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Extended formulations for convex envelopes

Martin Ballerstein · Dennis Michaels

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Abstract In this work we derive explicit descriptions for the convex envelope of nonlinear functions that are component-wise concave on a subset of the variables and convex on the other variables. These functions account for more than 30 % of all nonlinearities in common benchmark libraries. To overcome the combinatorial difficulties in deriving the convex envelope description given by the component-wise concave part of the functions, we consider an extended formulation of the convex envelope based on the Reformulation–Linearization-Technique introduced by Sherali and Adams (SIAM J Discret Math 3(3):411–430, 1990). Computational results are reported showing that the extended formulation strategy is a useful tool in global optimization.

Keywords Convex envelope · Edge-concave functions · Extended formulation · Reformulation–Linearization-Technique · Simultaneous convexification

1 Introduction

Many state-of-the-art global optimization algorithms (e.g., see BARON [39], COUENNE [7], SCIP [25]) rely on the ability to construct and solve convex relaxations. A key step in the construction is to determine a strong convex underestimator of a nonconvex function $f : D \subseteq \mathbf{R}^n \to \mathbf{R}$. The best possible convex underestimator is called the *convex envelope* of f over D (e.g., see [22,37]), and is denoted by $\text{vex}_D[f]$, in the following.

M. Ballerstein (✉)
Eidgenössische Technische Hochschule Zürich, Institut für Operations Research, Rämistrasse 101,
8092 Zurich, Switzerland
e-mail: martin.ballerstein@ifor.math.ethz.ch

D. Michaels
Fakultät für Mathematik, Technische Universität Dortmund, M/518, Vogelpothsweg 87,
44227 Dortmund, Germany
e-mail: dennis.michaels@math.tu-dortmund.de

The value of $\text{vex}_D[f]$ at $x \in D$ is given by (e.g., [24])

$$\inf \left\{ \sum_{i=1}^{n+1} \lambda_i f(x^i) \;\middle|\; x = \sum_{i=1}^{n+1} \lambda_i x^i,\ \sum_{i=1}^{n+1} \lambda_i = 1,\ \lambda_i \geq 0,\ x^i \in D \right\}. \tag{1}$$

In general, problem (1) is a nonconvex problem which is extremely difficult to solve. Over the last decade, many articles dealing with the computation of envelopes for several classes of functions have been published (e.g., see [5,14–16,20,21,35,37]). Usually, analytical and geometric properties of the functions are used to reduce the complexity and to derive alternative formulations of problem (1) that are much more tractable. We point out that the alternative formulations do not necessarily lead to explicit formulas for the convex envelope. Although favorable when designing global optimization algorithms, this is somehow not surprising due to the high complexity of problem (1).

The goal of this paper is to provide explicit formulas for the convex envelope of two classes of nonlinear functions in an extended space. Both classes consist of *continuous* functions

$$f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x+n_y} \to \mathbf{R}, \quad (x, y) \mapsto f(x, y), \tag{2}$$

that are *component-wise concave* in the x-variables over $[l^x, u^x]$ for each fixed $y \in [l^y, u^y]$, and that satisfy for each fixing of x to one of the *vertices* of $[l^x, u^x]$ the following assumptions:

Class 1: $n_y \leq 1$, and f is convex or concave along the y-direction. This behavior may be different for different fixings of the x-variables.

Class 2: $n_y \in \mathbf{Z}_{\geq 0}$ and f is *convex* on the space of the y-variables.

For example, the function $f(x, y) := xy^2$ over $[-1, 1] \times [0, 2]$ belongs to Class 1 but not to Class 2 since $f(-1, y)$ is concave in y and $f(1, y)$ is convex in y. The function $f(x, y_1, y_2) := x(y_1^2 + y_2^2)$ over the nonnegative orthant is contained in Class 2 but not in Class 1. The importance of the two classes of functions is reflected by their frequent occurrence in the benchmark libraries GLOBALLib [11] and MINLPLib [9]. In fact, Classes 1 and 2 account for more than 30 % of all nonlinear functions in these libraries [15, p. 392].

Convex envelopes are only known for subclasses and have been recently deduced by Khajavirad and Sahinidis [15,16]. They further assume that $f(x, y)$ is decomposable into the form $g(x) \cdot h(y)$, and that g is *submodular* and *convex-extendable* from the vertices of $[l^x, u^x]$. The latter assumption implies that an explicit description of the convex envelope of g over $[l^x, u^x]$ is given by the *Lovász* extension of g restricted to vertices of $[l^x, u^x]$ (see also [35]). The knowledge of $\text{vex}_{[l^x,u^x]}[g]$ is then used to determine the analytical formulas for $\text{vex}_{[l,u]}[f]$. In fact, it turns out that the ability to derive an explicit formula for $\text{vex}_{[l,u]}[f]$ requires at least a complete characterization of $\text{vex}_{[l^x,u^x]}[g]$ (see [36, Thm. 10] and [15,16]).

The convex envelope of a component-wise concave function g over a box $[l^x, u^x]$ is polyhedral, i.e., it can be expressed as a maximum of a finite number of linear functions (e.g., see [32]). Moreover, the corresponding optimization problem (1) reduces to a linear program (e.g., see [23,35]). However, a complete characterization is only available up to dimension three [23], and for some special cases in higher dimensions (e.g., [35]). This is caused by the fact that the determination of these convex envelopes corresponds to an investigation of all possible triangulations of the box $[l^x, u^x]$ (cf. [35]). In dimension four, this is already hard to analyze as the box can exhibit up to 879,594,48 possible regular triangulations which can be subdivided into 235,277 different symmetry classes [12, Thm. 2].

To avoid such impracticable case distinctions, workarounds are available for particular as well as general classes of functions. For the special case of multilinear functions, a *cutting-plane* algorithm that computes parts of the envelopes was suggested in Bao et al. [5]. This requires the solution of a linear program in each step of the algorithm whose size grows exponentially in the number of variables of the multilinear function (see also [35]). For the general class of decomposable functions, a generic approach is to reformulate a higher-dimensional function as the composition of lower-dimensional functions for which the convex envelopes are known (e.g., [22,38]). Such reformulations lead to relaxations in an extended space that are, in general, weaker than the convex envelope of the original function. We refer to the work [10] for a study of reformulation strategies for quadrilinear terms.

In order to handle the combinatorial variety given by the component-wise concave part of our functions $f(x, y)$, we consider an extended formulation based on the *Reformulation–Linearization-Technique* (RLT) by Sherali and Adams (e.g., see [2,26–28]). We will link $f(x, y)$ with a vector $\phi(x, y) = \big(\phi_1(x, y), \dots, \phi_K(x, y)\big)$ that consists of all monomials $\prod_{j\in J} x_j$ and $y_k \prod_{j\in J} x_j$, for $J \subseteq \{1, \dots, n_x\}$, and $k = 1, \dots, n_y$. An extended formulation for the convex envelope is then given by the following convex hull object

$$\begin{aligned}\operatorname{conv}\Big(\Big\{&(x, y, z, \mu) \in \mathbf{R}^{n_x+n_y+K+1} \mid z_i = \phi_i(x, y), \quad i = 1, \dots, K,\\ &\mu \geq f(x, y),\ x \in [l^x, u^x],\ y \in [l^y, u^y]\Big\}\Big).\end{aligned} \tag{3}$$

By construction, the projection of the convex hull object in Eq. (3) onto the (x, y, μ)-space equals the epigraph of $\text{vex}_{[l,u]}[f]$. It can therefore be interpreted as an extended formulation for $\text{vex}_{[l,u]}[f]$. For our classes of functions f, we show in Theorems 4 and 5 that the extended formulation for $\text{vex}_{[l,u]}[f]$ is completely given by the polytope $P := \operatorname{conv}(\{(x, y, z) \in \mathbf{R}^{n_x+n_y+K} \mid z_i = \phi_i(x, y),\ i = 1, \dots, K\}$ whose facet-description is known, and an additional cut $\mu \geq \Phi(x, y, z)$ that links the function f with the introduced monomials ϕ_i.

We remark that the extended formulation in Eq. (3) describes the simultaneous convexification of the epigraph of f with all graphs of the involved monomials ϕ_i. Such simultaneous convexifications usually lead to tighter relaxations than the individual relaxation of the involved functions by convex envelopes. Explicit formulas for the simultaneous convex hull are, however, only known for special sets of functions. As one important example, we mention the case when the set of functions consists of the set of all quadratic monomials in a given number of variables (e.g., see [3,8]). In particular, Burer and Letchford [8] give in their work a characterization of valid linear inequalities and provide conditions under which a given linear inequality is irredundant or dominated by others.

In a recent work, Tawarmalani [34] analyzes structural properties of the simultaneous convex hull of finitely many general functions. The author gives necessary conditions on the extreme points of such sets and shows that a certain part of the simultaneous convex hull is already described by all convex hulls of the single functions provided that each function is submodular.

The paper is structured as follows. In Sect. 2, we consider the special case when f is a component-wise concave function, i.e., $n_y = 0$. We will, in particular, discuss conditions on f under which the corresponding extended formulation (3) is polyhedral and relate these to existing literature. In Sect. 3, we deal with general functions $f(x, y)$ of Classes 1 and 2 and derive an explicit description for their convex envelopes in an extended space. In Sect. 4, computational results are presented that demonstrate the usefulness of the extended formulation. Parts of this paper were presented in Ballerstein and Michaels [4].

2 RLT-based formulations for the convex envelope of component-wise concave functions

In this section, we focus on component-wise concave functions $f : [l, u] \subseteq \mathbf{R}^n \to \mathbf{R}$ (i.e., $n_y = 0$). Thus, f belongs to Classes 1 and 2. In Sect. 2.1, we link f with all multilinear monomials in the x-variables to obtain an extended formulation for its convex envelope. We then present conditions on f such that the extended formulation is polyhedral and refer to existing literature. In Sect. 2.2, the extended formulation is applied to reduce the size of relaxations, based on the Reformulation Linearization Technique, for polynomial programs including component-wise concave monomials.

2.1 Polyhedral extended formulations for component-wise concave functions

Let $f : [l, u] \subseteq \mathbf{R}^n \to \mathbf{R}$ be a continuous function. We link f with the vector

$$F^{(n)} := \left(x_1, \ldots, x_n, x_1x_2, \ldots, x_{n-1}x_n, x_1x_2x_3, \ldots, \prod_{i=1}^{n} x_i \right)$$

of all multilinear monomials. The extended formulation for $\mathrm{vex}_{[l,u]}[f]$ is obtained by the simultaneous convexification of the epigraph of f with the graphs of all monomials $F^{(n)}$

$$\mathcal{U}_f := \mathrm{conv}(\{(z, \mu) \in \mathbf{R}^{2^n} \mid \mu \geq f(x),\ z = F^{(n)}(x),\ x \in [l, u]\}),$$

where $z_J \in \mathbf{R}$ is a newly introduced variable associated with the monomial $\prod_{j \in J} x_j$, for each $\emptyset \neq J \subseteq N := \{1, \ldots, n\}$, and the variable $\mu \in \mathbf{R}$ is associated with f. A crucial part of the description of $\mathcal{U}_f$ is given by the following convex hull object

$$\mathcal{S}^{(n)}_{[l,u]} := \mathrm{conv}\left(\left\{z \in \mathbf{R}^{2^n-1} \mid z = F^{(n)}(x),\ x \in [l, u]\right\}\right).$$

Sherali and Adams showed in [2,27] that $\mathcal{S}^{(n)}_{[l,u]}$ forms a *simplex* whose facets are given by the linearized version of the so-called *bound-factor product constraints*, i.e., by

$$\left[\prod_{i \in I} (x_i - l_i) \prod_{i \in N \setminus I} (u_i - x_i) \right]_L (z) \geq 0, \quad \text{for all } I \subseteq N, \tag{4}$$

where the operator $[\cdot]_L(z)$ substitutes each monomial $\prod_{j \in J} x_j$ by a new variable z_J, e.g., $[-3x_1 + 5x_1x_2]_L(z)$ denotes the linear function $-3z_{\{1\}} + 5z_{\{1,2\}}$.

In expanded form, the facet-defining system in Eq. (4) yields (e.g., cf. [2])

$$e_v(z) \geq 0, \qquad \text{for all } v \in \mathrm{vert}([l, u]), \tag{5}$$

where e_v denotes the linear function $e_v : \mathbf{R}^{2^n-1} \to \mathbf{R}$ given by

$$z \mapsto e_v(z) := \sum_{J \subseteq N} (-1)^{\alpha(v)+|J|} F^{(n)}_{N \setminus J}(v)\, z_J, \tag{6}$$

and $\alpha(v)$ denotes the number of components of v which attain their lower bound, i.e., $\alpha(v) := \#\{i \in N \mid v_i = l_i\}$. It is easy to verify that any facet of $\mathcal{S}^{(n)}_{[l,u]}$ is also a facet of $\mathcal{U}_f$ (see Lemma 2 in the "Appendix"). Thus, $(z, \mu) \in \mathcal{U}_f$ implies that $z \in \mathcal{S}^{(n)}_{[l,u]}$.

Our second ingredient to derive a polyhedral description for $\mathcal{U}_f$ is the following known lemma.

Lemma 1 (e.g., Cor. 6 in [37]) *Let $f : [l, u] \subseteq \mathbf{R}^n \to \mathbf{R}$ be a continuous function. There exists a unique multilinear function $m_f : [l, u] \subseteq \mathbf{R}^n \to \mathbf{R}$ which coincides with f at each vertex of the box $[l, u]$. This multilinear function reads $m_f(x) = \sum_{J\subseteq N} a_J \prod_{j\in J} x_j$ with coefficients*

$$a_J = \frac{\sum_{v\in \mathrm{vert}([l,u])} (-1)^{\alpha(v)+|J|} \ \ F^{(n)}(v)_{N\setminus J} \ f(\hat{v})}{\prod_{i\in N}(u_i - l_i)}. \tag{7}$$

The vector $\hat{v}$ denotes the vector opposite to v in the box, i.e., $\hat{v}_j = l_j$, if $v_j = u_j$, and $\hat{v}_j = u_j$, otherwise.

The RLT theory [2,26–28] implies the following necessary and sufficient conditions on f such that $\mathcal{U}_f$ is a polyhedral set defined by the vertices of $[l, u]$.

Theorem 1 *Let $f : [l, u] \subseteq \mathbf{R}^n \to \mathbf{R}$ be a continuous function. Then,*

$$\mathcal{U}_f = \left\{ (z, \mu) \in \mathbf{R}^{2^n} \mid z \in \mathcal{S}^{(n)}_{[l,u]}, \ \mu \geq [m_f]_L(z) = \sum_{J\subseteq N} a_J z_J \right\} \tag{8}$$

with coefficients a_J according to Eq. (7)*, if and only if $f(x) \geq m_f(x) := \sum_{J\subseteq N} a_J \prod_{j\in J} x_j$ for all $x \in [l, u]$. In particular, this condition is fulfilled for component-wise concave functions f.*

Proof We have already remarked that the facet-description of $\mathcal{S}^{(n)}_{[l,u]}$ is irredundant for $\mathcal{U}_f$ (cf. Lemma 2 of the "Appendix"). It remains to discuss the additional inequality $\mu \geq [m_f]_L(z)$. If $f = m_f$, the description for $\mathcal{U}_f$ in the theorem follows easily from the fact that m_f can be uniquely represented as a linear combination of all multilinear monomials (see Lemma 1) and the RLT-theory [2,26–28]. If $f(x) \geq m_f(x)$ for all $x \in [l, u]$, then $\mathcal{U}_f = \mathcal{U}_{m_f}$ as f and m_f coincide at the vertices of the box which correspond to the extreme points of the set $\mathcal{U}_f$ (cf. [26,34]).

To prove the converse direction assume that there is an $\bar{x} \in [l, u]$ with $f(\bar{x}) < m_f(\bar{x})$. Then, for $(z, \mu) = (F^{(n)}(\bar{x}), f(\bar{x})) \in \mathcal{U}_f$, the relation

$$\mu = f(\bar{x}) < m_f(\bar{x}) = \sum_{J\subseteq N} a_J F^{(n)}_J(\bar{x}) = \sum_{J\subseteq N} a_J z_J$$

holds. This implies that $(z, \mu) \notin \{(z, \mu) \in \mathbf{R}^{2^n} \mid z \in \mathcal{S}^{(n)}_{[l,u]}, \ \mu \geq \sum_{J\subseteq N} a_J z_J\}$. Thus, $\mathcal{U}_f$ is not given by Eq. (8). □

The 'if"-part in Theorem 1 has been already discussed by Sherali [26]. In that work, the author used a description for the set $\mathcal{U}_m$ associated with a multilinear function $m : \mathbf{R}^n \to \mathbf{R}$ on $[0, 1]^n$ to provide a theoretical framework for projecting the extended space representation onto the (x, μ)-space. For some classes of multilinear functions, explicit formulas for the convex envelope are obtained this way. He further mentioned that $\mathcal{U}_f = \mathcal{U}_{m_f}$ if $f \geq m_f$ over $[l, u]$. We also refer to Tawarmalani [34] in which this relation is indicated.

The condition $f \geq m_f$ on $[l, u]$ in Theorem 1 implies that f must have a so-called *vertex-polyhedral* convex envelope, i.e., the set of extreme points of the epigraph of $\mathrm{vex}_{[l,u]}[f]$ corresponds to the set of vertices of the underlying polyhedral domain (see [32,33]). In fact, we have that $\mathrm{vex}_{[l,u]}[f] = \mathrm{vex}_{[l,u]}[m_f]$ ([37, Cor. 6]). Furthermore, it has been shown in Tardella [33, Thm. 2] that $\mathrm{vex}_{[l,u]}[f]$ is vertex-polyhedral if and only if $f(x) \geq \mathrm{vex}_{\mathrm{vert}([l,u])}[f](x)$, for all $x \in [l, u]$. This means that for any function f on $[l, u]$ with a vertex-polyhedral convex envelope, its convex envelope is identical to $\mathrm{vex}_{[l,u]}[m_f]$. However, the extended formulation in Theorem 1 is only correct in the more restrictive case of $f(x) \geq m_f(x)$ for all $x \in [l, u]$. To illustrate this, we consider the following example.

Example 1 Consider $f : \mathbf{R}^2 \to \mathbf{R}$, $x \mapsto f(x) := (x_1^3 - 2x_1)(x_2^2 - 0.5)$, on $[l, u] := [-2, 1] \times [-0.75, 0.95]$. The corresponding multilinear function reads $m_f(x) = -0.425 + 0.2125x_1 - 0.4x_2 + 0.2x_1x_2$, and $\mathrm{vex}_{[l,u]}[f] \equiv \mathrm{vex}_{[l,u]}[m_f]$ is given by

$$\max\left\{\tfrac{1}{80}(5x_1 - 64x_2 - 58),\ \tfrac{1}{400}(161x_1 - 80x_2 - 246)\right\}.$$

For the point $\bar{x} = (-0.74, -0.25)$, we have that $f(\bar{x}) \approx -0.470 < -0.44525 = m_f(\bar{x})$. It follows that the point

$$(\bar{x}_1, \bar{x}_2, \bar{x}_1\bar{x}_2, f(\bar{x})) = (-0.74, -0.25, 0.185, -0.470) \in \mathcal{U}_f$$

does not satisfy the additional inequality $\mu \geq -0.425 + 0.2125z_{\{1\}} - 0.4z_{\{2\}} + 0.2_{\{1,2\}}$.

Next, we give the explicit description of $\mathcal{U}_f$ for two important classes of component-wise concave functions.

Example 2 For $d \in \mathbf{Z}^n_{\geq 0}$, consider the negative of a monomial $x^d := \prod_{j=1}^n x_i^{d_i}$ over a nonnegative box $[l, u] \subseteq \mathbf{R}^n_{\geq 0}$. Then,

$$\mathcal{U}_{-x^d} = \left\{(z, \mu) \in \mathbf{R}^{2^n} \mid z \in \mathcal{S}^{(n)}_{[l,u]},\ \mu \geq \sum_{J \subseteq N} a_J z_J\right\},$$

where for all $J \subseteq N$, the coefficient a_J is equal to

$$(-1)^{n-|J|+1} \prod_{j \in N\setminus J} l_j u_j \prod_{j \in J}\left(\sum_{r=0}^{d_j-1} l_j^{d_j-1-r} u_j^r\right) \prod_{j \in N\setminus J}\left(\sum_{r=0}^{d_j-2} l_j^{d_j-2-r} u_r^j\right).$$

Example 3 Consider the bivariate function $f(x) := a_{20}x_1^{d_1} + a_{11}x_1x_2 + a_{02}x_2^{d_2}$, where $d_i \in \mathbf{Z}_{>0}$, $a_{20}, a_{11}, a_{02} \in \mathbf{R}$. If f is component-wise concave over a box $[l, u] \subseteq \mathbf{R}^2$, then a facet-description of $\mathcal{U}_f$ is given by the description of $\mathcal{S}^{(2)}_{[l,u]}$ and the additional inequality

$$\begin{aligned}&\left(a_{20}\sum_{i=0}^{d_1-1} l_1^{d_1-1-i}u_1^i\right) z_{\{1\}} + \left(a_{02}\sum_{i=0}^{d_2-1} l_2^{d_2-1-i}u_2^i\right) z_{\{2\}} + a_{11}\, z_{\{1,2\}} - \mu\\ &\leq a_{20}\sum_{i=1}^{d_1-1} l_1^{d_1-i}u_1^i + a_{02}\sum_{i=1}^{d_2-1} l_2^{d_2-i}u_2^i.\end{aligned}$$

2.2 Reduced RLT relaxations for polynomial programs

Theorem 1 can be used to reduce the size of relaxations for certain polynomial programs based on the RLT [27,31].

We adapt the notation in [29,31] and consider the polynomial program

$$\min\ \phi_0(x) \quad \text{s.t.} \quad \phi_i(x) \leq 0, \quad \forall\, i = 1, \ldots, m, \quad x \in [l, u] \subseteq \mathbf{R}^n_{\geq 0}, \tag{PP}$$

where $\phi_i(x) = \sum_{t \in T_i} \alpha_{it} \prod_{j \in J_{it}} x_j$, for $i = 0, \ldots, m$. The index set T_i, $i = 0, \ldots, m$, indicates the monomials occurring in $\phi_i(x)$. Let δ denote the largest degree of a monomial occurring in (PP), and let $N := \{1, \ldots, n\}$ be the index set of variables. By $\overline{N}$ we denote the multiset which consists of δ copies of N, i.e., $\overline{N} = \{N, N, \ldots, N\}$. Then, $J_{it} \subseteq \overline{N}$ and $|J_{it}| \leq \delta$ for all $t \in T_i$ and $i = 0, 1, \ldots, m$. For instance, the multiset $\{1, 1, 2\}$ corresponds to the monomial $x_1^2 x_2$. The classical RLT relaxation of (PP) reads (cf. [29,31])

$$\begin{aligned} \min \quad & [\phi_0(x)]_L(z, w) \\ \text{s.t.} \quad & [\phi_i(x)]_L(z, w) \leq 0, \quad \forall\, i = 1, \ldots, m, \quad (z, w) \in R_{\text{RLT}}, \end{aligned} \tag{PP$_{\text{RLT}}$}$$

where the operator $[\cdot]_L(z, w)$ denotes the linearization of an expression such that all multilinear monomials defined by a multiset J are substituted by a new variable $z_J \in \mathbf{R}$, and all nonmultilinear monomials are substituted by a variable $w_J \in \mathbf{R}$. For example, $[-x_1^3 x_2 + 5x_1x_2]_L(z, w) = -w_{\{1,1,1,2\}} + 5z_{\{1,2\}}$. The vector $(z, w) \in \mathbf{R}^{\binom{n+\delta}{\delta}-1}$ corresponds to all monomials $\prod_{j\in J} x_j$ with $\emptyset \neq J \subseteq \overline{N}$ and $|J| \leq \delta$. The set $R_{\text{RLT}} \subseteq \mathbf{R}^{\binom{n+\delta}{\delta}-1}$ is defined as

$$\begin{aligned} R_{\text{RLT}} := \Bigg\{ (z, w) \in \mathbf{R}^{\binom{n+\delta}{\delta}-1} \,\Bigg|\, & \forall (J_1 \cup J_2) \subseteq \overline{N}, |J_1 \cup J_2| = \delta : \\ & \Big[\prod_{j\in J_1} (x_j - l_j) \prod_{j\in J_2} (u_j - x_j) \Big]_L (z, w) \geq 0 \Bigg\}. \end{aligned}$$

Example 4 Let (PP) be given as $\min\{x_1 - x_1^3 \mid x_1 \in [0, 1]\}$. Then, $\delta = 3$, $\overline{N} = \{1, 1, 1\}$, and (PP$_{\text{RLT}}$) reads $\min\{z_{\{1\}} - w_{\{1,1,1\}} \mid (z, w) \in R_{\text{RLT}}\}$, where

$$R_{\text{RLT}} = \left\{ (z, w) \,\middle|\, \begin{array}{l} 1 - 3z_{\{1\}} + 3w_{\{1,1\}} - w_{\{1,1,1\}} \geq 0,\ w_{\{1,1\}} - w_{\{1,1,1\}} \geq 0 \\ z_{\{1\}} - 2w_{\{1,1\}} + w_{\{1,1,1\}} \geq 0,\ w_{\{1,1,1\}} \geq 0 \end{array} \right\}.$$

For example, $w_{\{1,1\}} - w_{\{1,1,1\}} \geq 0$ is obtained from $[(x_1 - 0)^2(1 - x_1)^1]_L(z, w) = [x_1^2 - x_1^3]_L(z, w) \geq 0$.

The RLT relaxation is a strong tool to relax polynomial programs. However, it can lead to an explosion in the problem size for problems with many variables and a high degree δ.

One possibility to reduce the size of RLT relaxations is given in Sherali et al. [30], where the existence of a linear subsystem is exploited. Theorem 1 offers another possibility to reduce the relaxation size. If the coefficient α_{it} of a nonmultilinear monomial is negative, the corresponding term $\alpha_{it} \prod_{j\in J_{it}} x_j$ is component-wise concave and can be underestimated with the help of Theorem 1. We show that this term can be excluded from the determination of the largest degree δ of the program, yet yielding the same relaxation quality.

Example 5 (Example 4 cont'd) The component-wise concave term $-x^3$ is replaced by $w_{\{1,1,1\}}$. Let $f(x) := -x^3$. Theorem 1 yields the underestimator $-w_{\{1,1,1\}} \geq [m_f]_L(z) = -z_{\{1\}}$. Excluding the term $-x^3$, the largest degree is $\delta = 1$ and the RLT-relaxation is $z_{\{1\}} \in \mathcal{S}^{(1)}_{[0,1]} = [0, 1]$. We will show that the relaxation $\min\{z_{\{1\}} - w_{\{1,1,1\}} \mid (z, w_{1,1,1}) \in R^{\star}_{\text{mod}}\}$ with

$$R^{\star}_{\text{mod}} = \left\{ (z, w_{\{1,1,1\}}) \middle| -z_{\{1\}} + w_{\{1,1,1\}} \leq 0, z_{\{1\}} \geq 0, z_{\{1\}} \leq 1 \right\}$$

is as strong as the RLT-relaxation in Example 4 although the relaxation based on $R^{\star}_{\text{mod}}$ needs one variable and one constraint less.

We consider the extreme case with $\alpha_{it} < 0$ for all $t \in T_i$ and $i = 0, \ldots, m$ such that $J_{it} \not\subseteq N$, that is the coefficients of the nonmultilinear monomials are negative. Recall that we consider nonnegative domains $[l, u] \subseteq \mathbf{R}^n_{\geq 0}$ so that all summands of the involved functions $\phi_i(x) = \sum_{t \in T_i} \alpha_{it} \prod_{j \in J_{it}} x_j$ are component-wise concave. We refer to this class of polynomial programs as *component-wise concave polynomial programs* (PP^-). Further, we assume that $\delta > n$. Otherwise, we consider the subset of monomials involved in the nonmultilinear monomial with the largest degree, e.g., for the monomials $x_1^2 x_2$, $x_1 x_2$ and, $x_1 x_2 x_3 x_4$ we just consider the monomials $x_1^2 x_2$ and $x_1 x_2$.

Technically, we proceed as follows. The index set of all nonmultilinear monomials, for which a variable w_J is introduced is denoted by $I := \{J \subseteq \overline{N} \mid 1 \leq |J| \leq \delta,\ \prod_{j \in J} x_j \text{ is nonmultilinear}\}$. The index set of nonmultilinear monomials which actually occur in (PP^-) is given by $I^\star := \{J_{it} \mid J_{it} \in I \text{ for } t \in T_i,\ \ i = 0, 1, \ldots, m\}$ and the corresponding subvector of w is denoted by $w^\star$. The modified RLT relaxation reads

$$\begin{aligned} \min \quad & [\phi_0(x)]_L(z, w^\star) \\ \text{s.t.} \quad & [\phi_i(x)]_L(z, w^\star) \leq 0,\ \forall\, i = 1, \ldots, m, \quad (z, w^\star) \in R^\star_{\text{mod}}, \end{aligned} \tag{PP^-_{mod}}$$

where

$$R^\star_{\text{mod}} := \left\{ (z, w^\star) \in \mathbf{R}^{(2^n - 1) + |I^\star|} \mid z \in \mathcal{S}^{(n)}_{[l,u]},\ -w^\star_J \geq [m_{-x^J}(x)]_L(z)\ \forall J \in I^\star \right\}$$

with $x^J := \prod_{j \in J} x_j$.

The problem characteristics of the two sets R_{RLT} and $R^\star_{\text{mod}}$ in terms of number of variables and constraints are compared in Table 1. Although the problem characteristics are quite different, we prove that the two relaxations of (PP^-) based on R_{RLT} and $R^\star_{\text{mod}}$ return the same objective function value.

Theorem 2 $\min(\text{PP}^-_{\text{RLT}}) = \min(\text{PP}^-_{\text{mod}})$.

Proof The relation $\min(\text{PP}^-_{\text{RLT}}) \geq \min(\text{PP}^-_{\text{mod}})$ can be derived as follows. Given $(\bar{z}, \bar{w}) \in R_{\text{RLT}}$, assume that its subvector $(\bar{z}, \bar{w}^\star) \notin R_{\text{mod}}$. As the RLT theory implies that $\bar{z} \in \mathcal{S}^{(n)}_{[l,u]}$ (see [31]), it follows that there is a $J \in I^\star$ with $-\bar{w}^\star_J < [m_{-x^J}(x)]_L(\bar{z})$. By Theorem 1, there exists an $\bar{x} \in [l, u]$ with $\prod_{j \in J} \bar{x}_j < m_{x^J}(\bar{x})$. This contradicts that $-\prod_{j \in J} \bar{x}_j$ is component-wise concave over the underlying positive domain and thus, we can conclude that $(\bar{z}, \bar{w}^\star) \in R_{\text{mod}}$.

For the converse relation let $(\bar{z}, \bar{w}^\star)$ be an optimal solution of $\min(\text{PP}^-_{\text{mod}})$. We can assume that $-\bar{w}^\star_J$ is at its lower bound for all $J \in I^\star$, i.e., $-\bar{w}^\star_J = \sum_{S \subseteq N} a_{J,S} \bar{z}_S$ for all $J \in I^\star$, because $-\bar{w}^\star_J$ is not bounded from below by the constraints $[\phi_i(x)]_L(z, w^\star) \leq 0$, $i =$

Table 1 Problem characteristics of R_{RLT} and $R^\star_{\text{mod}}$. The formulas for R_{RLT} are from Sherali and Tuncbilek [31]

	R_{RLT}	$R^\star_{\text{mod}}$
# variables	$\binom{n+\delta}{\delta} - 1$	$(2^n - 1) + \lvert I^\star \rvert$
# constraints	$\sum_{k=0}^{\delta} \binom{n+k-1}{k} \binom{n+(\delta-k)-1}{\delta-k}$	$2^n + \lvert I^\star \rvert$
Case: $n = 4$ and $\delta = 5$		
# variables	125	$15 + \lvert I^\star \rvert \leq 15 + 110 = 125$
# constraints	792	$16 + \lvert I^\star \rvert \leq 16 + 110 = 126$

$1,\ldots,m$, and the minimization of the objective function $[\phi_0(x)]_L(z, w^\star)$ attains its optimal solution at the minimal $-\bar{w}^\star_J$ (if $-\bar{w}^\star_J$ occurs in the objective function). To construct a solution $(\bar{z}, \bar{w}) \in R_{\text{RLT}}$, we define $-\bar{w}_J := \sum_{S\subseteq N} a_{J,S}\bar{z}_S$ for all $J \in I \setminus I^\star$. As $\bar{z} \in \mathcal{S}^{(n)}_{[l,u]}$, it can be represented as $\bar{z} = \sum_{v\in V} \lambda_v F^{(n)}(v)$, where $V := \text{vert}([l,u])$. Let $G : \mathbf{R}^n \to \mathbf{R}^{|I|}$, with $G_J(x) := \prod_{j\in J} x_j$ for all $J \in I$, be the vector of nonmultilinear monomials. Then, $-\bar{w}_J = \sum_{S\subseteq N} a_{J,S}(\sum_{v\in V} \lambda_v F^{(n)}_S(v)) = \sum_{v\in V} \lambda_v \prod_{j\in J} v_j = \sum_{v\in V} \lambda_v G_J(v)$ for all $J \in I$. Therefore, the point $(\bar{z}, \bar{w})$ can be represented as convex combination of points $(F^{(n)}(v), G(v)) \in R_{\text{RLT}}$ which shows that $(\bar{z}, \bar{w}) \in R_{\text{RLT}}$. □

One can even show that the quality of the relaxations of (PP$^-$) based on R_{RLT} and $R^\star_{\text{mod}}$ is not only identical but best possible when dealing with polynomial programs and using a relaxation which is based on the substitution of monomials by new variables. The desired object in this context is given by the convex hull of all monomials with degree less or equal to δ and reads

$$\mathcal{C} := \text{conv}\left(\left\{(z, w) \mid z = F^{(n)}(x),\ w_J = \prod_{j\in J} x_j\ \forall J \in I,\ x \in [l,u]\right\}\right).$$

The description of $\mathcal{C}$ is not polyhedral and also not known in general. Let (PP$^-_{\mathcal{C}}$) denote the relaxation of component-wise concave polynomial programs (PP$^-$) based on $\mathcal{C}$. We can prove the following statement using the same arguments as in the proof of Theorem 2.

Theorem 3 $\min(\text{PP}^-_{\mathcal{C}}) = \min(\text{PP}^-_{\text{RLT}}) = \min(\text{PP}^-_{\text{mod}})$.

The strength of the RLT based relaxation for (PP$^-$) provides a possible explanation for an observation made by Sherali et al. in [29] for polynomial programs: The more the programs are of the form (PP$^-$), i.e., the more negative coefficients occur, the faster the computations. The authors generated random instances which are dense and sometimes dominated by the objective function, e.g., the place in the program files occupied by the objective function varies from 15 to 90 %. In particular, all monomials occur in the objective function while their occurrence in the constraints is determined randomly. The random instances are solved by the classical RLT approach and additionally by a combined approach of RLT and linear cuts derived from semidefinite programming (SDP). Table 2 displays their results and shows that a higher percentage of negative coefficients in the objective function leads to a tremendous acceleration of the computations. One reason for this acceleration is given by the tight RLT based relaxation in this case.

Table 2 The table presents the average CPU time of an RLT and a combined RLT+SDP based algorithm depending on the percentage of negative objective function coefficients. The figures are taken from Table 3 in Sherali et al. [29]

Algorithm	CPU time (depending on % of neg. obj. coef.)		
	10 %	50 %	90 %
RLT	1,173	1,850	138
RLT+SDP	674	1,055	45

3 Extended formulation for the convex envelope of nonlinear functions

In this section we present closed-form expressions for extended formulations for the convex envelope of functions $f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x+n_y} \to \mathbf{R},\ (x, y) \mapsto f(x, y)$ contained in Classes 1 and 2 (see Sect. 1). Similar to the case of component-wise concave functions, we show in Sects. 3.1 and 3.2 that the extended formulations are given by a polytope corresponding to the convex hull of the graph of a particular collection of multilinear monomials and one additional inequality. While this inequality is linear for component-wise functions, it can be *nonlinear* for functions belonging to Classes 1 and 2. In Sect. 3.3, we compare the extended formulations with available convex envelopes which are mainly due to recent results by Khajavirad and Sahinidis [15,16].

3.1 Class 1

Let $f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x+1} \to \mathbf{R},\ (x, y) \mapsto f(x, y)$ be a function that is component-wise concave in the x-variables, and that f is either convex or concave in y whenever x is fixed to one of the vertices of $[l^x, u^x]$. In the special case when f is concave in y for each fixing of x, the description of $\mathcal{U}_f$ is polyhedral and given by Theorem 1. Next, we show that for functions belonging to Class 1, the description of $\mathcal{U}_f$ is still given by the simplex $\mathcal{S}^{(n)}_{[l,u]}$ and one additional, possibly nonlinear restriction.

Theorem 4 *Consider a function* $f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x} \times \mathbf{R} \to \mathbf{R},\ (x, y) \mapsto f(x, y)$. *Let* $V_x := \mathrm{vert}([l^x, u^x])$ *and* $n := n_x + 1$. *Assume that* $f(x, y)$ *is component-wise concave in* x, *and that* V_x *can be partitioned into* V_1 *and* V_2 *such that* $f(x, y)$ *is convex but not linear in* y *for each* $x \in V_1$ *and concave in* y *for each* $x \in V_2$. *Then,*

$$\mathcal{U}_f = \left\{(z, \mu) \in \mathbf{R}^{2^n} \mid z \in \mathcal{S}^{(n)}_{[l,u]} \text{ and } \mu \geq \phi(z)\right\},$$

where $\phi(z) := \sum_{v \in V_1} \lambda_v f(v, y^v) + \sum_{v \in V_2} \lambda_{v,l} f(v, l^y) + \lambda_{v,u} f(v, u^y)$, *and where for* $v \in V_1$,

$$\lambda_v = \frac{e_{\hat{v}}(z^x)}{\prod_{j=1}^{n_x}(u_j - l_j)}, \quad y^v = \frac{\sum_{J \subseteq N_x} (-1)^{|J|+\alpha(\hat{v})}\ F^{(n_x)}_{N_x \setminus J}(\hat{v}) z_{J \cup \{n\}}}{e_{\hat{v}}(z^x)}, \tag{9}$$

and for $v \in V_2$

$$\lambda_{v,l} = \frac{e_{(\hat{v},u^y)}(z)}{\prod_{j=1}^{n}(u_j - l_j)} \quad \text{and} \quad \lambda_{v,u} = \frac{e_{(\hat{v},l^y)}(z)}{\prod_{j=1}^{n}(u_j - l_j)}. \tag{10}$$

Here, $\hat{v}$ *denotes the vector opposite to* v *in* $[l^x, u^x]$, z^x *denotes the subvector of* z*-variables with entries* z_J, $\emptyset \neq J \subseteq N_x$, *and* $e_{\hat{v}}(z^x)$ *according to* Eq. (6).

Proof Lemma 2 of the "Appendix" implies that the description of $\mathcal{S}^{(n)}_{[l,u]}$ is necessary to characterize $\mathcal{U}_f$. For the remaining constraint we can argue as follows. As f is component-wise concave in the x-variables and the multilinear monomials $\prod_{j \in J} x_j$ are linear in the x-variables, the set $\mathcal{U}_f$ can be represented as follows (see [34,37]):

$$\mathcal{U}_f = \mathrm{conv}\left(\bigcup_{v \in V_x} \left\{(F^{(n)}(v, y^v), \mu) \mid \mu \geq f(v, y^v),\ y^v \in [l^y, u^y]\right\}\right).$$

For each fixed $v \in V_x$ the set $\mathcal{U}_{f(v,y)}$ corresponds to the epigraph of the function $\mathrm{vex}_{[l^y,u^y]}[f_v]$, where $f_v(y) := f(v, y)$. If $v \in V_1$, then $f(v, y)$ is convex and

$\mathrm{vex}_{[l^y,u^y]}[f_v](y) = f(v,y)$. If $v \in V_2$, then $f(v,y)$ is concave and $\mathrm{vex}_{[l^y,u^y]}[f_v](y)$ is given by the secant connecting $(l^y, f_v(l_y))$ and $(u^y, f_v(u_y))$.

Disjunctive programming techniques imply that, for any given $\bar{z} \in \mathcal{S}^{(n)}_{[l,u]}$, the corresponding minimal value μ with $(\bar{z},\mu) \in \mathcal{U}_f$ can be computed by the following optimization problem

$$\begin{aligned}
\min\ & \sum_{v\in V_1} \lambda_v f(v,y^v) + \sum_{v\in V_2} \left(\lambda_{v,l} f(v,l^y) + \lambda_{v,u} f(v,u^y)\right)\\
\text{s.t.}\ & \bar{z} = \sum_{v\in V_1} \lambda_v F^{(n)}(v,y^v) + \sum_{v\in V_2} \left(\lambda_{v,l} F^{(n)}(v,l^y) + \lambda_{v,u} F^{(n)}(v,u^y)\right)\\
& 1 = \sum_{v\in V_1} \lambda_v + \sum_{v\in V_2} \left(\lambda_{v,l} + \lambda_{v,u}\right)\\
& \lambda_v \ge 0,\ v\in V_1,\quad \lambda_{v,l},\lambda_{v,u} \ge 0,\ v\in V_2,\quad y^v \in [l^y,u^y],\ v \in V_1.
\end{aligned}$$

We infer from Lemma 3 of the “Appendix” that the solution given in Eqs. (9) and (10) is optimal to the problem above, where $\lambda_v \ge 0,\ v \in V_1,\ \lambda_{v,l},\lambda_{v,u} \ge 0,\ v \in V_2$, and $1 = \sum_{v\in V_1}\lambda_v + \sum_{v\in V_2}(\lambda_{v,l}+\lambda_{v,u})$ follows from the fact that $\bar{z} \in \mathcal{S}^{(n)}_{[l,u]}$. This proves the claim. □

Theorem 1 is a special case of Theorem 4, namely for $V_1 = \emptyset$ and $V_2 = V_x$. Even though the two representations do not coincide at a first glance, it can be checked that the additional inequality in Theorem 4 reduces to the one in Theorem 1 in this special case.

The next example illustrates Theorem 4 and emphasizes its potential for simultaneous convexification purposes.

Example 6 Let $f(x) = x_1x_2/y,\ x_1 \in [-1,1], x_2 \in [0.1,1], y \in [0.1,1]$. This is Example 2 in [15]. The convex envelope over the subdomain $0.9x_1 + 2x_2 \ge 1.1$ reads

$$\mathrm{vex}_{[l,u]}[f](x,y) = \begin{cases}
\dfrac{(0.5x_1+1.1x_2-0.6)^2}{y+0.05x_1+0.11x_2-0.16} + 5x_1 - 1.1x_2 - 3.9, & \text{if } 0.1 \le y \le s_1,\\
\dfrac{(0.5x_1+0.76x_2-0.26)^2}{y+0.05x_1-0.05} + 5x_1 - 5, & \text{if } s_1 \le y \le s_2,\\
\dfrac{0.12(x_2-1)^2}{y-0.45x_1-1.1x_2+0.56} + 5.5x_1 + 1.1x_2 - 5.6, & \text{if } s_2 \le y \le s_3,\\
10y + x_1 + x_2 - 11, & \text{if } s_3 \le y \le 1,
\end{cases}$$

where $s_1 = 10y + x_1 + x_2 - 11,\ s_2 = 0.45x_1 + 0.76x_2 - 0.21$, and $s_3 = 0.45x_1 + 0.55$. The convex envelope over $0.9x_1 + 2x_2 \le 1.1$ reads

$$\mathrm{vex}_{[l,u]}[f](x,y) = \begin{cases}
\dfrac{0.5(x_1+1)^2}{20y+x_1-1} + 0.5x_1 - 10x_2 + 0.5, & \text{if } 0.1 \le y \le s_3,\\
y + 0.1x_1 - 10x_2, & \text{if } s_3 \le y \le 1.1 - x_2,\\
10y + 0.1x_1 - x_2 - 9.9, & \text{if } 1.1 - x_2 \le y \le 1.
\end{cases}$$

The extended formulation $\mathcal{U}_f$ is given by the facets of $\mathcal{S}^{(3)}_{[l,u]}$ and the inequality $\mu \ge \phi(z)$ with

$$\begin{aligned}
\phi(z) := &-5.5z_{\{2\}} + 5.5z_{\{1,2\}} + 5z_{\{2,3\}} - 5z_{\{1,2,3\}} - \frac{101}{81}\\
&+ \frac{\left(1 + z_{\{1\}} - z_{\{2\}} - z_{\{1,2\}}\right)^2}{18\left(z_{\{3\}} + z_{\{1,3\}} - z_{\{2,3\}} - z_{\{1,2,3\}}\right)} + \frac{\left(1 + z_{\{1\}} - 10z_{\{2\}} - 10z_{\{1,2\}}\right)^2}{180\left(-z_{\{3\}} - z_{\{1,3\}} + 10z_{\{2,3\}} + 10z_{\{1,2,3\}}\right)}.
\end{aligned}$$

The set $\mathcal{U}_f$ is the simultaneous convex hull of (z,μ) with $\mu \ge f(x,y)$ and the seven multilinear monomials in the x- and y-variables over $[l,u]$. Let $\mathcal{R}$ denote the convex relaxation, where f and each multilinear monomial are individually relaxed by their convex and concave envelope. We can bound component μ from above by $\max\{f(x, y) \mid (x, y) \in [l, u]\} = 10$. The volumes of the individually and simultaneously convexified sets are computed using the function `NIntegrate` in MATHEMATICA 8 [40], and are $\mathrm{Vol}(\mathcal{R}, \mu \leq 10) \approx 0.325$ and $\mathrm{Vol}(\mathcal{U}_f, \mu \leq 10) \approx 0.014$. This yields a gap of 2,120 %.

3.2 Class 2

Next, we consider functions $f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x} \times \mathbf{R}^{n_y} \to \mathbf{R},\ (x, y) \mapsto f(x, y)$, that are component-wise concave in the x-variables, and that are convex on the space of the y-variables for every fixed $x \in \mathrm{vert}([l^x, u^x])$.

The special case of $n_y = 1$ is already covered by Theorem 4. For $n_y \geq 2$, we proceed as follows. We set $N_x := \{1, \dots, n_x\},\ N_y := \{1, \dots, n_y\}$, and introduce

- for all $J \subseteq N_x,\ J \neq \emptyset$, the monomials $\prod_{j \in J} x_j$ and the variables $z_J \in \mathbf{R}$,
- for all $k \in N_y$ and for all $J \subseteq N_x$, the monomials $y_k \prod_{j \in J} x_j$ and the variables $w_J^k \in \mathbf{R}$, where we define $w^k := (w_\emptyset^k, w_{\{1\}}^k, \dots, w_{N_x}^k)$ which is associated with

$$y_k \left(1, F^{(n)}(x)\right) = \left(y_k, y_k x_1, \dots, y_k x_n, y_k x_1 x_2, \dots, y_k \prod_{j=1}^{n} x_j \right).$$

This collection of monomials ensures that for a fixed x all introduced monomials are either constant or linear. An extended formulation for the convex envelope of f is then given by the set

$$\begin{aligned}
\mathcal{E}_f \ := \ \mathrm{conv}\Big(\Big\{ \left(z, w^1, \dots, w^{n_y}, \mu\right) \in \mathbf{R}^{(2^{n_x}-1)+n_y \cdot 2^{n_x}+1} \ \Big|\ & \mu \geq f(x, y), \\
z = F^{(n_x)}(x),\ w^k = y_k \left(1, F^{(n_x)}(x)\right), \quad & \text{for all } k \in N_y, \\
z_{\{j\}} = x_j \in \left[l_j^x, u_j^x\right], \quad & j = 1, \dots, n_x, \\
w_\emptyset^k = y_k \in \left[l_k^y, u_k^y\right], \quad & k = 1, \dots, n_y \Big\}\Big).
\end{aligned}$$

By construction and our assumptions on f, $\mathcal{E}_{f(\bar{x},y)}$ corresponds to the epigraph of $\mathrm{vex}_{[l,u]}[f(\bar{x}, y)] = f(\bar{x}, y)$ for every fixed $\bar{x} \in \mathrm{vert}([l^x, u^x])$. Similar to the description of $\mathcal{U}_f$ which is based on $\mathcal{S}_{[l,u]}^{(n)}$, Lemma 2 of the "Appendix" implies that the description of the following set is needed for $\mathcal{E}_f$.

$$\begin{aligned}
\mathcal{L}_{[l,u]}^{(n_x,n_y)} := \mathrm{conv}\Big(\Big\{ \left(z, w^1, \dots, w^{n_y}\right) \in \mathbf{R}^{(2^{n_x}-1)+n_y \cdot 2^{n_x}} \ \Big|\ & z = F^{(n_x)}(x), \\
w^k = y_k \left(1, F^{(n_x)}(x)\right), \quad & \text{for all } k \in N_y, \\
z_{\{j\}} = x_j \in \left[l_j^x, u_j^x\right], \quad & j = 1, \dots, n_x, \\
w_\emptyset^k = y_k \in \left[l_k^y, u_k^y\right], \quad & k = 1, \dots, n_y \Big\}\Big).
\end{aligned}$$

Sherali and Adams analyzed this set in [28] and, in a more general setting, in [2] and showed that

$$\mathcal{L}_{[l,u]}^{(n_x,n_y)} = \bigcap_{k=1}^{n_y} \left\{ \left(z, w^1, \dots, w^{n_y}\right) \mid (z, w^k) \in \mathcal{S}_{[l^x,u^x] \times [l_k^y, l_k^y]}^{(n_x+1)} \right\}. \tag{11}$$

According to our definition, points in $\mathcal{S}_{[l^x,u^x] \times [l_k^y, l_k^y]}^{(n_x+1)}$ are labeled by subsets $J \subseteq \{1, \dots, n_x + 1\},\ J \neq \emptyset$, that follow the order of the vector $F^{(n_x+1)}$. This labeling might be different to the order of the vector (z, w^k). However, to keep the notation short and simple, we assume for Eq. (11) that the components of points (z, w^k) are permuted in the correct way when necessary.

We are now ready to give a description for $\mathcal{E}_f$.

Theorem 5 *Let* $f : [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x} \times \mathbf{R}^{n_y} \to \mathbf{R}$ *be a function that is component-wise concave in the* x*-variables for every fixed* $y \in [l^y, u^y]$ *and convex on the space of* y*-variables for every* $\bar{x} \in V := \text{vert}([l^x, u^x])$*. Then,*

$$\mathcal{E}_f = \left\{ (z, w^1, \ldots, w^k, \mu) \;\middle|\; \begin{array}{l} (z, w^k) \in \mathcal{S}^{(n_x+1)}_{[l^x,u^x]\times[l^y_k,u^y_k]}, \quad k = 1, \ldots, n_y, \\ \mu \geq \varphi(z, w) := \sum_{v \in V} \lambda_v \; f(v, y^v) \end{array} \right\},$$

where, for all $v \in V$ *and* $k \in N_y$,

$$\lambda_v = \frac{e_{\hat{v}}(z)}{\prod_{i=1}^{n_x}(u^x_i - l^x_i)}, \quad y^v_k = \frac{\sum_{J \subseteq N_x} (-1)^{|J|+\alpha(\hat{v})} \; F^{(n_x)}_{N_x \setminus J}(\hat{v}) w^k_J}{e_{\hat{v}}(z)}, \tag{12}$$

$e_{\hat{v}}(z)$ *according to* Eq. (6)*, and* $\hat{v}$ *is the vector opposite to* v *in* $[l^x, u^x]$.

Proof The constraints $(z, w^k) \in \mathcal{S}^{(n_x+1)}_{[l^x,u^x]\times[l^y_k,u^y_k]}$, $k \in N_y$, are implied by Lemmas 2 of the "Appendix" and Eq. (11). For the remaining constraint we can argue similar to the proof of Theorem 4. This way, we obtain for any given $(\bar{z}, \bar{w}^1, \ldots, \bar{w}^{n_y}) \in \mathcal{L}^{(n_x,n_x)}_{[l,u]}$ that the corresponding minimal value μ with $(\bar{z}, \bar{w}^1, \ldots, \bar{w}^{n_y}, \mu) \in \mathcal{E}_f$ is given by

$$\begin{array}{lllll} \min & \sum_{v \in \text{vert}([l^x,u^x])} \lambda_v f(v, y^v) & & & \\ \text{s.t.} & \sum_{v \in \text{vert}([l^x,u^x])} \lambda_v \; F^{(n_x)}(v) & = \bar{z}, & & \\ & \sum_{v \in \text{vert}([l^x,u^x])} \lambda_v & = 1, & & \\ & \lambda_v & \geq 0, & v \in \text{vert}([l^x, u^x]), & \\ & \sum_{v \in \text{vert}([l^x,u^x])} \lambda_v \; y^v_k \; F^{(n_x)}(v) & = \overline{w}^k, & k = 1, \ldots, n_y & \\ & y^v & \in [l^y, u^y]. & & \end{array} \tag{13}$$

The specific structure of the constraints set implies that the values of the multipliers λ_v are uniquely determined by the first three sets of constraints. For fixed λ_v, the remaining constraints decompose into n_y variable disjoint linear subsystems that can be solved independently from each other (see [2,28]). Thus, for each $k \in \{1, \ldots, n_y\}$, we can solve the system

$$\sum_{v \in \text{vert}([l^x,u^x])} \lambda_v F^{(n_x)}(v) = \bar{z}, \qquad \sum_{v \in \text{vert}([l^x,u^x])} \lambda_v \; y^v_k \; F^{(n_x)}(v) = \overline{w}^k.$$

This subsystem is a special case of the system considered in Lemma 3 (with $V_2 = \emptyset$). This gives rise to the solution as given in Eq. (12). Note that the solution for the λ_v-variables does not depend on the solution for y_k-variables and that the restrictions $\sum_{v \in \text{vert}([l^x,u^x])} \lambda_v = 1$, $\lambda_v \geq 0$ and $y^v_k \in [l^y_k, u^y_k]$ follow from the fact that $(\bar{z}, \bar{w}^1, \ldots, \bar{w}^{n_y}) \in \mathcal{L}^{(n_x,n_y)}_{[l,u]}$. $\square$

The next example illustrates Theorem 5 and compares the extended formulation to the convex envelope.

Example 7 Let $f := x/(y_1 y_2)$, $(x, y_1, y_2) \in [l, u] := [0.5, 2] \times [0.1, 1] \times [1.5, 2]$. This is Example 2 in [16], where the convex envelope of f is described by six different formulas, each of them valid over a specific subdomain of the box $[l, u]$. The extended formulation

$\mathcal{E}_f$ obtained by the simultaneous convexification with the monomials $y_1 x$ $(= w^1_{\{1\}})$ and $y_2 x$ $(= w^2_{\{1\}})$ is given by

$$\mathcal{E}_f = \left\{ (z, w^1, w^2, \mu) \in \mathbf{R}^5 \;\middle|\; \begin{array}{l} (z, w^1) \in \mathcal{S}^{(2)}_{[0.5,2]\times[0.1,1]}, \ (z, w^2) \in \mathcal{S}^{(2)}_{[0.5,2]\times[1.5,2]}, \\ \mu \geq \varphi(z, w^1, w^2) \end{array} \right\},$$

where

$$\varphi(z, w^1, w^2) := \frac{l^x (u^x - z)^3}{(u^x - l^x)\left(u^x w^1_{\emptyset} - w^1_{\{1\}}\right)\left(u^x w^2_{\emptyset} - w^2_{\{1\}}\right)} + \frac{u^x (z - l^x)^3}{(u^x - l^x)\left(l^x w^1_{\emptyset} - w^1_{\{1\}}\right)\left(l^x w^2_{\emptyset} - w^2_{\{1\}}\right)}.$$

The variable μ can be bounded from above by $\max\{f(x, y) \mid x \in [l, u]\} = 40/3$. MATHEMATICA 8 computes the volumes of $\mathcal{E}_f$ and its individual counterpart $\mathcal{R}$ as $\mathrm{Vol}(\mathcal{E}_f, \mu \leq 40/3) \approx 0.263$ and $\mathrm{Vol}(\mathcal{R}, \mu \leq 40/3) \approx 0.269$ which implies a gap of 2 %.

3.3 Comparison with available convex envelopes

In Examples 6 and 7, some advantages and disadvantages of the extended formulations $\mathcal{U}_f$ and $\mathcal{E}_f$ compared to the convex envelopes are indicated. The extended formulations have the disadvantage of introducing additional variables corresponding to certain multilinear monomials. Especially for higher dimensional functions, the exponential growth in the number of variables can lead to an explosion of the problem size. Nevertheless, for lower dimensional cases the growth of variables is reasonable and we noticed that the multilinear monomials often occur in the problem description, see e.g., problems `ex734` and `ex735` from GLOBALLib [11] and `eniplac`, `1252`, `nvs05`, and `pump` from MINLPLib [9]. Therefore, the extended formulations can lead to improved convex relaxations as indicated in Example 6. Furthermore, one can check that the formulas describing parts of the convex envelope are only valid over the specified subdomains. For instance, consider Example 6 and let $(\bar{x}_1, \bar{x}_2, \bar{y}) = (0, 0.5, 0.7)$. Then, $\mathrm{vex}_{[l,u]}[f](\bar{x}_1, \bar{x}_2, \bar{y}) = \bar{y} + 0.1\bar{x}_1 - 10\bar{x}_2 = -4.3$ while this is violated by the last formula, $10\bar{y} + 0.1\bar{x}_1 - \bar{x}_2 - 9.9 = -3.4$. Usually, convex relaxations are constructed and solved over the entire domain. Thus, the formulas of the convex envelope can be used in a cut-generation algorithm to construct valid linear cuts, but they cannot be added directly to the convex relaxation whereas this is possible with the extended formulation.

To conclude this section, we emphasize that the convex envelopes for the two classes of functions considered in this section are not known, in general. As mentioned in the introduction, Khajavirad and Sahinidis [15,16] derived explicit formulas of convex envelopes for special subclasses in the original space. They considered functions $f(x, y) = g(x)h(y)$, where

- $g(x)$ is a component-wise concave function such that its restriction to the vertices is submodular and has the same monotonicity in every argument,
- $h(y)$ is a nonnegative convex function of one of the two forms (i) $h(y) = y^a,\ a \in \mathbf{R}\backslash[0, 1]$ or (ii) $h(y) = a^y, a > 0$, and
- $g(x)$ is nonnegative or $h(y)$ is monotone.

For special cases they can relax some conditions but the assumptions above reflect their general setting.

First, the formulations presented in this work do not require that f can be written as $f(x, y) = g(x)\, h(y)$ as the following example illustrates.

Example 8 Let $f : \mathbf{R}^2 \to \mathbf{R}$, $(x, y) \mapsto f(x, y) = (y + 1)\exp(xy)$ be restricted to $[l, u] = [-1, 1]\times[-3, -1]$ so that the function belongs to Class 1. Thus, Theorem 4 yields $(x, z) \in \mathcal{U}_f$ if and only if $z \in \mathcal{S}^{(2)}_{[l,u]}$ and $\mu \geq \phi(z)$, where

$$\phi(z) := \frac{1 - z_{\{1\}} + z_{\{2\}} - z_{\{1,2\}}}{2}\exp(3) + \frac{1 + z_{\{1\}} + z_{\{2\}} + z_{\{1,2\}}}{2}\exp\left(\frac{z_{\{2\}} + z_{\{1,2\}}}{1 + z_{\{1\}}}\right).$$

Second, Khajavirad and Sahinidis state that the property of component-wise concavity of $g(x)$ can be relaxed to having a vertex-polyhedral convex envelope in their context. For the extended formulation, we discuss in the following remark that the component-wise concavity of $g(x)$ can be relaxed by $g(x) \geq m_g(x)$ for all $x \in [l^x, u^x]$. In this case, the assumptions by Khajavirad and Sahinidis are more general than ours. For example, consider the function $g : [0, 1]^2 \to \mathbf{R}$, $x \mapsto g(x) := \max\{-x_1 + 0.5, -x_2 + 0.5\}$, that is vertex-polyhedral, submodular, when restricted to the vertices of $[0, 1]^2$, and nonincreasing in each variable x_i. However, $g(x) < m_g(x) = -x_1x_2 + 0.5$ for all x in the interior of the box $[0, 1]^2$.

Remark 1 The condition of being component-wise concave in the x-variables in Theorems 4 and 5 can be relaxed to the condition $f(x, \bar{y}) \geq m_{f(x,\bar{y})}(x)$ for all $x \in [l^x, u^x]$ and all fixed values $\bar{y} \in [l^y, u^y]$, where $m_{f(x,\bar{y})}(x)$ is the multilinear function obtained in Lemma 1. If we consider the special case of $f(x, y) = g(x)h(y) \neq 0$ with $h(y)$ nonnegative and convex, we can strengthen Theorems 4 and 5 as follows. The extended formulation in Theorem 4 is valid if and only if $g(x) \geq m_g(x)$ for all $x \in [l^x, u^x]$. If $g(x)$ is further nonnegative, the extended formulation in Theorem 5 is valid if and only if $g(x) \geq m_g(x)$ for all $x \in [l^x, u^x]$.

Third, in the setting of the convex envelope the univariate variable y in the convex function $h(y)$ can be replaced by $c^T y+d$, where y is multivariate, if $g(x)$ is nonnegative. This extension is also covered by Theorem 5 because $f(x, c^T y + d)$ is the composition of a convex and a linear function and thus, it is convex [24].

Finally, Theorems 4 and 5 do not require that $g(x)$ is submodular restricted to the vertices and nondecreasing (or nonincreasing) in every argument. For instance, the convex envelope of the function $f(x, y) = g(x)h(y) = (x_1x_2)y^2$ cannot be determined by the framework of Khajavirad and Sahinidis as g is supermodular (cf. Section 4.1 in [16]) while the function satisfies all assumptions of Theorem 4. As an example consider the function over $[l, u] = [1, 2]^3$. Theorem 4 implies that $(z, \mu) \in \mathcal{U}_f$ if and only if $z \in \mathcal{S}^{(3)}_{[l,u]}$ and

$$\begin{aligned}\mu \geq\ & \frac{\left(4z_{\{3\}} - 2z_{\{1,3\}} - 2z_{\{2,3\}} + z_{\{1,2,3\}}\right)^2}{4 - 2z_{\{1\}} - 2z_{\{2\}} + z_{\{1,2\}}} + \frac{2\left(2z_{\{3\}} - z_{\{1,3\}} - 2z_{\{2,3\}} + z_{\{1,2,3\}}\right)^2}{-2 + z_{\{1\}} + 2z_{\{2\}} - z_{\{1,2\}}}\\ &+ \frac{2\left(2z_{\{3\}} - 2z_{\{1,3\}} - z_{\{2,3\}} + z_{\{1,2,3\}}\right)^2}{-2 + 2z_{\{1\}} + z_{\{2\}} - z_{\{1,2\}}} + \frac{4\left(z_{\{3\}} - z_{\{1,3\}} - z_{\{2,3\}} + z_{\{1,2,3\}}\right)^2}{1 - z_{\{1\}} - z_{\{2\}} + z_{\{1,2\}}}.\end{aligned}$$

4 Computations

The extended formulations presented in the previous sections are based on the introduction of an exponential amount of additional variables corresponding to multilinear monomials. In this section we show that the extended description can accelerate computations significantly not only for instances in which all these multilinear monomials occur in the problem formulation but also for instances in which only a few monomials appear. This indicates that the strength of the extended formulations can compensate the computational obstacles implied by the introduction of unnecessary variables (at least for low dimensional functions up to dimension four).

We focus on component-wise concave functions discussed in Sect. 2 because their extended formulation is polyhedral (see Theorem 1) and thus easier to implement. Yet, the computational results can hint at the computational behavior of the extended formulations for the other two classes of functions. In Sect. 4.1, our test set is presented which consists of instances of the Molecular Distance Geometry Problem. In Sect. 4.2, different relaxation strategies for this class of problems are investigated. In Sect. 4.3, we show the results of two separators within the open source, mixed-integer nonlinear optimization software SCIP [1] based on the relaxations $\mathcal{S}^{(n)}_{[l,u]}$ and $\mathcal{U}_f$.

4.1 Molecular distance geometry problem

The molecular distance geometry problem (MDGP) (see e.g., [19]) is to determine the three-dimensional structure of a molecule consisting of a finite set $A = \{1, \ldots, s\}$ of atoms and given distances $d_{i,j} \geq 0$ between two atoms $\{i, j\} \in E \subseteq A \times A$. This leads to the following unconstrained nonconvex optimization problem

$$\min \sum_{\{i,j\}\in E} \left(||\xi^i - \xi^j||^2 - d_{ij}^2\right)^2 \quad \text{s.t.} \quad \xi := (\xi^1, \ldots, \xi^s) \in \mathbf{R}^{3s}, \tag{14}$$

where $\xi^i := (\xi^i_1, \xi^i_2, \xi^i_3) \in \mathbf{R}^3$ represents the position of atom i in the three-dimensional space. A point $\xi \in \mathbf{R}^{3s}$ is a solution of the MDGP if and only if the corresponding objective function value at ξ is zero.

In the formulation of Eq. (14) the MDGP can be solved instantaneously by solvers like BARON or SCIP for low dimensional problems. In order to illustrate the impact of the proposed relaxation methods we follow [10] and analyze the *expanded model* formulation

$$\min \sum_{\{i,j\}\in E} s_{i,j} \quad \text{s.t.} \quad s_{i,j} \geq \text{EXPAND}\left[\left(||\xi^i - \xi^j||^2 - d_{ij}^2\right)^2\right], \ \xi \in \mathbf{R}^{3s}, \tag{15}$$

where the operator EXPAND[$\cdot$] expands each term $\left(||\xi^i - \xi^j||^2 - d_{ij}^2\right)^2$ such that it is given as the sum of 52 monomials of the following form:

$$x_1, \quad x_1x_2, \quad x_1x_2x_3, \quad x_1x_2x_3x_4, \quad x_1^2, \quad x_1^4, \quad -x_1^2x_2x_3, \quad -x_1^3x_2.$$

We consider two test sets related to the MDGP. Test set TS1 contains five MDGP instances lav6–lav20 which are characterized in Table 3. The instances differ in the number of atoms and edges, and the domains which are chosen such that the instances are feasible. All the instances (except for the domain) have been randomly generated as described in Lavor [18] and were given to us by Jon Lee. Test set TS2 consists of 50 randomly generated test instances

Table 3 Lavor instances: Each instance is characterized by the number of atoms, the number of edges between the atoms and the domain of each component ξ_i of an atom

Instance	lav6	lav7	lav8	lav10	lav20
# Atoms	6	7	8	10	20
# Edges	13	16	20	28	70
Domain	[0, 3]	[0, 4]	[0, 4]	[0, 5]	[0, 9]

where we construct 10 random instances for each of the five Lavor instances. For this it is decided uniformly at random if a summand is multiplied by zero or one. Thus, the instances of TS2 are sparser than the instances of TS1.

4.2 Different relaxation strategies applied to TS1

We consider four different linear relaxation strategies which are briefly summarized. Relaxation strategy StandRelax follows Cafieri et al. [10], where each term is reformulated into terms of products of univariate or bilinear/trilinear terms for which the formulas for their envelopes are applied. QHullRelax additionally computes the convex envelopes for all component-wise concave monomials by the algorithm Qhull [6]. In $\mathcal{S}$-Relax all multilinear terms, in particular the quadrilinear terms $x_1x_2x_3x_4$, are relaxed by $\mathcal{S}^{(4)}_{[l,u]}$. $\mathcal{U}$-Relax is based on $\mathcal{S}$-Relax and it further employs extended-space underestimators $\mathcal{U}_f$ for the component-wise concave monomials $f(x) = -x_1^3x_2$ and $f(x) = -x_1^2x_2x_3$.

All computations were accomplished in a SCIP 2.1.1 [1] framework using CPLEX 12.3 [13] as LP solver on a 2.67 GHz INTEL X5650 with 96GB RAM. Relaxation strategy QHullRelax uses Qhull 2012.1. The time limit for all computations was 1 h.

Table 4 displays the results of the relaxation strategies in a branch-and-bound algorithm with respect to the bound obtained at the root node, the final bound, and the number of iterations. Note that the optimal objective function value for all instances is zero.

Table 4 The table compares the behavior of the relaxation strategies with respect to their root node relaxation, the final bound, and the number of iterations in the branching procedure. All computations were stopped after 1 h

	StandRelax	QHullRelax	$\mathcal{S}$-Relax	$\mathcal{U}$-Relax
lav6				
Root	−36,871.1	−36,871.1	−14,770.3	−14,777.3
Bound	−15,554.0	−21,727.7	−7,212.0	−6,333.0
# iter	14,406	750	13,182	18,147
lav7				
Root	−141,278.7	−141,278.7	−56,698.8	−56,698.8
Bound	−69,754.6	−99,271.3	−32,564.3	−30,002.2
# iter	12,039	365	11,008	15,649
lav8				
Root	−176,869.1	−176,869.1	−70,946.4	−70,946.4
Bound	−100,891.1	−138,822.6	−46,212.7	−43,218.0
# iter	10,090	231	8,839	12,689
lav10				
Root	−602,754.7	−602,754.7	−241,694.4	−241,694.4
Bound	−423,748.9	−520,950.4	−184,078.4	−176,735.0
# iter	6,898	138	6,372	9,703
lav20				
Root	−15,840,033.3	−15,840,033.3	−6,367,589.5	−6,367,589.5
Bound	−13,291,564.3	−14,557,815.3	−5,618,446.6	−5,529,058.1
# iter	2,690	44	2,192	3,360

Table 5 Final bounds and computational time by StandRelax and QHullRelax after the same number of iterations

	Iterations	StandRelax		QHullRelax	
		Bound	Time (s)	Bound	Time (s)
lav6	750	−21,730.3	143	−21,727.7	3,600
lav7	635	−99,271.3	80	−99,271.3	3,600
lav8	231	−138,822.6	61	−138,822.6	3,600
lav10	138	−520,950.4	57	−520,950.4	3,600
lav20	44	−14,557,815.3	54	−14,557,815.3	3,600

The following comments are in order. First, the root node relaxations of $\mathcal{S}$-Relax and $\mathcal{U}$-Relax are twice as good as the relaxations of StandRelax and QHullRelax. As we start with lower bounds of zeros for the variables in the root node, StandRelax and QHullRelax, and $\mathcal{S}$-Relax and $\mathcal{U}$-Relax yield the same lower bound. Changing the lower bounds to 1, for instance, reveals that QHullRelax generates stronger bounds than StandRelax and $\mathcal{U}$-Relax is better than $\mathcal{S}$-Relax.

Second, the final bounds derived by the relaxations based on $\mathcal{S}$-Relax and $\mathcal{U}$-Relax are also always twice as good as the bound obtained by the relaxations based on StandRelax and QHullRelax. This shows that the extended-space relaxations are not only stronger but are also solvable in a reasonable time. For instance, $\mathcal{U}$-Relax performs always the highest number of iterations among all relaxation strategies and provides the best lower bounds. Compared to the bounds by $\mathcal{S}$-Relax the bounds by $\mathcal{U}$-Relax are about 10 % better for the smaller Lavor instances and still 3 % better for the larger instances.

Relaxation strategy QHullRelax returns the worst bounds. This is due to the expensive computation of the convex envelope by the Qhull algorithm as indicated in Table 5. The table compares bounds and computation times for StandRelax and QHullRelax after the same number of iterations. It turns out that StandRelax needs significantly less computation time in all cases, while the bounds are identical, except for instance lav6 where the bound by QHullRelax is slightly better.

4.3 A comparison of standard solvers applied to TS2

In this subsection we compare the computational results of the state-of-the-art solver BARON [39], the open-source solver SCIP [1], and SCIP with two separators based on extended-space underestimators. The separators are add-ons for SCIP and can be downloaded from http://www.ifor.math.ethz.ch/staff/balmarti. The separator SimMultMono is based on $\mathcal{S}^{(n)}_{[l,u]}$ while the separator EdgeConcaveMonomials uses $\mathcal{U}_f$, where f is a monomial over a non-negative domain. We denote the corresponding algorithms $\mathcal{S}$-SCIP and $\mathcal{U}$-SCIP, respectively.

All computations were accomplished in the GAMS 23.9.1 environment with BARON 11.1.0 and SCIP 3.0.0. We used the default settings of the separators except for the parameter “freq” which is set to 1 in order to apply the separators at every iteration. The current implementation of the separators requires to reformulate the problems such that additional variables are introduced corresponding to the monomials which are then linked to the monomials by additional constraints. We refer to this formulation as *reformulated model* formulation. Both BARON and SCIP were tested on the reformulated model and the expanded model formulation in Eq. (15). As both algorithms perform better on the expanded model formulation, we only state their results for this formulation subsequently.

Table 6 shows the computational results for test set TS2 consisting of 50 randomly modified Lavor instances. We compare the algorithms in terms of four criteria: The number of times a algorithm computes the best lower or upper bound on the problem or is at most 0.01 %

Table 6 Test set TS2 (50 randomized Lavor instances). The table compares the number of times an algorithm computes the best lower or upper bound or is in the range of the best bound, and reports the sum of the dual gaps over all instances where each summand is either bounded by 100 or 1,000 %

	BARON	SCIP	$\mathcal{S}$-SCIP	$\mathcal{U}$-SCIP
# best primal bound	18	10	22	22
# best dual bound	0	0	3	50
Dual gap (100 %)	84.65 %	97.73 %	58.50 %	55.19 %
Dual gap (1,000 %)	140.14 %	256.41 %	64.44 %	60.52 %

worse than the best bound. The dual gap is computed with respect to the best known feasible solution over all algorithms as the arithmetic sum over all instances where the gap for each instance is either bounded by 100 or 1,000 %.

Good primal bounds are computed by the algorithms BARON, $\mathcal{S}$-SCIP and $\mathcal{U}$-SCIP. The primal bounds of all algorithms deviate in average not more than 6 % from the best primal bound. The best dual bounds are obtained by $\mathcal{U}$-SCIP for all cases. The dual gaps show that $\mathcal{S}$-SCIP is almost as good as $\mathcal{U}$-SCIP. The dual gaps by algorithms $\mathcal{S}$-SCIP and $\mathcal{U}$-SCIP are two times better than the dual gap of BARON and four times better than the dual gap of SCIP with respect to 1,000 %. This comparison shows that SCIP can benefit from the separators and that using the separators in BARON may even yield better results.

Finally, we remark that the algorithms $\mathcal{S}$-SCIP and $\mathcal{U}$-SCIP introduce variables corresponding to the monomials needed by the relaxations $\mathcal{S}^{(n)}_{[l,u]}$ and $\mathcal{U}_f$. In contrast to test set TS1, not all of the corresponding monomials occur in the problem formulation of TS2. Yet, the results show that the proposed relaxations accelerate the computations.

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Appendix

The following elementary lemma shows that the facets of $\mathcal{S}^{(n)}_{[l,u]}$ and $\mathcal{L}^{(n_x,n_y)}_{[l,u]}$ are also facets of $\mathcal{U}_f$ and $\mathcal{E}_f$, respectively.

Lemma 2 *Let $h, g_i : D \subseteq \mathbf{R}^n \to \mathbf{R}$, $i = 1, \ldots, m$, be continuous functions over a convex, compact domain $D \subseteq \mathbf{R}^n$, and let $g : D \subseteq \mathbf{R}^n \to \mathbf{R}^m$ be the vector-valued function given by $g(x) := \big(g_1(x), \ldots, g_m(x)\big)^\top$. Furthermore, consider the two convex sets $\mathcal{L} := \operatorname{conv}(\{(x, \zeta) \in \mathbf{R}^{n+m} \mid \zeta = g(x),\ x \in D\})$ and $\mathcal{U} := \operatorname{conv}(\{(x, \zeta, \mu) \in \mathbf{R}^{n+m+1} \mid \zeta = g(x),\ \mu \geq h(x),\ x \in D\})$. Then, each facet-defining inequality of $\mathcal{L}$ also induces a facet for $\mathcal{U}$.*

Proof Let $a^\top x + b^\top \zeta \leq \gamma$ be an arbitrary facet-defining inequality for $\mathcal{L}$ with $a \in \mathbf{R}^n$, $b \in \mathbf{R}^m$, and $\gamma \in \mathbf{R}$. Then, $a^\top x + b^\top \zeta \leq \gamma$ is valid for $\mathcal{U}$. As $a^\top x + b^\top \zeta \leq \gamma$ is facet-defining for $\mathcal{L}$, there are $n+m$ points $x^r \in D$ such that the points $\big(x^r, g(x^r)\big)$, $r = 1, \ldots, n+m$, are affinely independent and each point satisfies $a^\top x + b^\top \zeta \leq \gamma$ with equality. Now, consider the set of points $(x^r, \zeta^r, \mu^r) := \big(x^r, g(x^r), h(x^r)\big) \in \mathcal{U}$, $r = 1, \ldots, n+m$, and the point $(x^{n+m+1}, \zeta^{n+m+1}, \mu^{n+m+1}) := \big(x^1, g(x^1), h(x^1)+1\big)$. Then, $a^\top x^r + b^\top \zeta^r = \gamma$ holds for all $r = 1, \ldots, n+m+1$. Furthermore, the points (x^r, ζ^r, μ^r), $r = 1, \ldots, n+m+1$ are affinely independent since the set $\{(x^r, \zeta^r) - (x^1, \zeta^1) \mid r = 2, \ldots, n+m+1\}$ is linearly independent. □

The next lemma gives the key argument to derive the extended formulations $\mathcal{U}_f$ and $\mathcal{E}_f$ for functions f belonging to Classes 1 and 2. It deals with a slight modification of the equation systems underlying the works [2,27,28] by Sherali and Adams to derive equivalent extended linear formulations for certain polynomial mixed-discrete programs. We adapt their proofs to our setting. For $V_1 = \emptyset$, the statement of Lemma 3 follows from the fact that the convex hull of $\{F^{n_x+1}(v, y) \mid (v, y) \in \mathrm{vert}([l^x, u^x] \times [l^y, u^y])\}$ equals $\mathcal{S}^{(n_x+1)}_{[l^x,u^x]\times[l^y,u^y]}$. The special case when $V_2 = \emptyset$ is discussed in Adams and Sherali [2].

Lemma 3 *Let $[l, u] := [l^x, u^x] \times [l^y, u^y] \subseteq \mathbf{R}^{n_x} \times \mathbf{R}$ be a full-dimensional box, $N_x := \{1, \ldots, n_x\}$, $V_x := \mathrm{vert}([l^x, u^x])$ and $n := n_x + 1$. Moreover, let $V_1, V_2 \subseteq V_x$ be a partition of V_x, i.e., $V_x = V_1 \cup V_2$, $V_1 \cap V_2 = \emptyset$. For a given $z \in \mathbf{R}^{2^n - 1}$, consider the following nonlinear system in the variables λ_v, y^v with $v \in V_1$, and $\lambda_{v,l}$, $\lambda_{v,u}$ with $v \in V_2$:*

$$z_J = \sum_{v \in V_1} \lambda_v F_J^{(n_x)}(v) + \sum_{v \in V_2} \big(\lambda_{v,l} F_J^{(n_x)}(v) + \lambda_{v,u} F_J^{(n_x)}(v)\big), \tag{16}$$

$$z_{J\cup\{n\}} = \sum_{v \in V_1} \lambda_v y^v F_J^{(n_x)}(v) + \sum_{v \in V_2} \big(\lambda_{v,l} l^y F_J^{(n_x)}(v) + \lambda_{v,u} u^y F_J^{(n_x)}(v)\big), \tag{17}$$

for all $J \subseteq N_x$. Its solution is given by

$$\lambda_v = \frac{e_{\hat v}(z^x)}{\prod_{j=1}^{n_x}(u_j - l_j)}, \quad y^v = \frac{\sum_{J\subseteq N_x} (-1)^{|J|+\alpha(\hat v)}\ F^{(n_x)}_{N_x\setminus J}(\hat v) z_{J\cup\{n\}}}{e_{\hat v}(z^x)}, \tag{18}$$

for $v \in V_1$, where $\hat v$ denotes the vector opposite to v in $[l^x, u^x]$, z^x denotes the subvector of z-variables with entries z_J, $\emptyset \neq J \subseteq N_x$, and $e_{\hat v}(z^x)$ according to Eq. (6)*. The solution of $\lambda_{v,l}$ and $\lambda_{v,u}$ with $v \in V_2$ reads*

$$\lambda_{v,l} = \frac{e_{(\hat v, u^y)}(z)}{\prod_{j=1}^{n}(u_j - l_j)} \quad \text{and} \quad \lambda_{v,u} = \frac{e_{(\hat v, l^y)}(z)}{\prod_{j=1}^{n}(u_j - l_j)}. \tag{19}$$

Proof We prove Lemma 3 in two steps. Initially, we consider subsystem (I) defined by Eq. (16) and subsystem (II) defined by Eq. (17) for all $J \subseteq N_x$ independently. Afterwards we combine the solutions of the two subsystems.

Let T be the matrix whose columns are given by the vectors $(1, F^{(n_x)}(v))$, $v \in V$. We can then bring both subsystems into the form $\zeta = T\xi$. This system has the unique solution (see [2,17,27])

$$\xi_v = \frac{e_{\hat v}(\zeta)}{\prod_{j=1}^{n_x}(u_j - l_j)}, \qquad v \in V.$$

For subsystem (I) we replace $\big(\lambda_{v,l} F_J^{(n_x)}(v) + \lambda_{v,u} F_J^{(n_x)}(v)\big)$ by $(\lambda_v F_J^{(n_x)}(v))$ in Eq. (16). Hence, we obtain the system $(1, z^x) = T\lambda$ with unique solution

$$\lambda_v = \frac{e_{\hat v}(z^x)}{\prod_{j=1}^{n_x}(u_j - l_j)}, \quad v \in V.$$

For subsystem (II) we first substitute

$$\left(\lambda_{v,l} l_n F_J^{(nx)}(v) + \lambda_{v,u} u_n F_J^{(nx)}(v)\right) \quad \text{by} \quad \left(\lambda_v y^v F_J^{(nx)}(v)\right)$$

in Eq. (17) and afterwards, $\lambda_v y^v$ by r_v. With $\zeta_J = z_{J\cup\{n\}}$ for all $J \subseteq N_x$, subsystem (II) is of the form $\zeta = Tr$ with unique solution $r_v = e_{\hat{v}}(\zeta)/\prod_{j=1}^{n_x}(u_j - l_j),\ v \in V$.

Finally, we consider the original system, where $r_v = \lambda_v y^v,\ v \in V_1$, and $r_v = \lambda_{v,l} l^y + \lambda_{v,u} u^y,\ \lambda_v = \lambda_{v,l} + \lambda_{v,u},\ v \in V_2$. To obtain $y^v,\ v \in V_1$, we can solve $r_v = \lambda_v y^v$ for y^v if $\lambda_v \neq 0$. Then, $y^v = r_v/\lambda_v = e_{\hat{v}}(\zeta)/e_{\hat{v}}(z^x)$. If $\lambda_v = 0$, y^v can take any value as its corresponding summand cancels out.

To derive $\lambda_{v,l}$ and $\lambda_{v,u},\ v \in V_2$, we solve the linear system $\lambda_v y^v = \lambda_{v,l} l^y + \lambda_{v,u} u^y$ and $\lambda_v = \lambda_{v,l} + \lambda_{v,u}$. Then, $\lambda_{v,l} = \lambda_v(u^y - y^v)/(u^y - l^y)$ and $\lambda_{v,u} = \lambda_v(y^v - l^y)/(u^y - l^y)$.

We prove the formula for $\lambda_{v,l}$ in Eq. (19). An analogous argument holds for $\lambda_{v,u}$. We get $\lambda_{v,l} = \lambda_v(u^y - y^v)/(u^y - l^y) = e_{\hat{v}}(z^x)(u^y - y^v)/\prod_{j\in N}(u_i - l_i)$. To deduce Eq. (19), it is thus sufficient to show that $e_{(\hat{v},u^y)}(z) = e_{\hat{v}}(z^x)(u^y - y^v)$. This follows because $e_{(\hat{v},u^y)}(z)$ can be rewritten as

$$\begin{aligned}
&\sum_{J\subseteq N} (-1)^{|J|+\alpha(\hat{v})} F_{N\setminus J}^{(n)}(\hat{v}, u^y) z_J \\
&= \sum_{J\subseteq N_x} (-1)^{|J|+\alpha(\hat{v})} F_{N\setminus J}^{(n)}(\hat{v}, u^y) z_J \\
&\quad + \sum_{J=T\cup\{n\}:T\subseteq N_x} (-1)^{|J|+\alpha(\hat{v})} F_{N\setminus J}^{(n)}(\hat{v}) z_J \\
&= \sum_{J\subseteq N_x} (-1)^{|J|+\alpha(\hat{v})} u^y F_{N_x\setminus J}^{(n_x)}(\hat{v}) z_J + \sum_{J\subseteq N_x} (-1)^{|J|+\alpha(\hat{v})+1} F_{N_x\setminus J}^{(n_x)}(\hat{v}) z_{J\cup\{n\}} \\
&= u^y e_{\hat{v}}(z^x) - y^v e_{\hat{v}}(z^x) = e_{\hat{v}}(z^x)(u^y - y^v).
\end{aligned}$$

This concludes the proof. □

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