex function ϕ is shown in solid black, its standard relaxation $\tilde{\phi}^S$ in dotted blue, and the proposed relaxation $\tilde{\phi}^G$ in dashed red.

2.8 Conclusions

This study 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 standard one. Finally, 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 the 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 its effect on the convergence rate of branch-and-bound algorithms.

Chapter 3

Convex envelopes generated from finitely many compact convex sets

In this chapter, we consider the problem of constructing the convex envelope of a lsc function defined over a compact convex set. We formulate the envelope representation problem as a convex optimization problem for functions whose generating sets consist of finitely many compact convex sets. In particular, we consider nonnegative functions that are products of convex and component-wise concave functions and derive closed-form expressions for the convex envelopes of a wide class of such functions. Several examples demonstrate that these envelopes reduce significantly the relaxation gaps of widely used factorable relaxation techniques.

3.1 Introduction

By definition, the tightest convex outer-approximation of a nonconvex set is obtained using its convex hull relaxation. The formal representation of the convex hull of a general nonconvex set and the study of its dimensionality date back to the works of Minkowski [42] and Carathéodory [9], respectively. A detailed treatment of this concept can be found in [47] and more recent results in [48, 18, 6]. In the context of combinatorial optimization, there is an extensive literature on constructing the convex hulls for problems with special structures [43]. In particular, characterizing the convex hull of the union of polyhedral sets has been pursued under the name of disjunctive programming and successfully employed to address many discrete problems [3, 4]. These results have been further extended to construct the convex hull of disjunctions of convex sets [10] and build relaxations for convex MINLPs [56, 15, 13]. In the special case where all disjunctions belong to orthogonal linear subspaces, Tawarmalani *et al.* [59] provide an explicit characterization of the convex hull of the union of the disjunctions in the space of the original variables.

In the context of nonconvex NLPs, there has been a line of similar research to construct the convex and concave envelopes of nonconvex functions that appear frequently in nonconvex optimization problems. However, until recently, convexification results in this area were restricted to a few classes of functions with polyhedral convex or concave envelopes [46, 57]; these results address bilinear [1], trilinear [39], three-dimensional edge-concave functions [40], and multilinear functions [53, 5]. Tawarmalani *et al.* [60] considered supermodular functions with polyhedral concave envelopes and derived explicit representations for the concave envelope of such functions over hyperrectangles and a variety of polyhedral subdivisions of hyperrectangles.

Non-polyhedral convex envelopes were first systematically studied by Tawarmalani and Sahinidis [62], who derived an explicit representation for the convex envelope of x/y over a subset of the nonnegative orthant. In another study, Tawarmalani and Sahinidis [61] proposed a convex formulation for constructing the convex envelope of $f(x, y)$ over a box under the assumption that f is concave in $y \in \mathbb{R}$ and convex in $x \in \mathbb{R}^n$. Jach *et al.* [20] considered $(n-1)$-convex functions with indefinite Hessians over a box, and showed that the convex envelope of such functions can be obtained by solving a series of lower-dimensional optimization problems. The latter work also derived analytical descriptions for the convex envelopes of some bivariate functions in this category; namely, bivariate functions of the form $f = g(xy)$ over a nonnegative box, where g is an increasing convex function, and bivariate indefinite quadratic functions. Tawarmalani *et al.* [60] utilized the orthogonal disjunctions theory of [59] to derive the convex envelope for a function of the form $xg(y)$ over the unit hypercube, where $g(\cdot)$ is a monotone convex function. An explicit representation for the convex envelopes of functions whose convex combinations are *pairwise complementary* was provided by Tawarmalani [58]. Moreover, the author of [58] considered the problem of simultaneous convexification of a collection of functions and provided sufficient conditions under which individual convexification of functions leads to the simultaneous convexification of the collection.

In this chaper, we formulate as a convex NLP, the problem of constructing the convex envelope of a lsc function whose generating set is representable as the union of a finite number of compact convex sets. Our convexification argument is based on the concept of the perspective transformation, which has also been employed in [10, 56, 15, 13] to derive a convex formulation for the convex hull relaxation of disjunctive programs. Our development unifies all prior results in the convexification of functions with non-polyhedral envelopes and extends to many additional classes of functions that appear frequently in nonconvex NLPs and MINLPs. We focus on functions of the form $\phi = f(x)g(y)$, $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ over a box, where $f(x)$ is a nonnegative convex function and $g(y)$ is a nonnegative component-wise concave function. While our approach extends to more general functions, we restrict our study to the case when $f(x)$, $x \in \mathbb{R}^m$ has a power or an exponential form and derive explicit characterizations for the convex envelope of a wide class of such functions. These functions appear frequently in the widely used `GLOBALLib` [14] and `MINLPLib` [8] collections of global optimization test problems. Through several examples, we demonstrate that our convex envelopes reduce significantly the relaxation gap of standard factorable relaxations.

The remainder of the chapter is structured as follows. We first provide preliminary material on constructing the convex envelopes of lsc functions in Section 3.2. In Section 3.3, we study nonnegative functions that are products of convex and component-wise concave functions. In Section 3.4, we restrict attention to products of convex functions with univariate concave and bivariate component-wise concave functions. We derive algebraic expressions for the convex envelopes of various functions that are building blocks of nonconvex optimization problems. Finally, conclusions are offered in Section 3.5.

3.2 Preliminaries

In this section, we present some basic properties of the convex envelopes and derive a basic formulation that we will use in the remainder of the chapter. Throughout the chapter, $\phi(x)$ represents a lsc function defined over a compact convex set $\mathcal{C} \subset \mathbb{R}^n$. The relative interior of $\mathcal{C}$ will be denoted by $\mathrm{ri}(\mathcal{C})$, and the epigraph of ϕ over $\mathcal{C}$ will be denoted by $\mathrm{epi}_{\mathcal{C}}\phi$. The convex envelope of ϕ over $\mathcal{C}$, denoted by $\mathrm{conv}_{\mathcal{C}}\phi$, is defined as the greatest convex function majorized by ϕ over $\mathcal{C}$. When the domain is clear from the context, we may drop the subscript $\mathcal{C}$ from $\mathrm{conv}_{\mathcal{C}}\phi$. Similarly, the concave envelope of ϕ over $\mathcal{C}$ is the lowest concave function minorized by ϕ over $\mathcal{C}$.

3.2.1 A convex formulation for the envelope representation problem

A closed convex set is the convex hull of its extreme points and extreme directions (cf. Theorem 18.5 in [47]). It follows that the convex envelope of a lsc function ϕ over a compact convex set $\mathcal{C}$ can be fully characterized by the set of extreme points of the convex hull of $\text{epi}_{\mathcal{C}}\phi$. We will therefore refer to the projection of this set on $\mathcal{C}$ as the *generating set* of the convex envelope of ϕ over $\mathcal{C}$ and will denote it by $\mathcal{G}_{\mathcal{C}}\phi$. To construct $\text{conv}_{\mathcal{C}}\phi$, by Carathéodory's theorem (cf. Theorem 17.1 in [47]), one needs to consider only $n+1$ or fewer points in the generating set, even when $\mathcal{G}_{\mathcal{C}}\phi$ is infinite. Hence, the value of $\text{conv}_{\mathcal{C}}\phi$ at a point $x \in \mathcal{C}$ can be found by solving the following optimization problem (see [62] for details):

$$\begin{aligned} \text{conv}_{\mathcal{C}}\phi(x) = \min_{z^i,\lambda_i} \Bigg\{ & \sum_{i=1}^{n+1} \lambda_i \phi(z^i) : \sum_{i=1}^{n+1} \lambda_i z^i = x, \ \sum_{i=1}^{n+1} \lambda_i = 1, \\ & z^i \in \mathcal{G}_{\mathcal{C}}\phi, \ \lambda_i \geq 0, \ i = 1, \ldots, n+1 \Big\}, \end{aligned} \tag{3.1}$$

where z^i denotes a point in the generating set of $\text{conv}_{\mathcal{C}}\phi$ and λ_i is the corresponding convex multiplier. The multipliers, in general, depend on the value of the particular x and, as a result, $z^i \in \mathcal{G}_{\mathcal{C}}\phi$ represents a semi-infinite nonconvex constraint. A significant simplification for Problem (3.1) is possible when the generating set can be expressed as a union of a *finite* number of closed *convex* sets, *i.e.* when $\mathcal{G}_{\mathcal{C}}\phi = \cup_{i\in I}\mathcal{S}_i$, where $\mathcal{S}_i \subset \mathcal{C}$ denotes a nonempty closed convex set for all $i \in I = \{1, \ldots, p\}$. By convexity of $\mathcal{S}_i$, to evaluate $\text{conv}_{\mathcal{C}}\phi(x)$, it suffices to consider p points in the generating set, each belonging to a different $\mathcal{S}_i$ (cf. Theorem 3.3 in [47]). Therefore, for such functions, the envelope representation problem simplifies to:

$$\text{conv}_{\mathcal{C}}\phi(x) = \min_{z^i,\lambda_i} \left\{ \sum_{i\in I} \lambda_i \phi(z^i) : \sum_{i\in I} \lambda_i z^i = x, \sum_{i\in I} \lambda_i = 1, z^i \in \mathcal{S}_i, \lambda_i \geq 0, \forall i \in I \right\}. \tag{3.2}$$

While $\phi(x)$ is nonconvex over $\mathcal{C}$, the condition $z^i \in \mathcal{S}_i \subset \mathcal{G}_{\mathcal{C}}\phi$ implies that $\phi(z^i)$ is convex over $\mathcal{S}_i$. However, Problem (3.2) is highly nonconvex due to the products of the form $\lambda_i\phi(z^i)$ in the objective and $\lambda_i z^i$ in the constraint set. In the special case where $\mathcal{S}_i$ is a singleton for all $i \in I$; *i.e.* when $\text{conv}_{\mathcal{C}}\phi$ is a polyhedral function, z^i is no longer an optimization variable and Problem (3.2) simplifies to an LP (see [5, 60]). We will henceforth assume that there exists a subset $\mathcal{S}_i$, for some $i \in I$, that is not a singleton. We also note that, if $\mathcal{S}_i$ is a singleton for $i \in I' \subset I$, then z^i, $i \in I'$ is fixed.

Next, we show that, under very mild assumptions, Problem (3.2) can be reformulated as a convex optimization problem. To this end, let $\mathcal{S}_i = \{u \in \mathcal{C} : g_i(u) \leq 0\}$, for all $i \in I$, where $g_i : \mathbb{R}^n \to \mathbb{R}^{m_i}$ is a vector mapping whose components g_{ij}, $j = 1, \ldots, m_i$ are closed convex functions. After introducing $x^i = \lambda_i z^i$ for all $i \in I$ and substituting in (3.2), the value of $\mathrm{conv}_{\mathcal{C}}\phi(x)$ can be found by solving the following convex problem:

$$
\begin{aligned}
\text{(CX)} \qquad \min_{x^i, \lambda_i} \quad & \sum_{i \in I} \lambda_i \phi\left(x^i / \lambda_i\right) \\
\text{s.t.} \quad & \sum_{i \in I} x^i = x \\
& \sum_{i \in I} \lambda_i = 1 \\
& \lambda_i \geq 0, \ \forall i \in I \\
& \lambda_i g_{ij}\left(x^i / \lambda_i\right) \leq 0, \ j = 1, \ldots, m_i, \ i \in I.
\end{aligned}
$$

Recall that ϕ is convex when restricted to $\mathcal{S}_i$, $i \in I$. Convexity of the objective of CX follows from the fact that, given a convex function $\phi(x^i)$ and $\lambda_i > 0$, the perspective of ϕ defined as $\Phi(x^i, \lambda_i) = \lambda_i \phi(x^i/\lambda_i)$ is convex [18]. By compactness of $\mathcal{C}$, when $\lambda_i = 0$, we have $x^i = 0$ and it can be shown that $\Phi(0, 0) = 0$ (see Proposition 2.2.2 in [18]). Hence, the objective function of CX is closed and bounded. Similar arguments hold for the functions g_{ij} and the last set of inequality constraints of CX.

In the sequel, we assume that ϕ and g_{ij} for $i \in \{1, \ldots, p\}$, $j \in \{1, \ldots, m_i\}$, are twice continuously differentiable (C^2) functions. Under these assumptions, it is simple to check that, while convex and continuous, CX is not differentiable at the points where $\lambda_i = 0$ for some $i \in I$. Thus, for gradient-based convex NLP solvers, the numerical solution of CX is plagued with numerical difficulties over the regions where some of the multipliers are approaching zero. For some special functional forms, the perspective constraints can be recast as second order cone constraints [16], and Problem CX can be reformulated as a second order conic optimization problem. Several solution techniques involving barrier methods [10] and perturbing the perspective transformations [15] have been proposed in the literature to address the non-differentiability of the general problem numerically.

Another difficulty in solving CX numerically is that its size depends on the number p of convex components in the generating set. In turn, p, in the worst case, increases exponentially in the number of original variables (n). However, as we detail in the following sections, for certain cases, algebraic and geometric properties of the functions involved can be exploited to solve Problem CX analytically and derive a closed-form expression for the convex envelope (see also [61, 20]).

3.2.2 Identifying the generating set of the convex envelope

As it follows from the above discussion, identifying the generating set of a function is a crucial step toward building its envelope. The following result (Theorem 7 in [62]) provides an exclusion criterion to identify regions that do not belong to the generating set.

Proposition 3.1. [62] Let $\phi(x)$ be a lsc function on a compact convex set $\mathcal{C}$. Consider a point $x_0 \in \mathcal{C}$. Then, $x_0 \notin \mathcal{G}_{\mathcal{C}}\phi$ if and only if there exists a convex subset $\mathcal{X}$ of $\mathcal{C}$ such that $x_0 \in \mathcal{X}$ and $x_0 \notin \mathcal{G}_{\mathcal{X}}\phi$.

If the subset $\mathcal{X}$ is a face of $\mathcal{C}$, the converse of the above result is also true (cf. Proposition 2.3.7 in [18]). This, so-called "transmission of extremality" property, leads to the following corollary, which, in combination with Proposition 3.1, provides a powerful tool for characterizing the generating set of many functions of practical interest.

Corollary 3.1. Let $\mathcal{X}$ denote a nonempty face of $\mathcal{C}$ and let φ denote the restriction of ϕ to $\mathcal{X}$. Then the restriction of $\mathcal{G}_{\mathcal{C}}\phi$ to $\mathcal{X}$ is the generating set of φ over $\mathcal{X}$.

For instance, given a C^2 function ϕ defined over a compact convex set $\mathcal{C}$, if the Hessian of ϕ is not positive semidefinite at $x_0 \in \mathrm{ri}(\mathcal{C})$, then x_0 does not belong to $\mathcal{G}_{\mathcal{C}}\phi$. Now, consider the major assumption in the derivation of Problem CX, namely that the generating set of the convex envelope of the function of interest is the union of a finite number of compact convex sets. There are many functions that do not satisfy this assumption. As a simple example, consider $\phi = x^2y$ over $\mathcal{C} = \{(x, y) : 0.01 \leq x \leq 1,\ 0.1 \leq y \leq \sqrt{x}\}$. The generating set in this case is: $\mathcal{G}_{\mathcal{C}}\phi = \mathcal{S}_1 \cup \mathcal{S}_2$, where $\mathcal{S}_1 = \{(x, y) : 0.01 \leq x \leq 1,\ y = 0.1\}$ and $\mathcal{S}_2 = \{(x, y) : 0.01 \leq x \leq 1,\ y = \sqrt{x}\}$. Obviously, $\mathcal{S}_2$ cannot be written as a union of finitely many convex sets. However, there also exists a multitude of functions of practical interest whose generating sets are amenable to such a representation. Some examples include:

1. Component-wise convex functions of the form $\phi = \prod_{i=1}^{n} f_i(x_i)$, $x_i \in \mathbb{R}^{m_i}$, over a box, where $f_i(x_i)$ is a nonnegative convex function and the Hessian of ϕ restricted to any face of the domain where two or more x_i are not fixed is indefinite:

   – $\phi = x_1^a x_2^b$, where $(a, b) \in \{\{(1, +\infty)^2\} \cup \{(-\infty, 0) \times (1, +\infty) : a + b < 1\}\}$, $x_1, x_2 \in \mathbb{R}$, $\phi \geq 0$;

   – $\phi = a^{x_1} x_2^b$, where $a > 0$, $b > 1$, $x_1, x_2 \in \mathbb{R}$, $x_2^b \geq 0$;

   – $\phi = \exp(x_1 x_2)$, where $x_1, x_2 \in \mathbb{R}$.

2. Products of nonnegative convex and component-wise concave functions, *i.e.* functions of the form $\phi = f(x)g(y)$, where $f(x)$ is nonnegative convex in $[\underline{x}, \bar{x}] \subset \mathbb{R}^m$ and $g(y)$ is component-wise concave in $[\underline{y}, \bar{y}] \subset \mathbb{R}^n$:

   – $\phi = x^a y^b$, where $a \in \{(-\infty, 0) \cup (1, \infty)\}$, $b \in (0, 1]$, $x^a \geq 0$;

   – $\phi = y\sqrt{1 + x^2}$, $\phi = ya^x$, $\phi = y/(x_1 x_2)$, where $a > 0$, $x, y \in \mathbb{R}$, $x_1, x_2 > 0$;

   – $\phi = y_1 y_2 / x$, $\phi = (y_1 + y_2)/x$, where $y_1, y_2 \in \mathbb{R}$, $x > 0$;

   – $\phi = x^2 y_1 y_2$, $\phi = x^2(y_1 + y_2)$, $\phi = y_1 y_2 \exp(-x)$, where $x, y_1, y_2 \in \mathbb{R}$.

3. Quasi-concave functions defined over a box (it follows from the definition of quasi-concave functions that they are not locally convex at any point in the interior of their domain and, as a result, this interior does not belong to the generating set):

   – $\phi = y/(1 + x_1^2)$, $1/(1 + x_1^2 + x_2^2)$, where $y \geq 0$, $x_1, x_2 \in \mathbb{R}$;

   – $\phi = \exp(x_1/x_2)$, where $x_1 \in \mathbb{R}$, $x_2 > 0$;

   – $\phi = 1/(x_1^2 + x_2^2 + x_3^2)^a$, where $a > 0$, $x_1, x_2, x_3 \in \mathbb{R}$, $x_1^2 + x_2^2 + x_3^2 > 0$.

Collectively, these three classes of functions constitute roughly 60% of the primitive functions appearing in the `GLOBALLib` [14] and `MINLPLib` [8] test problems. Class 2 functions, in particular, outnumber all others, since they constitute roughly 45% of the nonconvex functions in these two libraries. As these problems originate from diverse applications across science and engineering, this observation makes a strong argument for reducing the complexity of Problem CX for these functional classes and incorporating the results of this analysis in global optimization software technology. Below, we focus on functions in Class 2.

3.3 Products of nonnegative convex and component-wise concave functions

Consider the C^2 function $\phi = f(x)g(y)$, $x \in \mathcal{H}_x^m = [\underline{x}, \bar{x}] \subset \mathbb{R}^m$, $y \in \mathcal{H}_y^n = [\underline{y}, \bar{y}] \subset \mathbb{R}^n$. Define $\mathcal{C} = \mathcal{H}_x^m \times \mathcal{H}_y^n$. Let $f(x)$ be a convex function, and let $g(y)$ be a component-wise concave function; *i.e.* $g(y)$ is concave in y_k, $k = 1, \dots n$ when all $y_{k'}$, $k' \neq k$ are fixed to some arbitrary values in their domain. Further, assume that both $f(x)$ and $g(y)$ are nonnegative over $\mathcal{H}_x^m$ and $\mathcal{H}_y^n$, respectively. If $f(x)$ is affine, then by Proposition 3.1, we have $\mathcal{G}_{\mathcal{C}}\phi = \text{vert}(\mathcal{C})$, which in turn implies that $\text{conv}_{\mathcal{C}}\phi$ is polyhedral. We will henceforth assume that $f(x)$ is not affine. However, our analysis addresses the case where $g(y)$ is affine, or is affine with respect to a subset of its variables. Under these assumptions, it is easy to show that $\phi(x, y)$ is not strictly convex over any neighborhood in the interior of $\mathcal{C}$ and in the relative interior of any proper face of $\mathcal{C}$ for which all y variables are not fixed. Denote by $\hat{y}_i$, $i \in I = \{1, \dots, 2^n\}$ the vertices of $\mathcal{H}_y^n$. By Proposition 3.1 and Corollary 3.1, $\mathcal{G}_{\mathcal{C}}\phi$ is a subset of 2^n m-dimensional boxes:

$$\mathcal{G}_{\mathcal{C}}\phi \subseteq \{(x, \hat{y}_i), x \in \mathcal{H}_x^m, \forall i \in I\}.$$

Since, by assumption, $\phi(x, y)$ is continuously differentiable over $\mathcal{C}$, the above inclusion is strict when (i) $g(\hat{y}_i) = 0$ for some $i \in I$ or (ii) $f(x)$ is affine with respect to a subset of its variables. For example, if $\phi = x^2(1 - y^2)$, $0 \leq x \leq 1$, $-1 \leq y \leq 0.5$, then $\mathcal{G}_{\mathcal{C}}\phi = \{(0, -1) \cup (1, -1) \cup \{(x, 0.5), 0 \leq x \leq 1\}\}$. Thus, at a given $(x, y) \in \mathcal{C}$, the value of $\text{conv}_{\mathcal{C}}\phi(x, y)$ can be found by solving the following variant of CX:

$$
\begin{aligned}
\text{(CX1)} \qquad \min_{x^i,\lambda_i} \quad & \sum_{i\in I} \lambda_i f\left(x^i/\lambda_i\right) g(\hat{y}_i) \\
\text{s.t.} \quad & \sum_{i\in I} \lambda_i \hat{y}_i = y \\
& \sum_{i\in I} x^i = x && (3.3) \\
& \sum_{i\in I} \lambda_i = 1 && (3.4) \\
& \lambda_i \underline{x} \le x^i \le \lambda_i \bar{x}, \ \forall i \in I && (3.5) \\
& \lambda_i \ge 0, \ \forall i \in I,
\end{aligned}
$$

where the variables are x^i_j, $j = 1, \dots, m$ and λ_i for all $i \in I$, for a total of $(m+1)2^n$ variables. For a univariate $g(y)$, the multipliers vary linearly with the y variables and CX1 reduces to a convex problem with $2m$ variables (see [61]). Thus, in the following we assume $n \ge 2$. As noted in [61], the procedure for constructing the convex envelope of ϕ for a univariate concave $g(y)$ can be generalized to a multivariate (component-wise) concave $g(y)$ by convexifying the function sequentially, one y variable at a time. Sequential convexification would lead to a rapid growth of the number and complexity of the intermediate optimization problems to be solved, which makes it difficult to use even for simple functional forms. This growth can be avoided with the proposed approach. For the nonnegative convex $f(x)$, $x \in \mathcal{H}^m_x$, we study the following functional forms:

(i) $f(x) = (c^T x + d)^a$, $a \in \mathbb{R} \setminus \{[0,1]\}$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$,

(ii) $f(x) = a^{(c^T x + d)}$, $a > 0$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$.

The above expressions for $f(x)$ cover a large number of the Class 2 functions that appear in nonconvex problems. Furthermore, as we will detail later, they enjoy certain separability properties that are key to the derivation of the convex envelope of the corresponding function ϕ. Now, consider the component-wise concave $g(y)$, $y \in \mathcal{H}^n_y$. Denote by Λ' the set of optimal multipliers in the description of conv$g(y)$ over $\mathcal{H}^n_y$. As we will prove in Theorems 3.1 and 3.3, if the restriction of $g(y)$ to vert$(\mathcal{H}^n_y)$ is a submodular function that is nondecreasing (or nonincreasing) in every argument, then there exists $\Lambda^* \subseteq \Lambda'$ that is also optimal for the envelope representation problem of $\phi = f(x)g(y)$ over $\mathcal{C}$. Next, we review some basic properties of submodular functions that we will use in the remainder of the chapter. Recall that a real valued function $g(y)$ on a lattice $\mathcal{X}$ is said to be *submodular* if

$$g(y \wedge y') + g(y \vee y') \leq g(y) + g(y'), \quad \forall\, y, y' \in \mathcal{X}, \tag{3.6}$$

where $y \vee y'$ denotes the component-wise maximum and $y \wedge y'$ denotes the component-wise minimum of y and y' (see chapter 2 of [65] for an exposition). Similarly, $g(y)$ is said to be *supermodular*, if $g(y \wedge y') + g(y \vee y') \geq g(y) + g(y')$ for all $y, y' \in \mathcal{X}$. If $g(y)$ is both submodular and supermodular, then it is called *modular*. It can be shown that $g(y)$ is modular on $\mathcal{X} = \mathcal{X}_1 \times \ldots \times \mathcal{X}_n$, where $\mathcal{X}_k$ is a chain for all $k = 1, \ldots, n$, if and only if it is separable (Theorem 2.6.4 in [65]). For instance, if $\mathcal{X} = \mathbb{R}^n$, then $g(y) = \sum_{k=1}^{n} g_k(y_k)$, $y_k \in \mathbb{R}$. The following lemma provides sufficient conditions for the submodularity (supermodularity) of composite functions.

Lemma 3.1. ([65]) Let $g(y)$ be nondecreasing (or nonincreasing) over the lattice $\mathcal{X}$ and let $h(\cdot)$ be defined over an interval Z that contains the range of $g(y)$. Define the composite function $\psi = h(g(y))$. We have the following cases:

(i) if g is submodular over $\mathcal{X}$ and h is concave and nondecreasing over Z, then ψ is submodular over $\mathcal{X}$,

(ii) if g is supermodular over $\mathcal{X}$ and h is convex and nondecreasing over Z, then ψ is supermodular over $\mathcal{X}$.

In both parts of Lemma 3.1, if $g(y)$ is modular, then no monotonicity assumption on h is required. For example, consider $\psi(y) = h(\sum_{k=1}^{n} g_k(y_k))$, $y_k \in [\underline{y}_k, \bar{y}_k] \subset \mathbb{R}$, where $g_k(\bar{y}_k) - g_k(\underline{y}_k) \geq 0$ for all $k = 1, \ldots n$ (or $g_k(\bar{y}_k) - g_k(\underline{y}_k) \leq 0$ for all k). It follows from Lemma 3.1 that (i) if $h(\cdot)$ is concave, then $\psi(y)$, $y \in \mathrm{vert}(\mathcal{H}_y^n)$ is submodular and (ii) if $h(\cdot)$ is convex, then $\psi(y)$, $y \in \mathrm{vert}(\mathcal{H}_y^n)$ is supermodular. If $g(y)$ is a C^2 function and $\mathcal{X}$ is a subset of $\mathbb{R}^n$, then submodularity can be characterized as follows:

Lemma 3.2. ([65]) Suppose that $g(y)$ is twice continuously differentiable on $\mathcal{H}_y^n$. Then $g(y)$ is submodular (resp. supermodular) if and only if $\partial^2 g(y)/\partial y_i \partial y_j \leq 0$ (resp. ≥ 0), for all $y_i, y_j \in \mathcal{H}_y^n$ with $i \neq j$.

Obviously, if $g(y)$ is submodular over $\mathcal{H}_y^n$, then it is submodular over $\mathrm{vert}(\mathcal{H}_y^n)$, since the latter is a sublattice of the former.

Now, consider the component-wise concave $g(y)$, $y \in \mathcal{H}_y^n$. As discussed earlier, in this case we have $\mathcal{G}_{\mathcal{H}_y^n} g(y) = \mathrm{vert}(\mathcal{H}_y^n)$ and thus Problem (3.1) simplifies to the LP:

$$
\text{(CCV)} \qquad \begin{array}{ll} \min\limits_{\lambda_i} & \sum_{i \in I} \lambda_i g(\hat{y}_i) \\ \text{s.t.} & \left.\begin{array}{l} \sum_{i \in I} \lambda_i \hat{y}_i = y \\ \sum_{i \in I} \lambda_i = 1 \\ \lambda_i \geq 0, \ \forall i \in I. \end{array}\right\} \end{array} \tag{3.7}
$$

Let $\lambda' = \{\lambda'_i, \ i \in I\}$ denote a basic feasible solution of the above problem. Denote by V the index set of nonzero multipliers in λ'. Define b_{ik}, for all $i \in V$ and $k \in I \setminus V$, such that $\sum_{i \in V} b_{ik} = 1$ and $\sum_{i \in V} b_{ik} \hat{y}_i = \hat{y}_k$, for all $k \in I \setminus V$. Note that, for any $k \in I \setminus V$, the associated system of equations always has a unique solution since $\hat{y}_i$, $i \in V$ correspond to $n+1$ affinely independent vertices of $\mathcal{H}_y^n$. Then, from the optimality conditions for LPs, it follows that λ' is optimal for CCV if and only if

$$
\sum_{i \in V} b_{ik} g(\hat{y}_i) - g(\hat{y}_k) \leq 0, \quad \forall k \in I \setminus V. \tag{3.8}
$$

Now, suppose that $g(y)$ is submodular over the vertices of $\mathcal{H}_y^n$. As was shown in [60], the convex envelope of $g(y)$ in this case is given by its Lovász extension (see [33]). More precisely, we have the following result:

Proposition 3.2. (Theorem 3.3 in [60]) The convex (resp. concave) envelope of $g(y)$ over $\mathcal{H}_y^n$ is given by its Lovász extension if and only if (i) $g(y)$ is submodular (resp. supermodular) over $\mathrm{vert}(\mathcal{H}_y^n)$ and (ii) $\mathcal{G}_{\mathcal{H}_y^n} g(y) = \mathrm{vert}(\mathcal{H}_y^n)$.

Consequently, if the component-wise concave $g(y)$ is submodular over $\mathrm{vert}(\mathcal{H}_y^n)$, then an optimal solution for Problem (3.7) can be determined a priori, as follows. Let e^k denote the kth unit vector in $\mathbb{R}^n$. Given any $y \in \mathcal{H}_y^n$, let $\tilde{y}_k = (y_k - \underline{y}_k)/(\bar{y}_k - \underline{y}_k)$, $k \in \{1, \ldots, n\}$. Denote by π a permutation of $\{1, \ldots, n\}$ such that $\tilde{y}_{\pi(1)} \geq \tilde{y}_{\pi(2)} \geq ... \geq \tilde{y}_{\pi(n)}$. The region defined by this set of inequalities is a simplex $\Delta_\pi \subset \mathcal{H}_y^n$, whose vertices correspond to the vertices of $\mathcal{H}_y^n$ with nonzero optimal multipliers in (4.2). The set of these $n!$ simplices obtained from different permutations of $\{1, \ldots, n\}$ forms Kuhn's triangulation of $\mathcal{H}_y^n$. The vertices of Δ_π are: $\mathrm{vert}(\Delta_\pi) = \{\nu_j : \nu_j = \underline{y} + (\bar{y} - \underline{y}) \sum_{k=1}^{j-1} e^{\pi(k)}, \ j = 1, \ldots n+1\}$. Since, by construction, $y \in \Delta_\pi$, one can express y as a convex combination of $\mathrm{vert}(\Delta_\pi)$ as follows: $y = (1-\tilde{y}_{\pi(1)})\nu_1 + \sum_{j=2}^{n} (\tilde{y}_{\pi(j-1)} - \tilde{y}_{\pi(j)})\nu_j + \tilde{y}_{\pi(n)}\nu_{n+1}$. Thus, the nonzero optimal multipliers associated with $\mathrm{vert}(\Delta_\pi)$ are given by: $\tilde{\lambda}_1 = 1-\tilde{y}_{\pi(1)},\ \tilde{\lambda}_j = \tilde{y}_{\pi(j-1)} - \tilde{y}_{\pi(j)},\ j = 2,\ldots,n,\ \tilde{\lambda}_{n+1} = \tilde{y}_{\pi(n)}$. Let $\mathcal{I} = \{i \in I : \hat{y}_i = \nu_j,$ for some $j \in \{1,\ldots,n+1\}\}$ and, for each $i \in \mathcal{I}$, let $q(i)$ be equal to a j such that $\hat{y}_i = \nu_j$. Define λ^* as follows:

$$\lambda_i^* = \begin{cases} \tilde{\lambda}_{q(i)}, & \text{if } i \in \tilde{I}, \\ 0, & \text{otherwise.} \end{cases} \tag{3.9}$$

By Proposition 3.2 and relation (3.6), to check the optimality of λ^* for Problem (3.7), condition (3.8) simplifies to:

$$\delta(g) = g(\hat{y}_{i_1}) - g(\hat{y}_{i_2}) - g(\hat{y}_{i_3}) + g(\hat{y}_{i_4}) \leq 0, \quad \forall i_2, i_3 \in I, \tag{3.10}$$

where $\hat{y}_{i_1} = \hat{y}_{i_2} \wedge \hat{y}_{i_3}$, and $\hat{y}_{i_4} = \hat{y}_{i_2} \vee \hat{y}_{i_3}$. Let $\Omega(\lambda, g(\hat{y}))$ denote a differentiable function that is convex with respect to λ_i, $i \in I$. Consider an optimization problem of the following form:

$$\text{(GCV)} \qquad \begin{array}{ll} \min\limits_{\lambda_i} & \Omega(\lambda, g(\hat{y})) \\ \text{s.t.} & \text{Constraints (3.7).} \end{array}$$

Now, we examine the conditions under which the set λ^* given by (3.9), is optimal for the above problem. Since GCV is convex and differentiable, it suffices to show that λ^* satisfies the KKT conditions for this problem. Consider the set λ' defined in accordance with the optimality conditions (3.8). Since the feasible regions of CCV and GCV are identical, λ' is feasible for Problem GCV. Let $\gamma_i(\lambda, g(\hat{y}))$ denote the partial derivative of $\Omega(\lambda, g(\hat{y}))$ with respect to λ_i for all $i \in I$. It follows that λ' satisfies the KKT conditions for GCV if and only if:

$$\sum_{i \in V} b_{ik}\gamma_i(\lambda', g(\hat{y})) - \gamma_k(\lambda', g(\hat{y})) \leq 0, \quad \forall k \in I \setminus V, \tag{3.11}$$

where, as before, V denotes the index set of nonzero multipliers in λ' and b_{ik} is as defined in (3.8). Define the function $\gamma(g(\hat{y})) : \mathrm{vert}(\mathcal{H}_y^n) \to \mathbb{R}$, where $\gamma(g(\hat{y})) = \gamma_i(\lambda^*, g(\hat{y}))$ for all $\hat{y}_i \in \mathrm{vert}(\mathcal{H}_y^n)$. By (3.8), (3.10) and (3.11), the set λ^* is optimal for Problem GCV if and only if γ is submodular over $\text{vert}(\mathcal{H}_y^n)$, *i.e.*

$$\delta(\gamma(g(\hat{y}))) = \gamma(g(\hat{y}_{i_1})) - \gamma(g(\hat{y}_{i_2})) - \gamma(g(\hat{y}_{i_3})) + \gamma(g(\hat{y}_{i_4})) \leq 0, \quad \forall i_2, i_3 \in I, \tag{3.12}$$

where $\hat{y}_{i_1} = \hat{y}_{i_2} \wedge \hat{y}_{i_3}$ and $\hat{y}_{i_4} = \hat{y}_{i_2} \vee \hat{y}_{i_3}$. The above condition is key to the proof of following theorems. Next, we derive some relations that we will use to simplify the presentation in the following proofs. Define

$$\varphi_r(x) = \int_1^x v^{r-1} \mathrm{d}v = (x^r - 1)/r, \quad x > 0, \ r \in \mathbb{R} \setminus \{0\}. \tag{3.13}$$

It follows that $\lim_{r \to 0} \varphi_r(x) = \log x$. For notational simplicity, in the following, we denote $\lim_{r \to 0} \varphi_r(\cdot)$, by $\varphi_0(\cdot)$. Since $\varphi_r(x)$, $r \in (-\infty, 1)$ is an increasing function of r, we have:

$$\varphi_r(x) \leq x - 1, \quad r \in (-\infty, 1). \tag{3.14}$$

Define $\varphi_r(x, y) = \varphi_r(x) - \varphi_r(y)$, $r \in (-\infty, 1)$, $x, y > 0$. It is simple to show that

$$\varphi_r(x, y) \leq x - y, \ \forall \ (x, y) \in \{(0, 1]^2 : x \leq y\} \cup \{[1, \infty)^2 : y \leq x\}. \tag{3.15}$$

We are now in a position to prove the main results of this section. We consider the cases where $f(x)$ has power and exponential forms in turn.

Theorem 3.1. Let $f(x)$, $x \in \mathcal{H}_x^m$ be a nonnegative convex function of the form $f(x) = (c^T x + d)^a$, $a \in \mathbb{R} \setminus \{[0, 1]\}$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$ and, let $g(y)$, $y \in \mathcal{H}_y^n$ be a nonnegative component-wise concave function such that its restriction to the vertices of $\mathcal{H}_y^n$ is submodular and nondecreasing (or nonincreasing) in every argument. Then, for any (x, y) in the domain of $\phi = f(x)g(y)$, there exists an optimal solution of CX1 with at most $n + 1$ nonzero multipliers. Further, the values of these optimal multipliers are independent of the x variables and are given by (3.9).

Proof. We start by partially minimizing Problem CX1 with respect to x^i, $i \in I$. Let $\underline{x}_j < x_j < \bar{x}_j$ for all $j \in J = \{1, \ldots, m\}$. This assumption is without loss of generality since, for example, if $x_j = \underline{x}_j$ for some $j \in J$, then $x_j^i = \lambda_i \underline{x}_j$ for all $i \in I$. Thus, we can eliminate x_j^i, $i \in I$ from CX1 by updating $d = d + c_j \underline{x}_j$, $J = J \setminus \{j\}$. Furthermore, by nonnegativity of $f(x)$, if $x_j = \underline{x}_j$ or $x_j = \bar{x}_j$ for all $j \in J$, then CX1 reduces to the envelope representation problem for $g(y)$, which implies the optimality of λ^* given by (3.9). Let g_i, $i \in I$, denote the value of $g(y)$ at the vertices of $\mathcal{H}_y^n$ such that (i) if $a < 0$, then $g_1 \leq g_2 \leq \ldots \leq g_{2^n}$ and, (ii) if $a > 1$, then $g_1 \geq g_2 \geq \ldots \geq g_{2^n}$. In each case, we also rearrange $\hat{y}_i$, $i \in I$ accordingly. First, suppose that all multipliers are nonzero, $g_i > 0$ for all $i \in I$, and the inequalities given by (3.5) are inactive. Writing the KKT conditions for CX1 with respect to x^i, $i \in I$ yields:

$$\left(c^T x^i/\lambda_i + d\right)^{a-1} g_i = \left(c^T x^k/\lambda_k + d\right)^{a-1} g_k, \ \forall i, k \in I.$$

Substituting for $c^T x^i/\lambda_i + d$, $i \in I$ in the following surrogate of (3.3):

$$\sum_{i \in I} c^T x^i + d\lambda_i = c^T x + d, \tag{3.16}$$

we obtain

$$c^T x^i/\lambda_i + d = \frac{g_i^r}{\sum_{k \in I} \lambda_k g_k^r} \left(c^T x + d\right), \ \forall i \in I, \tag{3.17}$$

where $r = 1/(1-a)$. Let $l_j = \underline{x}_j$, $u_j = \bar{x}_j$, if $c_j > 0$, and $l_j = \bar{x}_j$, $u_j = \underline{x}_j$, if $c_j < 0$ for all $j \in J$. For notational simplicity, let $l = \sum_{j \in J} c_j l_j + d$, and $u = \sum_{j \in J} c_j u_j + d$. From (3.17) it follows that, if the inequality

$$\lambda_i l \leq c^T x^i + d\lambda_i \leq \lambda_i u, \tag{3.18}$$

is inactive for some $i \in I$, then there exists an optimal solution of Problem CX1, such that the corresponding inequalities in (3.5) are inactive. Conversely, if $c^T x^i + d\lambda_i \leq \lambda_i l$ (resp. $\geq \lambda_i u$) for some $i \in I$, then the only feasible solution for CX1 is $x_j^i = \lambda_i l_j$ (resp. $= \lambda_i u_j$) for all $j \in J$. Hence, instead of inequalities (3.5), we can equivalently study the bounds given by (3.18). Now suppose that $0 \leq l < u$. From (3.17), it follows that $c^T x^1/\lambda_1 \leq \ldots \leq c^T x^{2^n}/\lambda_{2^n}$. Partition I as $I = I_1 \cup I_2 \cup I_3$, where I_1 and I_3 denote the sets of indices whose corresponding $c^T x^i + d\lambda_i$ in (3.18) are at their lower and upper bounds, respectively. Suppose $I_2 \neq \emptyset$. As we will discuss later, this assumption is without loss of generality. Thus, let $I_1 = \{1, \ldots, s-1\}$, $I_2 = \{s, \ldots, t\}$ and, $I_3 = \{t+1, \ldots, 2^n\}$. For consistency, if $s = 1$, then we set $I_1 = \emptyset$ with $g_{s-1} = 0$, if $a < 0$ and $g_{s-1} = +\infty$, if $a > 1$. Similarly, if $t = 2^n$, then we set $I_3 = \emptyset$ with $g_{t+1} = +\infty$, if $a < 0$ and $g_{t+1} = 0$, if $a > 1$. Substituting $c^T x^i + d\lambda_i = \lambda_i l$ for all $i \in I_1$ and $c^T x^i + d\lambda_i = \lambda_i u$ for all $i \in I_3$ in CX1, and minimizing the resulting problem with respect to x^i, $i \in I_2$, yields:

$$c^T x^i/\lambda_i + d = \frac{g_i^r}{\sum_{k\in I_2}\lambda_k g_k^r}\left(c^T x + d - l\sum_{k\in I_1}\lambda_k - u\sum_{k\in I_3}\lambda_k\right), \ \forall i \in I_2. \tag{3.19}$$

From (3.18) and (3.19), it follows that:

$$c^T x + d \geq l\sum_{i\in I_1}\lambda_i + \max\left\{l/g_s^r,\ u/g_{t+1}^r\right\}\sum_{i\in I_2}\lambda_i g_i^r + u\sum_{i\in I_3}\lambda_i, \tag{3.20}$$

and

$$c^T x + d \leq l\sum_{i\in I_1}\lambda_i + \min\left\{l/g_{s-1}^r,\ u/g_t^r\right\}\sum_{i\in I_2}\lambda_i g_i^r + u\sum_{i\in I_3}\lambda_i, \tag{3.21}$$

where the lower bounds in (3.20) are obtained from the conditions $c^T x^s + d\lambda_s \geq \lambda_s l$ and $c^T x^{t+1} + d\lambda_{t+1} \geq \lambda_{t+1} u$, and the upper bounds in (3.21) follow from $c^T x^{s-1} + d\lambda_{s-1} \leq \lambda_{s-1} l$ and $c^T x^t + d\lambda_t \leq \lambda_t u$. Note that these inequalities are implied by the definitions of the index sets I_1, I_2, and I_3. For the above bounds to be consistent, the following should hold:

$$\left(g_t/g_s\right)^r \leq u/l \leq \left(g_{t+1}/g_{s-1}\right)^r. \tag{3.22}$$

Substituting (3.19) in Problem CX1, yields

$$\left.\begin{array}{ll}\min\limits_{\lambda_i} & l^a\sum_{i\in I_1}\lambda_i g_i + \left(c^T x + d - l\sum_{i\in I_1}\lambda_i - u\sum_{i\in I_3}\lambda_i\right)^a\left(\sum_{i\in I_2}\lambda_i g_i^r\right)^{1/r} \\ & +u^a\sum_{i\in I_3}\lambda_i g_i \\ \text{s.t.} & \text{Constraints (3.7).}\end{array}\right\} \tag{3.23}$$

We next show that λ^* given by (3.9) is optimal for Problem (3.23). It is simple to check that (3.23) is a special case of Problem GCV. Thus, to show the optimality of λ^*, it suffices to show that condition (3.12) is valid. First, let $I = I_2$. In this case, the objective function of (3.23) simplifies to $\Omega = f(x)(\sum_{i\in I}\lambda_i g_i^r)^{1/r}$. Obviously, given a submodular function ψ on a lattice $\mathcal{X}$, the function $\alpha\psi + \beta$, where $\alpha > 0$, $\beta \in \mathbb{R}$ is submodular on $\mathcal{X}$ as well. It follows that λ^* is optimal if and only if the function $\varphi_r(g(y))$, $r \in (-\infty, 0) \cup (0, 1)$, given by (3.13), is submodular over the vertices of $\mathcal{H}_y^n$. If $r \in (-\infty, 1)$, then $\varphi_r(u)$, $u > 0$ is concave and increasing in u. Further, by assumption, the restriction of $g(y)$ to $\text{vert}(\mathcal{H}_y^n)$ is submodular and component-wise nondecreasing (or nonincreasing). Hence, by Lemma 3.1, $\varphi_r(g(y))$, $r \in (-\infty, 0) \cup (0, 1)$ is submodular over $\mathrm{vert}(\mathcal{H}_y^n)$. Next, suppose that (i) I_1 or I_3 and (ii) I_2 are nonempty. Assumption (ii) is without loss of generality. To see this, consider a partitioning $\mathcal{I}$ of set I as $I = I_1 \cup I_3$, with $I_1 = \{1, \ldots, i'\}$ and $I_3 = \{i'+1, \ldots 2^n\}$ which corresponds to $c^T x + d = l \sum_{i \in I_1} \lambda_i + u \sum_{i \in I_3} \lambda_i$. It is simple to see that $\mathcal{I}$ is the limiting case between the two partitions (i) $I_1 = \{1, \ldots, i'\}$, $I_2 = \{i'+1\}$, $I_3 = \{i'+2, \ldots, 2^n\}$ and (ii) $I_1 = \{1, \ldots i'-1\}$, $I_2 = \{i'\}$, $I_3 = \{i'+1, \ldots, 2^n\}$. For the latter two partitions, we will demonstrate next that λ^* is optimal. Thus, by continuity of $\mathrm{conv}\phi$ over $\mathcal{C}$ (see Theorem 10.2 in [47]), λ^* is optimal for $\mathcal{I}$. Define

$$w_\lambda = \left(cx + d - l \sum_{i \in I_1} \lambda_i - u \sum_{i \in I_3} \lambda_i \right) / \left(\sum_{i \in I_2} \lambda_i g_i^r \right).$$

By (3.20) and (3.21), we have the following bounds on w_λ:

$$\max\left\{ l/g_s^r,\ u/g_{t+1}^r \right\} \leq w_\lambda \leq \min\left\{ l/g_{s-1}^r,\ u/g_t^r \right\}. \tag{3.24}$$

By (3.12), the set λ^* satisfies the KKT conditions for Problem (3.23) if and only if

$$\delta(\gamma(g)) = \gamma(g_{i_1}) - \gamma(g_{i_2}) - \gamma(g_{i_3}) + \gamma(g_{i_4}) \leq 0, \quad \forall i_2, i_3 \in I, \tag{3.25}$$

where $\hat{y}_{i_1} = \hat{y}_{i_2} \wedge \hat{y}_{i_3}$, $\hat{y}_{i_4} = \hat{y}_{i_2} \vee \hat{y}_{i_3}$, and $\gamma(g_i)$ denotes the partial derivative of the objective function of (3.23) with respect to λ_i at $\lambda = \lambda^*$, which is given by:

$$\gamma(g_i) = \begin{cases} l^a g_i - alw_{\lambda^*}^{a-1}, & \text{if } i \in I_1 \\ g_i^r w_{\lambda^*}^a / r, & \text{if } i \in I_2 \\ u^a g_i - auw_{\lambda^*}^{a-1}, & \text{if } i \in I_3. \end{cases} \tag{3.26}$$

Since, by assumption, the restriction of $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^n)$ is component-wise nondecreasing (or nonincreasing), without loss of generality, we assume (i) if $a < 0$, then $g_{i_1} \leq g_{i_2} \leq g_{i_3} \leq g_{i_4}$ and (ii) if $a > 1$, then $g_{i_1} \geq g_{i_2} \geq g_{i_3} \geq g_{i_4}$. Next, we consider all feasible combinations of bounds for Problem (3.23) and demonstrate in each case that

$$\text{(N)} \qquad \delta(g) \leq 0 \quad \Longrightarrow \quad \delta(\gamma(g)) \leq 0.$$

In the following, $\underline{w}$ and $\bar{w}$ denote a lower and an upper bound on w_{λ^*}, respectively, obtained from (3.24). By monotonicity of $c^T x_i/\lambda_i$, $i \in I$, the following cases arise:

I. $\{i_1, i_2, i_3\} \subseteq I_1$, $\{i_4\} \subseteq I_2$. Then, $\underline{w} = l/g_{i_4}^r$ and $\bar{w} = \min\{l/g_{i_3}^r,\ u/g_{i_4}^r\}$. In this case, $\delta(\gamma(g))$ is decreasing in w_{λ^*} and is given by:

$$\delta(\gamma(g)) = l^a(g_{i_1} - g_{i_2} - g_{i_3}) + alw_{\lambda^*}^{a-1} + g_{i_4}^r w_{\lambda^*}^a/r. \tag{3.27}$$

It suffices to show that the maximum of $\delta(\gamma(g))$ is non-positive. Substituting $w_{\lambda^*} = \underline{w}$ in (3.27), gives $\delta(g) \leq 0$. Thus, relation (N) holds. By symmetry, (N) is valid for $\{i_1\} \subseteq I_2$, $\{i_2, i_3, i_4\} \subseteq I_3$.

II. $\{i_1, i_2\} \subseteq I_1$, $\{i_3, i_4\} \subseteq I_2$. Then, $\underline{w} = l/g_{i_3}^r$ and $\bar{w} = \min\{l/g_{i_2}^r, u/g_{i_4}^r\}$. Again, $\delta(\gamma(g))$ is a decreasing function of w_{λ^*} and is given by:

$$\delta(\gamma(g)) = l^a\left(g_{i_1} - g_{i_2}\right) + \left(g_{i_4}^r - g_{i_3}^r\right) w_{\lambda^*}^a/r. \tag{3.28}$$

Substituting $w_{\lambda^*} = \underline{w}$ in $\delta(\gamma(g))$ and using $g_{i_1} - g_{i_2} \leq g_{i_3} - g_{i_4}$, yields

$$\varphi_r\left(g_{i_4}/g_{i_3}\right) \leq \left(g_{i_4}/g_{i_3}\right) - 1, \tag{3.29}$$

which follows from (3.14). By symmetry, (N) holds for $\{i_1, i_2\} \subseteq I_2$, $\{i_3, i_4\} \subseteq I_3$.

III. $\{i_1\} \subseteq I_1$, $\{i_2, i_3, i_4\} \subseteq I_2$. Then, $\underline{w} = l/g_{i_2}^r$ and $\bar{w} = \min\{l/g_{i_1}^r, u/g_{i_4}^r\}$. In this case, $\delta(\gamma(g))$ can be written as:

$$\delta(\gamma(g)) = l^a g_{i_1} - alw_{\lambda^*}^{a-1} + \left(-g_{i_2}^r - g_{i_3}^r + g_{i_4}^r\right) w_{\lambda^*}^a/r. \tag{3.30}$$

Over the region of interest, $\delta(\gamma(g))$ is a unimodal function of w_{λ^*} and has a local minimum if it possesses a stationary point in the interior of its domain. Thus, the maximum of $\delta(\gamma(g))$ is obtained at a boundary point. We have the following cases:

(i) $w_{\lambda^*} = \underline{w}$. Substituting for $\underline{w}$ in $\delta(\gamma(g))$ and using $\delta(g) \leq 0$, yields

$$\varphi_r\left(\left(g_{i_4}/g_{i_2}\right), \left(g_{i_3}/g_{i_2}\right)\right) \leq \left(g_{i_4}/g_{i_2}\right) - \left(g_{i_3}/g_{i_2}\right), \tag{3.31}$$

which follows from (3.15).

(ii) $w_{\lambda^*} = l/g_{i_1}^r$. Substituting for w_{λ^*} in $\delta(\gamma(g))$, gives $\delta(\varphi_r(g)) \leq 0$, which is valid since $\varphi_r(g)$ is submodular over $\text{vert}(\mathcal{H}_y^n)$.

By symmetry, (N) is valid for $\{i_1, i_2, i_3\} \subseteq I_2$, $\{i_4\} \subseteq I_3$.

IV. $\{i_1, i_2\} \subseteq I_1$, $\{i_3\} \subseteq I_2$, $\{i_4\} \subseteq I_3$. Then, $\underline{w} = \max\{l/g_{i_3}^r, u/g_{i_4}^r\}$ and $\bar{w} = \min\{l/g_{i_2}^r, u/g_{i_3}^r\}$. In this case, $\delta(\gamma(g))$ is decreasing in w_{λ^*}, and is given by:

$$\delta(\gamma(g)) = l^a(g_{i_1} - g_{i_2}) - g_{i_3}^r w_{\lambda^*}^a / r - auw_{\lambda^*}^{a-1} + u^a g_{i_4}. \tag{3.32}$$

It suffices to show $\delta(\gamma(g)) \leq 0$ for $w_{\lambda^*} = \underline{w}$. Using $\delta(g) \leq 0$, the following cases arise:

(i) If $l/u \leq (g_{i_3}/g_{i_4})^r$, then $\underline{w} = u/g_{i_4}^r$. Substituting for $\underline{w}$ in $\delta(\gamma(g))$ and using $l/u \leq (g_{i_3}/g_{i_4})^r$, gives (3.29).

(ii) If $l/u \geq (g_{i_3}/g_{i_4})^r$, then $\underline{w} = l/g_{i_3}^r$. Substituting for $\underline{w}$ in $\delta(\gamma(g))$, yields:

$$(u/l)^a \left(g_{i_4}/g_{i_3}\right) - a\left(u/l - 1\right) \leq g_{i_4}/g_{i_3}. \tag{3.33}$$

Over $1 \leq u/l \leq (g_{i_4}/g_{i_3})^r$, the left-hand side of (3.33) is decreasing in u/l. Therefore, its maximum is attained at $u/l = 1$ and is equal to the right-hand side of (3.33).

By symmetry, (N) holds for $\{i_1\} \subseteq I_1$, $\{i_2\} \subseteq I_2$, $\{i_3, i_4\} \subseteq I_3$.

V. $\{i_1\} \subseteq I_1$, $\{i_2, i_3\} \subseteq I_2$, $\{i_4\} \subseteq I_3$. Then, $\underline{w} = \max\{l/g_{i_2}^r, u/g_{i_4}^r\}$ and $\bar{w} = \min\{l/g_{i_1}^r, u/g_{i_3}^r\}$. In this case, $\delta(\gamma(g))$ can be written as:

$$\delta(\gamma(g)) = l^a g_{i_1} - a(l+u)w_{\lambda^*}^{a-1} - \left(g_{i_2}^r + g_{i_3}^r\right) w_{\lambda^*}^a / r + u^a g_{i_4}. \tag{3.34}$$

Over the region of interest, $\delta(\gamma(g))$ is a unimodal function that attains a minimum in the interior of its domain. Thus, the maximum of $\delta(\gamma(g))$ is attained at a boundary point. We have the following cases:

(i) If $l/u \leq (g_{i_2}/g_{i_4})^r$, then $\underline{w} = u/g_{i_4}^r$. Substituting for $\underline{w}$ in $\delta(\gamma(g))$, yields

$$\left(1 - \left(g_{i_2}/g_{i_4}\right)^r - \left(g_{i_3}/g_{i_4}\right)^r\right)/r \leq a\left(l/u\right) - \left(l/u\right)^a \left(g_{i_1}/g_{i_4}\right). \tag{3.35}$$

Over $(g_{i_1}/g_{i_4})^r \leq l/u \leq (g_{i_2}/g_{i_4})^r$, the right-hand side of (3.35) is decreasing in l/u. Substituting $l/u = (g_{i_2}/g_{i_4})^r$ in (3.35), and using $\delta(g) \leq 0$, yields (3.31). By symmetry, (N) holds for $w_{\lambda^*} = \bar{w} = l/g_{i_1}^r$.

(ii) If $l/u \geq (g_{i_1}/g_{i_3})^r$, then $\bar{w} = u/g_{i_3}^r$. Substituting for $\bar{w}$ in $\delta(\gamma(g))$, gives

$$(g_{i_4}/g_{i_3}) - 1 \leq (g_{i_2}/g_{i_3})^r / r + a\,(l/u) - (l/u)^a\,(g_{i_1}/g_{i_3})\,. \tag{3.36}$$

Over $(g_{i_1}/g_{i_3})^r \leq l/u \leq (g_{i_2}/g_{i_3})^r$, the right-hand side of (3.36) is decreasing in l/u. Substituting $l/u = (g_{i_2}/g_{i_3})^r$ in (3.36) and using $\delta(g) \leq 0$, yields $g_{i_2}/g_{i_3} \leq (g_{i_2}/g_{i_3})^r$ for $a < 0$, and $g_{i_2}/g_{i_3} \geq (g_{i_2}/g_{i_3})^r$ for $a > 1$, both of which are valid statements. By symmetry, the proof for $w = \underline{w} = l/g_{i_2}^r$ is similar.

Obviously, if $l < u \leq 0$, then the proof follows immediately from a similar line of arguments. Thus, suppose that $l < 0 < u$. By (3.17), if $c^T x + d \leq 0$ (resp. $c^T x + d \geq 0$), then $c^T x^i/\lambda_i + d \leq 0$ (resp. $c^T x^i/\lambda_i + d \geq 0$) for all $i \in I$, which implies the upper (resp. lower) bounds in (3.18) are always inactive. Thus, we partition the set I as $I = I_1 \cup I_2$ (resp. $I = I_2 \cup I_3$) and proceed accordingly. The remainder of the proof is quite similar to the proof for $0 \leq l < u$. $\square$

Employing a very similar line of arguments, we obtain the following result for the *concave envelope* of a closely related class of functions to those considered in Theorem 3.1:

Theorem 3.2. Consider $\phi(x,y) = (c^T x + d)^a g(y)$, $a \in (0,1)$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$, $x \in \mathcal{H}_x^m = \{[\underline{x}, \bar{x}] \subset \mathbb{R}^m : c^T x + d \geq 0\}$. Let $g(y)$, $y \in \mathcal{H}_y^n$ be a component-wise convex function such that its restriction to $\mathrm{vert}(\mathcal{H}_y^n)$ is nonnegative, supermodular and nondecreasing (or nonincreasing) in every argument. Then, any point in the graph of the concave envelope of $\phi(x,y)$ can be written as a convex combination of at most $n+1$ points in the hypograph of ϕ. Further, the corresponding optimal multipliers are given by (3.9).

Next, we consider the case where $f(x)$ is exponential. As we will show, several steps of the proof are derived by letting $\varphi_r \to \varphi_0$ in the proof of Theorem 3.1.

Theorem 3.3. Let $f(x) = a^{c^T x + d}$, $a > 0$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$, $x \in \mathcal{H}_x^m$, and let $g(y)$, $y \in \mathcal{H}_y^n$ be a nonnegative component-wise concave function. Assume that the restriction of $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^n)$ is submodular and nondecreasing (or nonincreasing) in every argument. Then, for any (x,y) in the domain of $\phi = f(x)g(y)$, there exists an optimal solution of CX1 with at most $n+1$ nonzero multipliers. Further, the values of these optimal multipliers are independent of the x variables and are given by (3.9).

Proof. As in the proof of Theorem 3.1, we start by partially optimizing CX1 with respect to x^i, $i \in I$, assuming all multipliers are nonzero. Without loss of generality, assume $\underline{x}_j < x_j < \bar{x}_j$ for all $j \in J = \{1, \ldots, m\}$. Let g_i, $i \in I$ denote the value of $g(y)$ at the vertices of $\mathcal{H}_y^n$ such that (i) if $0 < a < 1$, then $g_1 \leq g_2 \leq \ldots \leq g_{2^n}$ and (ii) if $a > 1$, then $g_1 \geq g_2 \geq \ldots \geq g_{2^n}$. First, suppose that the inequalities given by (3.5) are inactive. Writing the KKT conditions for CX1 with respect to x_i, $i \in I$, we obtain $c^T x^i/\lambda_i + \log_a g_i = c^T x^k/\lambda_k + \log_a g_k$, for all $i, k \in I$. Substituting for $c^T x^i/\lambda_i + d$ in (3.16), yields:

$$c^T x^i/\lambda_i + d = c^T x + d - \sum_{k \in I} \lambda_k \log_a (g_i/g_k), \ \forall i \in I.$$

Employing a similar argument as in the proof of Theorem 3.1, it follows that, instead of inequalities (3.5), we can equivalently analyze the bounds given by (3.18), where l and u are similarly defined. Partition I as $I = I_1 \cup I_2 \cup I_3$, where I_1 and I_3 denote the sets of indices whose corresponding $c^T x^i + d\lambda_i$ in (3.18) are at their lower and upper bounds, respectively. Letting $c^T x^i + d\lambda_i = \lambda_i l$ for all $i \in I_1$, and $c^T x^i + d\lambda_i = \lambda_i u$ for all $i \in I_3$ and minimizing CX1 with respect to x^i, $i \in I_2$, yields:

$$c^T x^i/\lambda_i + d = \left(c^T x + d - l \sum_{k \in I_1} \lambda_k - u \sum_{k \in I_3} \lambda_k - \sum_{k \in I_2} \lambda_k \log_a (g_i/g_k) \right) / \sum_{k \in I_2} \lambda_k, \qquad (3.37)$$

for all $i \in I_2$. It follows that $c^T x^1/\lambda_1 \leq c^T x^2/\lambda_2 \leq \ldots \leq c^T x^{2^n}/\lambda_{2^n}$. Thus, let $I_1 = \{1, \ldots, s-1\}$, $I_2 = \{s, \ldots, t\}$ and, $I_3 = \{t+1, \ldots, 2^n\}$. For consistency, if $s = 1$, then we set $I_1 = \emptyset$ with $g_{s-1} = 0$, if $0 < a < 1$ and $g_{s-1} = +\infty$, if $a > 1$. Similarly, if $t = 2^n$, then we set $I_3 = \emptyset$ with $g_{t+1} = +\infty$, if $0 < a < 1$ and $g_{t+1} = 0$, if $a > 1$. Define $\Gamma_2 = \sum_{i \in I_2} \lambda_i \log_a g_i$ Then, we have the following bounds on $c^T x + d$:

$$c^T x + d \geq l \sum_{i \in I_1} \lambda_i + \max \{l + \log_a g_s, \ u + \log_a g_{t+1}\} \sum_{i \in I_2} \lambda_i + u \sum_{i \in I_3} \lambda_i - \Gamma_2, \qquad (3.38)$$

and

$$c^T x + d \leq l \sum_{i \in I_1} \lambda_i + \min \{l + \log_a g_{s-1}, \ u + \log_a g_t\} \sum_{i \in I_2} \lambda_i + u \sum_{i \in I_3} \lambda_i - \Gamma_2, \qquad (3.39)$$

which, in turn, imply:

$$\log_a(g_s/g_t) \leq u - l \leq \log_a(g_{s-1}/g_{t+1}). \tag{3.40}$$

Finally, substituting (3.37) into CX1, yields:

$$\left.\begin{array}{ll} \min\limits_{\lambda_i} & a^l \sum_{i\in I_1} \lambda_i g_i \\ & + \left(\sum_{i\in I_2} \lambda_i\right) a^{\frac{c^T x + d - l\sum_{i\in I_1}\lambda_i - u\sum_{i\in I_3}\lambda_i}{\sum_{i\in I_2}\lambda_i}} \left(\prod_{i\in I_2} g_i^{\lambda_i}\right)^{\frac{1}{\sum_{i\in I_2}\lambda_i}} \\ & + a^u \sum_{i\in I_3} \lambda_i g_i \\ \text{s.t.} & \text{Constraints (3.7).} \end{array}\right\} \tag{3.41}$$

Next, we show that λ^* given by (3.9) is optimal for the above problem. As in the proof of Theorem 3.1, we will use the fact that (3.41) is an instance of Problem GCV. If $I = I_2$, then the objective function of (3.41) reduces to $\Omega = f(x)\prod_{i\in I} g_i^{\lambda_i}$, which can be equivalently replaced by $\Omega' = \sum_I \lambda_i \log g_i$. Since $\log(\cdot)$ is concave and increasing and the restriction of $g(y)$ over $\text{vert}(\mathcal{H}_y^n)$ is submodular and component-wise nondecreasing (or nonincreasing), by Lemma 3.1, $\log g(y)$, $y \in \text{vert}(\mathcal{H}_y^n)$ is submodular. Thus, λ^* is optimal. For all other feasible combinations of bounds, as in the proof of Theorem 3.1, the idea is to show that λ^* satisfies condition (3.25), where

$$\gamma(g_i) = \begin{cases} a^l g_i - l a^{w_{\lambda^*}} \log a, & \text{if } i \in I_1 \\ a^{w_{\lambda^*}} \left(1 + \log g_i - (\log a) w_{\lambda^*}\right), & \text{if } i \in I_2 \\ a^u g_i - u a^{w_{\lambda^*}} \log a, & \text{if } i \in I_3, \end{cases}$$

for all $i \in I$, and

$$w_\lambda = \left(c^T x + d - l\sum_{i\in I_1}\lambda_i - u\sum_{i\in I_3}\lambda_i + \sum_{i\in I_2}\lambda_i \log_a g_i\right) / \sum_{i\in I_2}\lambda_i.$$

Following a similar line of arguments as in the proof of Theorem 3.1, one needs to establish relation (N) for all feasible combinations of bounds of Problem (3.41). It is simple to check that the proofs follow from those of Theorem 3.1 by replacing u^a with a^u and letting $r \to 0$ in certain expressions. We will demonstrate this analogy for one set of bounds. Other cases are similarly proved. Without loss of generality, assume (i) if $0 < a < 1$, then $g_{i_1} \leq g_{i_2} \leq g_{i_3} \leq g_{i_4}$ and (ii) if $a > 1$, then $g_{i_1} \geq g_{i_2} \geq g_{i_3} \geq g_{i_4}$. In the following, $\underline{w}$ and

$\bar{w}$ denote a lower and an upper bound on w_{λ^*}, respectively.

Let $\{i_1, i_2\} \subseteq I_1$, $\{i_3\} \subseteq I_2$, $\{i_4\} \subseteq I_3$. Then, $\underline{w} = \max\{l + \log_a g_{i_3}, u + \log_a g_{i_4}\}$, and $\bar{w} = \min\{l + \log_a g_{i_2}, u + \log_a g_{i_3}\}$. In this case, $\delta(\gamma(g))$ is decreasing in w_{λ^*} and is given by

$$\delta(\gamma(g)) = a^l(g_{i_1} - g_{i_2}) - a^{w_{\lambda^*}}(1 + (\log a)(u - w_{\lambda^*}) + \log g_{i_3}) + a^u g_{i_4}.$$

It suffices to show that $\delta(\gamma(g))$ is non-positive for $w_{\lambda^*} = \underline{w}$. Using $\delta(g(y)) \leq 0$, the following cases arise:

(i) If $u - l \geq \log_a(g_{i_3}/g_{i_4})$, then $\underline{w} = u + \log_a g_{i_4}$. Substituting for $\underline{w}$ in $\delta(\gamma(g))$, and using $u - l \geq \log_a(g_{i_3}/g_{i_4})$, yields $\log(g_{i_4}/g_{i_3}) \leq g_{i_4}/g_{i_3} - 1$, which is always valid. Note that this inequality can be obtained by letting $r \to 0$ in (3.29).

(ii) If $u - l \leq \log_a(g_{i_3}/g_{i_4})$, then $\underline{w} = l + \log_a g_{i_3}$. Substituting $\underline{w}$ in $\delta(\gamma(g))$, yields (see (3.33)):

$$a^{u-l}(g_{i_4}/g_{i_3}) - (\log a)(u - l) \leq g_{i_4}/g_{i_3}.$$

Over $0 \leq u - l \leq \log_a(g_{i_3}/g_{i_4})$, the left-hand side of the above inequality is decreasing in $u - l$. Thus, its maximum is attained at $u - l = 0$, and is equal to the right-hand side.

By symmetry, (N) holds for $\{i_1\} \subseteq I_1$, $\{i_2\} \subseteq I_2$, $\{i_3, i_4\} \subseteq I_3$. □

Remark 3.1. Consider the concave function $g(y) = h(\sum_{k \in K} g_k(y_k))$, where $g_k(y_k)$, $y_k \in [\underline{y}_k, \bar{y}_k] \subset \mathbb{R}$ is concave for all $k \in K$ and $h(\cdot)$ is concave and nondecreasing over the range of $\sum_{k \in K} g_k(y_k)$. Suppose that $g_k(\bar{y}_k) - g_k(\underline{y}_k) \geq 0$, for all $k \in K_1 \subset K$ and $g_k(\bar{y}_k) - g_k(\underline{y}_k) \leq 0$ for all $k \in K \setminus K_1$. Obviously, $g(y)$ does not satisfy the submodularity and monotonicity assumptions of Theorems 3.1 and 3.3 (if $K = K_1$ or $K_1 = \emptyset$, then the conditions of Theorems 3.1 and 3.3 are met). Now, consider the affine mapping $T(y_k) = y_k$, for all $k \in K_1$ and $T(y_k) = \bar{y}_k + \underline{y}_k - y_k$, for all $k \in K \setminus K_1$. By Lemma 3.1, the concave function $g(T(y)) = h(\sum_{k \in K} g_k(T(y_k)))$, $y_k \in [\underline{y}_k, \bar{y}_k]$, is submodular and component-wise nondecreasing over $\mathrm{vert}(\mathcal{H}^n_y)$; hence, satisfying the conditions of Theorems 3.1 and 3.3. Let $\psi(x, y) = f(x)g(T(y))$. It is simple to show that $\mathrm{conv}_{\mathcal{C}}\phi(x, y) = \mathrm{conv}_{\mathcal{C}}\psi(x, T(y))$. Therefore, we first utilize Theorems 3.1 and 3.3, to construct $\mathrm{conv}_{\mathcal{C}}\psi(x, y)$ and then apply the inverse mapping to derive the convex envelope of $\phi(x, y)$ over $\mathcal{C}$. As another example, consider the component-wise convex function $g(y) = \prod_{k \in K} g_k(y_k)$, where $g_k(y_k)$,

$y_k \in [\underline{y}_k, \bar{y}_k] \subset \mathbb{R}$, is convex and nonnegative for all $k \in K$. Suppose that $g_k(\bar{y}_k) - g_k(\underline{y}_k) > 0$ for all $k \in K_1 \subset K$ and $g_k(\bar{y}_k) - g_k(\underline{y}_k) < 0$ for all $k \in K \setminus K_1$. Again, $g(y)$ does not satisfy the monotonicity and supermodularity assumptions of Theorem 3.2 (if $K = K_1$ or $K_1 = \emptyset$, then the assumptions of Theorem 3.2 are satisfied). However, if we let $T(y_k) = y_k$ for all $k \in K_1$ and $T(y_k) = \bar{y}_k + \underline{y}_k - y_k$, for all $k \in K \setminus K_1$, then $g(T(y))$ is component-wise convex over $\mathcal{H}_y^n$ and its restriction to $\mathrm{vert}(\mathcal{H}_y^n)$ is supermodular (cf. Lemma 2.6.4 in [65]) and component-wise increasing; thus satisfying the conditions of Theorem 3.2. For instance, this holds for $g(y) = \prod_{k \in K} y_k^{a_k}$, where $a_k \geq 1$, $y_k \geq 0$ for all $k \in K_1$ and $a_k < 0$, $y_k > 0$ for all $k \in K \setminus K_1$ (see Corollaries 3.14-3.16 in [60] for other examples).

Remark 3.2. Let $t = c^T x + d$, $x \in \mathcal{H}_x^m$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$, and let l and u denote the minimum and maximum of $c^T x + d$ over $\mathcal{H}_x^m$, respectively. Define $\psi(t, y) = f(t)g(y)$, over $\mathcal{D} = [l, u] \times \mathcal{H}_y^n$, where $f(t) = t^a$ or $f(t) = a^t$, and suppose that f and g satisfy the conditions of Theorems 3.1 and 3.3. From the proofs of these theorems, it follows that $\mathrm{conv}_{\mathcal{C}}\phi(x, y) = \mathrm{conv}_{\mathcal{D}}\psi(c^T x + d, y)$. It is important to note that such a recursive approach does not yield the convex envelope of the original function, in general. For example, as we will detail in Chapter 4, if we relax the nonnegativity assumption on $g(y)$, then this equivalence is no longer valid.

Throughout this section we assumed that $g(y)$ is component-wise concave over $\mathcal{H}_y^n$. Nonetheless, the results are valid for any $g(y)$ with a polyhedral convex envelope over $\mathcal{H}_y^n$. For the functions satisfying the conditions of Theorems 3.1 and 3.3, the envelope representation problem simplifies significantly, in that the optimal multipliers are independent of the x variables and are given by the set λ^*. In order to prove this decoupling, we derived explicit characterizations of the convex envelopes in both theorems. In the next section, we demonstrate the benefits of the proposed envelopes in closing the relaxation gaps of standard factorable techniques.

3.4 Closed-form expressions for the convex envelope of primitive functions

In this section, we present analytical expressions for the convex envelopes of selected functions of the form $\phi(x, y) = f(x)g(y)$, $x \in \mathcal{H}_x^m$, $y \in \mathcal{H}_y^n$, where $f(x)$ is nonnegative convex and $g(y)$ is component-wise concave. We consider the cases where $g(y)$ is univariate and bivariate in turn. All examples presented correspond to functions that occur frequently in applications. For numerical comparisons of the proposed envelopes and factorable relaxations, we compute the percentage of the gap closed by convϕ at a given point x as follows

$$(\mathrm{conv}\phi(x) - \tilde{\phi}(x))/(\phi(x) - \tilde{\phi}(x)) \times 100\%,$$

where $\tilde{\phi}$ is a convex underestimator of ϕ obtained by a conventional factorable relaxation scheme.

3.4.1 Univariate $g(y)$

In [61], the authors propose a convex formulation for evaluating the value of conv$\phi(x, y)$, where ϕ is convex in $x \in \mathcal{H}_x^m$ and concave in $y \in [\underline{y}, \bar{y}] \subset \mathbb{R}$. In [58], the author derives an explicit characterization of conv$\phi(x, y)$ provided that the convex combinations of ϕ are *pairwise complementary* (see Section 3 in [58] for details). In particular, it is shown that, if $\phi(x, \underline{y})$ is nondecreasing and convex and $\phi(x, \bar{y})$ is nonincreasing and convex, then the pairwise combinations of ϕ are complementary. In the following, we consider functions for which this condition is not satisfied. We further assume that ϕ can be written as $\phi(x, y) = f(x)g(y)$, $\mathcal{C} = \mathcal{H}_x^m \times \mathcal{H}_y^1$, where $f(x)$ is nonnegative convex and $g(y)$ is concave. First, let $g(y)$ be nonnegative. In the following two corollaries, we consider the cases where $f(x)$ has power and exponential forms in turn.

As it was shown in [60], if $g(\underline{y}) = 0$ (or $g(\bar{y}) = 0$), then the closed-form expressions for convϕ can be obtained in a more general setting. Namely, it suffices to assume that $f(x)$, $x \in \mathcal{H}_x^m$ is convex and monotone (see Theorem 4.1 in [60]). This generalization follows from to the fact that, if $f(x)$ is monotone and $g(\underline{y})g(\bar{y}) = 0$, then at any optimal solution of Problem CX1, if $\lambda_1 \underline{x}_j < x_j^1 < \lambda_1 \bar{x}_j$ (resp. $\lambda_2 \underline{x}_j < x_j^2 < \lambda_2 \bar{x}_j$) for some $j \in J$, then $x_j^2 = \lambda_2 \underline{x}$ or $x_j^2 = \lambda_2 \bar{x}$ (resp. $x_j^1 = \lambda_1 \underline{x}$ or $x_j^1 = \lambda_1 \bar{x}$). Thus, in the following, we assume that $g(y)$ is strictly positive. We state the results without proofs, since they follow directly from the proofs of Theorems 3.1 and 3.3. To simplify the notation, we denote $g(\underline{y})$ and $g(\bar{y})$ by $\underline{g}$ and $\bar{g}$, respectively, and $f(\underline{x})$ and $f(\bar{x})$ by $\underline{f}$ and $\bar{f}$, respectively.

Corollary 3.2. Consider $\phi = f(x)g(y)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$, $y \in [\underline{y}, \bar{y}] \subset \mathbb{R}$. Let $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0, 1]\}$ be nonnegative and convex and, let $g(y)$ be positive and concave. Define $\alpha = (\underline{g}/\bar{g})^{1/(1-a)}$. We have the following cases:

(i) if (1) $\alpha \geq 1$ and $\underline{x} \geq 0$, or (2) $\alpha \leq 1$ and $\bar{x} \leq 0$:

$$\text{conv}\phi = \begin{cases} \lambda_1^{1-a}(x - \lambda_2\underline{x})^a \underline{g} + \lambda_2 \underline{f}\bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1 \min\{\alpha\underline{x},\ \bar{x}\} + \lambda_2\underline{x}, \\ x^a \left(\lambda_1 \underline{g}^{\frac{1}{1-a}} + \lambda_2 \bar{g}^{\frac{1}{1-a}}\right)^{1-a}, & \text{if } (\lambda_1\alpha + \lambda_2)\underline{x} \leq x \leq (\lambda_1 + \lambda_2/\alpha)\bar{x}, \\ \lambda_1 \bar{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1\bar{x})^a \bar{g}, & \text{if } \lambda_1\bar{x} + \lambda_2 \max\{\underline{x},\ \bar{x}/\alpha\} \leq x \leq \bar{x}, \end{cases}$$

(ii) if (1) $\alpha \leq 1$ and $\underline{x} \geq 0$, or (2) $\alpha \geq 1$ and $\bar{x} \leq 0$:

$$\text{conv}\phi = \begin{cases} \lambda_1 \underline{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1\underline{x})^a \bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1\underline{x} + \lambda_2 \min\{\underline{x}/\alpha,\ \bar{x}\}, \\ x^a \left(\lambda_1 \underline{g}^{\frac{1}{1-a}} + \lambda_2 \bar{g}^{\frac{1}{1-a}}\right)^{1-a}, & \text{if } (\lambda_1 + \lambda_2/\alpha)\underline{x} \leq x \leq (\lambda_1\alpha + \lambda_2)\bar{x}, \\ \lambda_1^{1-a}(x - \lambda_2\bar{x})^a \underline{g} + \lambda_2 \bar{f}\bar{g}, & \text{if } \lambda_1 \max\{\underline{x},\ \alpha\bar{x}\} + \lambda_2\bar{x} \leq x \leq \bar{x}, \end{cases}$$

(iii) if $\alpha \geq 1$ and $\underline{x} < 0 < \bar{x}$:

$$\text{conv}\phi = \begin{cases} \lambda_1 \underline{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1\underline{x})^a \bar{g}, & \text{if } \underline{x} \leq x \leq (\lambda_1 + \lambda_2/\alpha)\underline{x}, \\ x^a \left(\lambda_1 \underline{g}^{\frac{1}{1-a}} + \lambda_2 \bar{g}^{\frac{1}{1-a}}\right)^{1-a}, & \text{if } (\lambda_1 + \lambda_2/\alpha)\underline{x} \leq x \leq (\lambda_1 + \lambda_2/\alpha)\bar{x}, \\ \lambda_1 \bar{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1\bar{x})^a \bar{g}, & \text{if } (\lambda_1 + \lambda_2/\alpha)\bar{x} \leq x \leq \bar{x}, \end{cases}$$

(iv) if $\alpha \leq 1$ and $\underline{x} < 0 < \bar{x}$:

$$\text{conv}\phi = \begin{cases} \lambda_1^{1-a}(x - \lambda_2\underline{x})^a \underline{g} + \lambda_2 \underline{f}\bar{g}, & \text{if } \underline{x} \leq x \leq (\lambda_1\alpha + \lambda_2)\underline{x}, \\ x^a \left(\lambda_1 \underline{g}^{\frac{1}{1-a}} + \lambda_2 \bar{g}^{\frac{1}{1-a}}\right)^{1-a}, & \text{if } (\lambda_1\alpha + \lambda_2)\underline{x} \leq x \leq (\lambda_1\alpha + \lambda_2)\bar{x}, \\ \lambda_1^{1-a}(x - \lambda_2\bar{x})^a \underline{g} + \lambda_2 \bar{f}\bar{g}, & \text{if } (\lambda_1\alpha + \lambda_2)\bar{x} \leq x \leq \bar{x}, \end{cases}$$

where $\lambda_1 = (\bar{y} - y)/(\bar{y} - \underline{y})$, $\lambda_2 = (y - \underline{y})/(\bar{y} - \underline{y})$.

Example 3.1. Let $\phi = \sqrt{y}/x^2$, $x \in [-2, -1]$, $y \in [1, 4]$. Then, $\alpha = (1/2)^{1/3} < 1$ and $\bar{x} = -1 < 0$. Thus, Part (i) of Corollary 3.2 is satisfied and convϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{(4-y)^3}{3(3x+2y-2)^2} + \frac{y-1}{6}, & \text{if } -2 \leq x \leq -0.14y - 1.45, \\ \frac{(0.09y+0.9)^3}{x^2}, & \text{if } -0.14y - 1.45 \leq x \leq -0.09y - 0.9, \\ \frac{2(y-1)^3}{3(3x-y+4)^2} + \frac{4-y}{3}, & \text{if } -0.09y - 0.9 \leq x \leq -1.0. \end{cases}$$

To construct a convex underestimator for ϕ using a standard factorable relaxation scheme [63], the concave function $g = \sqrt{y}$ is first replaced by its affine underestimator and the resulting expression is outer-linearized using bilinear envelopes to yield:

$$\tilde{\phi} = \max\left\{1/x^2 + (y-1)/12,\ 2/x^2 + (y-4)/3\right\}.$$

Figure 3.1(a) depicts the percentage of the gap closed by convϕ. Up to over 80% of the gap is closed by the convex envelope.

By checking more boundary conditions, Corollaries 3.2 can be easily generalized to the case where $f(x)$ is a nonnegative multivariate convex function of the form $f(x) = \prod_{j\in J} x_j^{a_j}$, where $x_j > 0$ and $a_j < 0$ for all $j \in J$. We show this through an example:

Example 3.2. Let $\phi = y/(x_1x_2)$, $x_1 \in [0.1, 1]$, $x_2 \in [1.5, 2]$, $y \in [0.5, 2]$. The convex envelope of ϕ is given by:

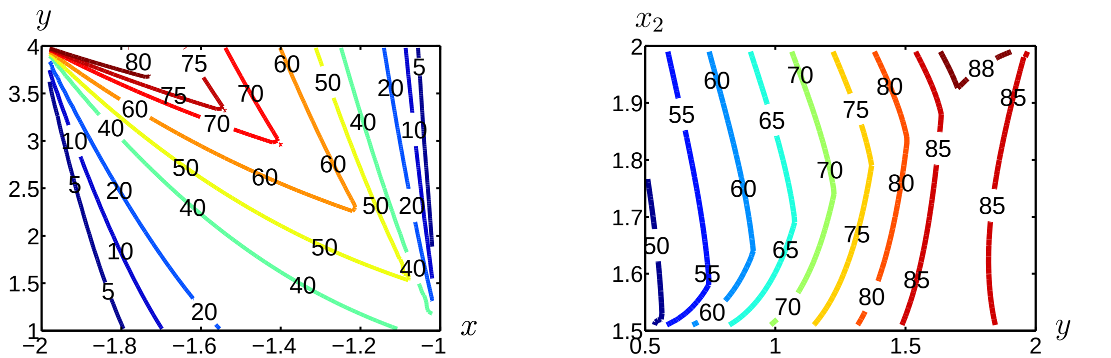
$$\begin{cases} \frac{10(2y-1)^3}{9(y+x_2-2)(y+15x_1-2)} - \frac{20}{9}(y-2), & \text{if } 0.1 \le x_1 \le 0.08+0.04y,\ 1.5 \le x_2 \le (y+4)/3, \\ \frac{20(y-2)^2}{3(3x_2-4y+2)} + \frac{5(2y-1)^2}{3(y+15x_1-2)}, & \text{if } 0.1 \le x_1 \le 0.08+0.04y,\ (y+4)/3 \le x_2 \le 2, \\ \frac{1}{x_1}\left(0.39(2-y) + \sqrt{\frac{2(2y-1)^3}{27(y+x_2-2)}}\right)^2, & \text{if } 0.08+0.04y \le x_1 \le 0.5+0.25y, \\ & \quad 1.5 \le x_2 \le (y+4)/3, \\ \frac{1}{x_1}\left(\frac{2y-1}{3} + \sqrt{\frac{4(2-y)^3}{9(3x_2-4y+2)}}\right)^2, & \text{if } 0.08+0.04y \le x_1 \le 0.5+0.25y, \\ & \quad (y+4)/3 \le x_2 \le 2, \\ \frac{4(2-y)^2}{9(-2y+3x_1+1)} + \frac{2(2y-1)^2}{9(y+x_2-2)}, & \text{if } 0.5+0.25y \le x_1 \le 1.0,\ 1.5 \le x_2 \le (y+4)/3, \\ \frac{4(2-y)^3}{3(3x_2-4y+2)(3x_1-2y+1)} + \frac{2y-1}{3}, & \text{if } 0.5+0.25y \le x_1 \le 1.0,\ (y+4)/3 \le x_2 \le 2. \end{cases}$$

A factorable relaxation of ϕ is obtained by letting $t = 1/(x_1x_2)$ and underestimating $\phi = yt$ using bilinear envelopes:

$$\tilde{\phi} = \max\{2/(x_1x_2) + 20(y-2)/3,\ 1/(2x_1x_2) + (2y-1)/4\}.$$

The gap closed by convϕ at $x_1 = 0.3$ is shown in Figure 3.1(b). Up to over 88% of the gap is closed by the convex envelope.

Corollary 3.3. Consider $\phi = f(x)g(y)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$, $y \in [\underline{y}, \bar{y}] \subset \mathbb{R}$. Let $f(x) = a^x$, $a > 0$ and, let $g(y)$ be concave and positive. Define $\alpha = \log_a(\bar{g}/\underline{g})$. Then, the convex envelope of ϕ is given by



(a) Example 3.1: $\phi = \sqrt{y}/x^2$ (b) Example 3.2: $\phi = y/(x_1x_2)$ at $x_1 = 0.3$

Figure 3.1: Gap closed by the convex envelopes for Examples 3.1 and 3.2

(i) if $\alpha \geq 0$:

$$\text{conv}\phi = \begin{cases} \lambda_1 a^{(x-\lambda_2\underline{x})/\lambda_1}\underline{g} + \lambda_2\underline{f}\bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1\min\{\underline{x}+\alpha,\ \bar{x}\} + \lambda_2\underline{x}, \\ a^x\underline{g}^{\lambda_1}\bar{g}^{\lambda_2}, & \text{if } \underline{x} + \lambda_1\alpha \leq x \leq \bar{x} - \lambda_2\alpha, \\ \lambda_1\bar{f}\underline{g} + \lambda_2 a^{(x-\lambda_1\bar{x})/\lambda_2}\bar{g}, & \text{if } \lambda_1\bar{x} + \lambda_2\max\{\underline{x},\ \bar{x}-\alpha\} \leq x \leq \bar{x}, \end{cases}$$

(ii) if $\alpha \leq 0$:

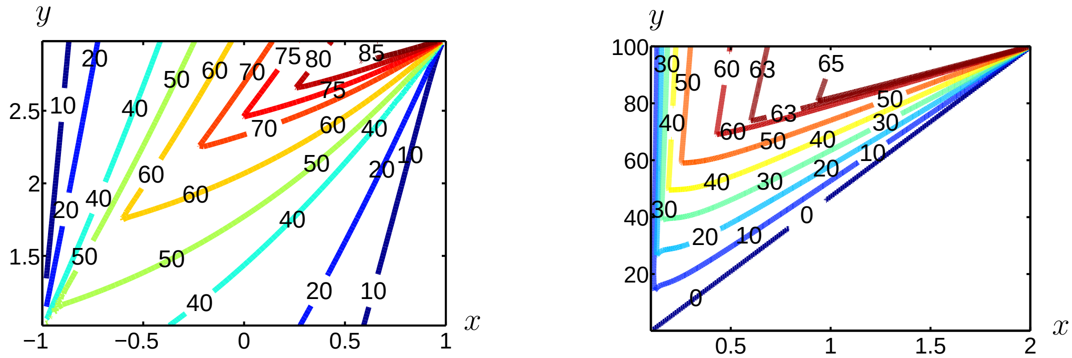
$$\text{conv}\phi = \begin{cases} \lambda_1\underline{f}\,\underline{g} + \lambda_2 a^{(x-\lambda_1\underline{x})/\lambda_2}\bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1\underline{x} + \lambda_2\min\{\underline{x}-\alpha,\ \bar{x}\}, \\ a^x\underline{g}^{\lambda_1}\bar{g}^{\lambda_2}, & \text{if } \underline{x} - \lambda_2\alpha \leq x \leq \bar{x} + \lambda_1\alpha, \\ \lambda_1 a^{(x-\lambda_2\bar{x})/\lambda_1}\underline{g} + \lambda_2\bar{f}\bar{g}, & \text{if } \lambda_1\max\{\underline{x},\ \bar{x}+\alpha\} + \lambda_2\bar{x} \leq x \leq \bar{x}, \end{cases}$$

where $\lambda_1 = (\bar{y}-y)/(\bar{y}-\underline{y})$, $\lambda_2 = (y-\underline{y})/(\bar{y}-\underline{y})$.

Example 3.3. Let $\phi = y\exp(-x)$, $x \in [-1,1]$, $y \in [1,3]$. Then, $\alpha = -\log 3 < 0$ and Part (ii) of Corollary 3.3 is valid. Thus, convϕ is given by:

$$\begin{cases} 1.5(y-1)\exp(\frac{-2x+y-3}{y-1}) + 1.36(3-y), & \text{if } -1 \leq x \leq 0.55y - 1.55, \\ 3^{(y-1)/2}\exp(-x), & \text{if } 0.55y - 1.55 \leq x \leq 0.55y - 0.65, \\ 0.5(3-y)\exp(\frac{-2x+y-1}{3-y}) + 0.55(y-1), & \text{if } 0.55y - 0.65 \leq x \leq 1. \end{cases}$$

To compare with a standard factorable relaxation, let $t = \exp(-x)$. Employing bilinear



(a) Example 3.3: $\phi = y\exp(-x)$ (b) Example 3.4: $\phi = \log_{10} y/x^2$

Figure 3.2: Gap closed by the convex envelopes for Examples 3.3 and 3.4

envelopes to underestimate $\phi = yt$, we obtain

$$\tilde{\phi} = \max\left\{3\exp(-x) + 2.72(y-3),\ \exp(-x) + 0.37(y-1)\right\}.$$

The two relaxations are compared in Figure 3.2(a). Up to over 85% of the gap of the standard relaxation is closed by the convex envelope.

Remark 3.3. In Parts (i) and (ii) of Corollary 3.2 and in Corollary 3.3, depending on the values of parameters $\mathcal{S} = \{\underline{x}, \bar{x}, \underline{g}, \bar{g}, a\}$, the convex envelope of ϕ can be composed of two or three convex pieces. For example, in Part (i) of Corollary 3.3, if $\bar{x} - \underline{x} \le \log_a(\bar{g}/\underline{g})$, then the second expression is not present in the graph of $\text{conv}_{\mathcal{C}}\phi$.

Next, we relax the nonnegativity requirement on $g(y)$. If $\underline{g}$ and $\bar{g}$ are both nonpositive, then $\text{conv}\phi$ is polyhedral. Thus, without loss of generality, let $\underline{g} < 0 < \bar{g}$. Denote by $\hat{x}_j$, $j \in \bar{J} = \{1, \ldots, 2^m\}$, the vertices of $\mathcal{H}^m_x$. In this case, we have:

$$\mathcal{G}_{\mathcal{C}}\phi \subseteq \{\{\hat{x}_j, \underline{y}\} \cup \{x, \bar{y}\},\ \forall j \in \bar{J},\ x \in \mathcal{H}^m_x\}.$$

We choose to first convexify ϕ over $\mathcal{L} = \{(x, \underline{y}), x \in \mathcal{H}^m_x\}$. Since the restriction of ϕ to $\mathcal{L}$ is concave, its convex envelope is polyhedral. First, let $f(x)$ be a univariate function. If $f(x)$ is nondecreasing (resp. nonincreasing) over $\mathcal{H}^1_x$, then $\text{conv}(f(x)\underline{g})$ is a nonincreasing (resp. nondecreasing) convex function and $f(x)\bar{g}$ is a nondecreasing (resp. nonincreasing) convex function. Thus, as discussed earlier, the pairwise complementarity property of [58] is satisfied, and the convex envelope of ϕ can be accordingly derived (see Proposition 3.3

in [58]). For completeness, we provide the expressions for convϕ in the following corollary.

Corollary 3.4. Consider $\phi = f(x)g(y)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$, $y \in [\underline{y}, \bar{y}] \subset \mathbb{R}$, where $f(x)$ is nonnegative, monotone and convex and $g(y)$ is concave with $\underline{g} < 0 < \bar{g}$. Then, conv$\phi$ is given by:

$$\text{conv}\phi = \begin{cases} \left(\frac{\bar{f}-\underline{f}}{\bar{x}-\underline{x}}\right)(x-\underline{x})\underline{g} + (\lambda_1\underline{g} + \lambda_2\bar{g})\underline{f}, & \text{if } \underline{x} \leq x \leq \lambda_1\bar{x} + \lambda_2\underline{x}, \\ \lambda_1\bar{f}\underline{g} + \lambda_2 f\left(\frac{x-\lambda_1\bar{x}}{\lambda_2}\right)\bar{g}, & \text{if } \lambda_1\bar{x} + \lambda_2\underline{x} \leq x \leq \bar{x}, \end{cases} \tag{3.42}$$

if $f(x)$ is nondecreasing, and by

$$\text{conv}\phi = \begin{cases} \lambda_1\underline{f}\underline{g} + \lambda_2 f\left(\frac{x-\lambda_1\underline{x}}{\lambda_2}\right)\bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1\underline{x} + \lambda_2\bar{x}, \\ \left(\frac{\bar{f}-\underline{f}}{\bar{x}-\underline{x}}\right)(x-\bar{x})\underline{g} + (\lambda_1\underline{g} + \lambda_2\bar{g})\bar{f}, & \text{if } \lambda_1\underline{x} + \lambda_2\bar{x} \leq x \leq \bar{x}, \end{cases} \tag{3.43}$$

if $f(x)$ is nonincreasing, where $\lambda_1 = (\bar{y} - y)/(\bar{y} - \underline{y})$, $\lambda_2 = (y - \underline{y})/(\bar{y} - \underline{y})$.

Example 3.4. Let $\phi = \log_{10} y/x^2$, $x \in [0.1, 2]$, $y \in [0.1, 10^2]$. In this case, $f(x) = 1/x^2$, $x \in [0.1, 2]$ is decreasing and convϕ is given by (3.43):

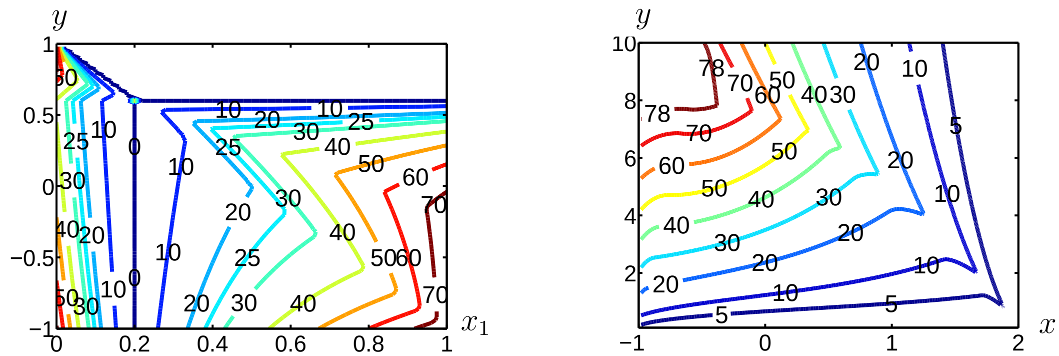
$$\text{conv}\phi = \begin{cases} 10^{-4}\frac{2(y-.1)^3}{(10x+0.01y-1)^2} + y - 100.1, & \text{if } 0.1 \leq x \leq 0.019y + 0.098, \\ 52.5x + 0.0075y - 105.251, & \text{if } 0.019y + 0.098 \leq x \leq 2. \end{cases}$$

To obtain a convex relaxation of ϕ using the standard method, let t_1 denote the affine underestimator of $\log_{10} y$, $y \in [0.1, 10^2]$ and let $t_2 = 1/x^2$. Employing the bilinear envelopes to underestimate $t_3 = t_1 t_2$, yields:

$$\tilde{\phi} = \max\left\{2/x^2 + 3(y - 100),\ 52.5x + 0.0075y - 105.251\right\}.$$

The two relaxations are compared in Figure 3.2(b). Up to over 65% of the relaxation gap is closed by the convex envelope of ϕ. Further, as can be seen from the figure, the two relaxations coincide over the region where convϕ is affine.

Example 3.5. Let $\phi = y\exp(x_1 - x_2)$, $y \in [-1, 1]$, $(x_1, x_2) \in [0, 1]^2$. The convex envelope



(a) Example 3.5: $\phi = y\exp(x_1 - x_2)$ at $x_2 = 0.8$

(b) Example 3.6: $\phi = x^2 \log_{10} y$

Figure 3.3: Gap closed by the convex envelopes for Examples 3.5 and 3.6

of ϕ is given by:

$$\begin{cases} \frac{y+1}{2}\exp(\frac{-2x_2}{y+1}) - 1.72x_1 + 0.5y - 0.5, & \text{if } 2x_1 + y \leq 1,\ 2x_2 - y \leq 1,\ x_1 + x_2 \leq 1, \\ -1.72x_1 + 0.63x_2 + 0.37y - 0.63, & \text{if } 2x_1 + y \leq 1,\ 2x_2 - y \geq 1,\ x_1 + x_2 \leq 1, \\ -0.63x_1 + 1.72x_2 + 0.37y - 1.72, & \text{if } 2x_1 + y \leq 1,\ 2x_2 - y \geq 1,\ x_1 + x_2 \geq 1, \\ \frac{y+1}{2}\exp(\frac{2x_1-2}{y+1}) + 1.72x_2 + 0.5y - 2.22, & \text{if } 2x_1 + y \geq 1,\ 2x_2 - y \geq 1,\ x_1 + x_2 \geq 1, \\ \frac{y+1}{2}\exp(\frac{2x_1-2x_2+y-1}{y+1}) + 1.36(y-1), & \text{if } 2x_1 + y \geq 1,\ 2x_2 - y \leq 1. \end{cases}$$

To compare with a factorable relaxation scheme, introduce $t_1 = x_1 - x_2$, and let $\tilde{\phi}$ denote the convex envelope of $t_2 = y\exp(t_1)$, given by Corollary 3.4:

$$\tilde{\phi} = \begin{cases} -1.175(x_1 - x_2 + 1) + 0.37y, & \text{if } -1 \leq x_1 - x_2 \leq -y, \\ \frac{y+1}{2}\exp\left(\frac{2x_1-2x_2+y-1}{y+1}\right) + 1.36(y-1), & \text{if } -y \leq x_1 - x_2 \leq 1. \end{cases}$$

The gap closed by convϕ at $x_2 = 0.8$ is depicted in Figure 3.3(a). As can be seen, convϕ closes up to 70% of the relaxation gap. To construct $\tilde{\phi}$, we used the convex envelope of $t_2 = y\exp(t_1)$, which is not implemented in current global solvers. Employing the standard relaxation method will lead to a much weaker relaxation than $\tilde{\phi}$.

Next, let $f(x)$ be non-monotone. In the following corollary, we consider the case where $f(x)$ is a monomial of even degree with $\underline{x} < 0 < \bar{x}$. A similar procedure can be employed to derive convϕ assuming other functional forms for $f(x)$.

Corollary 3.5. Consider $\phi = f(x)g(y)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$, $y \in [\underline{y}, \bar{y}] \subset \mathbb{R}$. Let $f(x) = x^a$,

$a = 2k$, $k = 1, \dots, n$, $\underline{x} < 0 < \bar{x}$ and, let $g(y)$ be concave with $\underline{g} < 0 < \bar{g}$. Define

$$\alpha = \operatorname{sgn}(\underline{f} - \bar{f}) \left| \frac{\underline{g}}{a\bar{g}} \frac{\bar{f} - \underline{f}}{\bar{x} - \underline{x}} \right|^{1/(a-1)}.$$

We then have the following cases:

1. if $|\underline{x}| \leq \bar{x}$ and $\alpha \leq \underline{x}$, then conv$\phi$ is given by (3.42),

2. if $\bar{x} \leq |\underline{x}|$ and $\alpha \geq \bar{x}$, then convϕ is given by (3.43),

3. otherwise, convϕ is given by:

$$\begin{cases} \lambda_1 \underline{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1 \underline{x})^a \bar{g}, & \text{if } \underline{x} \leq x \leq \lambda_1 \underline{x} + \lambda_2 \alpha, \\ \frac{\bar{f}-\underline{f}}{\bar{x}-\underline{x}}(x - \lambda_1 \underline{x} - \lambda_2 \alpha)\underline{g} + \lambda_1 \underline{f}\underline{g} + \lambda_2 \alpha^a \bar{g}, & \text{if } \lambda_1 \underline{x} + \lambda_2 \alpha \leq x \leq \lambda_1 \bar{x} + \lambda_2 \alpha, \\ \lambda_1 \bar{f}\underline{g} + \lambda_2^{1-a}(x - \lambda_1 \bar{x})^a \bar{g}, & \text{if } \lambda_1 \bar{x} + \lambda_2 \alpha \leq x \leq \bar{x}, \end{cases} \tag{3.44}$$

where $\lambda_1 = (\bar{y} - y)/(\bar{y} - \underline{y})$, $\lambda_2 = (y - \underline{y})/(\bar{y} - \underline{y})$.

Proof. As discussed earlier, to construct conv$_{\mathcal{C}}\phi$, we first convexify ϕ over $\mathcal{L} = \{(x, \underline{y}), x \in [\underline{x}, \bar{x}]\}$. Since by assumption $\underline{g} < 0$, the convex envelope of ϕ over $\mathcal{L}$ is affine: conv$_{\mathcal{L}}\phi = (m(x - \underline{x}) + \underline{f})\underline{g}$, where $m = (\bar{f} - \underline{f})/(\bar{x} - \underline{x})$. Subsequently, conv$_{\mathcal{C}}\phi$ is obtained by convexifying conv$_{\mathcal{L}}\phi$ and $\phi(x, \bar{y})$ over $\mathcal{C}$. It follows that, Problem CX simplifies to:

$$\left.\begin{array}{ll} \min\limits_{x^1} & \lambda_1(m(x^1/\lambda_1 - \underline{x}) + \underline{f})\underline{g} + \lambda_2^{1-a}(x - x^1)^a \bar{g} \\ \text{s.t.} & \max\{\lambda_1 \underline{x},\ x - \lambda_2 \bar{x}\} \leq x^1 \leq \min\{\lambda_1 \bar{x},\ x - \lambda_2 \underline{x}\}, \end{array}\right\} \tag{3.45}$$

where the multipliers vary linearly with the y variables and are given by $\lambda_1 = (\bar{y} - y)/(\bar{y} - \underline{y})$, $\lambda_2 = 1 - \lambda_1$. The derivative of the objective function of the above problem is zero at $x^1 = x - \lambda_2 \alpha$. Thus, two cases arise:

(i) $|\underline{x}| \leq \bar{x}$. In this case, α is negative. It follows that $x^1 = x - \lambda_2 \alpha \geq x$ and, thus, the bound $x - \lambda_2 \bar{x} \leq x^1$ is redundant. Further, if $\alpha \leq \underline{x}$, then the interior solution $x^1 = x - \lambda_2 \alpha$ is always greater than the upper bound $x - \lambda_2 \underline{x}$. Thus, the minimum of Problem (3.45) is attained at the upper bound on x^1 and convϕ is given by (3.42). For $\alpha \geq \underline{x}$, the constraint $x^1 \leq x - \lambda_2 \underline{x}$ is inactive. The following cases arise:

- if $x - \lambda_2 \alpha \leq \lambda_1 \underline{x}$, then $x^1 = \lambda_1 \underline{x}$,

- if $x - \lambda_2\alpha \geq \lambda_1\bar{x}$, then $x^1 = \lambda_1\bar{x}$,
- otherwise, $x^1 = x - \lambda_2\alpha$.

Substituting for x^1 in the objective function of (3.45), gives (3.44).

(ii) $|\underline{x}| \geq \bar{x}$. In this case, $\alpha \geq 0$, which implies $x^1 = x - \lambda_2\alpha \leq x$. Since by assumption $\underline{x} < 0$, it follows that the bound $x^1 \leq x - \lambda_2\underline{x}$ is redundant. Further, if $\alpha \geq \bar{x}$, then the minimum of Problem (3.45) is attained when x^1 hits its lower bound and convϕ is given by (3.43). If $\alpha \leq \bar{x}$, the constraint $x^1 \geq x - \lambda_2\bar{x}$ is inactive and we should solve the same problem as in Part (i) for $\alpha \geq \underline{x}$.

□

Example 3.6. Let $\phi = x^2 \log_{10} y$, $x \in [-1, 2]$, $y \in [0.1, 10]$. Then, $\alpha = -0.5$ and $\underline{x} < \alpha < \bar{x}$. Thus, Part 3 of Corollary 3.5 is satisfied and convϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{(9.9x-y+10)^2}{9.9(y-0.1)} + 0.1y - 1, & \text{if } -1 \leq x \leq 0.05y - 1.0, \\ -x + 0.18y - 2.02, & \text{if } 0.05y - 1.0 \leq x \leq 2.03 - 0.25y, \\ \frac{(9.9x+2y-20)^2}{9.9(y-0.1)} + 0.4y - 4, & \text{if } 2.03 - 0.25y \leq x \leq 2. \end{cases}$$

To obtain a convex relaxation of ϕ via a standard factorable method, let $t_1 = x^2$ and let t_2 denote the affine underestimator of $\log_{10} y$, $y \in [0.1, 10]$. Using bilinear envelopes to underestimate $t_3 = t_1 t_2$, we obtain:

$$\tilde{\phi} = \max\{0.81(y - 10) + x^2,\ -x - 2\}.$$

The two relaxations are compared in Figure 3.3(b), where it is seen that up to about 80% of the relaxation gap is closed by convϕ.

Similar to the case where $f(x)$ is monotone, the above result is easily generalizable for a multivariate $f(x)$.

3.4.2 Bivariate $g(y)$

In this section, we consider $\phi = f(x)g(y_1, y_2)$, $x \in \mathcal{H}_x^m$, $y \in \mathcal{H}_y^2$, where $f(x)$ is a nonnegative convex function with one of the forms considered in Theorems 3.1 and 3.3 and $g(y_1, y_2)$ is nonnegative and component-wise concave. We will show that, when $g(y)$

is bivariate, similar results to those of Theorems 3.1 and 3.3 can be obtained for much broader classes of $g(y)$. Namely, the restriction of $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^2)$ is not required to be submodular. This generalization follows the fact that, over $\mathrm{vert}(\mathcal{H}_y^2)$, there exist two possible triangulations:

(i) $\Delta_1 = \{(\underline{y}_1, \underline{y}_2), (\underline{y}_1, \bar{y}_2), (\bar{y}_1, \bar{y}_2)\}$ and $\Delta_2 = \{(\underline{y}_1, \underline{y}_2), (\bar{y}_1, \underline{y}_2), (\bar{y}_1, \bar{y}_2)\}$, which corresponds to $\mathrm{conv}g$ when the restriction of $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^2)$ is submodular,

(ii) $\Delta_1' = \{(\underline{y}_1, \underline{y}_2), (\underline{y}_1, \bar{y}_2), (\bar{y}_1, \underline{y}_2)\}$ and $\Delta_2' = \{(\underline{y}_1, \bar{y}_2), (\bar{y}_1, \underline{y}_2), (\bar{y}_1, \bar{y}_2)\}$, which corresponds to $\mathrm{conv}g$ when the restriction of $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^2)$ is *supermodular*.

Obviously, the restriction of a bivariate $g(y)$ to $\mathrm{vert}(\mathcal{H}_y^2)$ is either submodular or supermodular. Let h be a C^2 function which is concave and increasing over the range of $g(y)$. Since the composite function $h(g(y))$ is component-wise concave over $\mathcal{H}_y^2$, by Proposition 3.1, it has a polyhedral convex envelope. Denote by Λ' and Λ'' the sets of optimal multipliers in the descriptions of $\mathrm{conv}g(y)$ and $\mathrm{conv}h(g(y))$ over $\mathcal{H}_y^2$, respectively. Let $\Lambda^* = \Lambda' \cap \Lambda''$. In Propositions 3.3 and 3.5, by letting $h(g) = \varphi_r(g)$, where $\varphi_r(g)$ is given by (3.13), we show that, if Λ^* is nonempty, then it corresponds to the set of optimal multipliers in the description of the convex envelope of $\phi = f(x)g(y_1, y_2)$. In the following lemmas, we first present a simple criterion to evaluate the value of the optimal multipliers for $g(y_1, y_2)$, $y \in \mathcal{H}_y^2$. Subsequently, we derive a number of sufficient conditions under which Λ^* is nonempty and provide a characterization of it in each case. Define $\tilde{y}_1 = (y_1 - \underline{y}_1)/(\bar{y}_1 - \underline{y}_1)$, $\tilde{y}_2 = (y_2 - \underline{y}_2)/(\bar{y}_2 - \underline{y}_2)$. For notational simplicity, let $\tilde{g}_1 = g(\underline{y}_1, \underline{y}_2)$, $\tilde{g}_2 = g(\underline{y}_1, \bar{y}_2)$, $\tilde{g}_3 = g(\bar{y}_1, \underline{y}_2)$, and $\tilde{g}_4 = g(\bar{y}_1, \bar{y}_2)$. We have the following result:

Lemma 3.3. Consider the component-wise concave function $g(y_1, y_2)$, $y \in \mathcal{H}_y^2$. Define $\delta(g) = \tilde{g}_1 - \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4$. Then, the optimal multipliers in the description of the convex envelope of $g(y_1, y_2)$ are given by:

(i) if $\delta(g) \leq 0$:

$$\begin{cases} \lambda_1 = 1 - \tilde{y}_2, \ \lambda_2 = \tilde{y}_2 - \tilde{y}_1, \ \lambda_3 = 0, \ \lambda_4 = \tilde{y}_1, & \text{if } \tilde{y}_1 \leq \tilde{y}_2, \\ \lambda_1 = 1 - \tilde{y}_1, \ \lambda_2 = 0, \ \lambda_3 = \tilde{y}_1 - \tilde{y}_2, \ \lambda_4 = \tilde{y}_2, & \text{if } \tilde{y}_1 \geq \tilde{y}_2. \end{cases} \tag{3.46}$$

(ii) if $\delta(g) \geq 0$:

$$\begin{cases} \lambda_1 = 1 - \tilde{y}_1 - \tilde{y}_2,\ \lambda_2 = \tilde{y}_2,\ \lambda_3 = \tilde{y}_1,\ \lambda_4 = 0, & \text{if } \tilde{y}_1 + \tilde{y}_2 \leq 1, \\ \lambda_1 = 0,\ \lambda_2 = 1 - \tilde{y}_1,\ \lambda_3 = 1 - \tilde{y}_2,\ \lambda_4 = \tilde{y}_1 + \tilde{y}_2 - 1, & \text{if } \tilde{y}_1 + \tilde{y}_2 \geq 1. \end{cases} \tag{3.47}$$

In Lemma 3.3, $\delta(g) = 0$ implies that conv$g(y)$ is affine over $\mathcal{H}_y^2$ (*i.e.* $g(y)$, $y \in \text{vert}(H_y^2)$ is modular). It follows that any feasible set of multipliers is also optimal for conv$g(y)$ in this case. Note that $\delta(g) \leq 0$ (resp. $\delta(g) \geq 0$) is equivalent to the submodularity (resp. supermodularity) of $g(y)$ over vert$(\mathcal{H}_y^2)$. By Lemma 3.3, the set Λ^* defined before is nonempty when $\delta(g)\delta(h(g)) \geq 0$, where $\delta(h(g)) = h(\tilde{g}_1) - h(\tilde{g}_2) - h(\tilde{g}_3) + h(\tilde{g}_4)$. Let $\hat{g}(y)$ denote the restriction of $g(y)$ to the vertices of $\mathcal{H}_y^2$. Obviously, if $\hat{g}(y)$ is constant along any edge of $\mathcal{H}_y^2$, *i.e.* if $\tilde{g}_i = \tilde{g}_j$, for some $(i,j) \in \mathcal{E} = \{(1,2),(1,3),(2,4),(3,4)\}$, then $\delta(g)$ and $\delta(h(g))$ have the same sign and, as a result, Λ^* is nonempty. Thus, suppose that $\tilde{g}_i \neq \tilde{g}_j$ for all $(i,j) \in \mathcal{E}$. Consider $\hat{g}(y)$ with $\tilde{g}_2 \leq \tilde{g}_3 \leq \tilde{g}_1 \leq \tilde{g}_4$. It follows that $\delta(g) > 0$. As another example, consider the same function with $\tilde{g}_1 \leq \tilde{g}_2 \leq \tilde{g}_3 \leq \tilde{g}_4$. In this case, the sign of $\delta(g)$ cannot be determined by the ordering pattern of $\tilde{g}_i$, $i \in I$; *i.e.* depending on the values of $\tilde{g}_i$, $i \in I$, $\delta(g)$ can take both nonnegative and nonpositive values. Based on this simple observation, we introduce the following classification for $g(y_1, y_2)$, which we will use in the sequel:

C1. $\hat{g}(y)$ is non-monotone in at least one argument or is constant over at least one edge of $\mathcal{H}_y^2$. In this case, the sign of $\delta(g)$ is implied by the ordering pattern of $\tilde{g}_i$, $i \in I$. We have the following orderings: (i) $\min\{\tilde{g}_2, \tilde{g}_3\} \leq \min\{\tilde{g}_1, \tilde{g}_4\}$ and $\max\{\tilde{g}_2, \tilde{g}_3\} \leq \max\{\tilde{g}_1, \tilde{g}_4\}$, which implies $\delta(g) \geq 0$, (ii) $\min\{\tilde{g}_1, \tilde{g}_4\} \leq \min\{\tilde{g}_2, \tilde{g}_3\}$ and $\max\{\tilde{g}_1, \tilde{g}_4\} \leq \max\{\tilde{g}_2, \tilde{g}_3\}$, which implies $\delta(g) \leq 0$.

C2. $\hat{g}(y)$ is monotone in each argument and $\tilde{g}_i \neq \tilde{g}_j$, $\forall (i,j) \in \mathcal{E}$. In this case, the sign of $\delta(g)$ cannot be determined from the ordering pattern of $\tilde{g}_i$, $i \in I$. The feasible orderings are: (i) $\min\{\tilde{g}_1, \tilde{g}_4\} \leq \tilde{g}_2, \tilde{g}_3 \leq \max\{\tilde{g}_1, \tilde{g}_4\}$, which implies $\hat{g}(y)$ is nondecreasing (or nonincreasing) in y_1 and y_2 and (ii) $\min\{\tilde{g}_2, \tilde{g}_3\} \leq \tilde{g}_1, \tilde{g}_4 \leq \max\{\tilde{g}_2, \tilde{g}_3\}$, which implies $\hat{g}(y)$ is nonincreasing (resp. nondecreasing) in y_1 and nondecreasing (resp. nonincreasing) in y_2.

By the above classification, if $g(y)$ is in C1, then the sign of $\delta(h(g))$ follows from the ordering pattern of $\tilde{g}_i$, $i \in I$ for any h that is increasing. This, in turn, implies that Λ^*

is nonempty. It is simple to check that, if $g(y)$ is in C1, then $\delta(g) = 0$ if and only if $\delta(h(g)) = 0$. Thus, $\Lambda' = \Lambda''$. Next, suppose that $g(y)$ is in C2. If $\hat{g}(y)$ is component-wise nondecreasing (or nonincreasing), by Lemma 3.1, (i) if $\delta(g) \leq 0$, then $\delta(h(g)) \leq 0$ and (ii) if $\delta(h(g)) \geq 0$, then $\delta(g) \geq 0$. Thus, without loss of generality, let $\hat{g}(y)$ be nondecreasing in y_1 and nonincreasing in y_2. Consider the mapping $T(y_1) = y_1$ and $T(y_2) = \bar{y}_2 + \underline{y}_2 - y_2$. It follows that $\hat{g}(T(y))$ is component-wise nondecreasing and $\delta(g(T(y))) = -\delta(g(y))$. Thus, by Lemma 3.1, (i) if $\delta(g) \geq 0$, then $\delta(h(g)) \geq 0$ and (ii) if $\delta(h(g)) \leq 0$, then $\delta(g) \leq 0$. Hence, we have the following characterizations of Λ^*.

Lemma 3.4. Let $g(y)$, $y \in \mathcal{H}_y^2$, be component-wise concave and let $h(\cdot)$ be concave and increasing over the range of $g(y)$. Let Λ' and Λ'' denote the sets of optimal multipliers in the descriptions of conv$g$ and conv$h(g)$ over $\mathcal{H}_y^2$, respectively. Let $\Lambda^* = \Lambda' \cap \Lambda''$. Denote by $\hat{g}(y)$ the restriction of $g(y)$ to vert$(\mathcal{H}_y^2)$. We have the following cases:

(i) if $\hat{g}(y)$ is nonmonotone in at least one argument or is constant over any edge of $\mathcal{H}_y^2$, then submodularity (resp. supermodularity) of $\hat{g}(y)$ implies the submodularity (resp. supermodularity) of $h(\hat{g}(y))$; *i.e.* $\Lambda' = \Lambda''$, and Λ^* is given by Lemma 3.3,

(ii) if $\hat{g}(y)$ is submodular and nondecreasing (or nonincreasing) in every argument, then $h(\hat{g}(y))$ is submodular and Λ^* is given by (3.46),

(iii) if $h(\hat{g}(y))$ is submodular, nondecreasing in y_1 and nonincreasing in y_2, then $\hat{g}(y)$ is submodular and Λ^* is given by (3.46),

(iv) if $\hat{g}(y)$ is supermodular, nondecreasing in y_1 and nonincreasing in y_2, then $h(\hat{g}(y))$ is supermodular and Λ^* is given by (3.47),

(v) if $h(\hat{g}(y))$ is supermodular and nondecreasing (or nonincreasing) in every argument, then $\hat{g}(y)$ is supermodular and Λ^* is given by (3.47).

In all parts of Lemma 3.4, if $\delta(g) = \delta(h(g)) = 0$; *i.e.* $\tilde{g}_1 = \tilde{g}_2$ and $\tilde{g}_3 = \tilde{g}_4$ (or $\tilde{g}_1 = \tilde{g}_3$ and $\tilde{g}_2 = \tilde{g}_4$), then Λ^* consists of all feasible sets of multipliers for conv$g(y)$ over $\mathcal{H}_y^2$. For example, consider $g(y) = g_1(y_1)g_2(y_2)$, where g_1 and g_2 are nonnegative concave functions. Let (i) $h(u) = u^r$, $0 < r < 1$, $u \geq 0$ and (ii) $h(u) = \log u$, $u > 0$. It is simple to verify that, in both cases, (1) if $(g_1(\bar{y}_1) - g_1(\underline{y}_1))(g_2(\bar{y}_2) - g_2(\underline{y}_2)) \geq 0$, then Part (v) holds and, (2) if $(g_1(\bar{y}_1) - g_1(\underline{y}_1))(g_2(\bar{y}_2) - g_2(\underline{y}_2)) \leq 0$, then Part (iii) is satisfied. This example is of particular importance since $h(u) = u^r$, $0 < r < 1$ and $h(u) = \log u$ are indeed the functions we introduce in Propositions 3.3 and 3.5, respectively. As another example, consider $g(y) = g_1(y_1) + g_2(y_2)$, where g_1 and g_2 are concave functions and let h be any concave function which is increasing over the range of $g(y)$. In this case, (1) if $(g_1(\bar{y}_1) - g_1(\underline{y}_1))(g_2(\bar{y}_2) - g_2(\underline{y}_2)) \geq 0$, then Part (ii) holds and, (2) if $(g_1(\bar{y}_1) - g_1(\underline{y}_1))(g_2(\bar{y}_2) - g_2(\underline{y}_2)) \leq 0$, then Part (iv) is satisfied.

By adding the bivariate restriction on $g(y)$, we next relax the submodularity assumptions of Theorems 3.1 and 3.3 and prove that a similar result holds for many more functional classes. Since the proofs of Theorems 3.1 and 3.3 will be heavily used, we adopt the same notation and will not redefine the symbols.

Proposition 3.3. Let $f(x)$, $x \in \mathcal{H}_x^m$ be a nonnegative convex function of the form $f(x) = (c^T x + d)^a$, $a \in \mathbb{R} \setminus \{[0,1]\}$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$ and, let $g(y_1, y_2)$, $y \in \mathcal{H}_y^2$ be a nonnegative component-wise concave function. Define $\varphi_r(u) = (u^r - 1)/r$, $u \geq 0$, $r = 1/(1-a)$. Denote by Λ' and Λ'', the sets of optimal multipliers in the descriptions of conv$g$ and conv$\varphi_r(g)$ over $\mathcal{H}_y^2$, respectively. Let $\Lambda^* = \Lambda' \cap \Lambda''$. If Λ^* is nonempty then, for any (x, y) in the domain of $\phi = f(x)g(y_1, y_2)$ and any $\lambda^* \in \Lambda^*$, there exists an optimal solution of CX1 with the optimal multipliers given by λ^*.

Proof. We start from Problem (3.23) and will show that, if Λ^* is nonempty, then any $\lambda^* \in \Lambda^*$ is optimal for this problem. First, assume $\delta(g) \neq 0$ or $\delta(h(g)) \neq 0$; *i.e.* Λ^* consists of one set of optimal multipliers, denoted by λ^*. Suppose that $l \geq 0$, where l is as defined in Theorem 3.1. Let $I = I_2$. As it follows from the proof of Theorem 3.1, λ^* is optimal if and only if $\delta(g)\delta(\varphi_r(g)) \geq 0$, where $\delta(g) = \tilde{g}_1 - \tilde{g}_2 - \tilde{g}_3 + \tilde{g}_4$ and $\delta(\varphi_r(g)) = \varphi_r(\tilde{g}_1) - \varphi_r(\tilde{g}_2) - \varphi_r(\tilde{g}_3) + \varphi_r(\tilde{g}_4)$. By Lemma 3.3, this statement follows immediately from the definition of Λ^*. Thus, suppose that (i) I_1 or I_3 and (ii) I_2 are nonempty. To prove the optimality of λ^*, it suffices to show that $\delta(\gamma(g))\delta(g) \geq 0$ (or equivalently $\delta(\gamma(g))\delta(\varphi_r(g)) \geq 0$), where $\gamma(g)$ is given by (3.26) and $\delta(\gamma(g)) = \gamma(\tilde{g}_1) - \gamma(\tilde{g}_2) - \gamma(\tilde{g}_3) + \gamma(\tilde{g}_4)$. Let $\hat{g}(y)$ denote the restriction of $g(y)$ to vert$(\mathcal{H}_y^2)$. If Λ^* is nonempty, then one of the following conditions is satisfied:

1. $\hat{g}(y)$ is nonmonotone in at least one argument or is constant along any edge of $\mathcal{H}_y^2$; *i.e.* $g(y)$ is in C1.

2. $\hat{g}(y)$ is (i) nonincreasing (or nondecreasing) in y_1 and y_2, with $\delta(g) \leq 0$ and $\delta(\varphi_r(g)) \leq 0$ or, (ii) nondecreasing in y_1 and nonincreasing in y_2, with $\delta(g) \geq 0$ and $\delta(\varphi_r(g)) \geq 0$.

3. $\hat{g}(y)$ is (i) nonincreasing (or nondecreasing) in y_1 and y_2, with $\delta(g) \geq 0$ and $\delta(\varphi_r(g)) \geq 0$ or, (ii) nondecreasing in y_1 and nonincreasing in y_2, with $\delta(g) \leq 0$ and $\delta(\varphi_r(g)) \leq 0$.

First, let $g(y)$ be in C1. To prove $\delta(\gamma(g))\delta(g) \geq 0$, it suffices to show that $\gamma(\tilde{g}_i)$, $i \in I$, is nondecreasing in $\tilde{g}_i$; *i.e.* for any $i, j \in I$, if $\tilde{g}_i \leq \tilde{g}_j$, then $\gamma(\tilde{g}_i) \leq \gamma(\tilde{g}_j)$. This statement means that, if $g(y)$ is in C1, then the sign of $\delta(\gamma(g))$ is implied by the ordering pattern of $\tilde{g}_i$, $i \in I$, which in turn proves the optimality of λ^* for Problem (3.23). It is simple to check that, if $i, j \in I_k$, $k \in \{1, 2, 3\}$, then $\gamma(\tilde{g}_i)$ is increasing in $\tilde{g}_i$. Thus, the following cases arise:

(i) $i \in I_1$, $j \in I_2$. By (3.19), if $a < 0$, then $\tilde{g}_i \leq \tilde{g}_j$, while, if $a > 1$, then $\tilde{g}_i \geq \tilde{g}_j$. Consider

$$\gamma(\tilde{g}_j) - \gamma(\tilde{g}_i) = \tilde{g}_j^r w_{\lambda^*}^a / r + alw_{\lambda^*}^{a-1} - l^a \tilde{g}_i. \tag{3.48}$$

Since $i \in I_1$ and $j \in I_2$, by (3.24) we have $l/\tilde{g}_j^r \leq w_{\lambda^*} \leq l/\tilde{g}_i^r$. Over this region, (3.48) is decreasing in w_{λ^*}. Thus, we have the following bounds on $\gamma(\tilde{g}_j) - \gamma(\tilde{g}_i)$:

$$l^a \tilde{g}_i \varphi_r(\tilde{g}_j/\tilde{g}_i) \leq \gamma(\tilde{g}_j) - \gamma(\tilde{g}_i) \leq l^a(\tilde{g}_j - \tilde{g}_i).$$

Two cases arise:

- If $\tilde{g}_i \leq \tilde{g}_j$ (*i.e.* $a < 0$), then $0 < r < 1$. Since $\varphi_r(\cdot)$ is increasing in r, we have $\varphi_r(\tilde{g}_j/\tilde{g}_i) > \log(\tilde{g}_j/\tilde{g}_i) \geq 0$. By nonnegativity of $f(x)$ and $g(y)$ it follows that $l^a \tilde{g}_i \varphi_r(\tilde{g}_j/\tilde{g}_i) \geq 0$. Thus, $\gamma(\tilde{g}_i) \leq \gamma(\tilde{g}_j)$.
- If $\tilde{g}_j \leq \tilde{g}_i$ (*i.e.* $a > 1$), then $l^a(\tilde{g}_j - \tilde{g}_i) \leq 0$, which implies $\gamma(\tilde{g}_j) \leq \gamma(\tilde{g}_i)$.

By symmetry, similar result holds for $i \in I_2$ and $j \in I_3$.

(ii) $i \in I_1$, $j \in I_3$. If $a < 0$ (resp. $a > 1$), then there exists some $k \in I_2$ such that $\tilde{g}_i \leq \tilde{g}_k \leq \tilde{g}_j$. (resp. $\tilde{g}_i \geq \tilde{g}_k \geq \tilde{g}_j$). By Part (i), we have $\gamma(\tilde{g}_i) \leq \gamma(\tilde{g}_k)$ (resp. $\gamma(\tilde{g}_i) \geq \gamma(\tilde{g}_k)$) and $\gamma(\tilde{g}_k) \leq \gamma(\tilde{g}_j)$ (resp. $\gamma(\tilde{g}_k) \geq \gamma(\tilde{g}_j)$). Hence, $\gamma(\tilde{g}_i) \leq \gamma(\tilde{g}_j)$ (resp. $\gamma(\tilde{g}_i) \geq \gamma(\tilde{g}_j)$).

Next, suppose that $\hat{g}(y)$ satisfies one of the conditions of Part 2. If $\hat{g}(y)$ is submodular and component-wise nondecreasing (or nonincreasing) then, by Theorem 3.1, λ^* is optimal for Problem (3.23). Thus, let $\hat{g}(y)$ be nondecreasing in y_1 and nonincreasing in y_2, with

$\delta(g) \geq 0$ and $\delta(\varphi_r(g)) \geq 0$. Consider the mapping $T(y_1) = y_1$ and $T(y_2) = \underline{y}_2 + \bar{y}_2 - y_2$. It follows that $g'(y) = \hat{g}(T(y))$ is component-wise nondecreasing with $\delta(g') = -\delta(g)$. Thus, it suffices to show that $\delta(g') \leq 0$ implies $\delta(\gamma(g')) \leq 0$, which is precisely the statement proved in Theorem 3.1. Now, let $\hat{g}(y)$ satisfy one of the conditions of Part 3. Let g_i, $i \in I$ denote the value of $g(y)$ at the vertices of $\mathcal{H}_y^2$ such that (i) if $a < 0$, then $g_1 \leq \ldots \leq g_4$ and (ii) if $a > 1$, then $g_1 \geq \ldots \geq g_4$. Employing a similar argument as in Part 2, it follows that, to prove the optimality of λ^*, it suffices to show

$$\text{(P)} \qquad \delta(\varphi_r(g)) \geq 0 \quad \Longrightarrow \quad \delta(\gamma(g)) \geq 0,$$

where $\delta(\varphi_r(g)) = \varphi_r(g_1) - \varphi_r(g_2) - \varphi_r(g_3) + \varphi_r(g_4)$ and $\delta(\gamma(g)) = \gamma(g_1) - \gamma(g_2) - \gamma(g_3) + \gamma(g_4)$. Next, we consider all feasible combinations of bounds for Problem (3.23) which are derived from Cases I-V considered in Theorem 3.1, by letting $i_j = j$, $j = 1, \ldots, 4$. For each case, we prove that (P) holds. In the following, by $\underline{w}$ and $\bar{w}$, we denote the minimum and maximum of w_{λ^*}, respectively, given by (3.24).

I. $I_1 = \{1, 2, 3\}$, $I_2 = \{4\}$. Then, $\underline{w} = l/g_4^r$ and $\bar{w} = \min\{l/g_3^r, u/g_4^r\}$. It suffices to show that $\delta(\gamma(g))$ given by (3.27) is nonnegative for $w_{\lambda^*} = \bar{w}$ or some upper bound on $\bar{w}$. Substituting $w_{\lambda^*} = l/g_3^r$ in (3.27), and using $\delta(\varphi_r(g)) \geq 0$, yields

$$\varphi_r((g_1/g_3), (g_2/g_3)) \leq (g_1/g_3) - (g_2/g_3),$$

which follows from (3.15). By symmetry, (P) holds for $I_2 = \{1\}$, $I_3 = \{2, 3, 4\}$.

II. $I_1 = \{1, 2\}$, $I_2 = \{3, 4\}$. Then, $\underline{w} = l/g_3^r$ and $\bar{w} = \min\{l/g_2^r, u/g_4^r\}$. Since $\delta(\gamma(g))$ given by (3.28) is decreasing in w_{λ^*}, it suffices to show that (P) holds for $w_{\lambda^*} = l/g_2^r$. Substituting for w_{λ^*} in $\delta(\gamma(g))$, and using $\delta(\varphi_r(g)) \geq 0$, yields

$$\varphi_r(g_1/g_2) \leq (g_1/g_2) - 1, \tag{3.49}$$

which follows from (3.14). By symmetry, (P) holds for $I_2 = \{1, 2\}$, $I_3 = \{3, 4\}$.

III. $I_1 = \{1\}$, $I_2 = \{2, 3, 4\}$. Then, $\underline{w} = l/g_2^r$ and $\bar{w} = \min\{l/g_1^r, u/g_4^r\}$. By $\varphi_r(g_4) - \varphi_r(g_3) - \varphi_r(g_2) \geq -\varphi_r(g_1)$, it suffices to show that

$$l^a g_1 - a l w_{\lambda^*}^{a-1} - g_1^r w_{\lambda^*}^a / r \geq 0.$$

The left-hand side of the above inequality is decreasing in w_{λ^*} and a lower bound on it is attained at $w_{\lambda^*} = l/g_1^r$, which is equal to zero. By symmetry, (P) is valid for $I_2 = \{1, 2, 3\}$, $I_3 = \{4\}$.

IV. $I_1 = \{1, 2\}$, $I_2 = \{3\}$, $I_3 = \{4\}$. Then, $\underline{w} = \max\{l/g_3^r, u/g_4^r\}$ and $\bar{w} = \min\{l/g_2^r,\ u/g_3^r\}$. Since $\delta(\gamma(g))$ given by (3.32) is decreasing in w_{λ^*}, it suffices to show that $\delta(\gamma(g)) \geq 0$ for $w_{\lambda^*} = \bar{w}$ or an upper bound on $\bar{w}$. Substituting for $w_{\lambda^*} = l/g_2^r$ in $\delta(\gamma(g))$, gives:

$$(g_3/g_2)^r/r + a(u/l) - (u/l)^a (g_4/g_2) \leq (g_1/g_2) - 1.$$

Over $1 \leq u/l \leq (g_4/g_2)^r$, the left-hand side of the above inequality is increasing in u/l. Substituting $u/l = (g_4/g_2)^r$, and using $\delta(\varphi_r(g)) \geq 0$, yields (3.49). By symmetry, (P) holds for $I_1 = \{1\}$, $I_2 = \{2\}$, $I_3 = \{3, 4\}$.

V. $I_1 = \{1\}$, $I_2 = \{2, 3\}$, $I_3 = \{4\}$. Then, $\underline{w} = \max\{l/g_2^r, u/g_4^r\}$ and $\bar{w} = \min\{l/g_1^r,\ u/g_3^r\}$. It is simple to check that the minimum of $\delta(\gamma(g))$ given by (3.34) is attained at $w_{\lambda^*} = (l + u)/(g_2^r + g_3^r)$. Thus, it suffices to show that

$$(1 + u/l)^{-a} g_1 + (1 + l/u)^{-a} g_4 \geq (g_2^r + g_3^r)^{1/r}. \tag{3.50}$$

Over $(g_3/g_2)^r \leq u/l \leq (g_4/g_1)^r$, the left-hand side of (3.50) is decreasing in u/l. Substituting $u/l = (g_4/g_1)^r$ in (3.50), gives $(g_1^r + g_4^r)^{1/r} \geq (g_2^r + g_3^r)^{1/r}$, which follows from $\delta(\varphi_r(g)) \geq 0$. Thus, relation (P) is valid.

Finally, let us consider the case where Λ^* contains a set of four nonzero multipliers; *i.e.* $\delta(g) = \delta(\varphi_r(g)) = 0$. It follows that $\tilde{g}_1 = \tilde{g}_2$ and $\tilde{g}_3 = \tilde{g}_4$ (or $\tilde{g}_1 = \tilde{g}_3$ and $\tilde{g}_2 = \tilde{g}_4$), which in turn implies $\gamma(\tilde{g}_1) = \gamma(\tilde{g}_2)$ and $\gamma(\tilde{g}_3) = \gamma(\tilde{g}_4)$ (or $\gamma(\tilde{g}_1) = \gamma(\tilde{g}_3)$ and $\gamma(\tilde{g}_2) = \gamma((\tilde{g}_4))$. Hence, $\delta(\gamma(g)) = 0$ and any $\lambda^* \in \Lambda^*$ is optimal for Problem (3.23). As discussed in Theorem 3.1, the proofs for the cases where $u \leq 0$ and $l < 0 < u$ are straightforward. $\square$

As an interesting observation, if we let $a > 1$ and $g(y) = y_1 y_2$ in the statement of Proposition 3.3, then there exist regions over which all optimal multipliers in Problem CX1 are nonzero and their values depend on the x variables. This is due to the fact that, while $g(y) = y_1 y_2$, $y \in \mathcal{H}_y^2$ is supermodular, $\varphi_r(g(y))$ is *submodular* for $a > 1$ and is supermodular for $a < 0$. Thus, while it might seem counterintuitive, constructing the convex envelope of $\phi = y_1 y_2 x^2$ is considerably harder than constructing the convex envelope of $\phi = y_1y_2/x$. Employing a similar proof technique, we obtain the following result for the concave envelope of the functions considered in Theorem 3.2.

Proposition 3.4. Let $f(x) = (c^Tx + d)^a$, $a \in (0,1)$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$, $x \in \mathcal{H}_x^m = \{[\underline{x}, \bar{x}] \subset \mathbb{R}^m : c^Tx + d \geq 0\}$, and let $g(y_1, y_2)$, $y \in \mathcal{H}_y^2$ be a component-wise convex function whose restriction to $\text{vert}(\mathcal{H}_y^2)$ is nonnegative. Define $\varphi_r(u) = (u^r - 1)/r$, $u \geq 0$, $r = 1/(1-a)$. Denote by Λ' and Λ'' the sets of optimal multipliers in the descriptions of the concave envelopes of $g(y)$ and $\varphi_r(g(y))$ over $\mathcal{H}_y^2$, respectively. Let $\Lambda^* = \Lambda' \cap \Lambda''$. If Λ^* is nonempty, then it is contained in the set of optimal multipliers corresponding to the concave envelope of $\phi = f(x)g(y_1, y_2)$.

Next, we consider the case where $f(x)$ is exponential. We present the following proposition without proof, since it follows from a line of arguments similar to those in Proposition 3.3 by letting $\varphi_r \to \varphi_0$.

Proposition 3.5. Let $f(x) = a^{c^Tx+d}$, $x \in \mathcal{H}_x^m$, $c \in \mathbb{R}^m$, $d \in \mathbb{R}$, and let $g(y_1, y_2)$ be nonnegative and component-wise concave. Define $\varphi_0(u) = \log u$, $u > 0$. Denote by Λ' and Λ'' the sets of optimal multipliers in the descriptions of $\text{conv}g$ and $\text{conv}\varphi_0(g)$ over $\mathcal{H}_y^2$, respectively. Let $\Lambda^* = \Lambda' \cap \Lambda''$. If Λ^* is nonempty then, for any (x, y) in the domain of $\phi = f(x)g(y_1, y_2)$ and any $\lambda^* \in \Lambda^*$, there exists an optimal solution of CX1 with the optimal multipliers given by λ^*.

Remark 3.4. In Propositions 3.3 and 3.5, the function $\varphi_r(g)$, $r \leq 0$ is undefined at points $y \in \mathcal{H}_y^2$ such that $g(y) = 0$, yet the results are valid for such cases. This can be seen by replacing $g(y) = 0$ with $g(y) = \epsilon$ and letting $\epsilon \searrow 0$ or defining $\varphi_r = -\infty$, if $g(y) = 0$. In the latter case, one can check the nonemptyness of Λ^* using condition (3.6). Namely, Λ^* is nonempty if and only if the restrictions of $g(y)$ and $\varphi_r(g)$ to $\text{vert}(\mathcal{H}_y^2)$ are both submodular (supermodular).

We next present closed-form expressions for the convex envelopes of selected functions of the forms considered in Proposition 3.3 and 3.5. We state the next two corollaries without proofs, since the envelope expressions follow directly from the proofs of Theorems 3.1 and 3.3. In the following, the set $\{i, j, k\}$ denotes the indices of the nonzero optimal multipliers given by Lemma 3.3, rearranged such that (i) if $a < 0$, then $g_i \leq g_j \leq g_k$ and (ii) if $a > 1$, then $g_i \geq g_j \geq g_k$, where g_r, $r \in \{i, j, k\}$ denotes the value of $g(y_1, y_2)$ at the corresponding vertex of $\mathcal{H}_y^2$.

Corollary 3.6. Consider $\phi(x,y) = x^a g(y_1,y_2)$, $a \in \mathbb{R} \setminus \{[0,1]\}$, $0 < \underline{x} \le x \le \bar{x}$. Let $g(y_1,y_2)$ be a nonnegative component-wise concave function and suppose that $\phi(x,y)$ satisfies the conditions of Proposition 3.3. Define $r = 1/(1-a)$ and $\alpha = \lambda_i g_i^r + \lambda_j g_j^r + \lambda_k g_k^r$. Then, the convex envelope of ϕ is given by:

– if $\underline{x} \le x \le (1-\lambda_k)\underline{x} + \lambda_k \min\{(g_k/g_j)^r \underline{x},\ \bar{x}\}$:

$$\text{conv}\phi = (\lambda_i g_i + \lambda_j g_j)\underline{x}^a + \lambda_k^{1-a}(x - (\lambda_i + \lambda_j)\underline{x})^a g_k,$$

– if $(1-\lambda_k)\underline{x} + \lambda_k (g_k/g_j)^r \underline{x} \le x \le \min\{\alpha \underline{x}/g_i^r,\ \lambda_i \underline{x} + (\lambda_j (g_j/g_k)^r + \lambda_k)\bar{x}\}$:

$$\text{conv}\phi = \lambda_i \underline{x}^a g_i + (x - \lambda_i \underline{x})^a \Big(\lambda_j g_j^r + \lambda_k g_k^r\Big)^{1-a},$$

– if $\lambda_i \underline{x} + \lambda_j \max\{\underline{x},\ (g_j/g_k)^r \bar{x}\} + \lambda_k \bar{x} \le x \le \lambda_i \underline{x} + \lambda_j \min\{\bar{x},\ (g_j/g_i)^r \underline{x}\} + \lambda_k \bar{x}$:

$$\text{conv}\phi = \lambda_i \underline{x}^a g_i + \lambda_j^{1-a}(x - \lambda_i \underline{x} - \lambda_k \bar{x})^a g_j + \lambda_k \bar{x}^a g_k,$$

– if $\alpha \underline{x}/g_i^r \le x \le \alpha \bar{x}/g_k^r$: $\text{conv}\phi = x^a \alpha^{1-a}$,

– if $\max\{\alpha \bar{x}/g_k^r,\ (\lambda_i + \lambda_j (g_j/g_i)^r)\underline{x} + \lambda_k \bar{x}\} \le x \le (\lambda_i (g_i/g_j)^r + \lambda_j + \lambda_k)\bar{x}$:

$$\text{conv}\phi = (x - \lambda_k \bar{x})^a \Big(\lambda_i g_i^r + \lambda_j g_j^r\Big)^{1-a} + \lambda_k \bar{x}^a g_k,$$

– if $(1-\lambda_i)\bar{x} + \lambda_i \max\{\underline{x},\ (g_i/g_j)^r \bar{x}\} \le x \le \bar{x}$:

$$\text{conv}\phi = \lambda_i^{1-a}(x - (\lambda_j + \lambda_k)\bar{x})^a g_i + (\lambda_j g_j + \lambda_k g_k)\bar{x}^a.$$

Example 3.7. Let $\phi = y_1 y_2 / x$, $x \in [0.1, 1]$, $y_1 \in [0.1, 1]$, $y_2 \in [0.5, 1.5]$. By Lemma 3.2, $\varphi_r(g) = 2(\sqrt{y_1 y_2} - 1)$ is supermodular and increasing in each argument. Thus, Part (v) of Lemma 3.4 is satisfied and convϕ is can be computed from Corollary 3.6. It follows that, over $20y_1 + 18y_2 \geq 29$, the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{(20y_1+18y_2-29)^2}{12(18x+2y_1+1.8y_2-4.7)} - 5/3y_1 - 5y_2 + 55/6, & \text{if } 0.1 \leq x \leq r_1, \\ \frac{(12.25y_1+4.66y_2-8.21)^2}{9(9x+y_1-1)} - 5/3(y_1 - 1), & \text{if } r_1 \leq x \leq r_2, \\ \frac{(0.93y_1+0.52y_2-0.48)^2}{x}, & \text{if } r_2 \leq x \leq r_3, \\ \frac{(0.43y_1+0.71y_2-1.49)^2}{x-1.11y_1-y_2+1.61} + 1.67y_1 + 1.5y_2 - 2.42, & \text{if } r_3 \leq x \leq r_4, \\ \frac{0.18(y_1-1)^2}{x-1.11y_1+0.11} + 1.67y_1 + y_2 - 1.67, & \text{if } r_4 \leq x \leq 1, \end{cases}$$

where $r_1 = .08y_1 + 0.07y_2 - 0.02$, $r_2 = 0.24y_1 + 0.13y_2 - 0.12$, $r_3 = 0.76y_1 + 0.42y_2 - 0.39$, and $r_4 = 0.5y_1 + 0.5$. Over $20y_1 + 18y_2 \leq 29$, we have:

$$\text{conv}\phi = \begin{cases} \frac{0.5(1.11y_1-0.11)^2}{x+0.11y_1-0.11} + 0.56(0.1 - y_1) + y_2, & \text{if } 0.1 \leq x \leq r_5, \\ \frac{(0.79y_1+0.39y_2-0.27)^2}{(x+0.11y_1+0.1y_2-0.16)} - 0.56y_1 - 0.5y_2 + 0.8, & \text{if } r_5 \leq x \leq r_6, \\ \frac{(0.54y_1+0.16y_2+0.09)^2}{x}, & \text{if } r_6 \leq x \leq r_7, \\ \frac{(0.17-0.25y_1+0.16y_2)^2}{x-1.11y_1+0.11} + 0.55y_1 - 0.06, & \text{if } r_7 \leq x \leq r_8, \\ \frac{0.05(1.61-1.11y_1-y_2)^2}{x-1.11y_1-y_2+0.61} + 0.56y_1 + 0.15y_2 - 0.13, & \text{if } r_8 \leq x \leq 1, \end{cases}$$

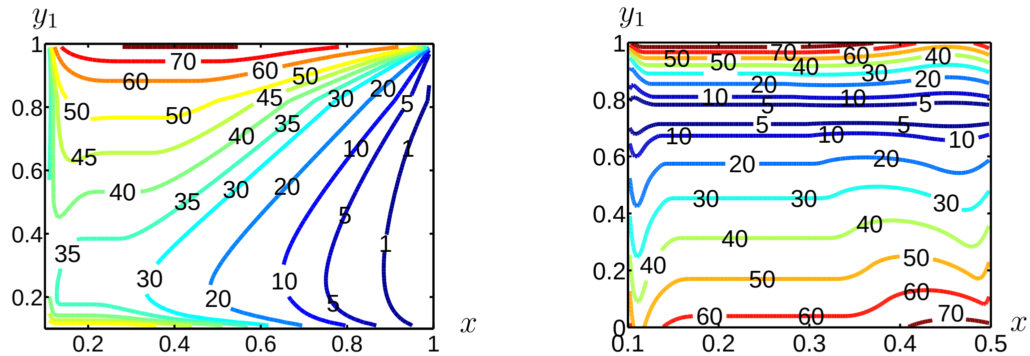
where $r_5 = 0.09y_1 + 0.09$, $r_6 = 0.24y_1 + 0.07y_2 + 0.04$, $r_7 = 0.76y_1 + 0.23y_2 + .12$, and $r_8 = 0.47y_1 + 0.42y_2 + 0.32$. To construct a convex underestimator of ϕ using a factorable relaxation method, let t_1 denote the convex envelope of y_1y_2 and denote by $\tilde{\phi}$ the convex envelope of $t_2 = t_1/x$ given by Corollary 3.2. Then, over $20y_1 + 18y_2 \leq 29$, we obtain:

$$\tilde{\phi} = \begin{cases} \frac{1.5(0.35y_1+0.07y_2-0.07)^2}{x+0.035y_1+0.007y_2-0.107} - 0.17y_1 - 0.035y_2 + 0.53, & \text{if } 0.1 \leq x \leq s_1, \\ \frac{(0.35y_1+0.07y_2+0.15)^2}{x}, & \text{if } s_1 \leq x \leq s_2, \\ \frac{0.024(0.5y_1+0.1y_2-1.55)^2}{x-0.34y_1-0.07y_2+0.07} + 0.52y_1 + 0.103(y_2 - 1), & \text{if } s_2 \leq x \leq 1, \end{cases}$$

where $s_1 = 0.15y_1 + 0.031y_2 + 0.0695$ and $s_2 = 0.28y_1 + 0.056y_2 + 0.13$. Over $20y_1 + 18y_2 \geq 29$, we obtain:

$$\tilde{\phi} = \begin{cases} \frac{1.5(1.03y_1+0.69y_2-1.07)^2}{(x+0.1y_1+0.07y_2-0.21)} - 0.52y_1 - 0.34y_2 + 1.03, & \text{if } 0.1 \leq x \leq s_3, \\ \frac{(1.04y_1+0.69y_2-0.85)^2}{x}, & \text{if } s_3 \leq x \leq s_4, \\ \frac{0.024(1.5y_1+y_2-3)^2}{x-1.03y_1-0.69y_2+1.07} + 1.55y_1 + 1.03y_2 - 1.6, & \text{if } s_4 \leq x \leq 1, \end{cases}$$

where $s_3 = 0.46y_1 + 0.31y_2 - 0.38$ and $s_4 = 0.85y_1 + 0.56y_2 - 0.69$. The gap closed by $\text{conv}\phi$ at $y_2 = 0.7$ is depicted in Figure 3.4(a). Up to over 70% of the relaxation gap is



(a) Example 3.7: $\phi = y_1 y_2 / x$ at $y_2 = 0.7$ (b) Example 3.8: $\phi = x^2\sqrt{y_1+y_2}$ at $y_2 = 1.25$

Figure 3.4: Gaps closed by the convex envelopes for Examples 3.7 and 3.8

closed by the convex envelope.

Example 3.8. Let $\phi = x^2\sqrt{y_1+y_2}$, $x \in [0.1, 0.5]$, $y_1 \in [0,1]$, $y_2 \in [0.5, 1.5]$. By Lemma 3.2, $g(y) = \sqrt{y_1+y_2}$ is submodular and increasing in each argument. Thus, Part (ii) of Lemma 3.4 is satisfied and convϕ is can be obtained from Corollary 3.6. It follows that over $y_2 - y_1 \geq 0.5$, we have:

$$\text{conv}\phi = \begin{cases} \frac{\sqrt{2}}{2}\frac{(x-0.1y_2+0.05)^2}{1.5-y_2} + 0.003(y_1+4y_2-2), & \text{if } 0.1 \leq x \leq r_1, \\ \frac{(x-0.1y_1)^2}{1.71-0.82y_1-0.6y_2} + 0.016y_1, & \text{if } r_1 \leq x \leq r_2, \\ \frac{x^2}{1.71-0.18y_1-0.6y_2}, & \text{if } r_2 \leq x \leq r_3, \\ \frac{(x+0.5y_2-0.75)^2}{-0.41-0.18y_1+0.82y_2} - 0.18y_2 + 0.26, & \text{if } r_3 \leq x \leq r_4, \\ 1.58\frac{(x+0.5y_1-0.5)^2}{y_1} - 0.31y_1 + 0.13y_2 + 0.11, & \text{if } r_4 \leq x \leq 0.5, \end{cases}$$

where $r_1 = 0.21 - 0.07y_2$, $r_2 = 0.27 - 0.03y_1 - 0.09y_2$, $r_3 = 0.6 - 0.06y_1 - 0.21y_2$, and $r_4 = 0.5 - 0.11y_1$. Over $y_2 - y_1 \leq 0.5$ the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{\sqrt{2}}{2}\frac{(x-0.1y_1)^2}{1-y_1} + 0.002(6y_1+2y_2-1), & \text{if } 0.1 \leq x \leq r_5, \\ \frac{(x-0.1y_2+0.05)^2}{1.82-0.6y_1-0.82y_2} + 0.016y_2 - 0.008, & \text{if } r_5 \leq x \leq r_6, \\ \frac{x^2}{1.51-0.6y_1-0.18y_2}, & \text{if } r_6 \leq x \leq r_7, \\ \frac{(x+0.5y_1-0.5)^2}{0.82y_1-0.18y_2+0.09} - 0.177(y_1-1), & \text{if } r_7 \leq x \leq r_8, \\ 1.58\frac{(x+0.5y_2-0.75)^2}{y_2-0.5} + 0.13y_1 - 0.31y_2 + 0.33, & \text{if } r_8 \leq x \leq 0.5, \end{cases}$$

where $r_5 = 0.17 - 0.07y_1$, $r_6 = 0.24 - 0.09y_1 - 0.03y_2$, $r_7 = 0.53 - 0.21y_1 - 0.06y_2$, and $r_8 = 0.56 - 0.11y_2$. To compare with a standard factorable relaxation, let $t_1 = y_1 + y_2$ and denote by $\tilde{\phi}$ the convex envelope of $t_2 = x^2\sqrt{t_1}$ given by Corollary 3.2. It follows that

$$\tilde{\phi} = \begin{cases} 0.003\frac{(y_1+y_2-20x-0.5)^2}{y_1+y_2-2.5} + 0.008(y_1+y_2-0.5), & \text{if } 0.1 \leq x \leq s_1, \\ \frac{x^2}{1.61-0.39(y_1+y_2)}, & \text{if } s_1 \leq x \leq s_2, \\ \frac{(4x+y_1+y_2-2.5)^2}{5(y_1+y_2-0.5)} - 0.09(y_1+y_2) + 0.22, & \text{if } s_2 \leq x \leq 1, \end{cases}$$

where $s_1 = 0.254 - 0.062(y_1+y_2)$ and $s_2 = 0.57 - 0.14(y_1+y_2)$. The gap closed by conv$\phi$ at $y_2 = 1.25$ is depicted in Figure 3.4(b). Up to over 70% of the relaxation gap is closed by the convex envelope.

Next, we present the envelope expressions for the case where $f(x)$ is exponential. In the following, the set $\{i,j,k\}$ denotes the indices of the nonzero optimal multipliers given by Lemma 3.3, rearranged such that (i) if $a < 1$, then $g_i \leq g_j \leq g_k$ and (ii) if $a > 1$, then $g_i \geq g_j \geq g_k$, where g_r, $r \in \{i,j,k\}$ denotes the value of $g(y_1,y_2)$ at the corresponding vertex of $\mathcal{H}_y^2$.

Corollary 3.7. Consider $\phi(x,y) = a^x g(y_1,y_2)$, $a > 0$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$. Let $g(y_1,y_2)$ be a nonnegative component-wise concave function and suppose that $\phi(x,y)$ satisfies the conditions of Proposition 3.5. Then, convϕ is given by:

– if $\underline{x} \leq x \leq \min\{(\lambda_i+\lambda_j)\underline{x} + \lambda_k\bar{x},\ \underline{x} + \lambda_k \log_a(g_j/g_k)\}$:

$$\text{conv}\phi = (\lambda_i g_i + \lambda_j g_j)a^{\underline{x}} + \lambda_k a^{(x-(\lambda_i+\lambda_j)\underline{x})/\lambda_k} g_k,$$

– if $\underline{x}+\lambda_k \log_a(g_j/g_k) \leq x \leq \min\{\underline{x}+\lambda_j \log_a(g_i/g_j)+\lambda_k \log_a(g_i/g_k),\ \lambda_i\underline{x}+\lambda_j \log_a(g_k/g_j)+(\lambda_j+\lambda_k)\bar{x}\}$:

$$\text{conv}\phi = \lambda_i a^{\underline{x}} g_i + (\lambda_j+\lambda_k)a^{(x-\lambda_i\underline{x})/(\lambda_j+\lambda_k)}(g_j^{\lambda_j} g_k^{\lambda_k})^{1/(\lambda_j+\lambda_k)},$$

– if $\lambda_i\underline{x} + \lambda_j \max\{\underline{x},\ \bar{x} + \log_a(g_k/g_j)\} + \lambda_k\bar{x} \leq x \leq \lambda_i\underline{x} + \lambda_j \min\{\underline{x} + \log_a(g_i/g_j),\ \bar{x}\} + \lambda_k\bar{x}$:

$$\text{conv}\phi = \lambda_i a^{\underline{x}} g_i + \lambda_j a^{(x-\lambda_i\underline{x}-\lambda_k\bar{x})/\lambda_j} g_j + \lambda_k a^{\bar{x}} g_k,$$

– if $\underline{x} + \lambda_j \log_a(g_i/g_j) + \lambda_k \log_a(g_i/g_k) \leq x \leq \bar{x} + \lambda_i \log_a(g_k/g_i) + \lambda_j \log_a(g_k/g_j)$:

$$\text{conv}\phi = g_i^{\lambda_i} g_j^{\lambda_j} g_k^{\lambda_k} a^x,$$

– if $\max\{\bar{x} + \lambda_i \log_a(g_k/g_i) + \lambda_j \log_a(g_k/g_j),\ (\lambda_i + \lambda_j)\underline{x} + \lambda_k \bar{x} + \lambda_j \log_a(g_i/g_j)\} \le x \le \bar{x} + \lambda_i \log_a(g_j/g_i)$:

$$\text{conv}\phi = (\lambda_i + \lambda_j) a^{(x-\lambda_k \bar{x})/(\lambda_i+\lambda_j)} (g_i^{\lambda_i} g_j^{\lambda_j})^{1/(\lambda_i+\lambda_j)} + \lambda_k a^{\bar{x}} g_k,$$

– if $\max\{\bar{x} + \lambda_i \log_a(g_j/g_i),\ \lambda_i \underline{x} + (\lambda_j + \lambda_k)\bar{x}\} \le x \le \bar{x}$:

$$\text{conv}\phi = \lambda_i a^{(x-(\lambda_j+\lambda_k)\bar{x})/\lambda_i} g_i + (\lambda_j g_j + \lambda_k g_k) a^{\bar{x}}.$$

Example 3.9. Let $\phi = (2y_1 - y_2)\exp(-x)$, $x \in [-0.5, 1.0]$, $y_1 \in [0.6, 1.5]$, $y_2 \in [0.1, 1.0]$. Then $g(y)$ is modular, increasing in y_1 and decreasing in y_2. Thus, Part (iv) of Lemma 3.4 holds and convϕ is given by Corollary 3.7. Hence, over $y_1 + y_2 \le 1.6$, we have

$$\text{conv}\phi = \begin{cases} \frac{1-y_2}{0.19}\exp\left(\frac{-0.9x-0.45}{1-y_2}\right) + 3.3y_1 + 3.66y_2 - 5.31, & \text{if } 0.1 \le x \le r_1, \\ \frac{y_1-0.6}{0.9}\exp\left(\frac{-0.9x+0.025y_1-0.37y_2-0.72}{y_1-0.6}\right) - 0.37y_1 + 0.55, & \text{if } r_1 \le x \le r_2, \\ \frac{y_1+y_2-1.6}{0.45}\exp\left(\frac{-0.9x+0.5y_1-y_2+0.25}{y_1+y_2-1.6}\right) - 0.37y_1 - 1.18y_2 + 1.73, & \text{if } r_2 \le x \le r_3, \\ \frac{1.5-y_1}{4.5}\exp\left(\frac{-0.9x+y_1-0.6}{1.5-y_1}\right) + 0.82y_1 - 0.37y_2 - 0.12, & \text{if } r_3 \le x \le 1.0, \end{cases}$$

where $r_1 = -0.41y_2 - 0.09$, $r_2 = 1.25y_1 - 0.41y_2 - 0.84$, and $r_3 = 2.56y_1 - 2.84$. Over $y_1 + y_2 \ge 1.6$, the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{y_1-0.6}{0.31}\exp\left(\frac{-0.9x+0.5y_1-0.75}{y_1-0.6}\right) - 2.01y_1 - 1.65y_2 + 3.19, & \text{if } 0.1 \le x \le r_5, \\ \frac{1-y_2}{0.55}\exp\left(\frac{-0.9x+0.97y_1-0.09y_2-0.88}{1-y_2}\right) - 0.74y_2 + 1.07, & \text{if } r_5 \le x \le r_6, \\ \frac{1.6-y_1-y_2}{0.82}\exp\left(\frac{-0.9x+y_1+0.5y_2-1.1}{1.6-y_1-y_2}\right) + 1.18y_1 + 0.37y_2 - 0.75, & \text{if } r_6 \le x \le r_7, \\ \frac{y_2-0.1}{4.5}\exp\left(\frac{-0.9x-y_2+1}{y_2-0.1}\right) + 0.74y_1 - 0.45y_2 + 0.008, & \text{if } r_7 \le x \le 1.0, \end{cases}$$

where $r_5 = 1.08y_1 - 1.15$, $r_6 = 1.08y_1 - 0.59y_2 - 0.56$, and $r_7 = 1.19 - 1.89y_2$. Alternatively, defining $t_1 = 2y_1 - y_2$ and employing the result of Corollary 3.3 to underestimate $t_2 = t_1 \exp(-x)$, we obtain:

$$\tilde{\phi} = \begin{cases} 2.9s\exp\left(\frac{0.5(s-1)-x}{s}\right) + 0.33(1-s), & \text{if } -0.5 \le x \le -0.5 + 2.67s, \\ 0.2\exp(-x)14.5^s, & \text{if } -0.5 + 2.67s \le x \le 1 + 2.67(1-s), \\ 0.2(1-s)\exp\left(\frac{s-x}{1-s}\right) + 1.07s, & \text{if } 1 + 2.67(1-s) \le x \le 1.0, \end{cases}$$

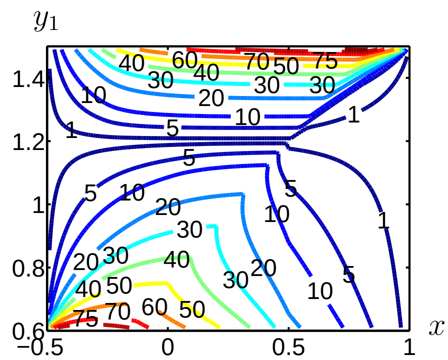


Figure 3.5: Gap closed by the convex envelope of $\phi = (2y_1 - y_2)\exp(-x)$ at $y_2 = 0.4$ for Example 3.9

where $s = 0.37(2y_1 - y_2 - 0.2)$. As shown in Figure 3.5, convϕ at $y_2 = 0.4$ closes up to over 75% of the relaxation gap in comparison to the recursive relaxation.

In Examples 3.8 and 3.9, in order to construct $\tilde{\phi}$, we utilized the convex envelopes of $t_2 = x^2\sqrt{t_1}$ and $t_2 = t_1 \exp(-x)$ that are not currently implemented in global solvers. Standard factorable relaxations are much weaker than $\tilde{\phi}$ for both examples.

3.5 Conclusions

In this chapter, we studied the problem of constructing the convex envelope of a lsc function defined over a compact convex set. We showed that, if the generating set of the convex envelope of the function under consideration can be expressed as the union of a finite number of closed convex sets, then the envelope representation problem can be recast as a convex optimization problem via a nonlinear change of variables. While characterizing the generating set is not an easy task, in general, we identified several important functional classes for which the aforementioned condition is satisfied. At the computational level, and in particular for general-purpose global solvers, it is highly advantageous to have closed-form expressions for the envelopes of functions that appear frequently as building blocks in nonconvex problems. With this goal in mind, we further studied nonnegative functions that are products of convex and component-wise concave functions and derived closed-form expressions for the convex envelopes of various functional forms in this category. In addition to extending this type of analysis to other important functional classes, future research should investigate the computational implications of integrating the proposed envelopes in a global solver and study their effect on the convergence rate of branch-and-bound algorithms in applications.

Chapter 4

Convex envelopes of products of convex and component-wise concave functions

In this chapter, we consider functions of the form $\phi(x, y) = f(x)g(y)$ over a box, where $f(x)$, $x \in \mathbb{R}$ is a nonnegative monotone convex function with a power or an exponential form, and $g(y)$, $y \in \mathbb{R}^n$ is a component-wise concave function which changes sign over the vertices of its domain. Utilizing the results of Chapter 3, we derive closed-form expressions for convex envelopes of various functions in this category. We demonstrate via numerical examples that the proposed envelopes are significantly tighter than popular factorable programming relaxations.

4.1 Introduction

In Chapter 3, we derived a sufficient condition under which the envelope representation problem is equivalent to a certain *convex* optimization problem. Namely, the generating set of the function under consideration is representable as a union of finitely many closed convex sets. We then studied functions of the form $\phi(x, y) = f(c^T x + d)g(y)$, $c, x \in \mathbb{R}^m$, $d \in \mathbb{R}$, $y \in \mathbb{R}^n$ over a box, where $f(\cdot)$ is a nonnegative convex function with a power or an exponential form and $g(y)$ is a *nonnegative* component-wise concave function. Motivated by diverse applications [8, 14], in this chapter, we relax the nonnegativity requirement on $g(y)$, *i.e.* , we permit $g(y)$, $y \in \mathbb{R}^n$, to take both negative and positive values over the vertices of the box over which the function is defined. The convex function $f(x)$ is required to be nonnegative, univariate, and monotone with a power or an exponential form. Under these assumptions, we present closed-form expressions for the convex envelopes of a wide class of functions of the form $\phi(x, y) = f(x)g(y)$. Together with the results of Chapter 3, the proposed envelopes cover over 30% of the nonconvex functions that appear in the popular `GLOBALLib` [14] and `MINLPLib` [8] collections.

The remainder of the chapter is organized as follows. In Section 4.2, we present a brief review of the material from Chapter 3 that we will use in this chapter. In Section 4.3, we derive closed-form expressions for convex envelopes of functions of the form $\phi = f(x)g(y)$ over a box, where $f(x)$, $x \in \mathbb{R}$ is a nonnegative convex function and $g(y)$, $y \in \mathbb{R}^n$ is a component-wise concave function. In Section 4.4, we focus on functions that are products of univariate convex and bivariate component-wise concave functions, and present explicit characterizations of convex envelopes for various functional types that appear frequently in nonconvex optimization problems.

4.2 Preliminaries

Throughout this chapter, ϕ denotes a lsc function defined over a compact convex set $\mathcal{C}$. The set of extreme points of $\mathcal{C}$ will be denoted by $\text{vert}(\mathcal{C})$, and the epigraph of ϕ over $\mathcal{C}$ will be denoted by $\text{epi}_{\mathcal{C}}\phi$. The convex envelope of ϕ over $\mathcal{C}$, denoted by $\text{conv}_{\mathcal{C}}\phi$, is defined as the highest convex function that lies below ϕ on $\mathcal{C}$, and is given by $\text{conv}_{\mathcal{C}}\phi = \inf\{t : (x, t) \in \Phi\}$, where Φ is the convex hull of $\text{epi}_{\mathcal{C}}\phi$. When the domain is clear from the context, we may drop the subscript $\mathcal{C}$ from $\text{conv}_{\mathcal{C}}\phi$. Since ϕ is lsc and $\mathcal{C}$ is compact, the set of extreme points of the convex hull of $\text{epi}_{\mathcal{C}}\phi$ is the minimal set sufficient to characterize $\text{conv}_{\mathcal{C}}\phi$ (cf. Theorem 18.5 in [47]). In the global optimization literature, the projection of this set on $\mathcal{C}$ is often referred to as the *generating set* of ϕ over $\mathcal{C}$ and will be denoted by $\mathcal{G}_{\mathcal{C}}\phi$.

As we discussed in Chapter 3, unless the generating set is finite (*i.e.* the convex envelope is polyhedral), employing the standard disjunctive programming approach for constructing $\text{conv}_{\mathcal{C}}\phi$ leads to a highly nonconvex optimization problem. In a similar vein to Chapter 3, we assume that $\mathcal{G}_{\mathcal{C}}\phi$ is representable as a union of finitely many closed convex sets, *i.e.* $\mathcal{G}_{\mathcal{C}}\phi = \cup_{i \in I}\mathcal{S}_i$, where $\mathcal{S}_i \subset \mathcal{C}$ is a nonempty closed convex set that can be algebraically expressed by a collection of closed convex functions g_{ij} such that

$\mathcal{S}_i = \{u \in \mathcal{C} : g_{ij}(u) \leq 0,\ j = 1, \ldots, m_i\}$ for all $i \in I = \{1, \ldots, p\}$. Under these assumptions, for any $x \in \mathcal{C}$, the value of $\mathrm{conv}_{\mathcal{C}}\phi(x)$ is equal to the optimal value of the following *convex* NLP:

$$\left.\begin{array}{ll} \min\limits_{x^i, \lambda_i} & \sum_{i \in I} \lambda_i \phi\left(x^i / \lambda_i\right) \\ \text{s.t.} & \sum_{i \in I} x^i = x \\ & \sum_{i \in I} \lambda_i = 1 \\ & \lambda_i \geq 0,\ \forall i \in I \\ & \lambda_i g_{ij}\left(x^i/\lambda_i\right) \leq 0,\ j = 1, \ldots, m_i,\ i \in I, \end{array}\right\} \tag{4.1}$$

where x^i is a point in the set $\lambda_i \mathcal{S}_i$ and $\lambda_i \in [0, 1]$ denotes the convex multiplier associated with $\mathcal{S}_i$. Now, consider a continuously differentiable function $g(y)$ over a box $\mathcal{H}_y^n \subset \mathbb{R}^n$. Let the convex envelope of $g(y)$ over $\mathcal{H}_y^n$ be polyhedral. By Proposition 3.1, $\mathcal{G}_{\mathcal{H}_y^n} g(y) = \mathrm{vert}(\mathcal{H}_y^n)$. Thus, Problem (4.1) simplifies to the following LP:

$$\left.\begin{array}{ll} \min\limits_{\lambda_i} & \sum_{i \in I} \lambda_i g(\hat{y}_i) \\ \text{s.t.} & \sum_{i \in I} \lambda_i \hat{y}_i = y \\ & \sum_{i \in I} \lambda_i = 1 \\ & \lambda_i \geq 0,\ \forall i \in I, \end{array}\right\} \tag{4.2}$$

where $\hat{y}_i$, $i \in I = \{1, \ldots, 2^n\}$ denote the vertices of $\mathcal{H}_y^n$. By Proposition 3.2, if $g(y)$, $y \in \mathrm{vert}(\mathcal{H}_y^n)$ is submodular, then an optimal solution of (4.2) can be obtained as follows. Given any $y \in \mathcal{H}_y^n$, let $\tilde{y}_k = (y_k - \underline{y}_k)/(\bar{y}_k - \underline{y}_k)$, $k \in \{1, \ldots, n\}$. Denote by π a permutation of $\{1, \ldots, n\}$ such that $\tilde{y}_{\pi(1)} \geq \tilde{y}_{\pi(2)} \geq \ldots \geq \tilde{y}_{\pi(n)}$. Let e^k denote the kth unit vector in $\mathbb{R}^n$. Then, the set of $n+1$ vertices of $\mathcal{H}_y^n$ with nonzero optimal multipliers are $\nu = \{\nu_j : \nu_j = \underline{y} + (\bar{y} - \underline{y}) \sum_{k=1}^{j-1} e^{\pi(k)},\ j = 1, \ldots n+1\}$. Finally, the values of the optimal multipliers associated with ν_j are given by $\tilde{\lambda}_1 = 1 - \tilde{y}_{\pi(1)}$, $\tilde{\lambda}_j = \tilde{y}_{\pi(j-1)} - \tilde{y}_{\pi(j)}$, $j = 2, \ldots, n$, $\tilde{\lambda}_{n+1} = \tilde{y}_{\pi(n)}$. Let $\tilde{I} = \{i \in I : \hat{y}_i = \nu_j, \text{for some } j \in \{1, \ldots, n+1\}\}$ and, for each $i \in \tilde{I}$, let $q(i)$ be equal to a j such that $\hat{y}_i = \nu_j$. Then, the set λ^* given by:

$$\lambda_i^* = \begin{cases} \tilde{\lambda}_{q(i)}, & \text{if } i \in \mathcal{I} \\ 0, & \text{otherwise,} \end{cases} \tag{4.3}$$

is an optimal solution of Problem (4.2).

4.3 Convex envelopes of products of convex and component-wise concave functions

Consider a function $\phi(x,y) = f(x)g(y)$ on a box $\mathcal{C} = [\underline{x}, \bar{x}] \times [\underline{y}, \bar{y}]$. Let $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ be a nonnegative monotone convex function with one of the following forms: (i) $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0,1]\}$ and (ii) $f(x) = a^x$, $a > 0$. Let the function $g(y)$, $y \in \mathcal{H}_y^n = [\underline{y}, \bar{y}] \subset \mathbb{R}^n$ be component-wise concave In Chapter 3, we considered the case where $g(y)$ is nonnegative. It is simple to check that $\mathrm{conv}_{\mathcal{C}}\phi$ is polyhedral if $g(y)$ is nonpositive over the vertices of $\mathcal{H}_y^n$. Thus, in the following, we assume that the sign of $g(y)$ changes over $\mathrm{vert}(\mathcal{H}_y^n)$. It should be noted that the results of this section are applicable for $\phi(x,y) = \tilde{f}(x)g(y)$, where $\tilde{f}(x) = f(cx+d)$, for some $c, d \in \mathbb{R}$, by letting $u = cx + d$, $\underline{u} = \min\{c\underline{x}, c\bar{x}\} + d$, $\bar{u} = \max\{c\underline{x}, c\bar{x}\} + d$, and using the fact that, if $\psi = f(u)g(y)$, $\mathcal{D} = [\underline{u}, \bar{u}] \times \mathcal{H}_y^n$, then $\mathrm{conv}_{\mathcal{C}}\phi(x,y) = \mathrm{conv}_{\mathcal{D}}\psi(cx+d, y)$. Denote by $\hat{y}_i$, $i \in I = \{1, \ldots, 2^n\}$, the vertices of $\mathcal{H}_y^n$. Let $I_N = \{i \in I : g(\hat{y}_i) < 0\}$, $I_P = I \setminus I_N$, and $I_0 = \{i \in I_P : g(\hat{y}_i) = 0\}$. Then, by Proposition 3.1 and Corollary 3.1, the generating set of ϕ over $\mathcal{C}$ is given by:

$$\mathcal{G}_{\mathcal{C}}\phi = \{(x, \hat{y}_i),\ \underline{x} \le x \le \bar{x},\ i \in I_P \setminus I_0\} \cup \{\{x, \hat{y}_i\},\ x \in \{\underline{x}, \bar{x}\},\ i \in I_0 \cup I_N\}.$$

It follows that the number p of convex components in $\mathcal{G}_{\mathcal{C}}\phi$ and, hence, the size of Problem (4.1) increase exponentially in the dimension of $\mathcal{C}$. In order to construct $\mathrm{conv}_{\mathcal{C}}\phi$, we employ a sequential convexification approach. We first convexify $\phi(x,y)$ over the vertices of $\mathcal{H}_y^n$ where $g(y)$ is negative. Since $\phi(x, \hat{y}_i) = f(x)g(\hat{y}_i)$ is a univariate concave function for all $i \in I_N$, the convex envelope of $\phi(x, \hat{y}_i)$, $i \in I_N$ over $[\underline{x}, \bar{x}]$ is affine. For notational simplicity, let $\Delta x = \bar{x} - \underline{x}$ and $\Delta f = f(\bar{x}) - f(\underline{x})$. Then, it follows from (4.1) that, for any $(x, y) \in \mathcal{C}$, the value of $\text{conv}_{\mathcal{C}}\phi(x, y)$ can be found by solving

$$
\begin{aligned}
\text{(CN)} \qquad \min_{x^i,\lambda_i} \quad & \sum_{i\in I_N} \left(\frac{\Delta f}{\Delta x} x^i + \frac{\bar{x} f(\underline{x}) - \underline{x} f(\bar{x})}{\Delta x} \lambda_i \right) g(\hat{y}_i) + \sum_{i\in I_P} \lambda_i f\left(x^i/\lambda_i\right) g(\hat{y}_i) \\
\text{s.t.} \quad & \sum_{i\in I} x^i = x && (4.4) \\
& \sum_{i\in I} \lambda_i \hat{y}_i = y \\
& \sum_{i\in I} \lambda_i = 1 \\
& \lambda_i \underline{x} \leq x^i \leq \lambda_i \bar{x}, \ \forall i \in I && (4.5) \\
& \lambda_i \geq 0, \ \forall i \in I,
\end{aligned}
$$

where, as in (4.1), the variables are x^i and λ_i for all $i \in I$, for a total number of 2^{n+1} variables. Problem CN is convex and continuous. However, due to the presence of perspective expressions $\lambda_i f(\cdot/\lambda_i)$, the objective function of CN is not differentiable at any point where $\lambda_i = 0$ for some $i \in I_P$. As we will demonstrate later, over a large region of $\mathcal{C}$, optimal solutions of CN are in fact points of non-differentiability. Thus, efficient gradient-based convex solvers cannot be easily employed to solve Problem CN. Motivated by this discussion, in the remainder of this chapter, we are interested in solving CN analytically to derive explicit characterization of $\text{conv}_{\mathcal{C}}\phi$. In Section 3.4.1 of Chapter 3, we addressed the case where $g(y)$ is a univariate function. We will henceforth assume that $n \geq 2$.

Before proceeding further, we recall the concept of generalized means (see Chapter III of [17] for an exposition), which we will use in the following proofs to simplify the formulas. Let $b = \{b_s, \ s \in \mathcal{S}\}$ denote a set of nonnegative numbers with a set of nonnegative weighting coefficients given by $\mu = \{\mu_s, \ s \in \mathcal{S}\}$. Let $\omega(x)$, $\min_{s\in\mathcal{S}} b_s \leq x \leq \max_{s\in\mathcal{S}} b_s$, be a continuous and strictly monotonic function. The weighted mean of the set b associated with $\omega(\cdot)$ is defined as:

$$
\Omega_\omega(b, \mu, \mathcal{S}) = \omega^{-1}\left(\frac{\sum_{s\in\mathcal{S}} \mu_s \omega(b_s)}{\sum_{s\in\mathcal{S}} \mu_s} \right), \tag{4.6}
$$

where $\omega^{-1}(\cdot)$ denotes the inverse function. For example, if we let $\omega(x) = x$ or $\omega(x) = \log x$, then (4.6) simplifies to the weighted arithmetic and geometric means of b, respectively.

Define

$$\varphi_r(x) = \int_1^x v^{r-1}\mathrm{d}v = \frac{x^r - 1}{r}, \quad x > 0,\ r \in \mathbb{R} \setminus \{0\}. \tag{4.7}$$

It follows that $\lim_{r\to 0} \Omega_{\varphi_r(x)}(b, \mu, \mathcal{S}) = \Omega_{\log(x)}(b, \mu, \mathcal{S})$. For notational simplicity, we denote $\Omega_{\varphi_r}(\cdot)$, by $\Omega_r(\cdot)$, in the sequel. In particular, $\varphi_0(x) = \log(x)$ and $\Omega_0(\cdot) = \Omega_{\log(x)}(\cdot)$. Since $\varphi_r(x)$ is an increasing function of r, for $-\infty < r < 1$, we have:

$$\varphi_r(x) \leq x - 1. \tag{4.8}$$

We now present the main result of this section. To wit, under certain assumptions, we solve Problem CN analytically and derive closed-form expressions for the convex envelope of $\phi(x, y)$ over $\mathcal{C}$.

Theorem 4.1. Let the convex function $f(x)$, $x \in [\underline{x}, \bar{x}] \in \mathbb{R}$ be nonnegative and monotone with one of the following forms: (i) $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0, 1]\}$ and (ii) $f(x) = a^x$, $a > 0$. Suppose that $g(y)$, $y \in \mathcal{H}_y^n$ is a component-wise concave function such that its restriction to $\mathrm{vert}(\mathcal{H}_y^n)$ is submodular and nondecreasing (or nonincreasing) in every argument. Then, given any $(x, y) \in \mathcal{C}$, there exists an optimal solution of Problem CN with the optimal multipliers λ^* given by (4.3).

Proof. If $I_N = \emptyset$, the result follows from the proofs of Theorem 3.1. We will henceforth assume that $I_N \neq \emptyset$. We start by partially minimizing CN with respect to x^i, $i \in I$, assuming the last two sets of inequalities are inactive. First, consider the case $I_P \setminus I_0 \neq \emptyset$. Writing the KKT conditions for CN with respect to x^i, $i \in I$, yields:

$$\Delta f g(\hat{y}_i)/\Delta x = f'\left(x^j/\lambda_j\right) g(\hat{y}_j), \quad \forall i \in I_N,\ j \in I_P \setminus I_0, \tag{4.9}$$

where $f'(x)$ denotes the derivative of $f(x)$. By monotonicity of $f(x)$ over $[\underline{x}, \bar{x}]$, it follows that the expressions in the right- and left-hand sides of (4.9) have opposite signs. Thus, no optimal solution of CN is attained in the relative interior of its feasible region. We next present the proof for the case where $f(x)$ is decreasing. By symmetry, a similar line of arguments holds for an increasing $f(x)$. Denote by g_i, $i \in I$ the value of $g(y)$ at the vertices of $\mathcal{H}_y^n$ such that $g_1 \leq g_2 \leq \ldots \leq g_{2^n}$. Let $I_N = \{1, \ldots, r-1\}$ and $I_P = \{r, \ldots, 2^n\}$. Since by assumption I_N and I_P are nonempty, we have $2 \leq r \leq 2^n$. From (4.5) and (4.9), it follows that at any optimal solution of CN (i) if $\lambda_i \underline{x} < x^i < \lambda_i \bar{x}$ for some $i \in I_N$, then

$x^i = \lambda_i \bar{x}$ for all $i \in I_P \setminus I_0$ and (ii) if $\lambda_i \underline{x} < x^i < \lambda_i \bar{x}$ for some $i \in I_P \setminus I_0$, then $x^i = \lambda_i \underline{x}$ for all $i \in I_N$. Thus, two cases arise:

- $x^i = \lambda_i \bar{x}$ for all $i \in I_P \setminus I_0$. First, suppose that $I_0 = \emptyset$ and $g_{i_1} \neq g_{i_2}$ for all $i_1, i_2 \in I_N$. By (4.4), (4.5), and (4.9), over

$$\underline{x} \sum_{i=1}^{r-j} \lambda_i + \bar{x} \sum_{i=r-j+1}^{2^n} \lambda_i \leq x \leq \underline{x} \sum_{i=1}^{r-j-1} \lambda_i + \bar{x} \sum_{i=r-j}^{2^n} \lambda_i, \quad \forall\, j = 1, \ldots, r-1, \tag{4.10}$$

we have $x^i = \lambda_i \underline{x}$, for all $i = 1, \ldots r-j-1$, $x^i = x - \underline{x} \sum_{k=1}^{r-j-1} \lambda_k - \bar{x} \sum_{k=r-j+1}^{2^n} \lambda_k$ for $i = r-j$, and $x^i = \lambda_i \bar{x}$, for all $i = r-j+1, \ldots, r-1$. Substituting for x^i, $i \in I$ in Problem CN, we obtain the following LP:

$$\left.\begin{array}{ll} \min\limits_{\lambda_i} & \sum_{i=1}^{r-j} \lambda_i \left(f(\underline{x}) g_i - \frac{\Delta f}{\Delta x} \underline{x} g_{r-j} \right) + \sum_{i=r-j+1}^{2^n} \lambda_i \left(f(\bar{x}) g_i - \frac{\Delta f}{\Delta x} \bar{x} g_{r-j} \right) \\ & + \frac{\Delta f}{\Delta x} x g_{r-j} \\ \text{s.t.} & \sum_{i \in I} \lambda_i \hat{y}_i = y \\ & \sum_{i \in I} \lambda_i = 1 \\ & \lambda_i \geq 0, \ \forall i \in I. \end{array}\right\} \tag{4.11}$$

By Proposition 3.2, the set λ^* given by (4.3) is optimal for Problem (4.11), if and only if the function $\kappa(g) : \mathrm{vert}(\mathcal{H}_y^n) \to \mathbb{R}$, given by

$$\kappa(g) = \begin{cases} f(\underline{x}) g_i - \frac{\Delta f}{\Delta x} \underline{x} g_{r-j}, & \text{if } i \in \{1, \ldots, r-j\} \\ f(\bar{x}) g_i - \frac{\Delta f}{\Delta x} \bar{x} g_{r-j}, & \text{if } i \in \{r-j+1, \ldots, 2^n\}. \end{cases} \tag{4.12}$$

is submodular. Since $f(x)$ is nonnegative, it follows that $\kappa(g)$ is increasing in g_i, $i \in I$. Denote by $\hat{\kappa}(u)$, a continuous extension of $\kappa(g)$ over the interval $u \in [g_1, g_{2^n}]$, defined as follows:

$$\hat{\kappa}(u) = \begin{cases} f(\underline{x}) u - \frac{\Delta f}{\Delta x} \underline{x} g_{r-j}, & \text{if } u \in [g_1, g_{r-j}] \\ f(\bar{x}) u - \frac{\Delta f}{\Delta x} \bar{x} g_{r-j}, & \text{if } u \in [g_{r-j}, g_{2^n}]. \end{cases} \tag{4.13}$$

Note that $\hat{\kappa}(u) = \kappa(g)$ at all $u = g_i$, $i \in I$. By (4.13), $\hat{\kappa}(u)$ consists of two affine segments intersecting at $u = g_{r-j}$. Furthermore, since $f(x)$ is decreasing by assumption, the slope of the second segment is less than the slope of the first one. It follows that $\hat{\kappa}(\cdot)$ is concave and increasing over an interval which contains the range of g_i, $i \in I$. Hence, by Part (i) of Lemma 3.1, $\kappa(g)$ is submodular and λ^* is optimal for (4.11).

Next, let $I_0 \neq \emptyset$. Define $I' = \{1, \ldots, r-j\} \cup I_0$, for some $j \in \{1, \ldots, r-1\}$. Then, over

$$\underline{x} \sum_{i \in I'} \lambda_i + \bar{x} \sum_{i \in I \setminus I'} \lambda_i \leq x \leq \underline{x} \sum_{i=1}^{r-j-1} \lambda_i + \bar{x} \sum_{i=r-j}^{2^n} \lambda_i,$$

we have $x^i = \lambda_i \underline{x}$, for all $i = 1, \ldots r-j-1$, $x^i = x - \sum_{k \in I_0} x^k - \underline{x} \sum_{k=1}^{r-j-1} \lambda_k - \bar{x} \sum_{k \in I \setminus I'} \lambda_k$ for $i = r-j$, and $x^i = \lambda_i \bar{x}$, for all $i \in I \setminus I'$. Since the objective function of CN is increasing in x^i for all $i \in I_N$, we conclude that its minimum is attained when $x^k = \lambda_k \bar{x}$ for all $k \in I_0$. Thus, the result follows. Now, suppose that $g_l = \ldots = g_q$, for some $\{l, \ldots, q\} \subseteq I_N$. Then, over $\underline{x} \sum_{i=1}^{q} \lambda_i + \bar{x} \sum_{i=q+1}^{2^n} \lambda_i \leq x \leq \underline{x} \sum_{i=1}^{l-1} \lambda_i + \bar{x} \sum_{i=l}^{2^n} \lambda_i$, we have $x^i = \lambda_i \underline{x}$, for all $i \in \{1, \ldots, l-1\}$, $\sum_{i=l}^{q} x^i = x - \underline{x} \sum_{i=1}^{l-1} \lambda_i - \bar{x} \sum_{i=q+1}^{2^n} \lambda_i$, and $x^i = \lambda_i \bar{x}$, for all $i \in \{q+1, \ldots, r-1\}$. Substituting for x^i, $i \in I$ in Problem CN, we obtain (4.11) with $r - j = q$. Thus, λ^* is optimal.

We now consider the case $I_P = \emptyset$, *i.e.* $r = 2^n + 1$. As we discussed earlier, $\mathrm{conv}_C \phi$ is polyhedral in this case. In addition, as it follows from the above argument, over the regions defined by (4.10), this polyhedral envelope is given by the objective function of (4.11), where the optimal multipliers are given by (4.3).

– $x^i = \lambda_i \underline{x}$ for all $i \in I_N$. First, suppose that all multipliers are nonzero and the inequalities $\lambda_i \underline{x} \leq x^i \leq \lambda_i \bar{x}$ are inactive for all $i \in I' = I_P \setminus I_0$. From (4.4) and (4.9)

$$x^i/\lambda_i = \frac{g_i^{1/(1-a)}}{\sum_{j \in I'} \lambda_j g_j^{1/(1-a)}} \left(x - \underline{x} \sum_{j \in I_N} \lambda_j - \sum_{j \in I_0} x^j \right), \ \forall i \in I', \tag{4.14}$$

if $f(x) = x^a$, and

$$x^i/\lambda_i = \left(\sum_{j \in I'} \lambda_j \log_a (g_j/g_i) + x - \underline{x} \sum_{j \in I_N} \lambda_j - \sum_{j \in I_0} x^j \right) / \sum_{j \in I'} \lambda_j, \ \forall i \in I', \tag{4.15}$$

if $f(x) = a^x$. From (4.14) and (4.15) it follows that x^i, $i \in I'$ is decreasing in $\sum_{j \in I_0} x^j$. Since the objective function of CN is decreasing in x^i for all $i \in I'$, at any optimal solution of CN, we have $x^i = \lambda_i \underline{x}$ for all $i \in I_0$. Define $r = 1/(1-a)$, if $f(x) = x^a$ and $r = 0$, if $f(x) = a^x$. For notational simplicity, we will denote $\Omega_r(g, \lambda, J)$, $J \subseteq I$, as defined in (4.6), by $\Omega_r(J)$. Substituting $x^i = \lambda_i \underline{x}$, $i \in I_0$ in (4.14) and (4.15), we obtain:

$$x^i/\lambda_i = \tau_a\left(\Omega_r(I')\tau_a^{-1}\left(\left(x - \underline{x}\sum_{j\in I_N\cup I_0}\lambda_j\right)/\sum_{j\in I'}\lambda_j\right)/g_i\right), \quad \forall i \in I', \tag{4.16}$$

where (i) $\tau_a(u) = u^{1/(a-1)}$, if $f(x) = x^a$ and (ii) $\tau_a(u) = \log_a u$, if $f(x) = a^x$. Furthermore, $\tau_a^{-1}(\cdot)$ denotes the inverse of $\tau_a(\cdot)$. Now, partition I_P as $I_P = I_1 \cup I_2 \cup I_3$, where I_1 and I_3 denote the sets of indices with the associated x^i in (4.5) at their lower and upper bounds, respectively. Since $f(x)$ is decreasing by assumption, it follows that $\tau_a(u)$ is decreasing in u. Hence, by (4.16) we have $x^r/\lambda_r \le x^{r+1}/\lambda_{r+1} \le \ldots \le x^{2^n}/\lambda_{2^n}$. Consequently, let $I_1 = \{r,\ldots,s-1\}$, $I_2 = \{s,\ldots,t\}$ and, $I_3 = \{t+1,\ldots,2^n\}$. For consistency, if $s = r$, we set $I_1 = \emptyset$ with $g_{s-1} = 0$. Similarly, if $t = 2^n$, then $I_3 = \emptyset$ with $g_{t+1} = +\infty$. Moreover, suppose that I_2 is nonempty. As discussed in the proof of Theorem 3.1, this assumption is without loss of generality. Define

$$x_\lambda = \left(x - \underline{x}\sum_{i\in I_N\cup I_1}\lambda_i - \bar{x}\sum_{i\in I_3}\lambda_i\right)/\sum_{i\in I_2}\lambda_i.$$

Substituting $x^i = \lambda_i\underline{x}$ for all $i \in I_N \cup I_1$, $x^i = \lambda_i\bar{x}$ for all $i \in I_3$ in CN, and minimizing the resulting problem with respect to x^i, $i \in I_2$, yields:

$$x^i/\lambda_i = \tau_a\left(\Omega_r(I_2)\tau_a^{-1}(x_\lambda)/g_i\right), \quad \forall i \in I_2. \tag{4.17}$$

From (4.5) and (4.17), it follows that:

$$x_\lambda \ge \max\left\{\tau_a\left(g_s\tau_a^{-1}(\underline{x})/\Omega_r(I_2)\right),\ \tau_a\left(g_{t+1}\tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right)\right\}, \tag{4.18}$$

and

$$x_\lambda \le \min\left\{\tau_a\left(g_{s-1}\tau_a^{-1}(\underline{x})/\Omega_r(I_2)\right),\ \tau_a\left(g_t\tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right)\right\}, \tag{4.19}$$

where the lower bounds in (4.18) are obtained from the conditions $x^s \ge \lambda_s\underline{x}$ and $x^{t+1} \ge \lambda_{t+1}\bar{x}$, and the upper bounds in (4.19) correspond to $x^{s-1} \le \lambda_{s-1}\underline{x}$ and $x^t \le \lambda_t\bar{x}$.

Substituting (4.17) in Problem CN, yields

$$\left.\begin{array}{ll}\min\limits_{\lambda_i} & f(\underline{x})\sum_{i\in I_N\cup I_1}\lambda_i g_i + \left(\sum_{i\in I_2}\lambda_i\right) f\left(x_\lambda\right)\Omega_r(I_2) + f(\bar{x})\sum_{i\in I_3}\lambda_i g_i \\ \text{s.t.} & \sum_{i\in I}\lambda_i\hat{y}_i = y \\ & \sum_{i\in I}\lambda_i = 1 \\ & \lambda_i \geq 0,\ \forall i\in I.\end{array}\right\} \tag{4.20}$$

We now prove that λ^* given by (4.3) is optimal for (4.20) by demonstrating that it satisfies the KKT conditions for this problem. Since the feasible regions of Problems (4.2) and (4.20) are identical, λ^* is feasible for (4.20). It is simple to show that (see the proof of Theorem 3.1 for details), λ^* satisfies the KKT conditions for Problem (4.20), if and only if the function $\gamma(g) : \text{vert}(\mathcal{H}_y^n) \to \mathbb{R}$, where $\gamma(g_i)$ is the partial derivative of the objective function of (4.20) with respect to λ_i, and is given by

$$\gamma(g_i) = \begin{cases} f(\underline{x})g_i - \underline{x}f'(x_{\lambda^*})\Omega_r(I_2), & \text{if } i\in I_N\cup I_1 \\ \left(f(x_{\lambda^*})\left(1+\varphi_r(g_i/\Omega_r(I_2))\right) - x_{\lambda^*}f'(x_{\lambda^*})\right)\Omega_r(I_2), & \text{if } i\in I_2 \\ f(\bar{x})g_i - \bar{x}f'(x_{\lambda^*})\Omega_r(I_2), & \text{if } i\in I_3, \end{cases} \tag{4.21}$$

is submodular. We first show that $\gamma(g)$ is a nondecreasing function of g_i, $i\in I$, *i.e.* for any $i,j\in I$, if $g_i\leq g_j$, then $\gamma(g_i)\leq\gamma(g_j)$. Since $f(x)$ is nonnegative and $\varphi_r(u)$, $u\geq 0$ as defined in (4.7), is increasing in u, we conclude that if $i,j\in I_N\cup I_1$, or $i,j\in I_k$, $k\in\{2,3\}$, then $\gamma(g_i)$ is increasing in g_i. Thus, the following cases arise:

(i) $i\in I_N\cup I_1$, $j\in I_2$. In this case, $\Delta\gamma = \gamma(g_j)-\gamma(g_i)$ is given by

$$\Delta\gamma = \left(f(x_{\lambda^*})\left(1+\varphi_r(g_j/\Omega_r(I_2))\right) - (x_{\lambda^*}-\underline{x})f'(x_{\lambda^*})\right)\Omega_r(I_2) - f(\underline{x})g_i. \tag{4.22}$$

Since $j\in I_2$, by (4.18), we have $x_{\lambda^*}\geq\tau_a\left(g_j\tau_a^{-1}(\underline{x})/\Omega_r(I_2)\right)$. Over this region, the right-hand side of (4.22) is decreasing in x_{λ^*}. First, consider the case $i\in I_1$. By (4.19), $x_{\lambda^*}\leq\tau_a\left(g_i\tau_a^{-1}(\underline{x})/\Omega_r(I_2)\right)$. Thus, a lower bound on $\Delta\gamma$ can be obtained by letting $x_{\lambda^*}=\tau_a\left(g_i\tau_a^{-1}(\underline{x})/\Omega_r(I_2)\right)$, which is given by $\Delta\gamma\geq f(\underline{x})g_i\varphi_r(g_j/g_i)$. Since $f(x)$ is decreasing by assumption, $g_i\leq g_j$ and $0\leq r<1$. From (4.7), it follows that $\varphi_r(g_j/g_i)\geq\log(g_j/g_i)\geq 0$. Thus, we have $\gamma(g_i)\leq\gamma(g_j)$. Now, consider the case $i\in I_N$. Clearly, if $I_1\neq\emptyset$, then the result follows from the above argument by noting that $\gamma(g_i)$ is increasing in g_i, $i\in I_N\cup I_1$. Thus, let

$I_1 = \emptyset$. By (4.19), a lower bound on $\Delta\gamma$ is attained at $x_{\lambda^*} = \tau_a\left(g_j \tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right)$. Substituting for x_{λ^*} in (4.22), yields $\Delta\gamma \geq (f(\bar{x}) - f'(\bar{x})\Delta x)g_j - f(\underline{x})g_i > 0$, where the second inequality holds since $f'(x)$ and g_i are both negative by assumption.

(ii) $i \in I_2$, $j \in I_3$. In this case, $\Delta\gamma$, as defined in Part (i), is given by

$$\Delta\gamma = f(\bar{x})g_j - \left(f(x_{\lambda^*})\left(1 + \varphi_r(g_i/\Omega_r(I_2))\right) + (\bar{x} - x_{\lambda^*})f'(x_{\lambda^*})\right)\Omega_r(I_2). \tag{4.23}$$

By (4.18) and (4.19), $\tau_a\left(g_j \tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right) \leq x_{\lambda^*} \leq \tau_a\left(g_i \tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right)$. Over this region, the right-hand side of (4.23) is decreasing in x_{λ^*}. Substituting $x_{\lambda^*} = \tau_a\left(g_i \tau_a^{-1}(\bar{x})/\Omega_r(I_2)\right)$ in (4.23), gives $\Delta\gamma \geq f(\bar{x})(g_j - g_i) \geq 0$. Thus, $\gamma(g_i) \leq \gamma(g_j)$.

(iii) $i \in I_N \cup I_1$, $j \in I_3$. In this case, there exists some $k \in I_2$ such that $g_i \leq g_k \leq g_j$. By Part (i), $\gamma(g_i) \leq \gamma(g_k)$ and by Part (ii), $\gamma(g_k) \leq \gamma(g_j)$. Hence, we have $\gamma(g_i) \leq \gamma(g_j)$.

As in the previous part, we now introduce a continuous extension of $\gamma(g)$, denoted by $\hat{\gamma}(\cdot)$ which is concave and nondecreasing over an interval that contains the range of g_i, $i \in I$, with $\hat{\gamma}(u) = \gamma(g)$ for all $u = g_i$, $i \in I$. It follows that λ^* is optimal for (4.20). Consider the function $\hat{\gamma}(u)$, $u \in [g_1, g_{2^n}]$, defined as follows:

$$\hat{\gamma}(u) = \begin{cases} f(\underline{x})u - \underline{x}f'(x_{\lambda^*})\Omega_r(I_2), & \text{if } u \in [g_1, g_{s-1}] \\ \gamma(g_{s-1}) + \frac{\gamma(g_s) - \gamma(g_{s-1})}{g_s - g_{s-1}}(u - g_{s-1}), & \text{if } u \in [g_{s-1}, g_s] \\ \left(f(x_{\lambda^*})\left(1 + \varphi_r(u/\Omega_r(I_2))\right) - x_{\lambda^*}f'(x_{\lambda^*})\right)\Omega_r(I_2), & \text{if } u \in [g_s, g_t] \\ \gamma(g_t) + \frac{\gamma(g_{t+1}) - \gamma(g_t)}{g_{t+1} - g_t}(u - g_t), & \text{if } u \in [g_t, g_{t+1}] \\ f(\bar{x})u - \bar{x}f'(x_{\lambda^*})\Omega_r(I_2), & \text{if } u \in [g_{t+1}, g_{2^n}]. \end{cases} \tag{4.24}$$

As we showed earlier, $\gamma(g_i)$ is nondecreasing in g_i, $i \in I$. It follows that $\hat{\gamma}(u)$ is also nondecreasing over $u \in [g_1, g_{2^n}]$. Further, since $\varphi_r(\nu)$, $\nu \geq 0$ is a concave function, $\hat{\gamma}(u)$ is piece-wise concave. Namely, $\hat{\gamma}(u)$ is concave over $u \in [g_s, g_u]$, and is affine over $u \in [g_i, g_j]$, for all $(i,j) \in \{(1, s-1), (s-1, s), (t, t+1), (t+1, 2^n)\}$. Denote by $d^-(u_0)$ and $d^+(u_0)$, respectively, the left and right derivatives of $\hat{\gamma}(u)$ at some $u_0 \in [g_1, g_{2^n}]$. It is simple to check that, to establish the concavity of $\hat{\gamma}(u)$, it suffices to show that $d^+(u_0) \leq d^-(u_0)$ for all $u_0 \in \{g_{s-1},\ g_s,\ g_t,\ g_{t+1}\}$; namely, $\hat{\gamma}(u)$ has a nonincreasing slope over $[g_1, g_{2^n}]$. By symmetry, one needs to only consider $u_0 = g_{s-1}$ and $u_0 = g_s$.

First, let $u_0 = g_{s-1}$. In this case, it suffices to show that

$$\left(f(x_{\lambda^*})\left(1+\varphi_r(g_s/\Omega_r(I_2))\right) - (x_{\lambda^*} - \underline{x})f'(x_{\lambda^*})\right)\Omega_r(I_2) \le f(\underline{x})g_s. \tag{4.25}$$

By (4.18), it follows that the left-hand side of (4.25) is nonincreasing in x_{λ^*}. Thus, an upper bound on it is attained at $x_{\lambda^*} = \tau_a(g_s\tau_a^{-1}(\underline{x})/\Omega_r(I_2))$ and equals the right-hand side of (4.25). Thus, (4.25) is valid and, as a result, $d^+(u_0) \le d^-(u_0)$ at $u_0 = g_{s-1}$. Next, let $u_0 = g_s$. By (4.24), we need to show that the following relation is valid:

$$f(x_{\lambda^*})\left(1+\varphi_r(\hat{g}) - (x_{\lambda^*} - \underline{x})f'(x_{\lambda^*})\right)\Omega_r(I_2) - f(x_{\lambda^*})\hat{g}^{r-1}\Delta g \ge f(\underline{x})g_{s-1}, \tag{4.26}$$

where $\hat{g} = g_s/\Omega_r(I_2)$ and $\Delta g = g_s - g_{s-1}$. It can be shown that, as a function of x_{λ^*}, the left-hand side of (4.26) attains a local maximum in the interior of the domain. Thus, it suffices to check the following cases:

(i) $x_{\lambda^*} = \tau_a(g_{s-1}\tau_a^{-1}(\underline{x})/\Omega_r(I_2))$. Substituting for x_{λ^*} in (4.26), we obtain

$$\varphi_r\left(g_{s-1}/g_s\right) \le (g_{s-1}/g_s) - 1,$$

which follows from (4.8).

(ii) $x_{\lambda^*} = \tau_a(g_s\tau_a^{-1}(\underline{x})/\Omega_r(I_2))$. It is simple to check that, in this case, the left-hand side of (4.26) equals its right-hand side.

It follows from the above arguments that $\hat{\gamma}(\cdot)$ is concave and nondecreasing over the range of g. Hence, by Part (i) of Lemma 3.1, $\gamma(g_i)$, $i \in I$ is submodular and, as a result, λ^* is optimal for (4.20). This completes the proof.

$\square$

Remark 4.1. The result of Theorem 4.1 is valid for any function $g(y)$ with a polyhedral convex envelope over $\mathcal{H}_y^n$. It is important to note that component-wise concavity is only a *sufficient* condition for polyhedrality of $\text{conv}_{\mathcal{H}_y^n} g(y)$. However, recognition of component-wise concave functions is relatively simple and these functional forms appear frequently in nonconvex optimization problems.

Now, let us revisit the case where $g(y)$ is nonpositive over the vertices of $\mathcal{H}_y^n$; *i.e.* $\text{conv}_{\mathcal{C}}\phi(x,y)$ is polyhedral. As it follows from the proof of Theorem 4.1, to derive the closed-form expression for the convex envelope, no assumption on the form of the convex function $f(x)$ is required. More precisely, we have the following corollary.

Corollary 4.1. Consider the function $\phi = f(x)g(y)$, $(x,y) \in \mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^n$. Let $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ be nonnegative convex and let $g(y)$, $y \in \mathcal{H}_y^n$ be a component-wise concave function such that its restriction to $\mathrm{vert}(\mathcal{H}_y^n)$ is nonpositive, submodular and nondecreasing (or nonincreasing) in every argument. Denote by g_i, $i \in I$, the value of $g(y)$ at the vertices of $\mathcal{H}_y^n$ such that (i) if $f(\underline{x}) \geq f(\bar{x})$, then $g_1 \leq g_2 \leq \ldots \leq g_{2^n}$, and (ii) if $f(\underline{x}) \leq f(\bar{x})$, then $g_1 \geq g_2 \geq \ldots \geq g_{2^n}$. Let $q(j) = 2^n - j + 1$ for all $j \in I$. Then, over

$$\underline{x} \sum_{i=1}^{q(j)} \lambda_i^* + \bar{x} \sum_{i=q(j)+1}^{2^n} \lambda_i^* \leq x \leq \underline{x} \sum_{i=1}^{q(j)-1} \lambda_i^* + \bar{x} \sum_{i=q(j)}^{2^n} \lambda_i^*, \quad \forall\, j \in I,$$

the convex envelope of ϕ over $\mathcal{C}$ is given by:

$$\sum_{i=1}^{q(j)} \lambda_i^* \left(f(\underline{x}) g_i - \frac{\Delta f}{\Delta x} \underline{x} g_{q(j)} \right) + \sum_{i=q(j)+1}^{2^n} \lambda_i^* \left(f(\bar{x}) g_i - \frac{\Delta f}{\Delta x} \bar{x} g_{q(j)} \right) + \frac{\Delta f}{\Delta x} x g_{q(j)},$$

where the set λ^* is given by (4.3).

For functions satisfying the conditions of Theorem 4.1, the closed-form expressions for the convex envelopes are given by the objective functions of (i) Problem (4.11) over the regions defined by (4.10), and (ii) Problem (4.20) over the regions given by inequalities (4.18) and (4.19). In the following section, we will investigate the strength of these envelopes in comparison to standard factorable relaxations.

4.4 Convex envelopes of products of convex and bivariate component-wise concave functions

In this section, we consider functions of the form $\phi(x,y) = f(x)g(y_1,y_2)$ over $\mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^2$, where, as in Section 4.3, $f(x)$, $[\underline{x}, \bar{x}] \subset \mathbb{R}$ is a nonnegative convex function with a power or an exponential form. However, we restrict our attention to the case of a *bivariate* component-wise concave $g(y)$ that takes both negative and positive values over $\mathcal{H}_y^2$. In Theorem 4.1, in addition to component-wise concavity, we assume that the restriction of $g(y)$ to the vertices of $\mathcal{H}_y^n$ is submodular and nondecreasing (or nonincreasing) in every argument. These assumptions were key in proving the decoupling between the optimal multipliers λ^* and x variables. For the bivariate $g(y)$, however, similar results can be obtained in a more general setting. This generalization is due to the fact that, over $\mathcal{H}_y^2$, there exist two candidate sets of multipliers for Problem (4.2), and the optimality of each can be stated in terms of submodularity or supermodularity of $g(y)$ over $\text{vert}(\mathcal{H}_y^2)$, as given by Lemma 3.3.

Let $\hat{g}(y)$ denote the restriction of $g(y)$ to the vertices of $\mathcal{H}_y^2$. Suppose that $\hat{g}(y)$ is supermodular, nondecreasing in y_1 and nonincreasing in y_2. Consider the mapping $T(y_1) = y_1$ and $T(y_2) = \underline{y}_2 + \bar{y}_2 - y_2$. It follows that the restriction of $g'(y) = g(T(y))$ to $\text{vert}(\mathcal{H}_y^2)$ is submodular and nondecreasing in both arguments. Thus, the result of Theorem 4.1 is valid for this case. Now, let $\hat{g}(y)$ be nonmonotone in at least one argument or be constant over at least one edge of $\mathcal{H}_y^2$ (*i.e.* $\tilde{g}_i = \tilde{g}_j$ for some $(i,j) \in \{(1,2),(1,3),(2,4),(3,4)\}$). It follows that one of the following cases arises:

(i) $\min\{\tilde{g}_2, \tilde{g}_3\} \leq \min\{\tilde{g}_1, \tilde{g}_4\}$, and $\max\{\tilde{g}_2, \tilde{g}_3\} \leq \max\{\tilde{g}_1, \tilde{g}_4\}$,

(ii) $\min\{\tilde{g}_1, \tilde{g}_4\} \leq \min\{\tilde{g}_2, \tilde{g}_3\}$, and $\max\{\tilde{g}_1, \tilde{g}_4\} \leq \max\{\tilde{g}_2, \tilde{g}_3\}$.

It is simple to verify that, for all above configurations, the sign of $\delta(g)$, as defined in the statement of Lemma 3.3, is *implied* by the ordering pattern of $\tilde{g}_i$, $i \in I$. For example, consider the supermodular function $g(y) = y_1 y_2$, where $\underline{y}_1 < 0 < \bar{y}_1$ and $0 < \underline{y}_2 < \bar{y}_2$. It follows that $\tilde{g}_2 < \tilde{g}_1 < \tilde{g}_3 < \tilde{g}_4$, which implies $\delta(g) > 0$. More generally, if $g(y) = g_1(y_1)g_2(y_2)$, where $g_1(y_1)$ is a nonnegative affine function and $g_2(y_2)$ is a concave function with $g_2(\underline{y}_2) < 0 < g_2(\bar{y}_2)$, then we have $\delta(g) > 0$ (resp. $\delta(g) < 0$), if g_1 is increasing (resp. decreasing). As another example, consider the bilinear function $g(y) = y_1 y_2$ with $\underline{y}_1 < 0 < \bar{y}_1$ and $\underline{y}_2 < 0 < \bar{y}_2$. In this case, we have $\max\{\tilde{g}_2, \tilde{g}_3\} < \min\{\tilde{g}_1, \tilde{g}_4\}$, which in turn implies $\delta(g) > 0$. We can further generalize this example to $g(y) = g_1(y_1)g_2(y_2)$, where $g_1(y_1)$ and $g_2(y_2)$ are affine functions both of which change sign over their domains. It follows that (i) if $g(\bar{y}_1)g(\bar{y}_2) \geq 0$, then $\delta(g) > 0$, and (ii) if $g(\bar{y}_1)g(\bar{y}_2) \leq 0$, then $\delta(g) < 0$. Motivated by these examples, we now show that, if the sign of $\delta(g)$ is implied by the ordering pattern of $\tilde{g}_i$, $i \in I$, then the optimal multipliers corresponding to $\text{conv}_{\mathcal{H}_y^2} g(y)$ are also optimal for the envelope representation problem of $\phi(x,y) = f(x)g(y_1,y_2)$ over $\mathcal{C}$.

The proof of Theorem 4.1 involved two main steps: (i) the function $\kappa(g)$ defined in accordance with Problem (4.11) is submodular over $\text{vert}(\mathcal{H}_y^n)$, and (ii) the function $\gamma(g)$

given by (4.21) and associated with Problem (4.20) is submodular over $\mathrm{vert}(\mathcal{H}_y^n)$. Under the submodularity and monotonicity assumptions on $g(y)$, $y \in \mathrm{vert}(\mathcal{H}_y^n)$, it follows that the set λ^* given by (4.3) is optimal for CN. For bivariate $g(y)$, let $\delta(\kappa) = \kappa(\tilde{g}_1) - \kappa(\tilde{g}_2) - \kappa(\tilde{g}_3) + \kappa(\tilde{g}_4)$ and $\delta(\gamma) = \gamma(\tilde{g}_1) - \gamma(\tilde{g}_2) - \gamma(\tilde{g}_3) + \gamma(\tilde{g}_4)$. By Lemma 3.3, if $\delta(g)\delta(\kappa) \geq 0$ and $\delta(g)\delta(\gamma) \geq 0$, there exists an optimal set of multipliers corresponding to $\mathrm{conv}_{\mathcal{H}_y^2} g(y)$ that is also optimal for the envelope representation problem of $\phi(x, y)$ over $\mathcal{C}$. In the proof of Theorem 4.1, in order to prove the submodularity of $\kappa(g)$ and $\gamma(g)$, we first demonstrated that both functions are nondecreasing in g_i, $i \in I$. This implies that, if $\hat{g}(y_1, y_2)$ is nonmonotone in at least one argument or is constant along any edge of $\mathcal{H}_y^2$, the signs of $\delta(\kappa)$ and $\delta(\gamma)$ are also implied by the ordering pattern of $\tilde{g}_i$, $i \in I$, and hence are the same as the sign of $\delta(g)$. Let $\delta(g) = 0$. It is simple to check that $\tilde{g}_{i_1} = \tilde{g}_{i_2}$ and $\tilde{g}_{i_3} = \tilde{g}_{i_4}$, where $I = \{i_1, i_2, i_3, i_4\}$. Since by assumption $I_N \neq \emptyset$, we have (i) $|I_N| = 2$ with $I_N = \{i_1, i_2\}$ and $I_2 = \{i_3, i_4\}$ or (ii) $|I_N| = 4$. It can be shown that, in both cases, $\delta(\kappa) = \delta(\gamma) = 0$, *i.e.* any feasible solution of Problem (4.2) is optimal for the envelope representation problem of $\phi(x, y)$ over $\mathcal{C}$. Thus, we have

Proposition 4.1. Let the convex function $f(x)$, $x \in [\underline{x}, \bar{x}] \in \mathbb{R}$ be nonnegative and monotone with one of the following forms (i) $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0, 1]\}$, (ii) $f(x) = a^x$, $a > 0$. Let $g(y_1, y_2)$, $y \in \mathcal{H}_y^2$ be component-wise concave with $I_N \neq \emptyset$. Denote by $\hat{g}(y)$ the restriction of $g(y_1, y_2)$ to vertices of $\mathcal{H}_y^2$. We have the following cases:

(i) If $\hat{g}(y)$ is submodular and nondecreasing (or nonincreasing) in both arguments, then the set of multipliers given by (3.46) is optimal for the envelope representation problem of $\phi = f(x)g(y_1, y_2)$ over $\mathcal{C}$.

(ii) If $\hat{g}(y)$ is supermodular, nondecreasing in y_1 and nonincreasing in y_2, then the set of multipliers given by (3.47) is optimal for the envelope representation problem of $\phi = f(x)g(y_1, y_2)$ over $\mathcal{C}$.

(iii) If $\hat{g}(y)$ is nonmonotone in at least one argument or is constant over any edge of $\mathcal{H}_y^2$, then the optimal multipliers in the description of $\mathrm{conv}_{\mathcal{H}_y^2} g(y)$ are also optimal for the envelope representation problem of $\phi = f(x)g(y_1, y_2)$ over $\mathcal{C}$.

Next, we present closed-form expressions for the convex envelope of $\phi = f(x)g(y_1, y_2)$ over $\mathcal{C}$, assuming $g(y)$ attains negative values over one, two, three, and all four vertices of $\mathcal{H}_y^2$ in turn. We state several corollaries without proofs since the results are immediate from the proof of Theorem 4.1. In the following, $\{i,j,k\}$ denotes the index set of nonzero multipliers given by Proposition 4.1, such that $g_i \le g_j \le g_k$, where g_i, $i \in I$ denotes the value of $g(y)$ at $\text{vert}(\mathcal{H}_y^2)$. As in the proof of Theorem 4.1, let (i) $\tau_a(u) = u^{1/(a-1)}$, if $f(x) = x^a$ and (ii) $\tau_a(u) = \log_a u$, if $f(x) = a^x$. For notational simplicity, we denote $\Omega_r(\lambda, g, I')$, $I' = \{i_1, \dots i_k\}$, by $\Omega_r(i_1, \dots, i_k)$, where, as before, $r = 1/(1-a)$, if $f = x^a$ and $r = 0$, if $f(x) = a^x$. We provide the envelope expressions for the case where $f(x)$ is decreasing. By symmetry, the formulas for the increasing $f(x)$ can be similarly obtained. For a quantitative comparison of the proposed envelopes and conventional factorable relaxations, we compute the percentage of the gap closed by $\text{conv}_{\mathcal{C}}\phi$ at $x \in \mathcal{C}$ as

$$(\text{conv}_{\mathcal{C}}\phi(x) - \tilde{\phi}(x))/(\phi(x) - \tilde{\phi}(x)) \times 100\%,$$

where $\tilde{\phi}$ denotes a convex underestimator of ϕ obtained by a standard factorable relaxation scheme.

Corollary 4.2. Consider $\phi = f(x)g(y_1, y_2)$, $\mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^2$, where $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ is nonnegative convex and decreasing with one of the following forms: (i) $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0,1]\}$ and (ii) $f(x) = a^x$, $a > 0$. Suppose that $g(y)$, $y \in \mathcal{H}_y^2$, is a component-wise concave function with $g_1 < 0 \le g_2 \le g_3 \le g_4$, and $\hat{g}(y)$ satisfies one of the conditions of Proposition 4.1. Then, the convex envelope of $\phi(x,y)$ over $\mathcal{C}$ is given by:

- $\underline{x} \le x \le (1-\lambda_k)\underline{x} + \lambda_k \min\{\bar{x}, \tau_a(g_j/g_k)\underline{x}\}$:

$$\text{conv}\phi = (\lambda_i g_i + \lambda_j g_j) f(\underline{x}) + \lambda_k f\left(\frac{x - (\lambda_i + \lambda_j)\underline{x}}{\lambda_k}\right) g_k,$$

- $(1-\lambda_k)\underline{x} + \lambda_k \min\{\bar{x}, \tau_a(g_j/g_k)\underline{x}\} \le x \le \lambda_i \underline{x} + \lambda_j \max\{\underline{x}, \tau_a(g_k/g_j)\bar{x}\} + \lambda_k \bar{x}$:

$$\text{conv}\phi = \lambda_i f(\underline{x}) g_i + (\lambda_j + \lambda_k) f\left(\frac{x - \lambda_i \underline{x}}{\lambda_j + \lambda_k}\right) \Omega_r(j,k),$$

- $\lambda_i \underline{x} + \lambda_j \max\{\underline{x}, \tau_a(g_k/g_j)\bar{x}\} + \lambda_k \bar{x} \le x \le \lambda_i \underline{x} + (1-\lambda_i)\bar{x}$:

$$\text{conv}\phi = \lambda_i f(\underline{x}) g_i + \lambda_j f\left(\frac{x - \lambda_i \underline{x} - \lambda_k \bar{x}}{\lambda_j}\right) g_j + \lambda_k f(\bar{x}) g_k,$$

- $\lambda_i \underline{x} + (1-\lambda_i)\bar{x} \le x \le \bar{x}$: $\text{conv}\phi = \Delta f/\Delta x (x - \bar{x}) g_i + (\lambda_i g_i + \lambda_j g_j + \lambda_k g_k) f(\bar{x})$.

Example 4.1. Let $\phi = (y_1 + y_2)/x$, $x \in [1,5]$, $y_1 \in [-2,1]$, $y_2 \in [1,3]$. Then, by Part (i) of Proposition 4.1, the convex envelope of ϕ is given by Corollary 4.2. Thus, over $3y_2 - 2y_1 \geq 7$, we have:

$$\text{conv}\phi = \begin{cases} \frac{4(y_1+2)^2}{3(3x+y_1-1)} - y_1/3 + y_2 - 8/3, & \text{if } 1 \leq x \leq (y_1+5)/3, \\ \frac{(2y_1+3y_2+1)^2}{18(2x+y_2-3)} + 0.5(y_2-3), & \text{if } (y_1+5)/3 \leq x \leq s_1, \\ \frac{(2y_1-3y_2+7)^2}{6(6x-10y_1+3y_2-29)} + 4/15y_1 + 0.5y_2 - 29/30, & \text{if } s_1 \leq x \leq 2y_2 - 1, \\ 0.2(x+y_1+y_2) - 1, & \text{if } 2y_2 - 1 \leq x \leq 5, \end{cases}$$

where $s_1 = (10y_1 + 9y_2 + 23)/12$. Over $3y_2 - 2y_1 \leq 7$, convϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{2(y_2-1)^2}{(2x+y_2-3)} + y_1 - y_2 + 2, & \text{if } 1 \leq x \leq 0.21y_2 + 0.79, \\ \frac{3(0.47y_1+0.29y_2+0.65)^2}{3x+y_1-1} + (y_1-1)/3, & \text{if } 0.21y_2 + 0.79 \leq x \leq s_2, \\ \frac{(2y_1-3y_2+7)^2}{3(6x+2y_1-15y_2+13)} + y_1/3 + 0.4y_2 - 11/15, & \text{if } s_2 \leq x \leq (4y_1+11)/3, \\ 0.2(x+y_1+y_2) - 1, & \text{if } (4y_1+11)/3 \leq x \leq 5, \end{cases}$$

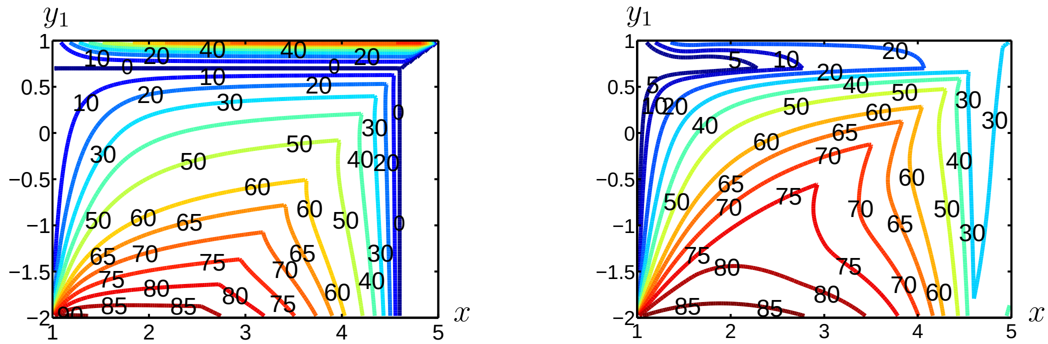
where $s_2 = 0.85y_1 + 0.73y_2 + 1.96$. To compare with a standard factorable relaxation, let $t = y_1 + y_2$. Utilizing the convex envelope of the fractional term t/x [25, 61], we obtain the following convex underestimator for ϕ:

$$\tilde{\phi}_1 = \begin{cases} 0.2(y_1+y_2-4) + \frac{0.16(y_1+y_2+1)^2}{x+0.2(y_1+y_2-4)}, & \text{if } 1 \leq x \leq 0.8(y_1+y_2) + 1.8, \\ 0.2(y_1+y_2+x) - 1, & \text{if } 0.8(y_1+y_2) + 1.8 \leq x \leq 5. \end{cases}$$

Alternatively, a convex underestimator of ϕ can be constructed by first disaggregating ϕ as $\phi = y_1/x + y_2/x$, and then employing the convex envelope of the fractional term to obtain $\tilde{\phi}_2 = \text{conv}(y_1/x) + \text{conv}(y_2/x)$. The percentage of relaxation gaps of $\tilde{\phi}_1$ and $\tilde{\phi}_2$ closed by convϕ at $y_2 = 2.8$ are depicted in Figures 4.1(a) and 4.1(b), respectively. Up to over 85% of the gap is closed by the convex envelope in both cases.

Corollary 4.3. Consider $\phi = f(x)g(y_1, y_2)$, $\mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^2$, where $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ is a nonnegative convex and decreasing function with one of the following forms: (i) $f(x) = x^a$, $a \in \mathbb{R} \setminus \{[0,1]\}$ and (ii) $f(x) = a^x$, $a > 0$. Suppose that $g(y)$, $y \in \mathcal{H}_y^2$ is a component-wise concave function with $g_1 \leq g_2 < 0 \leq g_3 \leq g_4$, and $\hat{g}(y)$ satisfies one of the conditions of Proposition 4.1. We have the following cases:

(i) If $\hat{g}(y)$ is nonmonotone in both arguments, then $\text{conv}_{\mathcal{C}}\phi(x,y)$ is given by:



(a) aggregated recursive relaxation

(b) disaggregated recursive relaxation

Figure 4.1: Gap closed by the convex envelope of $\phi = (y_1+y_2)/x$ at $y_2 = 2.8$ in Example 4.1

- $\underline{x} \le x \le \lambda_k \bar{x} + (1-\lambda_k)\underline{x}$:

$$\operatorname{conv}\phi = (\lambda_i g_i + \lambda_j g_j) f(\underline{x}) + \lambda_k f\left(\frac{x-(1-\lambda_k)\underline{x}}{\lambda_k}\right) g_k,$$

- $\lambda_k \bar{x} + (1-\lambda_k)\underline{x} \le x \le \lambda_i \underline{x} + (1-\lambda_i)\bar{x}$:

$$\operatorname{conv}\phi = \lambda_i f(\underline{x}) g_i + \Delta f/\Delta x (x - \lambda_i \underline{x} - (1-\lambda_i)\bar{x}) g_j + (\lambda_j g_j + \lambda_k g_k) f(\bar{x}),$$

- $\lambda_i \underline{x} + (1-\lambda_i)\bar{x} \le x \le \bar{x}$: $\operatorname{conv}\phi = \Delta f/\Delta x (x - \bar{x}) g_i + (\lambda_i g_i + \lambda_j g_j + \lambda_k g_k) f(\bar{x})$.

(ii) Otherwise, over the triangular sub-region of $\mathcal{H}_y^2$ as defined by Lemma 3.3, where $g(y)$ is negative over one vertex, the convex envelope of ϕ over $\mathcal{C}$ is given by Corollary 4.2, and over the sub-region where $g(y)$ attains negative values over two vertices, $\operatorname{conv}_{\mathcal{C}}\phi$ is given by the expressions in Part (i).

Example 4.2. Let $\phi = y_1 y_2 / x$, $x \in [0.1, 1]$, $y_1 \in [-1, 1]$, $y_2 \in [0.1, 1]$. In this case, $g(y)$ is nonmonotone in y_2. Thus, Part (iii) of Proposition 4.1 and Part (ii) of Corollary 4.3 are satisfied. Then, over $0.9y_1 + 2y_2 \ge 1.1$, we have

$$\operatorname{conv}\phi = \begin{cases} \frac{(0.5y_1+1.1y_2-0.6)^2}{x+0.05y_1+0.11y_2-0.16} + 5y_1 - 1.1y_2 - 3.9, & \text{if } 0.1 \le x \le s_1, \\ \frac{(0.5y_1+0.76y_2-0.26)^2}{x+0.05y_1-0.05} + 5y_1 - 5, & \text{if } s_1 \le x \le s_2, \\ \frac{0.12(y_2-1)^2}{x-0.45y_1-1.1y_2+0.56} + 5.5y_1 + 1.1y_2 - 5.6, & \text{if } s_2 \le x \le s_3, \\ 10x + y_1 + y_2 - 11, & \text{if } s_3 \le x \le 1, \end{cases}$$

where $s_1 = 0.11y_1 + 0.24y_2 - 0.03$, $s_2 = 0.45y_1 + 0.76y_2 - 0.21$, and $s_3 = 0.45y_1 + 0.55$.

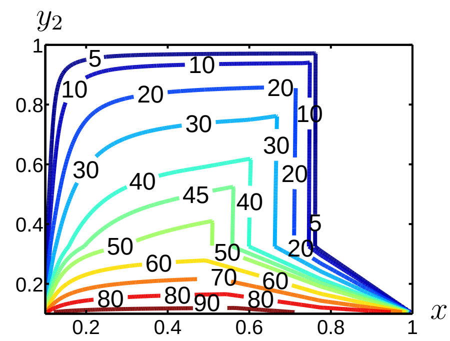


Figure 4.2: Gap closed by the convex envelope of $\phi = y_1y_2/x$ at $y_1 = 0.5$ in Example 4.2

Over $0.9y_1 + 2y_2 \leq 1.1$, the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} \frac{0.5(y_1+1)^2}{20x+y_1-1} + 0.5y_1 - 10y_2 + 0.5, & \text{if } 0.1 \leq x \leq s_3, \\ x + 0.1y_1 - 10y_2, & \text{if } s_3 \leq x \leq 1.1 - y_2, \\ 10x + 0.1y_1 - y_2 - 9.9, & \text{if } 1.1 - y_2 \leq x \leq 1. \end{cases}$$

Now, let $\tilde{t}$ denote the convex envelope of the bilinear term y_1y_2. Then, employing the convex envelope of the fractional term [61, 25], we obtain $\tilde{\phi} = \text{conv}(\tilde{t}/x)$, which is a convex underestimator of ϕ and is given by:

$$\tilde{\phi} = \begin{cases} \frac{5(y_1+y_2)^2}{20x+y_1+y_2-2} + 5(y_1 + y_2 - 2), & \text{if } 0.1 \leq x \leq r_1, \\ 10x + y_1 + y_2 - 11, & \text{if } r_1 \leq x \leq 1, \end{cases}$$

over $0.9y_1 + 2y_2 \geq 1.1$, where $r_1 = 0.1 + 0.45(y_1 + y_2)$, and by

$$\tilde{\phi} = \begin{cases} \frac{0.05(y_1-10y_2+11)^2}{20x+0.1y_1-y_2-0.9} + 0.5y_1 - 5y_2 - 4.5, & \text{if } 0.1 \leq x \leq r_2, \\ 10x + 0.1y_1 - y_2 - 9.9, & \text{if } r_2 \leq x \leq 1, \end{cases}$$

over $0.9y_1 + 2y_2 \leq 1.1$, where $r_2 = 0.595 + 0.045(y_1 - 10y_2)$. Compared to the factorable relaxation, the gap closed by the convex envelope of ϕ at $y_1 = 0.5$ is depicted in Figure 4.2. As can be seen, up to 90% of the relaxation gap is closed by convϕ.

Now, suppose that $g_1 \leq g_2 \leq g_3 < 0 < g_4$. From the proof of Theorem 4.1, it follows that, given any nonnegative nonincreasing convex $f(x)$ over $x \leq (1 - \lambda_4)\underline{x} + \lambda_4\bar{x}$, we have $x^i = \lambda_i\underline{x}$, $i \in \{1, 2, 3\}$ and $x^4 = x - (1 - \lambda_4)\underline{x}$. First, let $\hat{g}(y)$ be submodular and nondecreasing (or nonincreasing) in both arguments. In this case, $\delta(\gamma) = \gamma(g_1) - \gamma(g_2) -$

$\gamma(g_3) + \gamma(g_4)$, where $\gamma(g_i)$ is given by (4.21), simplifies to:

$$\delta(\gamma) = f(\underline{x})(g_1 - g_2 - g_3) + (f(x_{\lambda^*}) - (x_{\lambda^*} - \underline{x})f'(x_{\lambda^*}))\, g_4. \tag{4.27}$$

It is simple to check that $\delta(\gamma)$ is nonincreasing in x_{λ^*}. Thus, an upper bound on δ is obtained by letting $x_{\lambda^*} = \underline{x}$ in (4.27). This gives $\delta(\gamma) \leq f(\underline{x})\delta(g)$, which in turn implies $\delta(g)\delta(\gamma) \geq 0$. We can further relax the assumptions on $g(y)$ for this case as well. In Proposition 4.1, we did not address two cases: (i) $\hat{g}(y)$ is supermodular and nondecreasing (or nonincreasing) in both arguments and (ii) $\hat{g}(y)$ is submodular, nondecreasing in y_1 and nonincreasing in y_2. First, note that the two cases are equivalent after applying an affine transformation. Thus, let $\hat{g}(y)$ be supermodular and nondecreasing in each argument, *i.e.* $\delta(g) = g_1 - g_2 - g_3 + g_4 \geq 0$. First, consider the function $\delta(\gamma)$, given by (4.27). We are interested in finding a sufficient condition under which $\delta(\gamma) \geq 0$ (*i.e.* $\delta(g)\delta(\gamma) \geq 0$). Recall that $\delta(\gamma)$ is nonincreasing in x_{λ^*}. Thus, if $\delta(\gamma) \geq 0$ for $x_{\lambda^*} = \bar{x}$, then the result follows. Substituting for x_{λ^*} in (4.27), we conclude that, if

$$g_1 - g_2 - g_3 + (f(\bar{x}) - f'(\bar{x})\Delta x)\,/f(\underline{x})g_4 \geq 0, \tag{4.28}$$

then $\delta(\gamma)$ is nonnegative. Since $(f(\bar{x}) - f'(\bar{x})\Delta x)/f(\underline{x}) \leq 1$ and $g_4 > 0$, the above inequality does not follow from supermodularity of $g(y)$. Next, consider the function $\kappa(g)$ defined by (4.12). It is simple to check that $\kappa(g_i)$, $i \in I$ is supermodular when

$$g_1 - g_2 + f(\bar{x})/f(\underline{x})(-g_3 + g_4) \geq 0. \tag{4.29}$$

We now show that, condition (4.28) is implied by condition (4.29). Since $g_3 < 0$, and $f(x)$ is nonincreasing, we have $g_1 - g_2 - g_3 + f(\bar{x})/f(\underline{x})g_4 > g_1 - g_2 + f(\bar{x})/f(\underline{x})(-g_3 + g_4)$. Further, since $g_4 > 0$, it follows that $g_1 - g_2 - g_3 + (f(\bar{x}) - f'(\bar{x})\Delta x)/f(\underline{x})g_4 \geq g_1 - g_2 - g_3 + f(\bar{x})/f(\underline{x})g_4$. Hence, the left-hand side of (4.28) is always greater than the left-hand side of (4.29). Thus, we have the following result:

Corollary 4.4. Consider $\phi = f(x)g(y_1, y_2)$, $\mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^2$, where $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ is a nonnegative convex and nonincreasing function. Suppose that $g(y)$, $y \in \mathcal{H}_y^2$ is a component-wise concave function with $g_1 \leq g_2 \leq g_3 < 0 < g_4$, and that either (1) $\hat{g}(y)$ satisfies one of the conditions of Proposition 4.1, or (2) $g_1 - g_2 + f(\bar{x})/f(\underline{x})(-g_3 + g_4) \geq 0$.

Then, we have the following cases:

(i) If $\hat{g}(y)$ satisfies the conditions of Part (i) or Part (ii) of Proposition 4.1, then $\text{conv}_{\mathcal{C}}\phi$ is given by Part (i) of Corollary 4.3.

(ii) Otherwise, over the triangular sub-region of $\mathcal{H}_y^2$ given by Lemma 3.3, where $g(y)$ is negative over all three vertices, the convex envelope of ϕ over $\mathcal{C}$ is affine, and over the other sub-region, $\text{conv}_{\mathcal{C}}\phi$ is given by the expressions in Part (i) of Corollary 4.3.

Example 4.3. Let $\phi = (\sqrt{y_1} - y_2)\exp(-x)$, $x \in [0,1]$, $y_1 \in [0,1]$, $y_2 \in [0.1, 2]$. Then, Part (ii) of Proposition 4.1 and Part (ii) of Corollary 4.4 are satisfied. It follows that, over $1.9y_1 + y_2 \geq 2$, the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} (0.95 - 0.47y_2)\exp\left(\frac{-x}{1.05-0.53y_2}\right) + y_1 - 0.53y_2 - 0.95, & \text{if } 0 \leq x \leq s_1, \\ 0.63x + y_1 - 0.37y_2 - 1.26, & \text{if } s_1 \leq x \leq y_1, \\ 1.26x + 0.37(y_1 - y_2) - 1.26, & \text{if } y_1 \leq x \leq 1, \end{cases}$$

where $s_1 = 1.05 - 0.53y_2$. Over $1.9y_1 + y_2 \leq 2$, we have

$$\text{conv}\phi = \begin{cases} 0.9y_1 \exp\left(-x/y_1\right) + 0.1y_1 - y_2, & \text{if } 0 \leq x \leq y_1, \\ 0.063x + 0.37y_1 - y_2, & \text{if } y_1 \leq x \leq s_1, \\ 1.26x + 0.37(y_1 - y_2) - 1.26, & \text{if } s_1 \leq x \leq 1. \end{cases}$$

To construct a factorable relaxation, let $t_1 = \sqrt{y_1}$ and $t_2 = \tilde{t}_1 - y_2$, where $\tilde{t}_1$ is the affine underestimator of t_1 over $y_1 \in [0,1]$. Then, the convex envelope of $t_2\exp(-x)$ given by Corollary 3 in [25], is a convex underestimator of ϕ:

$$\tilde{\phi} = \begin{cases} 0.31(y_1 - y_2 + 2)\exp\left(\frac{-2.9x}{y_1-y_2+2}\right) + 0.69(y_1 - y_2) - 0.62, & \text{if } 0 \leq x \leq r_1, \\ 1.26x + 0.37(y_1 - y_2) - 1.26, & \text{if } r_1 \leq x \leq 1, \end{cases}$$

where $r_1 = 0.34(y_1 - y_2 + 2)$. The two relaxations are compared in Figure 4.3 at $y_2 = 0.2$. Up to over 70% of the relaxation gap of the factorable underestimator is closed by the convex envelope. Relaxation $\tilde{\phi}$ employs the convex envelope of $t_2\exp(-x)$ and is stronger than the factorable relaxations currently implemented in global solvers.

Finally, consider the case where $g(y)$ is nonpositive over the vertices of $\mathcal{H}_y^2$. It follows from the proof of Theorem 4.1 that, if $\delta(\kappa(g))\delta(g) \geq 0$, there exists an optimal set of

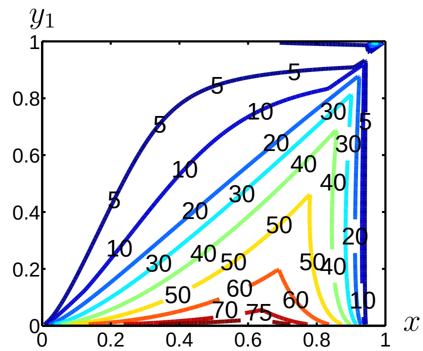


Figure 4.3: Gap closed by the convex envelope of $\phi = (\sqrt{y_1} - y_2)\exp(-x)$ at $y_2 = 0.2$ in Example 4.3

multipliers in the description of $\text{conv}_{\mathcal{H}_y^2} g(y)$ that is also optimal for the convex envelope of $\phi(x, y)$ over $\mathcal{C}$. A similar line of arguments as in the case $|I_N| = 3$ gives

Corollary 4.5. Consider $\phi = f(x)g(y_1, y_2)$, $\mathcal{C} = [\underline{x}, \bar{x}] \times \mathcal{H}_y^2$, where $f(x)$, $x \in [\underline{x}, \bar{x}] \subset \mathbb{R}$ is a nonnegative convex function. Suppose that $g(y)$, $y \in \mathcal{H}_y^2$ is a component-wise concave function with (i) $g_1 \leq \ldots \leq g_4 \leq 0$ if $f(\bar{x}) \leq f(\underline{x})$, and (ii) $g_4 \leq \ldots \leq g_1 \leq 0$ if $f(\underline{x}) \leq f(\bar{x})$. Moreover, assume that one of the following conditions is met:

(1) $\hat{g}(y)$ satisfies one of the conditions of Proposition 4.1,

(2) $f(\underline{x})(g_1 - g_2) + f(\bar{x})(-g_3 + g_4) \geq 0$.

Then, the convex envelope of ϕ over $\mathcal{C}$ is given by:

- $\underline{x} \leq x \leq (1-\lambda_k)\underline{x} + \lambda_k \bar{x}$: $\text{conv}\phi = (\lambda_i g_i + \lambda_j g_j + \lambda_k g_k) f(\underline{x}) + \Delta f/\Delta x (x - \underline{x}) g_k$,
- $(1-\lambda_k)\underline{x} + \lambda_k \bar{x} \leq x \leq: \lambda_i \underline{x} + (1-\lambda_i)\bar{x}$:

$$\text{conv}\phi = (\lambda_i g_i + \lambda_j g_j) f(\underline{x}) + \Delta f/\Delta x \left(x - (1-\lambda_k)\underline{x} - \lambda_k \bar{x}\right) g_j + \lambda_k f(\bar{x}) g_k,$$

- $\lambda_i \underline{x} + (1-\lambda_i)\bar{x} \leq x \leq \bar{x}$: $\text{conv}\phi = \Delta f/\Delta x (x - \bar{x}) g_i + (\lambda_i g_i + \lambda_j g_j + \lambda_k g_k) f(\bar{x})$,

where $\{i, j, k\}$ is the index set of nonzero multipliers in Proposition 4.1, rearranged such that (i) if $f(\underline{x}) \leq f(\bar{x})$, then $g_k \leq g_j \leq g_i$, and (ii) if $f(\bar{x}) \leq f(\underline{x})$, then $g_i \leq g_j \leq g_k$.

Example 4.4. Let $\phi = (y_1y_2 - 2)/\log x$, $x \in [10, 100]$, $y_1 \in [0, 1]$, $y_2 \in [1, 2]$. Then, Part 2 of Corollary 4.5 is satisfied and over $y_1 + y_2 \geq 2$, the convex envelope of ϕ is given by:

$$\text{conv}\phi = \begin{cases} (2y_1 + y_2 - 4)/\log(10), & \text{if } 10 \leq x \leq s_1, \\ 0.5(0.01x + 3y_1 + y_2 - 6.11)/\log(10), & \text{if } s_1 \leq x \leq 10(9y_1 + 1), \\ (0.01x + y_1 + 0.5y_2 - 3.11)/\log(10), & \text{if } 10(9y_1 + 1) \leq x \leq 100, \end{cases}$$

where $s_1 = 90(y_1 + y_2) - 17$. Over $y_1 + y_2 \leq 2$, we have

$$\text{conv}\phi = \begin{cases} (0.006x + y_1 - 2.06)/\log(10), & \text{if } 10 \leq x \leq 10(9y_1 + 1), \\ 0.063x + 0.37y_1 - y_2, & \text{if } 10(9y_1 + 1) \leq x \leq s_2, \\ (0.01x + 0.5y_1 - 2.11)/\log(10), & \text{if } s_2 \leq x \leq 100, \end{cases}$$

where $s_2 = 90(y_1 + y_2) - 80$. To construct a factorable relaxation, let $t_1 = \text{conv}(y_1y_2) - 2$, $t_2 = \log x$ and let $\tilde{\phi} = \text{conv}(t_1/x)$. Then, over $y_1 + y_2 \geq 2$, we have

$$\tilde{\phi} = \begin{cases} (2y_1 + y_2 - 4)/\log(10), & \text{if } 10 \leq x \leq r_1, \\ (0.01x + y_1 + 0.5y_2 - 3.11)/\log(10), & \text{if } r_1 \leq x \leq 100, \end{cases}$$

where $r_1 = 45(2y_1 + y_2) - 80$ and over $y_1 + y_2 \leq 2$, $\tilde{\phi}$ is given by:

$$\tilde{\phi} = \begin{cases} (y_1 - 2)/\log(10), & \text{if } 10 \leq x \leq 5(9y_1 + 2), \\ (0.01x + 0.5y_1 - 2.11)/\log(10), & \text{if } 5(9y_1 + 2) \leq x \leq 100, \end{cases}$$

The two relaxations are compared in Figure 4.4 at $y_2 = 1.2$. Up to over 50% of the relaxation gap is closed by the convex envelope.

4.5 Conclusions

We derived explicit characterizations for the convex envelopes of various functions that are products of convex and component-wise concave functions. These functional types appear frequently as sub-expressions in nonconvex optimization problems. In particular, we assumed that the component-wise concave function takes both negative and positive values over the domain of definition, which complements our earlier work in Chapter 3. Via several examples, we demonstrated that the proposed envelopes reduce significantly

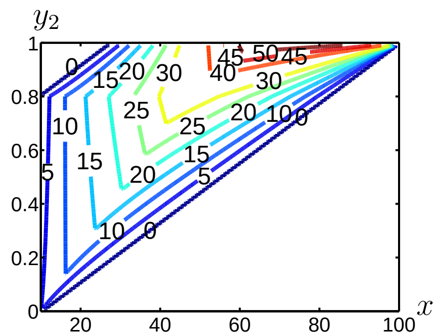


Figure 4.4: Gap closed by the convex envelope of $(y_1y_2 - 2)/\log x$ at $y_2 = 1.2$ in Example 4.4

the relaxations gaps of conventional factorable relaxations. In future work, we plan to incorporate the new envelopes into a global optimization solver and investigate their computational implications in the context of solving a variety of applications.

Chapter 5

A Lagrangian-based global optimization approach for quasi-separable nonconvex nonlinear optimization problems

In this chapter, we develop a deterministic approach for global optimization of nonconvex quasi-separable problems encountered frequently in engineering systems design. Our branch-and-bound based optimization algorithm applies Lagrangian decomposition to generate tight lower bounds by exploiting the structure of the problem and enable parallel computing of subsystems and use of efficient dual methods. We apply the approach to two product design applications: (i) product family optimization with a fixed platform configuration and (ii) product design using an integrated marketing-engineering framework. Results show that Lagrangian bounds are much tighter than the factorable programming bounds implemented by the global solver `BARON`, and the proposed lower bounding scheme shows encouraging scalability, enabling solution of some highly nonlinear problems that cause difficulty for existing solvers.

5.1 Introduction

Large-scale quasi-separable optimization problems arise frequently in mechanical design applications [67, 30, 28]. Several decomposition methods have been introduced for solving these problems efficiently. However, all existing approaches employ either local solvers [30, 27, 66, 32] or stochastic global techniques [24]. In the context of deterministic global optimization, the special structure of quasi-separable problems can be exploited to develop sharp bounding schemes that improve the convergence rate of the algorithm significantly. In this chapter, we develop an efficient algorithm for global optimization of nonconvex quasi-separable problems [22]. For obtaining tight lower bounds, the original problem is converted to a block-separable formulation by relaxing the coupling constraints using Lagrangian relaxation. The separable dual function is then decomposed into smaller subproblems, which can be solved for global optimality efficiently using a commercial global solver. The approximate dual optimal value, provides a tight lower bound for the branch-and-bound tree.

While the algorithmic constructs employed here are based on known Lagrangian relaxation and branch-and-bound techniques, the main contributions of this study are twofold. First, we show that the lower bounds generated by the proposed approach are much tighter than those created via convexification of the all-in-one problem using factorable programming techniques that are implemented in a commercial global optimization solver. Second, we are able to solve for the first time some realistic and highly nonconvex mechanical engineering design problems, for which we demonstrate that global solutions are significantly better than those obtained by prior approaches.

The remainder of this chapter proceeds as follows. In Section 5.2, the general formulation for lower bounding through Lagrangian decomposition is developed. The product family optimization problem is formulated in Section 5.3 and solved for a family of electric motors. The joint marketing-engineering product design problem is defined in Section 5.4 and demonstrated through a weight scale design case study. Finally, conclusions and future work are discussed in Section 5.5.

5.2 Proposed method

Using the concept of functional dependence table (FDT) [67], we define a quasi-separable problem as one with a block arrowhead FDT structure (see Figure 5.1). Let x_i and $\mathcal{X}_i$ with $i \in \{1, \ldots, n\}$ denote the local variables and the ground set for the ith sub-problem, respectively, where n is the total number of sub-problems. Define y and g as the linking variables and constraints, that couple the subproblems. For the system

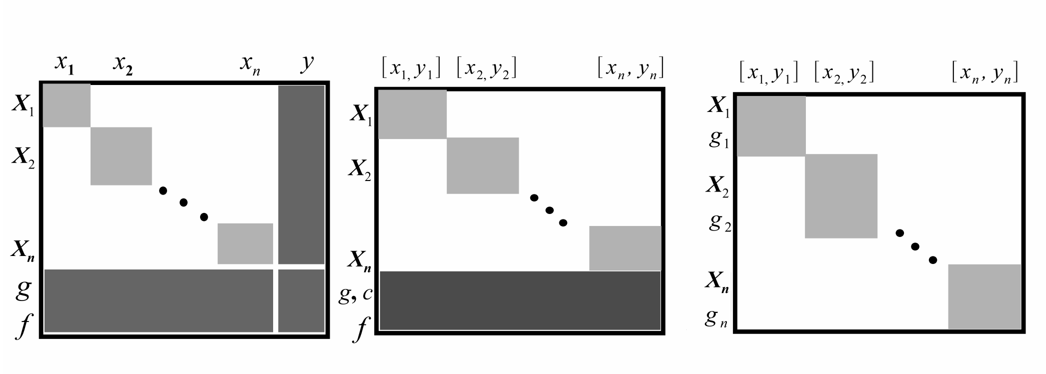


Figure 5.1: Functional dependence table: (a) arrowhead structure for the original problem, (b) introducing local copies of linking variables y_i and consistency constraints c, and (c) relaxing the coupling constraints (g, c) and applying Lagrangian decomposition

to be decomposable, both the objective and linking constraints are assumed to have an additive structure. Hence, one can formulate a quasi-separable problem as follows:

$$\begin{aligned} \min \quad & \sum_{i=1}^{n} f_i(x_i, y) \\ \text{s.t.} \quad & x_i \in \mathcal{X}_i, \quad \forall i \in \{1, \ldots, n\} \\ & \sum_{i=1}^{n} g_i(x_i, y) \leq 0 \end{aligned} \tag{5.1}$$

To allow for decomposition, Problem (5.1) should be reformulated to make the FDT block diagonal. First, local copies of linking variables are introduced in each subproblem $(y_i, \forall i \in \{1, \ldots, n\})$. Next, consistency constraints (c) are added to ensure all copies attain equal values at the optimal solution:

$$\begin{aligned} \min \quad & \sum_{i=1}^{n} f_i(x_i, y_i) \\ \text{s.t.} \quad & x_i \in \mathcal{X}_i \quad \forall i \in \{1, \ldots, n\} \\ & \sum_{i=1}^{n} g_i(x_i, y_i) \leq 0 \\ & c(y_1, \ldots, y_n) = 0. \end{aligned} \tag{5.2}$$

The next step is to relax the coupling constraints. This will be explained in the next section. Similar to any branch-and-bound based method, main steps are lower bounding, upper bounding, and branching. We shall detail on each of these stages in the following sections.

5.2.1 Lower bounding

Let $\tilde{x}_i = [x_i,\ y_i]$, and $\tilde{g} = [\sum_i g(x_i, y_i),\ c(y_1, \ldots, y_n)]$. Applying Lagrangian relaxation to the coupling constraints in Problem (5.2), we obtain the following Lagrangian function:

$$L(\tilde{x}, \lambda) = \sum_{i=1}^{n} f_i(\tilde{x}_i) + \lambda^T \tilde{g}_i(\tilde{x}_i).$$

Hence, the dual function is given by

$$q(\lambda) = \sum_{i=1}^{n} \inf_{\tilde{x}_i \in \mathcal{X}_i} (f_i(\tilde{x}_i) + \lambda^T \tilde{g}_i(\tilde{x}_i)), \tag{5.3}$$

where $\lambda \in \mathbb{R}_+^{|\tilde{g}|}$ denotes the vector of Lagrange multipliers. From (5.3) it follows that for a fixed λ, the dual function is separable and therefore decomposes into n independent sub-problems. Thus, the dual problem can be written as:

$$\max_{\lambda \in \mathbb{R}_+^{|\tilde{g}|}} \quad \sum_{i=1}^{n} q_i(\lambda), \tag{5.4}$$

where

$$q_i(\lambda) = \inf_{\tilde{x}_i \in \mathcal{X}_i} (f_i(\tilde{x}_i) + \lambda^T \tilde{g}_i(\tilde{x}_i)).$$

By the weak duality theorem, any dual value is a lower bound for the optimal primal value [7]. Thus, solving the dual problem (even approximately) provides a lower bound for the branch-and-bound algorithm. Further, the separable structure of the dual function allows for fast computation of the dual subproblems, which is an important feature for efficiency of dual methods [7]. An approximate optimal value of (5.4) can be found using any non-differentiable convex optimization approach. Subgradient methods are among the most popular non-differentiable convex optimization methods [54], and they have been used extensively for solving the dual problems by generating a sequence of dual feasible points using a single subgradient at each iteration:

$$\lambda^{k+1} = P_+(\lambda^k + \alpha^k \bar{g}^k), \tag{5.5}$$

where $\bar{g}^k$ denotes a subgradient of the dual function at λ^k and α^k is a positive step size at the kth iteration. P_+ represents the projection over the nonnegative orthant. There are several schemes for selecting α^k; we adopt a diminishing step size rule, which converges to a maximizing point of (5.4), if the following conditions are met [7]:

$$\lim_{k\to\infty} \alpha^k = 0, \quad \sum_{k=1}^{\infty} \alpha^k \to \infty, \quad \sum_{k=1}^{\infty} (\alpha^k)^2 \leq \infty.$$

In each iteration, all sub-problems are solved in parallel globally. Next, the multipliers are updated according to (5.5), and the iterative procedure continues for $k_{\max}$ number of iterations. Therefore, a lower bound for (5.1) is given by:

$$LB = \max_{k\in K} \left(\sum_{i=1}^{n} q_i(\lambda^k) \right), \quad K = \{1, \ldots, k_{\max}\}. \tag{5.6}$$

5.2.2 Upper bounding

In general, any feasible point of (5.1) can serve as an upper bound (UB) to the global minimum. These bounds enhance the algorithmic convergence by pruning the nodes of the branch-and-bound tree that do not contain any solution better than the best known feasible point. In the proposed approach, in every node of the branch-and-bound tree, after lower bounding, Problem (5.1) is locally optimized using the dual optimal value as the starting point, the local solution is compared with the incumbent, and UB is updated accordingly.

5.2.3 Branching

In any node of the branch-and-bound tree, if the difference between the lower and upper bounds falls within a user-specified tolerance, that node is pruned and the upper bound is updated. Otherwise, the feasible region is partitioned into two subsets, and the two new nodes are added to the list of open nodes. We adopt a depth-first search rule for node selection. Branching decisions can be made by computing a violation that measures the dual infeasibility introduced by relaxing the coupling constraints. For instance, if the coupling constraints are consistency constraints, the variance of each linking variable among its subproblems is calculated and the one with the maximum violation is selected as the branching variable, using the mean value of that variable among its copies as the branching point.

5.3 Application No. 1: product families

A product family is a set of products that share some components to reduce the manufacturing cost while maintaining variant distinctiveness to attract a range of market segments. Among more than forty approaches in the literature [55], there exists no approach that guarantees global optimality for the general problem. Existing methods either use local optimization techniques or rely on stochastic global optimizers. In this study, we assume that the platform configuration is selected a priori.

Consider a family of n products with r platforms. Let x_i, $i \in I = \{1, \ldots, n\}$ be the ith variant distinct components and y_j, $j \in J = \{1, \ldots, r\}$ be the platform components, each shared among a subset of variants. Define $\mathcal{S}_j$ for all $j \in J$ as the index set of variants present in the jth platform and $\mathcal{U}_i$ as the index set of shared components present in the ith variant $\mathcal{U}_i = \{j \in J : i \in \mathcal{S}_j\}$. Let f_i and g_i denote the objective function and constraints for the ith product, respectively. The product family optimization problem is formulated as follows:

$$\begin{aligned} \max \quad & \sum_{i \in I, j \in \mathcal{U}_i} f_i(x_i, y_j) \\ \text{s.t.} \quad & g_i(x_i, y_j) \leq 0, \quad \forall j \in \mathcal{U}_i,\ \forall i \in I. \end{aligned}$$

Hence, individual product designs are coupled through the platform components. First, we introduce copies of common components for each variant present in that platform: y_{jk} for all $k \in \mathcal{S}_j$ and $j \in J$. Next, we add the consistency constraints enforcing these copies to be equal:

$$\begin{aligned}
\max \quad & \sum_{i \in I, j \in \mathcal{U}_i} f_i(x_i, y_{ji}) \\
\text{s.t.} \quad & g_i(x_i, y_{ji}) \leq 0, \ \forall j \in \mathcal{U}_i, \ \forall i \in I \\
& y_{jk} = \frac{1}{|\mathcal{S}_j|} \sum_{k' \in \mathcal{S}_j} y_{jk'}, \ \forall k \in \mathcal{S}_j, \ \forall j \in J.
\end{aligned}$$

The above consistency constraints require that each copy of a shared component be equal to the average of all of its copies. Relaxing the consistency constraints and applying Lagrangian decomposition, the *ith* Lagrangian subproblem is given by:

$$\begin{aligned}
\max \quad & f_i(x_i, y_{ji}) + \sum_{j \in \mathcal{U}_i} y_{ji} \Big(\lambda_{ji} - \sum_{u \in \mathcal{U}_i} \frac{\lambda_{ui}}{|\mathcal{S}_u|} \Big) \\
\text{s.t.} \quad & g_i(x_i, y_{ji}) \leq 0, \ \forall j \in \mathcal{U}_i, \ \forall i \in I,
\end{aligned} \tag{5.7}$$

where $\lambda_{jk} \in \mathbb{R}$ for all $j \in J$ and $k \in \mathcal{S}_j$ denote the Lagrange multipliers associated with the consistency constraints. The lower bounding step involves global optimization of individual variants in parallel followed by a subgradient update of the multipliers using (5.5) for a predefined number of iterations. We select as the branching variable, the y element with the largest variance among its copies and the corresponding mean value as the branching point.

5.3.1 Case study: universal electric motors

The universal electric motor product family example has been applied as a case study to compare the efficiency of various approaches in the product family optimization literature [55]. In this example, the goal is to design a family of electric motors that satisfy a variety of torque requirements while reducing manufacturing cost through sharing components. Among the existing objective-function formulations, the following are considered for comparison purposes:

(i) Goal programming [38]: the objective is to minimize undesirable deviation of mass and efficiency from their targets, given by 0.5 kg and 70%, respectively. Namely, the deviation value for any motor that weighs less than 0.5 kg and has an efficiency of 70% or more is set to zero.

(ii) Direct optimization of mass and efficiency [24]: the objective function is defined as the weighted sum of mass and efficiency over the entire family

$$f = \sum_{i=1}^{n} w_1(1 - \eta_i) + w_2 m_i^*,$$

where η_i and m_i^* denote efficiency and normalized mass for the *ith* motor, respectively, and w_1 and w_2 are weight coefficients.

Comparison of alternative optimizers

To highlight the need for deterministic global optimization, two examples employing a local solver and a stochastic global optimizer were selected from the literature and solved for global optimality using `BARON`. Throughout this section, the relative termination tolerance between upper and lower bounds is set to 0.01%.

(i) Messac et al. [37] used physical programming for optimizing a family of ten electric motors treating radius and thickness as platform variables along with the goal programming objective function. The same problem was solved using `BARON`. Results are compared in Table 5.1; by switching from a local to a global optimizer, the optimal family on average is 8.0% more efficient and weighs 7.4% less.

(ii) Simpson et al. [55] used genetic algorithm (GA) to optimize a family of ten electric motors to jointly determine the optimal platform selection and variant design using the direct objective function formulation. To compare the solution quality, one of the Pareto optimal solutions with radius and thickness shared among all products was selected and optimized using `BARON` holding the platform configuration fixed (see Table 5.1). The GA-reported solution is a product family that on average is 7.9% less efficient and weighs 9.2% more than the global optimum.

Scalability and decomposition

In both previous examples, the all-in-one problem was solved using `BARON` without Lagrangian decomposition because both cases are relatively small-scale problems. In this section, we demonstrate the effect of increasing the problem size on the convergence rate of the global solver. The electric motor product family was optimized for 5, 10, 15, and 20

Table 5.1: Average mass and efficiency for the electric motor product family using alternative optimization schemes

	Example 1		Example 2	
	Ref. [37]	BARON	Ref. [55]	BARON
Mass (kg)	0.672	0.622	0.660	0.599
Efficiency (%)	0.629	0.684	0.621	0.674

products, respectively, under various platform configurations. First, for all cases, the all-in-one formulation was solved using `BARON`. Computational time for each family is listed in Table 5.2. Results show that while `BARON` is quite efficient for relatively small problems, it slows down significantly when increasing the size of the problem. Namely, by increasing the number of products from 5 to 15, the computational time increases exponentially, and the solver fails to find a feasible solution for 20 products. As we shall detail next, this undesirable trend is due to weak lower bounds created by convex underestimations.

Next, we apply the proposed Lagrangian-based approach to solve the same problem using a randomized incremental subgradient method for lower bounding. In each iteration, one individual motor is selected randomly and optimized globally using `BARON`. Next, the multipliers are updated using relation (5.1) and the process is repeated for 20 iterations. `CONOPT` was used as the local solver for upper bounding, using the dual solution as the starting point. Table 5.2 shows that while the proposed method is slower than `BARON` for five products, it outperforms the commercial solver as the number of products increases, showing an almost linear complexity within this range. The key feature of the decomposed algorithm is that it only uses `BARON` for optimizing a single product at a time, for which the solver is quite fast and efficient, to generate lower bounds using Lagrangian decomposition. These tight lower bounds then enable fast convergence of the branch-and-bound tree for the entire family.

Table 5.3 compares the lower bounds at the root node of the branch-and-bound tree for the families of Table 5.1 using Lagrangian versus factorable bounds generated by `BARON`. The Lagrangian bounds at the root node are within 1% of the optimal solution whereas factorable programming bounds are much weaker. Therefore, although computing Lagrangian bounds are more expensive than the factorable bounds, their high quality reduces the overall execution time significantly.

Table 5.2: Computational time of the electric motor product family for all-in-one versus decomposition approach

	Computational time (s)	
No. of products	`BARON` (all-in-one)	Proposed method
5	26	31
10	690	77
15	2725	108
20	–	156

Table 5.3: Factorable versus Lagrangian bounds at the root node for electric motor product family

No. of products	Optimal solution	Lagrangian bounds	Factorable bounds
5	1.748	1.736	0.167
10	3.426	3.419	0.323
15	5.112	5.101	0.265
20	6.646	6.638	0.015

5.4 Application No. 2: design for maximum profit

Designing products for the maximum profit through simultaneous consideration of consumers preferences and engineering constraints has received great attention in recent years [41, 31, 29]. However, prior approaches have employed either local solvers [41] or GAs [31, 29] to solve the nonconvex problem and therefore do not guarantee global optimality. In this example, we adapt the formulation proposed in [41] to solve the joint marketing-engineering product design problem. Using the logit function for demand modeling and the latent class model for capturing preference heterogeneity, the all-in-one problem can be formulated as follows:

$$
\begin{aligned}
\max_{x,\eta} \quad & \Pi = q(p - c_v) - c_I \\
\text{s.t.} \quad & g(x) \leq 0, \quad h(x) = 0 \\
& z = r(x) \\
& x_{\min} \leq x \leq x_{\max},\ p_{\min} \leq p \leq p_{\max} \\
& z_{\min} \leq z \leq z_{\max} \\
& \Delta\hat{z}_{\zeta\omega}\eta_{\zeta\omega} \leq y_{\zeta\omega} \leq \Delta\hat{z}_{\zeta\omega}\eta_{\zeta(\omega-1)},\ \forall\omega \in \{2, \ldots \Omega_\zeta - 1\} \\
& \Delta\hat{z}_{\zeta 2}\eta_{\zeta 1} \leq y_{\zeta 2} \leq \Delta\hat{z}_{\zeta 2}, \quad 0 \leq y_{\zeta\Omega_\zeta} \leq \Delta\hat{z}_{\zeta\Omega_\zeta}\eta_{\zeta(\Omega_\zeta-1)} \\
& \eta_{\zeta\omega} \in \{0, 1\}, \quad \forall\zeta \in \{1, \ldots, Z\},\ \forall\omega \in \{2, \ldots, \Omega_\zeta - 1\},
\end{aligned}
\tag{5.8}
$$

where

$$
\begin{aligned}
& \Delta\hat{z}_{\zeta\omega} = \hat{z}_{\zeta\omega} - \hat{z}_{\zeta(\omega-1)}, \quad \forall\omega \in \{2, \ldots \Omega_\zeta - 1\} \\
& q = Q\Big(\sum_{i=1}^{m} s_i \frac{e^{v_i}}{1 + e^{v_i}}\Big), \quad v_i = v_{i0}(\beta_{i0}, \hat{p}) + \sum_{\zeta=1}^{Z} v_{i\zeta}(\beta_{i\zeta}, \hat{z}_\zeta) \\
& v_{i\zeta} = \beta_{i\zeta 1} + \sum_{\omega=2}^{\Omega_\zeta} \Big(\frac{\beta_{i\zeta\omega} - \beta_{i\zeta(\omega-1)}}{\hat{z}^M_{\zeta\omega} - \hat{z}^M_{\zeta(\omega-1)}}\Big) y_{\zeta\omega}, \quad z_\zeta = \hat{z}_{\zeta 1} + \sum_{\omega=2}^{\Omega_\zeta} y_{\zeta\omega} \\
& v_{i0} = \beta_{i01} + \sum_{\omega=2}^{\Omega_\zeta} \Big(\frac{\beta_{i0\omega} - \beta_{i0(\omega-1)}}{\hat{p}_\omega - \hat{p}_{(\omega-1)}}\Big) y_{0\omega}, \quad p = \hat{p}_1 + \sum_{\omega=2}^{\Omega_\zeta} y_{0\omega},
\end{aligned}
$$

and Π denotes the profit; q is the product demand, which is a function of product attributes z and price p. c_V and c_I are unit variable and investment costs, respectively. s_i denotes the size of the ith market segment and Q is the overall market size. Product utility in each segment v_i is assumed to have a continuous form using piecewise linear interpolation over the discrete part-worths (β), obtained from conjoint analysis. The incremental cost formulation [44] is applied to represent piecewise linear functions, which requires introduction of intermediate continuous y and binary z variables. x denotes the design variables; g and h are inequality and equality engineering constraints, respectively. Product attributes are related to the engineering variables through equality constraints $z = r(x)$. As we will illustrate in the next section, `BARON` cannot close the relaxation gap of all-in-one formulation in a reasonable time.

Following the same scheme introduced in [41], Problem (5.8) can be decomposed into marketing and engineering subproblems, by first introducing marketing z_M and engineering z_E product attribute copies along with the consistency constraints $z_M = z_E$, and subsequently relaxing the consistency constraints in the Lagrangian decomposition framework. Applying the aforementioned steps, we obtain:

(i) Marketing sub-problem:

$$\begin{aligned}
\max_{p, z_M} \quad & \Pi = q(p - c_v) - c_I - \sum_{\zeta=1}^{Z} \lambda_\zeta z_\zeta^M \\
\text{s.t.} \quad & p_{\min} \le p \le p_{\max}, \quad z_{\min} \le z^M \le z_{\max} \\
& \Delta \hat{z}_{\zeta\omega}^M \eta_{\zeta\omega} \le y_{\zeta\omega} \le \Delta \hat{z}_{\zeta\omega}^M \eta_{\zeta(\omega-1)}, \ \forall \omega \in \{2, \dots \Omega_\zeta - 1\} \\
& \Delta \hat{z}_{\zeta 2}^M \eta_{\zeta 1} \le y_{\zeta 2} \le \Delta \hat{z}_{\zeta 2}^M, \quad 0 \le y_{\zeta \Omega_\zeta} \le \Delta \hat{z}_{\zeta \Omega_\zeta}^M \eta_{\zeta(\Omega_\zeta - 1)} \\
& \eta_{\zeta\omega} \in \{0, 1\}, \quad \forall \zeta \in \{1, \dots, Z\}, \ \forall \omega \in \{2, \dots, \Omega_\zeta - 1\},
\end{aligned} \tag{5.9}$$

where

$$\begin{aligned}
& \Delta \hat{z}_{\zeta\omega}^M = \hat{z}_{\zeta\omega}^M - \hat{z}_{\zeta(\omega-1)}^M, \quad \forall \omega \in \{2, \dots \Omega_\zeta - 1\} \\
& q = Q\Big(\sum_{i=1}^{m} s_i \frac{e^{v_i}}{1 + e^{v_i}} \Big), \quad v_i = v_{i0}(\beta_{i0}, \hat{p}) + \sum_{\zeta=1}^{Z} v_{i\zeta}(\beta_{i\zeta}, \hat{z}_\zeta) \\
& v_{i\zeta} = \beta_{i\zeta 1} + \sum_{\omega=2}^{\Omega_\zeta} \Big(\frac{\beta_{i\zeta\omega} - \beta_{i\zeta(\omega-1)}}{\hat{z}_{\zeta\omega}^M - \hat{z}_{\zeta(\omega-1)}^M} \Big) y_{\zeta\omega}, \quad z_\zeta = \hat{z}_{\zeta 1} + \sum_{\omega=2}^{\Omega_\zeta} y_{\zeta\omega} \\
& v_{i0} = \beta_{i01} + \sum_{\omega=2}^{\Omega_\zeta} \Big(\frac{\beta_{i0\omega} - \beta_{i0(\omega-1)}}{\hat{p}_\omega - \hat{p}_{(\omega-1)}} \Big) y_{0\omega}, \quad p = \hat{p}_1 + \sum_{\omega=2}^{\Omega_\zeta} y_{0\omega}.
\end{aligned}$$

(ii) Engineering sub-problem:

$$\begin{aligned}
\max_{x} \quad & \sum_{\zeta=1}^{Z} \lambda_\zeta z_\zeta^E \\
\text{s.t.} \quad & g(x) \le 0, \quad h(x) = 0 \\
& z^E = r(x) \\
& x_{\min} \le x \le x_{\max}, \ p_{\min} \le p \le p_{\max} \\
& z_{\min} \le z^E \le z_{\max}.
\end{aligned} \tag{5.10}$$

In each iteration, Problems (5.9) and (5.10) are solved in parallel, followed by a subgradient update of the multipliers. Moreover, the branching variable and branching point selection are defined similar to the first example.

5.4.1 Case study: dial read-out weight scale

The weight scale design problem was introduced in [41] as a case study for the integrated marketing-engineering approach. The same example is used here to show the efficiency of the decomposition approach. Each scale is represented by 5 product attributes, denoted by z, 8 design variables, denoted by x, and 14 engineering constraints. First, the all-in-one problem (5.8) was optimized using `BARON`. After 24 hours, the upper bound was 87.76 with a relative gap of 32.1% from the lower bound. However, using the proposed decomposition method with a relative gap tolerance of 0.1%, the algorithm terminated after 4 hours and 26 minutes (Table 5.4). `BARON` and `DICOPT` were employed to solve the upper bounding and lower bounding problems, respectively. Upper bounds generated at the root node, using factorable technique and Lagrangian decomposition, are compared in Table 5.5. Lagrangian bounds are reported after 20 subgradient iterations: while requiring more computation than the factorable approach, the tightness of Lagrangian bounds lowers the overall execution time significantly, consistent with the conclusion from the first example.

Table 5.4: Optimal scale design marketing attributes

Attributes (z)	Lower bound	Optimal value	Upper bound
z_1 : weight capacity	200.0	250.0	400.0
z_2 : aspect ratio	0.75	1.040	1.33
z_3 : platform area	100.0	140.0	140.0
z_4 : tick mark gap	0.0625	0.1237	0.1875
z_5 : number size	0.75	1.432	1.750
p : price	10.0	25.0	30.0
Lower bound: 66.436		Upper bound: 66.497	
Relative gap: % 0.092			

Table 5.5: Factorable versus Lagrangian bounds at the root node for scale design

Upper bound (millions)- Relative gap (%)	
All-in-one (`BARON`)	Proposed method
122.530-84.43	68.850-3.63
Global optimum (millions): 66.436	

5.5 Conclusions

We presented a deterministic method for global optimization of nonconvex quasi-separable problems. The decomposable structure of the problem was exploited to provide tight lower bounds for the branch-and-bound algorithm using Lagrangian decomposition. Two important mechanical design applicaions were considered and demonstrated through case studies taken from the literature. Results were compared with those obtained from solving the all-in-one problem using `BARON`. While `BARON` is efficient for the small-scale problems, the computational effort increases exponentially with the size of the problem. In contrast, the proposed approach proved to be scalable, and the Lagrangian lower bounding scheme was capable of generating tight bounds in both examples. Results show that solutions reported in the literature using local solvers and stochastic global methods are significantly suboptimal, and without a lower bound the modeler cannot be sure of the solution quality. However, this guaranteed global optimality comes with a considerable increase in the computational cost compared with local solvers. Thus, deterministic global solvers are preferable when the computational cost is affordable.

Chapter 6

Conclusions and future research

We conclude by summarizing the main contributions of this thesis and outlining some directions of future research.

In Chapter 2, we proposed a new method to outer-approximate convex transformable or G-convex functions. For a given G-convex function, there exist infinitely many choices for the transforming function, and the tightness of the proposed relaxation depends on the form of the transforming function. We developed a simple criterion to compare the sharpness of resulting relaxations, and demonstrated that the tightest possible relaxation has a well-defined mathematical description. This is the key advantage of the proposed method over existing transformation techniques in the global optimization literature, all of which suffer from too many degrees of freedom and unknown theoretical properties. We then applied the proposed relaxation to a wide class of functions that appear frequently in nonconvex problems. Namely, we considered signomials, product and ratios of convex and/or concave functions and log-concave functions. We provided theoretical and numerical comparisons of the proposed approach with a widely used factorable relaxation scheme. In all instances, new relaxations were considerably tighter.

At the numerical level, in addition to a generic implementation of the proposed relaxations in a global solver, the new convexification technique can be employed to develop customized algorithms for solving a variety of challenging applications to global optimality. Some examples include, training artificial neural networks, portfolio optimization, and positioning product lines for the maximum profit. At the theoretical level, it would be interesting to further investigate the favorable properties of other classes of generalized convex functions in the context of global optimization. For instance, by definition, a function is quasi-convex if and only if its sub-level sets are convex. Quasi-convex functions are the broadest class of generalized convex functions and frequently appear as component functions of nonconvex optimization problems. In the context of factorable programming, we exploit the convexity of the *epigraph* of intermediate expressions and generate supporting hyperplanes that bound nonconvex functions. An interesting question is how one can exploit the convexity of the *sub-level sets* of quasi-convex functions to generate *lifting inequalities* that serve as strong cuts for the epigraph of the function.

In Chapters 3 and 4, we studied the problem of constructing the convex envelope of a nonconvex function over a compact convex set. We proposed a convex formulation for constructing the convex envelope of a lsc function whose generating set is representable as a union of finite number of closed convex sets. We conducted an extensive survey in `GLOBALLib` and `MINLPLib` test problems and identified three major functional classes that satisfy this sufficient condition. These functions constitute over 60% of nonconvex functions that appear in these two libraries. We then focused on one class, namely, functions that are products of convex and component-wise concave functions. We derived explicit characterizations for the convex envelopes of a wide range of such functions. Through numerous examples, all taken from real-world applications, we demonstrated that the proposed envelopes reduce significantly the relaxation gaps of standard factorable relaxations. A natural future direction is to consider the other two functional categories and reduce the complexity of the envelope representation problem (ideally solve it) for those functions. On the numerical side, implementing these new classes of cutting planes would have an immediate impact on the efficiency of global solvers.

Finally, in Chapter 5, we studied a rather different convexification approach, namely, Lagrangian relaxation. We considered nonconvex quasi-separable optimization problems, a structure that occurs frequently in engineering systems design applications. The decomposable structure of the problem was exploited to provide tight lower bounds for the branch-and-bound algorithm using Lagrangian decomposition. We considered two applications in mechanical design, product family optimization and design for maximum profit. The proposed approach proved to be scalable, and the Lagrangian lower bounding scheme was capable of generating tight bounds in both examples. An interesting future direction is to equip a general-purpose global solver with such alternative bounding schemes and study the empirical properties of Lagrangian bounds in a variety of applications.

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