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Explicit convex and concave envelopes through polyhedral subdivisions

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Abstract In this paper, we derive explicit characterizations of convex and concave envelopes of several nonlinear functions over various subsets of a hyper-rectangle. These envelopes are obtained by identifying polyhedral subdivisions of the hyper-rectangle over which the envelopes can be constructed easily. In particular, we use these techniques to derive, in closed-form, the concave envelopes of concave-extendable supermodular functions and the convex envelopes of disjunctive convex functions.

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1 Introduction and motivation

A significant amount of research has been devoted to developing concave overestimators and convex underestimators of nonlinear functions $f(x)$ over the hypercube. One of the motivations for such research is that, whenever an optimization problem involves maximizing $f(x)$ (resp. minimizing $f(x)$) or contains an inequality $f(x) \geq r$ (resp. $f(x) \leq r$), replacing $f(x)$ by a concave overestimator (resp. convex underestimator) yields a convex relaxation of the problem. Such a relaxation can, for instance,

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be used in branch-and-bound algorithms for global optimization where convex relaxations must be constructed over successively refined partitions of the original variable space; see [40] for an exposition.

In order for branch-and-bound algorithms to produce globally optimal solutions, certain mild technical conditions are typically needed; see [16]. In particular, if one can guarantee that for a minimization problem the node with the lowest lower bound is chosen periodically, the volume of partition elements tends to zero, and the relaxations approach the original functions when the volume of the partition elements goes down to zero, branch-and-bound converges to a globally optimal solution. It is well-known, see for example [3], that the concave (resp. convex) envelope, i.e., the lowest (resp. highest) concave overestimator (resp. convex underestimator) of a function over a specified region, converges to this function as partition elements become smaller. As a result, deriving concave and convex envelopes of nonlinear functions over partition elements is a problem that is commonly encountered in the implementation of branch-and-bound algorithms for nonlinear programs. Further, since among all partitioning schemes in branch-and-bound algorithms, the rectangular partitioning scheme in which partition elements are hyper-rectangles is used most often, computing convex and concave envelopes of general functions $f(x)$ over a hyper-rectangle is a problem of crucial practical importance.

Since it is NP-Hard to maximize/minimize a multilinear function, a multivariate function that is a linear function of each variable when the other variables are given fixed values, over the unit hypercube, see [9], finding the concave/convex envelope of a generic function $f(x)$ is provably hard. Nevertheless, for many practically useful functions, such as bilinear terms [1], various types of multilinear functions [3,5,25,28,31], and the fractional terms [38], concave envelopes have been derived in the literature. Further, general theoretical frameworks for the construction of such envelopes [2,7,10,22,24,32,33,39] have been proposed. It is remarkable however that, despite recent progress in the field, there remain many practically useful functions for which concave envelopes are not known. As an example, consider the function $d(x) = \frac{1}{a_0+\sum_{i=1}^n a_i x_i}$ over the unit hypercube. This function appears, for instance, in the formulation of the consistent biclustering problem [6]. If we assume that $a_0 + \sum_{i=1}^n a_i x_i > 0$ whenever $0 \le x \le 1$, then f is well-defined over the relevant domain. A standard procedure to relax $z = d(x)$ is to first introduce a new variable $y = a_0 + \sum_{i=1}^n a_i x_i$ and then to relax $z = \frac{1}{y}$ by constructing the convex and concave envelopes of $\frac{1}{y}$. This leads to the relaxation $z \ge \frac{1}{y}$ and $z \le \frac{1}{y^L} + \frac{y^L - y}{y^U y^L}$. Here, y^L and y^U are computed respectively by minimizing and maximizing $a_0 + \sum_{i=1}^n a_i x_i$ over the unit hypercube. Assuming $a_i \ne 0$ for $i = 1, \dots, n$ and $n > 1$, this procedure yields a concave overestimator of $d(x)$ that is weaker than the concave envelope of $d(x)$. We shall elaborate on this fact in the ensuing paragraphs.

In this paper, we develop techniques for identifying the convex/concave envelopes of nonlinear functions over hyper-rectangles or specific subsets of hyper-rectangles by investigating polyhedral subdivisions of their domain. Following this approach, we provide streamlined and unified generalizations of a variety of results from the literature and expose new convex/concave envelope characterizations and separation results for them. In Sect. 2, we develop a general set of tools for the convexification of polyhedral functions providing a common framework for the derivation of earlier results in [3,25,31]. In particular, we show that computing the value of the concave envelope at a point is equivalent to solving a certain optimization problem. Insights derived from this result allow us to relate concave envelopes to polyhedral subdivisions of hyper-rectangles and to describe polynomial separation procedures for a variety of functions. For example, we show that the concave (resp. convex) envelope of a maximum (resp. minimum) of a collection of functions is polynomially separable if the concave (resp. convex) envelopes of the individual functions are polynomially separable. The remainder of the paper studies a variety of polyhedral subdivisions of the hyper-rectangle and gives insights into the classes of functions for which they describe the convex/concave envelopes.

In Sect. 3, we show that by combining the results of [20,39,43] concave envelopes of supermodular concave-extendable functions can be developed over a lattice family. This result generalizes the explicit characterizations of convex/concave envelopes for specific functions described in [5,8,22,27,31]. In addition, we show that this result has many unrealized applications in improving relaxations of factorable programs beyond the classical technique of [21] and its more recent variants implemented in global optimization software [4,19,42]. To support this claim, consider the function $d(x)$ described above. This function is of the form $f(x) = c\left(a_0 + \sum_{i=1}^n a_i x_i\right)$. Our results allow the derivation of the concave (resp. convex) envelope of f over a hyper-rectangle if $c(\cdot)$ is a convex (resp. concave) function. In factorable programming, products of variables are replaced with new variables until a function of the form of $f(x)$ is obtained. Then, a variable, say y, is introduced to replace $a_0 + \sum_{i=1}^n a_i x_i$ and $c(y)$ is overestimated using a linear function over $[y^L, y^U]$ where the bounds y^L and y^U are derived from the bounds on x_i and the defining expression for y. Assume $n > 1$, $c(\cdot)$ is strictly convex, and without loss of generality that $a_i > 0$ for all i. Then, the factorable relaxation is clearly weaker than the aforementioned envelope because the concave envelope matches the function value at $(x_1^U, \ldots, x_{n-1}^U, x_n^L)$ whereas the factorable relaxation overestimates the function value. This illustrates that exploiting the closed-form concave envelopes we develop in this paper will help strengthen the relaxations used in commercial global optimization solvers.

In Sect. 4, we show that the orthogonal disjunctions theory [24] can be used to develop convex envelopes of functions of the form $xg(y)$ over the unit hypercube when $g(\cdot)$ is a non-increasing convex function. These relaxations are piecewise-conic and have a multitude of applications in global optimization. For example, we show that a variety of fractional, logarithmic, and polynomial functions can be convexified using the approach. We also develop polyhedral subdivisions to convexify a symmetric function of binary variables generalizing prior results in [31]. We conclude the section by illustrating, using two extreme situations, that the polyhedral partitions characterizing the envelope of a function over a hyper-rectangle and over its subsets are not always related. In the first situation, the envelope changes over the entire subregion requiring an entirely new proof. In the second situation, the envelope remains the same over a portion of the feasible region allowing us to leverage the proof given for the hyper-rectangle. Throughout the section, we provide illustrations of our results. We conclude in Sect. 5 with comments on the applicability of the results developed in this paper and directions of future research.

2 Preliminaries

In this section, we review and unify existing literature regarding the derivation of concave envelopes over hyper-rectangles.

Definition 2.1 For a function $f : S \mapsto \mathbb{R}$, where S is a nonempty convex subset of $\mathbb{R}^n$, the function $g(x) : S \to \mathbb{R}$ is the concave envelope of $f(x)$ over S if

1. $g(x)$ is concave over S
2. $g(x) \geq f(x)$ for all $x \in S$
3. If $h(x)$ is any concave function over S that satisfies $h(x) \geq f(x)$ for all $x \in S$, then $h(x) \geq g(x)$ for all $x \in S$.

We denote the concave envelope of f over a set S by $\text{conc}_S(f)$. When the set S is clear from the context, we often will omit the subscript S.

In words, $\text{conc}_S(f)$ is the lowest concave overestimator of the function $f(x)$ over S. Similarly, the convex envelope of a function over S is the highest convex underestimator of the function f over S. In the remainder of the text, we will denote the convex envelope of f over S by $\text{conv}_S(f)$. Often, we will derive the concave envelope of a function f both over a convex set S, and a convex subset S' of S. In such a situation, we will often write that $\text{conc}_S(f)(x) \geq \text{conc}_{S'}(f)(x)$. This expression must be understood as holding for all $x \in S'$ and is verified because the restriction of $\text{conc}_S(f)(x)$ to S' is a concave overestimator of f over S'. The concave envelopes $g(x)$ we derive will often be expressed as a minimum of a finite number of affine functions. In such a situation, we will say that $\alpha^\intercal x + \beta$ is a nonvertical facet of $g(x)$ if $z \leq \alpha^\intercal x + \beta$ is a facet-defining inequality of the hypograph of g, i.e., $\text{hyp}(g) = \{(x, z) \in \mathbb{R}^{n+1} \mid z \leq g(x)\}$. We will refer to facet-defining inequalities of $\text{hyp}(g)$ of the form $0 \leq \alpha^\intercal x + \beta$ as vertical facets of $g(x)$.

Consider a continuous function $f(x) = f(x_1, x_2, \ldots, x_n)$ over the hyper-rectangle $x_i^L \leq x_i \leq x_i^U$. We denote the conjugate of f as f^*. We assume *w.l.o.g.* that $x_i^U > x_i^L$ for $i = 1, \ldots, n$. Otherwise, the dimension of x can be reduced by fixing variables x_i with $x_i^U = x_i^L$. We further assume that, for every i, $x_i^U = 1$ and $x_i^L = 0$, or else, the following linear transformation can be used to transform x into x':

$$x' = T(x) = T(x_1, \ldots, x_n) = \left(\frac{x_1 - x_1^L}{x_1^U - x_1^L}, \ldots, \frac{x_n - x_n^L}{x_n^U - x_n^L} \right) \tag{1}$$

where $0 \leq x' \leq 1$. Transformation (1) will typically be without loss of generality for our study although we mention that it might not preserve all useful properties of f. We will make remarks when the assumed property of the function is not necessarily preserved after transformation.

Concave envelopes can often be constructed by considering only the values of f over the extreme points of its domain of definition. Definition 2.2, which is inspired by previous work on convex extensions [40], formalizes this notion.

Definition 2.2 A function $f(x) : P \to \mathbb{R}$, where P is a polytope, is said to be concave-extendable (resp. convex-extendable) from $X \subseteq P$ if the concave (resp. convex) envelope of $f(x)$ is determined by X only, i.e., the concave envelopes of f and $\hat{f}$ over P are identical, where $\hat{f}$ is the restriction of f to X that is defined as:

$$\hat{f}(x) = \begin{cases} f(x) & x \in X \\ -\infty & \text{otherwise.} \end{cases}$$

□

It follows from Definition 2.2 that $\text{conv}(X) = P$. In the remainder of this paper, we will often encounter functions that are concave-extendable or convex-extendable from the vertices of the unit hypercube, i.e., $P = [0, 1]^n$ and $X = \text{vert}([0, 1]^n)$, where we use the notation $\text{vert}(P)$ to denote the set of vertices of the polytope P. Clearly, convex functions are concave-extendable from vertices. Examples of functions that are not convex but still concave-extendable from the vertices of a hypercube include multilinear functions [25] and, more generally, functions that are convex when restricted to the space of each variable, i.e., the space created when all other variables are assigned fixed values within their domain. The concave envelope of any function that is concave-extendable from vertices is polyhedral since it is completely determined by a finite number of points. A partial converse is also known to be true: all continuously differentiable functions that have a polyhedral concave envelope over the unit hypercube are concave-extendable from vertices; see Theorem 1.1 in [25].

Concave envelopes of functions that are concave-extendable from the vertices of P are intimately related to certain partitions of P. We describe these relations next.

Definition 2.3 ([17]) Let $S \subseteq \mathbb{R}^n$. A set of n-dimensional polyhedra $S_1, \ldots, S_m \subseteq S$ is a polyhedral subdivision of S if $S = \bigcup_{i=1}^m S_i$ and $S_i \cap S_j$ is a (possibly empty) face of both S_i and S_j. □

In particular, if each polyhedron in the subdivision is a simplex, then the polyhedral subdivision is called a *triangulation*. In the optimization literature, triangulations are also known as *simplicial covers*; see [5] for example. Observe that there is no requirement in Definition 2.3 that the extreme points of S_i are also extreme points of S. However, in this paper, we will be most interested in subdivisions where the extreme points of each polyhedron are also extreme points of S. We say that these subdivisions *do not add vertices*.

Let $v_1, \ldots, v_m$ form a collection of points in $\mathbb{R}^n$ such that $\text{aff}(v_1, \ldots, v_m) = \mathbb{R}^n$. Consider the corresponding matrix, V, in $\mathbb{R}^{n \times m}$, whose j^{th} column V_j satisfies $V_j = v_j$, We denote the submatrix of V that consists of columns whose indices belong to the set J as $V(J)$. For simplicity of notation and because it will be clear from the context, we also denote the set of points v_j corresponding to the index set J as $V(J)$ and therefore we use $\text{conv}(V(J))$ to represent $\text{conv}(\bigcup_{j \in J} v_j)$. Let $f(V) = (f(v_1), \ldots, f(v_m))^\intercal$ and let e denote a column vector of all ones of appropriate dimension. Consider the following primal-dual pair of linear programming problems:

$$\begin{array}{llll} P(x): \min_{(a,b)} & ax+b & \quad D(x): \max_{\lambda} & f(V)^{\mathsf{T}}\lambda \\ \text{s.t.} & aV+be \geq f(V) & \quad \text{s.t.} & V\lambda = x \\ & a\in\mathbb{R}^n,\ b\in\mathbb{R} & & e^{\mathsf{T}}\lambda = 1 \\ & & & \lambda \geq 0. \end{array}$$

The constraints of the primal problem $P(x)$ express that in order for the affine function $l(x) = ax + b$ to majorize the concave envelope of f over $\operatorname{conv}(V)$, its value at each of the points v_j must be larger than $f(v_j)$. Given a point $x \in \mathbb{R}^n$, the dual problem searches to find, among all ways of describing x as a convex combination of vectors v_j, one that yields the largest interpolated value. Let F denote the feasible region of $P(x)$. Observe that F does not depend on x and that F is nonempty since b can be chosen arbitrarily large. Since $D(x)$ is feasible if $x \in \operatorname{conv}(V)$ and since the feasible region of $D(x)$ is bounded, it follows from strong duality in linear programming that the optimal values of $P(x)$ and $D(x)$ are finite and are equal for each $x \in \operatorname{conv}(V)$. We denote this common optimal value by $z(x)$. For a given $(a, b) \in F$, we let $J(a, b)$ denote the index set of constraints of F that are tight at (a, b) and let $R(a, b) = \operatorname{conv}(V(J(a, b)))$. It follows from complementarity slackness conditions that if (a, b) is optimal for $P(x)$, then all optimal solutions λ to $D(x)$ are such that their support is restricted to $J(a, b)$. Therefore, $x \in R(a, b)$. In the following theorem, we record some relations between the above primal-dual pair and the concave envelope of f over $\operatorname{conv}(V)$. Similar results have appeared in the literature. We will discuss these connections after the proof.

Theorem 2.4 *Consider a function $f : V \mapsto \mathbb{R}^n$ and let* $\operatorname{conc}(f)$ *be its concave envelope over* $\operatorname{conv}(V)$. *Also define* $\mathcal{R} = \{R(a', b') \mid (a', b') \in \operatorname{vert}(F)\}$. *Then,*

- (i) $z(x) = \operatorname{conc}(f)(x)$ *for* $x \in \operatorname{conv}(V)$.
- (ii) *Let* $(a^*, b^*) \in \operatorname{vert}(F)$. *Then,* (a^*, b^*) *is optimal for* $P(x)$ *if and only if* $x \in R(a^*, b^*)$. *Further, the extreme points of F are in one-to-one correspondence with the nonvertical facets of* $\operatorname{conc}(f)(x)$.
- (iii) *For each* $(a', b') \in \operatorname{vert}(F)$, $a'x + b'$ *defines a nonvertical facet of* $\operatorname{conc}(f)$ *over* $R(a', b')$.
- (iv) $\mathcal{R}$ *is a polyhedral subdivision of* $\operatorname{conv}(V)$. *Further,* $\operatorname{conc}(f)$ *can be computed by interpolating f affinely over each element of* $\mathcal{R}$.

Proof To prove (i), we consider $x' \in \operatorname{conv}(V)$. Let λ' be any feasible solution of $D(x')$, then

$$\operatorname{conc}(f)(x') = \operatorname{conc}(f)(V\lambda') \geq \operatorname{conc}(f)(V)^{\mathsf{T}}\lambda' \geq f(V)^{\mathsf{T}}\lambda' \tag{2}$$

where the equality follows from feasibility of λ', the first inequality holds from concavity of $\operatorname{conc}(f)$ and the second inequality is satisfied because $\operatorname{conc}(f)(x) \geq f(x)$ for all $x \in \operatorname{conv}(V)$. This implies that $\operatorname{conc}(f)(x') \geq z(x')$ since λ' can be chosen to be an optimal solution of $D(x')$ in (2). Further, if (a', b') is feasible to F, then

$a'x+b' \geq f(x)$ for all $x \in \{v_1, \ldots, v_m\}$. Since affine functions are concave, we know that $a'x'+b' \geq \mathrm{conc}(f)(x')$. This implies that $\mathrm{conc}(f)(x') \leq z(x')$ since (a', b') can be chosen to be an optimal solution of $P(x')$. We conclude that $\mathrm{conc}(f)(x') = z(x')$.

We now prove (ii). Since $\mathrm{aff}(v_1, \ldots, v_m) = \mathbb{R}^n$ and $\mathrm{rank}(V^\mathsf{T} \mid e) = n+1$, by Minkowski's representation theorem (see Theorem 4.8 in [23]), there exists an optimal solution (a^*, b^*) to $P(x)$ that is an extreme point of F. Consider any point $x'' \in R(a^*, b^*)$. Since x'' can be expressed as a convex combination of v_j, $j \in J(a^*, b^*)$, there exists a solution λ'' that is feasible to $D(x'')$ and that satisfies complementary slackness conditions with (a^*, b^*). Therefore, (a^*, b^*) must be optimal to $P(x)$ for every $x \in R(a^*, b^*)$. Further, since (a^*, b^*) is an extreme point of F, at least $n+1$ of the points in $V\big(J(a^*, b^*)\big)$ are affinely independent. This implies that a^*x+b^* defines a nonvertical facet of $\mathrm{conc}(f)$. On the other hand, if $x'' \notin R(a^*, b^*)$, then (a^*, b^*) cannot be optimal to $P(x'')$ since there does not exist a complementary dual feasible solution.

Consider a non-vertical facet G of $\mathrm{hyp}(\mathrm{conc}(f)) = \{(z, x) \mid z \leq \mathrm{conc}(f)(x)\}$ which is defined by $\tilde{a}x + \tilde{b} \geq z$ and consider a point $(\tilde{x}, \tilde{a}\tilde{x} + \tilde{b})$ in the relative interior of this facet. First, note that $(\tilde{a}, \tilde{b})$ is feasible to F and $\tilde{a}\tilde{x} + \tilde{b} = \mathrm{conc}(f)(\tilde{x}) = z(\tilde{x})$. Therefore, $(\tilde{a}, \tilde{b})$ is optimal to $P(\tilde{x})$. Since any overestimating inequality of $f(x)$ that is tight at $(\tilde{x}, \tilde{a}\tilde{x} + \tilde{b})$ is also tight everywhere on G and $\dim(G) = n$, it is unique. Consequently, the optimal solution for $P(\tilde{x})$ is unique. Since $P(\tilde{x})$ has an extreme point solution, $(\tilde{a}, \tilde{b})$ must be an extreme point of F. Hence, there is a one-to-one correspondence between extreme points of F and nonvertical facets of $\mathrm{conc}(f)$. This completes the proof of (ii) and also proves (iii).

We now prove (iv). We have shown that for each $x \in \mathrm{conv}(V)$ there is an extreme point of F that optimizes $P(x)$ and has objective value $z(x)$. Therefore, $\mathcal{R}$ is the subdivision of $\mathrm{conv}(V)$ obtained by projecting the hypograph of $z(x)$ to the x-space. As proven above, the concave envelope is affine over each $R(a, b)$ if $(a, b) \in \mathrm{vert}(F)$ and $ax + b > \mathrm{conc}(f)(x)$ whenever $x \notin R(a, b)$. Projecting the hypograph of a polyhedral function yields a (regular) polyhedral subdivision of the domain; see [17]. Now, we show the last statement of (iv). Consider any polyhedron $R_i \in \mathcal{R}$ that is obtained as a projection into the x-space of a nonvertical facet of $\mathrm{hyp}(\mathrm{conc}(f))$. As shown in (ii), there exists $(a', b') \in \mathrm{vert}(F)$, such that this facet is defined by $z \leq a'x + b'$, $R_i = R(a', b')$, and $V(J(a', b')) \subseteq R_i$. Then,

$$\mathrm{vert}(R_i) = \mathrm{vert}\Big(\mathrm{conv}\Big(V\big(J(a', b')\big)\Big)\Big) \subseteq V\big(J(a', b')\big),$$

where the equality follows from the definition of $R(a', b')$ and the inclusion because convexification does not add vertices. Let $J' = \{j \mid v_j \in \mathrm{vert}(R_i)\}$. Since $\mathrm{vert}(R_i) \subseteq V(J(a', b')) \subseteq V$, it follows that $V(J') = \mathrm{vert}(R_i)$ and $J' \subseteq J(a', b')$. Further, there are exactly $n+1$ affinely independent points in $V(J')$ since $\mathrm{aff}(R_i) = \mathrm{aff}(V(J')) = \mathbb{R}^n$. Let J'' be the index set of these points. Then, (a', b') can be computed by solving $a'V(J'')+b'e(J'') = f(V(J''))$, where $e(J'')$ is a row vector of all ones in $\mathbb{R}^{|J''|}$. This shows the affine interpolation necessary to recover (a', b') from every polyhedron in $\mathcal{R}$. $\square$

Any polyhedral subdivision can be refined into a triangulation [17]. Therefore, by Theorem 2.4 there exists a triangulation of the domain that is such that $\mathrm{conc}(f)$ is affine over each simplex of the triangulation and $\mathrm{conc}(f)(x) = f(x)$ at all extreme points x of the simplices of the triangulation. Theorem 2.4 can be partially extended to general nonlinear functions by expanding the set of constraints to include an inequality for each feasible point (or, more precisely, each point in the generating set); see [40] for details. The main idea is that since $b \geq f(x) - ax$ for all x, it follows that the optimal value of b is obtained by maximizing $f(x) - ax$ over all x, yielding $b = (-f)^*(-a)$; see [26]. Then, $\inf_{a,b}\{ax + b \mid (a, b) \in F\} = \inf_a\{ax + (-f)^*(-a)\} = -\sup_a \{-ax - (-f)^*(-a)\} = -(-f)^{**}(x)$. If the underlying set is compact and $f(x)$ is upper-semicontinuous, $f(x)$ is bounded from above. Therefore, $-(-f)^{**}(x) = \mathrm{conc}\, f(x)$ by Theorem 1.3.5 in [14]. The advantage of restricting the result to finite point sets is that F has finitely many constraints, and, as a result, one can identify the facets of the concave envelope as well as the simplices of the corresponding triangulation by studying the basic feasible solutions of F. When Theorem 2.4 is applied to functions that are concave-extendable from vertices of a hypercube, the number of constraints defining F is exponentially large, since a constraint is created for each extreme point of the hypercube. As a result, identifying the basic feasible solutions of F can be computationally difficult. In this paper, we identify situations where these basic feasible solutions can be identified explicitly.

We next relate Theorem 2.4 to existing results in the literature. Concave-extendability has been used in [3] to develop an algorithmic approach for the derivation of concave envelopes. In particular, the authors designed a column-generation algorithm to find a facet of the concave envelope of a function that is concave-extendable from vertices by separating the envelope from a pre-specified point. They also proved, using a slightly different proof technique, the following result that establishes the correspondence between the facets of the concave envelope and the basic solutions of $P(x)$.

Corollary 2.5 (Theorem 2.4 in [3]) *The affine function $a^*x + b^*$ defines a non-vertical facet of the concave envelope of the multilinear function $f(x)$ over $P = \prod_{i=1}^n [l_i, u_i]$ if and only if (a^*, b^*) is a basic feasible solution of the following linear programming problem:*

$$\begin{aligned} \min_{(a,b)} \quad & ax + b \\ s.t. \quad & av^j + b \geq f(v^j) \quad \forall\, v^j \in \mathrm{vert}(P) \\ & a \in \mathbb{R}^n, b \in \mathbb{R}. \end{aligned} \tag{3}$$

Proof Multilinear functions are concave-extendable from vertices of hypercubes; see [25]. Letting $V = \mathrm{vert}(P)$, the result follows directly from Theorem 2.4. □

Corollary 2.6 (Lemma 1.1 in [25]) *Let $f(x)$ be a continuously differentiable function on an n-dimensional convex polytope P. Assume* $\mathrm{conc}(f)(x)$ *over P is a polyhedral function. Let $h(x) = ax + b$ be an affine function and assume that there exist $v^i, i = 1, \ldots, n+1, n+1$ affinely independent vertices of P, such that $h(v^i) =$*

$f(v^i), i = 1, \ldots, n+1$ and $h(x) \geq f(x)$ for all $x \in \mathrm{vert}(P)$. Then, $h(x)$ is an element of $\mathrm{conc}(f)$ *and, in particular, $h(x)$ defines the concave envelope of $f(x)$ over* $\mathrm{conv}(v^1, \ldots, v^{n+1})$.

Proof For a continuously differentiable function, $\mathrm{conc}(f)$ is polyhedral if and only if f is concave-extendable from vertices; see Theorem 1.1 in [25]. Note that $ax+b \geq f(x)$ for all $x \in \mathrm{vert}(P)$ and $av^i + b = f(v^i)$ for $n+1$ affinely independent vertices establish that (a, b) is an extreme point of F. Since $\mathrm{conv}(v^1, \ldots, v^{n+1}) \subseteq R(a, b)$, the result follows from Theorem 2.4. □

Motivated by Theorem 2.4, we now turn our attention to functions constructed by affine interpolations over triangulations. Formally, let $\mathcal{S} = \{S_1, \ldots, S_m\}$ be a triangulation of $\mathrm{conv}(V)$ that does not add vertices, where S_i is a simplex for each i and J_i denotes the index set of vertices of S_i. We construct the function $f^{\mathcal{S}} : S \mapsto \mathbb{R}$ by interpolating the function f affinely over each simplex S_i. More precisely, given a point $x \in S$, there exists an index i (not necessarily unique) such that $x \in S_i$. Since S_i is a simplex, there exists a unique λ that is feasible to $D(x)$ and is such that $\lambda_j = 0$ for all $j \notin J_i$. For this λ, we define $f^{\mathcal{S}}(x) = f(V)^{\intercal}\lambda$. Note that this definition is consistent because if $x \in S_i \cap S_{i'}$, then x belongs to a common face of S_i and $S_{i'}$, and $\lambda_j = 0$ for all $j \notin J_i \cap J_{i'}$.

Corollary 2.7 *Consider a function $f : V \mapsto \mathbb{R}$, and let $\mathcal{S}$ be a triangulation of* $\mathrm{conv}(V)$ *that does not add vertices. Then, $f^{\mathcal{S}}$ is the concave envelope of f over* $\mathrm{conv}(V)$ *if and only if $f^{\mathcal{S}}$ is concave.*

Proof Clearly, $f^{\mathcal{S}}$ is a concave envelope of f only if it is concave. Now, we show the converse. By construction, $f^{\mathcal{S}}(x)$ is the objective value of a feasible solution in $D(x)$ and so $f^{\mathcal{S}}(x) \leq z(x)$. Then, it follows from Theorem 2.4 (i) that for any $x \in \mathrm{conv}(V)$, $f^{\mathcal{S}}(x) \leq \mathrm{conc}(f)(x)$. Further, $f^{\mathcal{S}}(x) = f(x)$ whenever $x \in V$ and so $f^{\mathcal{S}}(x) \geq f(x)$. Since $f^{\mathcal{S}}$ is concave, $f^{\mathcal{S}}(x) \geq \mathrm{conc}(f)(x)$. Therefore, for any $x \in \mathrm{conv}(V)$, $f^{\mathcal{S}}(x) = \mathrm{conc}(f)(x)$. □

The ideas in Corollary 2.7 can be extended to more general settings using the notion of barycentric coordinates or inclusion certificates; see [35]. Theorem 2.4 was proven for a finite point set and can be used to construct concave envelopes of functions restricted to this set. It can also help in determining if functions defined over $\mathrm{conv}(V)$ are concave-extendable from vertices as formalized below.

Corollary 2.8 *Consider a function $f : \mathrm{conv}(V) \mapsto \mathbb{R}$. Then, there exists a triangulation $\mathcal{S}$ that does not add vertices such that $f^{\mathcal{S}}$ is the concave envelope of f over* $\mathrm{conv}(V)$ *if and only if f is concave-extendable from V.*

Proof If f is concave-extendable from V, then the result follows directly from Theorem 2.4 and the fact that any polyhedral subdivision can be refined into a triangulation; see [17]. For the converse, let $\mathcal{S}$ be a triangulation for which $f^{\mathcal{S}}$ is the concave envelope of f over $\mathrm{conv}(V)$. It follows that, $f^{\mathcal{S}}(x) \leq z(x) \leq \mathrm{conc}(f)(x) = f^{\mathcal{S}}(x)$, where the first inequality is satisfied because $f^{\mathcal{S}}(x)$ corresponds to a feasible solution for $D(x)$, the second inequality follows from Theorem 2.4 where it is shown that $z(x)$

is the concave envelope of f restricted to V, and the last equality holds because of our assumption. Therefore, equality holds throughout. In particular, $z(x) = \mathrm{conc}(f)(x)$, which implies by Theorem 2.4 (i) that f is concave-extendable from V. □

Consider the problem $M(r, s) = \max\{f(x) - r^\intercal x - s \mid x \in V\}$. The ability to construct the concave envelope of $f(x)$ is closely related to the ability to solve $M(r, s)$.

Corollary 2.9 *If $M(r, s)$ can be solved in polynomial time, then $P(x)$ can also be solved in polynomial time. Further, if* (i) *there is a polynomial-time separation algorithm for* $\mathrm{conv}(V)$*,* (ii) *there exists a polynomial-time algorithm to find an optimal solution for $D(x)$, and* (iii) *there is a polynomial-time algorithm to solve $P(x)$, then $M(r, s)$ can be solved in polynomial time.*

Proof We start by showing the first statement of the corollary. Assume there exists a polynomial-time algorithm to solve $M(r, s)$. We show that a polynomial-time separation algorithm can be constructed for $P(x)$. For any solution (a, b), we solve $M(a, b)$. If the optimal value $M(a, b)$ is nonpositive, then $f(x) \leq av + b$ for all $v \in V$ and therefore $(a, b) \in F$. Otherwise, the optimal solution of $M(a, b)$ gives a hyperplane separating (a, b) from F. Therefore, the optimization oracle for $M(r, s)$ yields a separation oracle for $P(x)$. The result then follows from Theorem 6.4.9 in [12].

We now prove the second statement of the corollary. Define $M'(r, s)$ as $\max\{\mathrm{conc}(f)(x) - r^\intercal x - s \mid x \in \mathrm{conv}(V)\}$, where $\mathrm{conc}(f)(x)$ is the concave envelope of $f(x)$ over $\mathrm{conv}(V)$. We show that the optimal value of $M(r, s)$ is the same as that of $M'(r, s)$. Clearly, the optimal value of $M(r, s)$ is no larger than that of $M'(r, s)$. For the converse, consider an optimal solution x' to $M'(r, s)$. Because x' is optimal for $M'(r, s)$ and $\mathrm{conc}(f)(v_i) \geq f(v_i)$ for all i, we write $\big(\mathrm{conc}(f)(x') - r^\intercal x' - s\big)e^\intercal \geq f(V)^\intercal - r^\intercal V - se^\intercal$, where $e \in \mathbb{R}^m$ is a column vector of all ones. Consider now λ' to be an optimal solution to $D(x')$, i.e., $e^\intercal \lambda' = 1$, $V\lambda' = x'$, and $\mathrm{conc}(f)(x') = z(x') = f(V)^\intercal \lambda'$. It follows that $\mathrm{conc}(f)(x') - r^\intercal x' - s = \big(f(V)^\intercal - r^\intercal V - se^\intercal\big)\lambda'$. We conclude that $\mathrm{conc}(f)(x') - r^\intercal x' - s = f(v) - r^\intercal v - s$ for any v in the support of λ', showing that the optimal value of $M(r, s)$ is no smaller than that of $M'(r, s)$.

Further, given an optimal solution to $M'(r, s)$, λ' can be computed using the algorithm for $D(x)$ in polynomial time and, as a result, a solution to $M(r, s)$ can be computed. Now, we solve $M'(r, s)$ by reformulating it as $M''(r, s)$ which is defined as $\max\{t \mid \mathrm{conc}(f)(x) - r^\intercal x - s - t \geq 0, x \in \mathrm{conv}(V)\}$. Using Theorem 6.4.9 in [12], it suffices to construct a strong separation oracle for $M''(r, s)$. Given $(\bar{t}, \bar{x})$, if $\bar{x} \notin \mathrm{conv}(V)$ we can use the separation algorithm for $\mathrm{conv}(V)$. Otherwise, solve $P(\bar{x})$ and let $(\bar{a}, \bar{b})$ be an optimal solution. Then, define $a' = \bar{a} - r$ and $b' = \bar{b} - s - \bar{t}$. It follows that $a'x + b' \geq \mathrm{conc}(f)(x) - r^\intercal x - s - \bar{t}$ for all $x \in \mathrm{conv}(V)$ and $a'\bar{x} + b' = \mathrm{conc}(f)(\bar{x}) - r^\intercal \bar{x} - s - \bar{t}$. Therefore, $a'\bar{x} + b' \geq 0$ if and only if $(\bar{t}, \bar{x})$ is feasible. Otherwise, if $a'\bar{x} + b' < 0$, we find a separating hyperplane $a'x + \bar{b} - s - t \geq 0$ that separates the feasible region of $M''(r, s)$ from $(\bar{t}, \bar{x})$. □

Although the proof that an algorithm to solve $M(r, s)$ can be used to solve $P(x)$ uses the ellipsoid algorithm through the application of Theorem 6.4.9 in [12], it is possible to develop a Dantzig-Wolfe decomposition algorithm (albeit without polynomial time complexity) for the solution of $D(x)$ using the algorithm for $M(r, s)$; see [3] for details. The proof technique used to show that $M(r, s)$ can be solved using algorithms for separation of $\operatorname{conv}(V)$ and optimization routines for $D(x)$ and $P(x)$ is similar to that used in [12] for showing that submodular function minimization is polynomially solvable. Corollary 2.9 is also related to Theorem 1 in [34] in that the author discusses the equivalence of the concave envelopes of two functions f and f' if the optimization problems $\max\{f(x) - r^\mathsf{T}x - s \mid x \in V\}$ and $\max\{f'(x) - r^\mathsf{T}x - s \mid x \in V\}$ have the same optimal value.

The formulation of the concave envelope described in Theorem 2.4 enables us to compute the concave envelope for functions defined as a maximum of other functions. Consider $f_i : V \mapsto \mathbb{R}$, for $i = 1, \ldots, k$. When associated with f_i, we denote $P(x)$, $D(x)$, and F by $P(f_i, x)$, $D(f_i, x)$, and $F(f_i)$ respectively.

Corollary 2.10 *Consider a collection of functions $f_i : V \mapsto \mathbb{R}$, for $i = 1, \ldots, k$. If there exists a polynomial-time algorithm to solve $P(f_i, x)$ for each i and for each $x \in \operatorname{conv}(V)$, and there exists a polynomial-time strong separation algorithm for $\operatorname{conv}(V)$, then there exists a polynomial-time algorithm to optimize a linear function over $F\big(\max\{f_1, \ldots, f_k\}\big)$, and hence to solve $P\big(\max\{f_1, \ldots, f_k\}, x\big)$.*

Proof Consider the optimization problem $P'(f_i, x, r)$ defined as $\min\{ax + br \mid (a, b) \in F(f_i)\}$ and denote its optimal value by $z(f_i, x, r)$. We first construct a strong optimization oracle for $P'(f_i, x, r)$ [12], i.e., an oracle that provides an optimal solution if one exists, otherwise it returns a recession direction of $F(f_i)$ in which the objective function decreases. Since $F(f_i) \neq \emptyset$, the recession cone of $F(f_i)$, denoted as $0^+\big(F(f_i)\big)$, is given by $\big\{(a, b) \;\big|\; av + b \geq 0 \text{ for all } v \in V\big\}$.

Since $z(f_i, x, r)$ is positively homogeneous in (x, r) we may assume by scaling that r is 1, -1, or 0. If $x \in \operatorname{conv}(V)$ and $r = 1$, the oracle is assumed to be available. If $x \notin \operatorname{conv}(V)$ and $r = 1$, then using the separation routine for $\operatorname{conv}(V)$ we can find in polynomial time a ρ such that $\rho^\mathsf{T}x < c$ and $\rho^\mathsf{T}v \geq c$ for all $v \in V$. Then, $(\rho^\mathsf{T}, -c) \in 0^+\big(F(f_i)\big)$ and is the desired recession direction. Now, we assume that $r = 0$. If $x = 0$ then the optimal solution of $P(f_i, 0)$ is optimal to $P'(f_i, x, r)$. Otherwise, there exists an x_k such that $x_k \neq 0$. If $x_k < 0$, use the strong separation oracle for $\operatorname{conv}(V)$ to compute $x_k^L = \min\big\{x'_k \mid x' \in \operatorname{conv}(V)\big\}$, where the minimum exists since V is assumed to be of finite size; see Theorem 6.4.9 in [12]. Then, $v_k - x_k^L \geq 0$, for all $v \in V$ and therefore $(e_k^\mathsf{T}, -x_k^L) \in 0^+(F)$ is the desired recession direction, where e_k is the k^{th} principal vector. On the other hand, if $x_k > 0$, then compute $x_k^U = \max\big\{x'_k \mid x' \in \operatorname{conv}(V)\big\}$ and, as before, $(-e_k^\mathsf{T}, x_k^U)$ is the desired recession direction. Now, assume that $r = -1$. Then, $(0, 1) \in 0^+\big(F(f_i)\big)$ is the desired recession direction.

Since $F\big(\max\{f_1, \ldots, f_k\}\big) = \bigcap_{i=1}^k F(f_i)$, the strong optimization oracles can be used to optimize a linear function over $F\big(\max\{f_1, \ldots, f_k\}\big)$ and hence to solve $P\big(\max\{f_1, \ldots, f_k\}, x\big)$ using the ellipsoid algorithm; see Corollary 14.1d in [29]. □

In most applications, the underlying polyhedron $\operatorname{conv}(V)$ will be simple and so the corresponding separation algorithm will be trivial. We will describe, in the forthcoming sections, various types of functions for which concave envelopes can be obtained in polynomial time. Corollary 2.10 states that the concave envelope of the maximum of any subset of these functions can also be computed in polynomial time.

The above algorithm is polynomial-time only if k is treated as part of the input. Otherwise, as we will describe later, the convex envelope over $[0, 1]^n$ of a function that is submodular when restricted to $\{0, 1\}^n$ can be expressed as a maximum of exponentially many linear functions. Since $\text{conv}(f) \le f$, it follows easily that $\text{conc}(\text{conv}(f)) \le \text{conc}(f)$. Further, since each point in $\{0, 1\}^n$ belongs to $\text{vert}([0, 1]^n)$, it follows that $\text{conv}(f) = f$ at each $v \in V$. Therefore, $\text{conc}(\text{conv}(f)) \ge \text{conc}(f)$. Combining, we obtain that $\text{conc}(\text{conv}(f)) = \text{conc}(f)$. If k was not part of input, Corollary 2.10 would imply that $P(x)$ can be solved in polynomial time for a submodular function, thereby providing a polynomial-time separation routine for maximizing a submodular function. This, in turn, is not possible unless $P = NP$.

Corollary 2.10 can also be proven using disjunctive programming if an explicit polynomial-sized characterization of the facets of f_i is available for each i. The main idea would be to express the hypograph of $\max\{f_1, \dots, f_k\}$ as the convex hull of the union of hypographs for each f_i in a lifted space; see Theorem 16.5 in [26]. This would provide an explicit polynomial-sized polyhedral representation of the concave envelope in a higher-dimensional space.

3 Supermodular function that is concave-extendable from vertices

In this section, we use a result of [20] to derive the triangulation associated with the concave envelope of supermodular functions. This allows us to construct closed-form expressions for the concave envelopes of supermodular functions over the hypercube assuming that these functions are concave-extendable from vertices. We then demonstrate the utility of this construction in two ways. First, we provide a direct and unified derivation of many recent results in the literature (each of which was initially proven using a different technique) as a consequence of this simple construction. Second, we show that it can be used to improve the relaxations currently used in existing factorable programming solvers; see [4,19,41]. In particular, during the construction of relaxations, factorable programming techniques [21] typically use variable substitution to relax functions expressed as a composition of a convex function and a linear function. We will show, among many other examples, that the techniques described in this section apply to this structure.

It follows from our discussion in Sect. 2 that the facets of the concave envelope of any function that is concave-extendable from the vertices of a polytope P can be obtained through the solution of a linear program, $P(x)$, which has a constraint for every vertex of P. As a result, the linear program $P(x)$ typically has an exponential number of constraints, limiting the applicability of the technique. However, if the function under study is well-structured, we show that it is sometimes possible to deduce the triangulation defining its concave envelope by explicitly characterizing the set of optimal solutions of the linear program. Supermodularity is one such function structure that permits an a-priori derivation of the corresponding triangulation.

Definition 3.1 ([43]) A function $f(x) : S \subseteq \mathbb{R}^n \to \mathbb{R}$ is said to be supermodular if $f(x' \vee x'') + f(x' \wedge x'') \ge f(x') + f(x'')$ for all $x', x'' \in S$, where $x' \vee x''$ denotes the component-wise maximum and $x' \wedge x''$ denotes the component-wise minimum of x' and x''. $\square$

An important special case of the above definition is encountered when $S = \{0, 1\}^n$. In this case, any element x of S is of the form $x = \sum_{i \in K} e_i$ where e_i is the i^{th} principal vector in $\mathbb{R}^n$ and $K \subseteq \{1, \dots, n\}$. Then, f can also be viewed as a set function in the following way. We define $f' : 2^N \to \mathbb{R}$ as $f'(K) = f(\sum_{j \in K} e_j)$. Then, $f(x)$ is supermodular if and only if $f'(A \cup B) + f'(A \cap B) \geq f'(A) + f'(B)$.

Given a function $f : \{0, 1\}^n \mapsto \mathbb{R}$ that is supermodular, it follows from Theorem 2.4 that there is a triangulation of the hypercube that yields the concave envelope of f. We show in Theorem 3.3 that this triangulation is in fact Kuhn's triangulation. A triangulation $\mathcal{K} = \{\Delta_1, \dots, \Delta_{n!}\}$ is said to be *Kuhn's triangulation* of the hypercube $[0, 1]^n$, if the simplices of $\mathcal{K}$ are in a one-to-one correspondence with the permutations of $\{1, \dots, n\}$ as discussed next. Given a permutation π of $\{1, \dots, n\}$, the $n+1$ vertices of the corresponding simplex Δ_π are $\left\{(0, \dots, 0) + \sum_{j=1}^{k} e_{\pi(j)} \mid k = 0, \dots, n\right\}$; see [17]. Observe that both the vectors $(0, \dots, 0)$ and $(1, \dots, 1)$ are vertices of each of the simplices composing Kuhn's triangulation.

We define the *Lovász extension* [20] of a function $f(x)$ as $f^{\mathcal{K}}(x)$, where $\mathcal{K}$ is Kuhn's triangulation of the unit hypercube. Given any $x \in [0, 1]^n$, we can find a permutation π of $\{1, \dots, n\}$ such that $x_{\pi(1)} \geq x_{\pi(2)} \geq \cdots \geq x_{\pi(n)}$ by sorting the components of x. It is clear that x belongs to Δ_π since it can be expressed as the following convex combination of its extreme points:

$$x = (1 - x_{\pi(1)})0 + \sum_{j=1}^{n-1} (x_{\pi(j)} - x_{\pi(j+1)}) \left(\sum_{r=1}^{j} e_{\pi(r)} \right) + x_{\pi(n)} \left(\sum_{r=1}^{n} e_{\pi(r)} \right).$$

It follows that:

$$\begin{aligned} f^{\mathcal{K}}(x) &= (1 - x_{\pi(1)}) f(0) + \sum_{j=1}^{n-1} \left(x_{\pi(j)} - x_{\pi(j+1)}\right) f\left(\sum_{r=1}^{j} e_{\pi(r)} \right) \\ &\quad + x_{\pi(n)} f\left(\sum_{r=1}^{n} e_{\pi(r)} \right) = \sum_{i=1}^{n} \left(f\left(\sum_{j=1}^{i} e_{\pi(j)} \right) - f\left(\sum_{j=1}^{i-1} e_{\pi(j)} \right) \right) x_{\pi(i)} \\ &\quad + f(0) \end{aligned} \tag{4}$$

for all $x \in \Delta_\pi$.

We next present a result that is crucial in developing the concave envelope of a supermodular function that is concave-extendable from the vertices of the unit hypercube. Because it plays an important role in the subsequent development, we provide here a self-contained proof using the techniques of Sect. 2. We note however that this lemma was first stated, although not explicitly proven, in [20].

Lemma 3.2 (Proposition 4.1 in [20]) *$f^{\mathcal{K}}$ is concave if and only if f restricted to $\{0, 1\}^n$ is supermodular.*

Proof Given $S \subseteq \{1, \dots, n\}$, let $\chi(S)$ be the indicator vector of S. Consider two arbitrary subsets, X and Y, of $\{1, \dots, n\}$. The following argument shows that, if $f^{\mathcal{K}}$ is concave, the restriction of f to $\{0, 1\}^n$ is supermodular:

$$\frac{1}{2}f\big(\chi(X)\big)+\frac{1}{2}f\big(\chi(Y)\big)=\frac{1}{2}f^{\mathcal{K}}\big(\chi(X)\big)+\frac{1}{2}f^{\mathcal{K}}\big(\chi(Y)\big) \le f^{\mathcal{K}}\left(\frac{1}{2}\big(\chi(X)+\chi(Y)\big)\right)$$
$$= f^{\mathcal{K}}\left(\frac{1}{2}\chi(X\cup Y)+\frac{1}{2}\chi(X\cap Y)\right) = \frac{1}{2}f\big(\chi(X\cup Y)\big)+\frac{1}{2}f\big(\chi(X\cap Y)\big).$$

In the above derivation, the first equality holds because $f(x) = f^{\mathcal{K}}(x)$ for $x \in \{0, 1\}^n$, the first inequality follows from concavity of $f^{\mathcal{K}}(x)$, the second equality is satisfied since $\chi(X) + \chi(Y) = \chi(X \cup Y) + \chi(X \cap Y)$, and the last equality holds because $f^{\mathcal{K}}$ is affine over the line segment $\big[\chi(X \cap Y), \chi(X \cup Y)\big]$ since this line segment is completely contained in at least one of the simplices Δ_π.

Now, we argue that if f restricted to $\{0, 1\}^n$ is supermodular then $f^{\mathcal{K}}(x)$ is concave. To this end, we will show that $f^{\mathcal{K}}(x) = z(x)$, where $z(x)$ is the optimal value of $P(x)$. Since $z(x)$ is the minimum of affine functions of x, one for each $(a, b) \in F$, it will follow that $f^{\mathcal{K}}(x)$ is concave. Consider $x' \in [0, 1]^n$ and assume without loss of generality, by reordering the components of x' if necessary that $x'_1 \ge \cdots \ge x'_n$. Since the multipliers $(1 - x'_1), (x'_1 - x'_2), \dots, (x'_{n-1} - x'_n), x'_n$ yield a feasible solution to $D(x')$, it follows from weak duality that $f^{\mathcal{K}}(x') \le z(x')$.

To show that $z(x') \le f^{\mathcal{K}}(x')$, we will prove that $a'_i = f(\sum_{r=1}^{i} e_r) - f(\sum_{r=1}^{i-1} e_r)$ for $i = 1, \dots, n$ and $b' = f(0)$ is feasible for $P(x')$ and has objective value $f^{\mathcal{K}}(x')$. First, we show that $(a', b') \in F$, i.e., $a'v + b' \ge f(v)$ for all $v \in \{0, 1\}^n$ by induction on $||v||_1$. The base case is clear since $v = 0$ is the only vector with $||v||_1 = 0$ and since $b' = f(0)$. For the inductive step, consider $v \in \{0, 1\}^n$ and assume that the result holds for all $w \in \{0, 1\}^n$ with $||w||_1 < ||v||_1$. Define k to be the largest index for which $v_k = 1$. Then,

$$a'v + b' = a'(v - e_k) + b' + a'e_k \ge f\big(v - e_k\big) + f\left(\sum_{r=1}^{k} e_r\right) - f\left(\sum_{r=1}^{k-1} e_r\right)$$
$$= f\left(v \wedge \sum_{r=1}^{k-1} e_r\right) + f\left(v \vee \sum_{r=1}^{k-1} e_r\right) - f\left(\sum_{r=1}^{k-1} e_r\right) \ge f(v),$$

where the first inequality follows from the inductive hypothesis and the definition of a'_k, the second equality follows from the definition of k, and the second inequality holds because of the supermodularity of f. By construction, see also (4), $a'x' + b' = f^{\mathcal{K}}(x')$ and therefore $z(x') \le f^{\mathcal{K}}(x')$. □

It seems that Lemma 3.2 was originally motivated by [11]'s greedy algorithm for optimizing linear functions over extended polymatroids [11]. Although, in the proof of Lemma 3.2, we replaced this optimization problem with $P(x)$, the proof still makes use of [11]'s algorithm implicitly. We discuss the connections next. First, note that F reduces to an extended polymatroid when b is restricted to be zero and $V = \{0, 1\}^n$.

In general, if b is assumed to be zero in $P(x)$, then the optimal value function $z(x)$ of $P(x)$ yields the tightest positively homogeneous concave overestimator of f instead of its concave envelope; see, for example, Proposition 2 in [24]. If $f(x)$ is supermodular, the concave envelope is positively homogeneous as long as $f(0) = 0$, an assumption that can be made without loss of generality by translating f if necessary. For more general functions, however, the concave envelope may not be positively homogeneous over the domain and assuming $b = 0$ would be restrictive in those cases. If $f(x)$ is supermodular, in light of Theorem 2.4, the above proof shows that $f^{\mathcal{K}}(x) = \text{conc}(f)(x)$. This fact can be derived from Lemma 3.2 using Corollary 2.7.

Theorem 3.3 *Consider a function* $f : [0, 1]^n \mapsto \mathbb{R}^n$. *The concave envelope of* f *over* $[0, 1]^n$ *is given by* $f^{\mathcal{K}}(x)$ *if and only if* f *is supermodular when restricted to* $\{0, 1\}^n$ *and concave-extendable from the vertices of* $[0, 1]^n$.

Proof If f is concave-extendable from the vertices of $[0, 1]^n$ and supermodular when restricted to $\{0, 1\}^n$ then it follows from Lemma 3.2 and Corollary 2.7 that $f^{\mathcal{K}}(x)$ is the concave envelope of $f(x)$. On the other hand, if $f^{\mathcal{K}}(x)$ is the concave envelope of $f(x)$, then it follows from Lemma 3.2 and Corollary 2.8 that f restricted to $\{0, 1\}^n$ is supermodular and f is concave-extendable from $\{0, 1\}^n$. □

Theorem 3.3 establishes that the concave envelope of a function that is concave-extendable from the vertices of the unit hypercube and that is supermodular when restricted to $\{0, 1\}^n$ is its Lovász extension. It follows from the proof of Lemma 3.2 that each of the linear functions (4) is valid for $\text{conc}_{[0,1]^n} f(x)$ and therefore

$$\operatorname*{conc}_{[0,1]^n} f(x) = \min_{\pi\in\Pi_n} \sum_{i=1}^{n} \left(f\left(\sum_{j=1}^{i} e_{\pi(j)}\right) - f\left(\sum_{j=1}^{i-1} e_{\pi(j)}\right)\right) x_{\pi(i)} + f(0), \tag{5}$$

where Π_n is the set of permutations of $\{1, \ldots, n\}$. By encoding the permutations differently, we can also establish that

$$\operatorname*{conc}_{[0,1]^n} f(x) = \min_{\hat{\pi}\in\Pi_n} \sum_{i=1}^{n} \left(f\left(\sum_{j|\hat{\pi}(j)\le\hat{\pi}(i)} e_j\right) - f\left(\sum_{j|\hat{\pi}(j)<\hat{\pi}(i)} e_j\right)\right) x_i + f(0), \tag{6}$$

an expression that is sometimes easier to use. In particular, it is simple to verify that expressions (5) and (6) match when $\hat{\pi}(j) = \pi^{-1}(j)$.

Theorem 3.3 applies in a straightforward manner for developing concave envelopes over general hypercubes by transforming the variables using (1). However, in typical applications, it is often more convenient to establish the supermodularity and concave-extendability from vertices without carrying out the transformation first. In particular, supermodularity can be established using the standard definition for checking this condition over real lattices, i.e., $f(x^1)+f(x^2) \le f(\min(x^1, x^2))+f(\max(x^1, x^2))$. Here x^1 and x^2 are any extreme points of the hypercube and min and max are assumed to be taken coordinatewise. Then, it follows easily that the transformed function is supermodular. Further, (1) maps the vertices of the hypercube to $\{0, 1\}^n$. Therefore, concave-extendability of the transformed function also follows from that of the original function. Then, Theorem 3.3 shows that Kuhn's triangulation, transformed to the hypercube in consideration, yields the concave envelope of the associated function. We will provide an application of Theorem 3.3 over general hypercubes in Corollary 3.13.

Next, we show that supermodularity can also help to obtain the concave envelope of certain functions over sets other than the unit hypercube (or more generally hyperrectangles). To this end, consider a directed graph $G = (V, E)$ where $V = \{1, \ldots, n\}$ and let I_0 and I_1 be non-intersecting subsets of $\{1, \ldots, n\}$. Consider the sets $C = \bigcap_{(i,j)\in E}\{x \mid x_i \geq x_j\}$, $C_0 = \bigcap_{i\in I_0}\{x \mid x_i = 0\}$, and $C_1 = \bigcap_{i\in I_1}\{x \mid x_i = 1\}$. Define

$$S = [0, 1]^n \cap C \cap C_0 \cap C_1 \tag{7}$$

and assume that $S \neq \emptyset$. The matrix associated with the constraints in $C \cap [0, 1]^n$ is composed of the node-edge incidence matrix of a directed graph appended with identity matrices. Therefore, it is totally unimodular and so, its vertices are binary. Further, Kuhn's triangulation gives a polyhedral subdivision of S. This can be seen by considering a point $x \in S$. Sort the coordinates of x in a non-increasing order extending the pre-order defined by G. If σ is the corresponding permutation of $\{1, \ldots, n\}$, then x clearly belongs to the associated simplex Δ_σ of Kuhn's triangulation. Let T be the face of Δ_σ such that $x \in \mathrm{ri}(T)$. Let $v \in \mathrm{vert}(T)$. Then, it can be verified that $v \in \{0, 1\}^n \cap S$. Further, note that if x and y belong to S, then so do $x \vee y$ and $x \wedge y$. Thus, the set S is the convex hull of the incidence vectors of a lattice family, where a lattice family is a family of sets $\mathcal{C}$ such that if $A, B \in \mathcal{C}$, then $A \cap B$ and $A \cup B$ also belong to $\mathcal{C}$. By a slight modification of Proposition 10.3.3 in [12], it can be shown that the incidence vectors of a finitely-sized lattice family can be expressed as the vertices of S by appropriately defining C, C_0, and C_1. A function f is said to be supermodular over a lattice family $\mathcal{C}$ or the corresponding incidence vectors, $\mathrm{vert}(S)$, if $f(A \cap B) + f(A \cup B) \geq f(A) + f(B)$ for all $A, B \in \mathcal{C}$.

Corollary 3.4 *Let $f : S \mapsto \mathbb{R}^n$ be supermodular when restricted to* $\mathrm{vert}(S)$ *and concave-extendable from the vertices of S defined in (7). Then, for any $x \in S$, $f^{\mathcal{K}}(x)$ is well-defined and forms the concave envelope of f over S.*

Proof Because of the form of S and the corollary's assumption, f restricted to $\mathrm{vert}(S)$ can be extended to $\bar{f} : \{0, 1\}^n \mapsto \mathbb{R}$ in such a way that $\bar{f}$ is supermodular when restricted to $\{0, 1\}^n$; see Theorem 49.2 in [30]. Let $x' \in S$. Then, $x' \in \mathrm{ri}(T)$ where T is a face of Δ_σ and σ is an ordering of coordinates of x' in non-increasing order that is consistent with the pre-ordering of coordinates defining S. Since the vertices of T belong to S, $f^{\mathcal{K}}(x')$ is obtained as an interpolation of $f(\cdot)$ evaluated at points in S. Therefore, $f^{\mathcal{K}}(x')$ is well-defined and $\bar{f}^{\mathcal{K}}(x') = f^{\mathcal{K}}(x')$. Let $h(x)$ be the concave envelope of $f(x)$ over S. By Theorem 3.3, $\bar{f}^{\mathcal{K}}(x)$ is the concave envelope of $\bar{f}$ over $[0, 1]^n$. Therefore, by concave-extendability of f from $\mathrm{vert}(S)$, it follows that

$f^{\mathcal{K}}(x') = \bar{f}^{\mathcal{K}}(x') \geq h(x')$. However, $f^{\mathcal{K}}(x')$ is also a feasible solution to $D(x')$ for $V = \text{vert}(S)$. Therefore, $f^{\mathcal{K}}(x') \leq h(x')$. In other words, $f^{\mathcal{K}}(x') = h(x')$. □

As was exploited in the proof of Corollary 3.4, an extension of f restricted to $\text{vert}(S)$ to $[0, 1]^n$, say $\bar{f}$, can be constructed that is supermodular when restricted to $\{0, 1\}^n$. Instead, if f itself can be extended to $[0, 1]^n$ such that the resulting function is not only supermodular when restricted to $\{0, 1\}^n$ but is also concave-extendable from $\{0, 1\}^n$, then the concave-extendability of f from $\text{vert}(S)$ follows. This is because $\bar{f}^{\mathcal{K}}(x) = \text{conc}_{[0,1]^n} \bar{f}(x) \geq \text{conc}_S f(x) \geq f^{\mathcal{K}}(x)$, where the first equality follows from Theorem 3.3, the first inequality is satisfied since $S \subseteq [0, 1]^n$, and the second inequality holds since $f^{\mathcal{K}}(x)$ is a feasible solution to $D(x)$. But, as argued above, $f^{\mathcal{K}}(x) = \bar{f}^{\mathcal{K}}(x)$. Therefore, the equality holds throughout and, as a result, f is concave-extendable from $\text{vert}(S)$.

Remark 3.5 Let $f(x) : V \mapsto \mathbb{R}^n$. Consider a polyhedral subdivision of $\text{conv}(V)$, namely $\mathcal{S} = \{S_1, \ldots, S_k\}$, which defines the concave envelope of $f(x)$ over $\text{conv}(V)$. For each i, let S'_i be a polytope that is a subset of S_i, such that the vertices of S'_i belong to V and for each $v \in \text{vert}(S'_i)$, $\text{conc}_{\text{conv}(V)}(f)(v) = f(v)$. As an example, it follows from Theorem 2.4 (iv) that S_i itself satisfies these requirements. Then, for any $x \in S'_i$:

$$\underset{\text{conv}(V)}{\text{conc}}(f)(x) \geq \underset{S'_i}{\text{conc}}(f)(x) \geq \underset{S_i}{\text{conc}}(f)(x) = \underset{\text{conv}(V)}{\text{conc}}(f)(x),$$

where the first inequality follows since $S'_i \subseteq \text{conv}(V)$; the second inequality since $\text{conc}_{S_i}(f)$ is affine, $\text{conv}_{S'_i}(f)$ is concave, and $\text{conc}_{S_i}(f)(v) = f(v)$ for all $v \in \text{vert}(S'_i)$; and the equality follows from the assumption that $\mathcal{S}$ defines the concave envelope of f over $\text{conv}(V)$. Therefore, equality holds throughout. Consequently, for any $X \subseteq \mathbb{R}^n$, such that $S'_i \subseteq X \subseteq \text{conv}(V)$ and any $x \in S'_i$, it follows that $\text{conc}_{S'_i}(f)(x) = \text{conc}_X(f)(x)$ since $\text{conc}_{\text{conv}(V)}(f)(x) \geq \text{conc}_X(f)(x) \geq \text{conc}_{S'_i}(f)(x)$ for $x \in S'_i$. Therefore, if $\mathcal{S}' = \{S'_1, \ldots, S'_k\}$ is a polyhedral subdivision of X then $\mathcal{S}'$ defines the concave envelope of f over X. This envelope can also be obtained by restricting $\text{conc}_{\text{conv}(V)}(f)$ to X. The idea behind this remark was the key to the proof of Corollary 3.4. We will encounter various other applications of this observation in the remainder of the paper. □

Theorem 3.3 and Corollary 3.4 generalize many results that have been developed for specific functions. To demonstrate the applicability of Theorem 3.3, we will now derive a variety of results from the literature as a consequence. Theorem 3.3 asserts that, for a given f, the concave envelope of f over the unit hypercube is $f^{\mathcal{K}}(x)$ if and only if f is supermodular and concave-extendable from vertices. Proofs in the literature typically demonstrate that $f^{\mathcal{K}}(x)$ is the concave envelope directly. However, the latter properties are often much easier to prove as we illustrate below. In these discussions, the following result is useful in establishing the supermodularity of nonlinear functions.

Lemma 3.6 (Lemma 2.6.4 in [43]) *Consider a lattice X and let $K = \{1, \ldots, k\}$. For $i \in K$, let $f_i(x)$ be increasing supermodular (resp. submodular) functions on X and*

Z_i be convex subsets of $\mathbb{R}$. Assume $Z_i \supseteq \{f_i(x) \mid x \in X\}$. Let $g(z_1, \ldots, z_k, x)$ be supermodular in $(z_1, \ldots, z_k, x)$ on $Z_1 \times \cdots \times Z_k \times X$. If for all $i \in K$, $\bar{z}_{i'} \in Z_{i'}$ for $i' \in K \backslash \{i\}$, and $\bar{x} \in X$, $g(\bar{z}_1, \ldots, \bar{z}_{i-1}, z_i, \bar{z}_{i+1}, \ldots, \bar{z}_k, \bar{x})$ is increasing (decreasing) and convex in z_i on Z_i, then $g\big(f_1(x), \ldots, f_k(x), x\big)$ is supermodular on X. □

By choosing $g(z_1, \ldots, z_k, x)$ appropriately as $z_1 z_2 \cdots z_k$ or $-z_1 z_2 \cdots z_k$, it follows easily that a product of nonnegative, increasing (decreasing) supermodular functions is also nonnegative increasing (decreasing) and supermodular; see Corollary 2.6.3 in [43]. Also, it follows trivially that a conic combination of supermodular functions is supermodular.

We now use Theorem 3.3 and Corollary 3.4 to derive the concave envelope of some multilinear functions over certain polytopes and apply this general result to derive various results of the literature. More precisely, we define $G \subseteq \mathbb{R}^{\sum_{i=1}^n d_i}$, where each $y \in G$ is expressed as $(y_1, \ldots, y_n)$, and $y_i = (y_{i1}, \ldots, y_{id_i}) \in \mathbb{R}^{d_i}$ for $i = 1, \ldots, n$, as:

$$G = \left\{ y \in \mathbb{R}^{\sum_{i=1}^n d_i} \;\middle|\; \sum_{r=1}^{d_i} y_{ir} \leq 1 \,\forall i;\;\; y_{ir} \geq 0 \,\forall (i, r) \right\}, \tag{8}$$

i.e., G is a set of points in $\mathbb{R}^{\sum_{i=1}^n d_i}$ that satisfy n non-overlapping generalized upper bound constraints. Note that since we can choose $d_i = 1$ for all i, G can also represent a hypercube. For each i, let $D_i = \{1, \ldots, d_i\}$ and T_i be a chain (by inclusion) of subsets of D_i where $\emptyset = T_{i0} \subset \cdots \subset T_{id_i} = D_i$. Without loss of generality, by relabeling the variables if necessary, we assume that $T_{ir} = \{1, \ldots, r\}$. Consider the multiset M where each i in $\{1, \ldots, n\}$ has d_i copies. Let Π denote the set of distinct arrangements of M. Then, each $\pi \in \Pi$ is a permutation of $\{1, \ldots, \sum_{i=1}^n d_i\}$, where we may additionally assume that, for each $i \in \{1, \ldots, d_i\}$, $\pi_{i1} \geq \cdots \geq \pi_{id_i}$. For $r \in \{1, \ldots, d_i\}$, we let $e(i, r) \in \mathbb{R}^{\sum_{i=1}^n d_i}$ represent the r^{th} principal vector in the i^{th} subspace. Further, let $e(i, d_i + 1)$ be the zero vector in $\mathbb{R}^{\sum_{i=1}^n d_i}$. For a given π, i, and i' in $\{1, \ldots, n\}$, and $r \in \{1, \ldots, d_i\}$, if there exists an index $j \in \{1, \ldots, d_{i'}\}$ such that $\pi_{i'j} \leq \pi_{ir}$, we define $w_\pi^{ir}(i') = \min\{j \mid \pi_{i'j} \leq \pi_{ir}\}$, otherwise we set $w_\pi^{ir}(i') = d_{i'} + 1$.

Next we introduce an example that we will use to illustrate the above notation and the result of Theorem 3.8.

Example 3.7 Consider the function

$$\hat{f}(y_{11}, y_{12}, y_{21}, y_{22}) = 2(1 + y_{11})(2 + y_{21} + y_{22}) + 3(y_{11} + y_{12})y_{21}$$

over the polytope

$$\hat{G} = \{y \in \mathbb{R}^4_+ \mid y_{11} + y_{12} \leq 1, y_{21} + y_{22} \leq 1\}.$$

For the set above, the arrangements $(\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22})$ in Π are $(2, 1, 4, 3), (3, 1, 4, 2)$, $(3, 2, 4, 1)$, $(4, 1, 3, 2)$, $(4, 2, 3, 1)$ and $(4, 3, 2, 1)$. In particular, for $\pi = (4, 1, 3, 2)$, we have $w_\pi^{11}(1) = 1, w_\pi^{12}(1) = 2, w_\pi^{21}(1) = 2, w_\pi^{22}(1) = 2$ and $w_\pi^{11}(2) = 1, w_\pi^{12}(2) = 3, w_\pi^{21}(2) = 1, w_\pi^{22}(2) = 2$. □

Theorem 3.8 *Consider the function* $f(y) = \sum_{k\in K} a_k \prod_{i=1}^{n}(b_{ik} + \sum_{j\in T_{ir_{ik}}} y_{ij})$ *over* G*, where for each* k*,* $r_{ik} \in D_i \cup \{0\}$*,* $a_k \geq 0$*, and* $b_{ik} \geq 0$*. Then, the concave envelope of* $f(y)$ *over* G *is given by:*

$$\min_{\pi\in\Pi} \sum_{i=1}^{n}\sum_{j=1}^{d_i}\left[\sum_{p=j}^{d_i}\left(f\left(\sum_{i'=1}^{n} e\big(i', w_\pi^{ip}(i')\big)\right)\right.\right.$$
$$\left.\left. -f\left(\sum_{i'=1}^{n} e\big(i', w_\pi^{ip}(i')\big) - e(i,p) + e(i,p+1)\right)\right)\right] y_{ij} + f(0). \tag{9}$$

In particular, consider $h(y) = \sum_{k\in K} a_k \prod_{i\in I_k} \sum_{j\in T_{ir_{ik}}} y_{ij}$*, where, for each* k*,* $I_k \subseteq \{1,\ldots,n\}$*. Then, the concave envelope of* h *over* G *is:*

$$\sum_{k\in K} a_k \min_{i\in I_k}\left(\sum_{j\in T_{ir_{ik}}} y_{ij}\right). \tag{10}$$

Proof Consider the invertible linear transformation G' of G obtained by defining $Y_{ir} = \sum_{j=1}^{r} y_{ij}$ for $r = 1,\ldots,d_i$ and by setting Y_{i0} to zero for notational convenience. Then,

$$G' = \left\{Y \in \mathbb{R}^{\sum_{i=1}^{n} d_i} \;\middle|\; 0 \leq Y_{i1} \leq \cdots \leq Y_{id_i} \leq 1\, \forall i = 1,\ldots,n\right\}.$$

Let $L_i \in \mathbb{R}^{d_i\times d_i}$ be the lower triangular matrix of all ones. It is easily verified that:

$$L_i^{-1} = \begin{bmatrix} 1 & & & \\ -1 & 1 & & 0 \\ & \ddots & \ddots & \\ 0 & & -1 & 1 \end{bmatrix}.$$

Then, let L be as shown below and L^{-1} be computed as:

$$L = \begin{bmatrix} L_1 & & \\ & L_2 & & 0 \\ 0 & & \ddots & \\ & & & L_n \end{bmatrix} \text{ and } L^{-1} = \begin{bmatrix} L_1^{-1} & & \\ & L_2^{-1} & & 0 \\ 0 & & \ddots & \\ & & & L_n^{-1} \end{bmatrix}.$$

Define Y to be the column vector $\left[Y_{11}, Y_{12}, \ldots, Y_{1d_1}, \ldots, Y_{n1}, \ldots, Y_{nd_n}\right]^\mathsf{T}$ and y to be the column vector $\left[y_{11}, y_{12}, \ldots, y_{1d_1}, \ldots, y_{n1}, \ldots, y_{nd_n}\right]^\mathsf{T}$. Also, define $\bar{f}$: $\mathbb{R}^{\sum_{i=1}^{n} d_i} \mapsto \mathbb{R}$ such that $\bar{f}(Y) = \sum_{k\in K} a_k \prod_{i=1}^{n}\left(b_{ik} + Y_{ir_{ik}}\right)$. Observe that $\bar{f}(Y) = f(y) = f(L^{-1}Y)$. Clearly $\bar{f}$ is supermodular since it is a conic combination of multilinear terms (see Lemma 3.6 and the following discussion) and concave-extendable over $0 \le Y \le 1$ (see Theorem 2.1 in [25]). It follows from Corollary 3.4 and Remark 3.5 that the concave envelope of $\bar{f}$ over G' is obtained as $\bar{f}^{\mathcal{K}}(Y)$. Therefore, for any permutation π in Π, we obtain a corresponding facet $\bar{f}(0) + \beta^\pi Y$ of the concave envelope in the space of Y variables using expression (6). In particular, for $i \in \{1, \ldots, n\}$ and $j \in \{1, \ldots, d_i\}$, the coefficient β^π_{ij} of variable Y_{ij} is given by

$$\begin{aligned}\beta^\pi_{ij} = \bar{f}\big(E(i,j)\big) - \bar{f}\big(E(i,j) - e(i,j)\big) = f\big(L^{-1}E(i,j)\big)\\ -f\Big(L^{-1}\big(E(i,j) - e(i,j)\big)\Big),\end{aligned}$$

where

$$E(i,j) = \sum_{i'=1}^{n} \sum_{j' | \pi_{i'j'} \le \pi_{ij}} e(i',j') = \sum_{i'=1}^{n} \sum_{j'=w^{ij}_\pi(i')}^{d_{i'}} e(i',j').$$

A direct computation shows that $L^{-1}E(i,j) = \sum_{i'=1}^n e(i', w^{ij}_\pi(i'))$ and $L^{-1}(E(i,j) - e(i,j)) = \sum_{i'=1}^n e(i', w^{ij}_\pi(i')) - e(i,j) + e(i,j+1)$. Since $\bar{f}(0) + \beta^\pi Y = f(0) + \beta^\pi L y$, it follows that the coefficient of y_{ij} in each overestimating hyperplane is $\alpha^\pi_{ij} = \sum_{p=j}^{d_i} \beta^\pi_{ip}$ yielding expression (9).

We now prove (10). To this end, we focus on the term $h_k(y) = a_k \prod_{i \in I_k} (\sum_{j \in T_{ir_{ik}}} y_{ij})$ of h and show that the coefficient $\alpha^{\pi,k}_{ip}$ of variable y_{ip} in its concave envelope is a_k. Then, $h_k(\sum_{i'=1}^n e(i', w^{ip}_\pi(i'))) = a_k$ if $w^{ip}_\pi(i') \le r_{i'k}$ for all $i' \in I_k$, (or equivalently $\pi_{i' r_{i'k}} \le \pi_{i,p}$ for all $i' \in I_k$) and 0 otherwise. Similarly,

$$\begin{aligned} &h_k\left(\sum_{i'=1}^n e\big(i', w^{ip}_\pi(i')\big) - e(i,p) + e(i,p+1)\right)\\ &= \begin{cases} 0 & \pi_{i' r_{i'k}} > \pi_{i,p} \text{ for some } i' \in I_k \backslash i \; or \; p \ge r_{ik} \\ a_k & \text{otherwise.}\end{cases}\end{aligned}$$

It follows that $\beta^{\pi,k}_{ip} = h_k(\sum_{i'=1}^n e(i', w^{ip}_\pi(i'))) - h_k(\sum_{i'=1}^n e(i', w^{ip}_\pi(i')) - e(i,p) + e(i,p+1))$ takes the value a_k when $p = r_{ik}$ and $\pi_{ir_{ik}} = \max_{i' \in I_k} \pi_{i' r_{i'k}}$ or else takes the value 0. In turn, we conclude that $\alpha^{\pi,k}_{ij} = \sum_{p=j}^{d_i} \beta^{\pi,k}_{ip}$ takes value a_k when $j \le r_{ik}$ and $\pi_{ir_{ik}} = \max_{i' \in I_k} \pi_{i' r_{i'k}}$ or else takes the value 0. Simplifying (9), the result follows, □

Note that (9) gives the concave envelope over a lattice family G' of any function that is concave-extendable from the vertices of G' and supermodular in Y_{ir} for $i = 1, \ldots, n$ and $r = 1, \ldots, d_i$ over G'.

Example 3.9 Consider the function $\hat{f}$ of Example 3.7. Applying the result of Theorem 3.8, we obtain for $\pi = (4, 1, 3, 2)$ that

$$
\begin{aligned}
\alpha_{12}^{\pi} &= \beta_{12}^{\pi} = \hat{f}[e(1,2) + e(2,3)] - \hat{f}[e(1,3) + e(2,3)] = 0 \\
\alpha_{11}^{\pi} &= \beta_{11}^{\pi} + \alpha_{12}^{\pi} = 0 + \hat{f}[e(1,1) + e(2,1)] - \hat{f}[e(1,2) + e(2,1)] = 6 \\
\alpha_{22}^{\pi} &= \beta_{22}^{\pi} = \hat{f}[e(1,2) + e(2,2)] - \hat{f}[e(1,2) + e(2,3)] = 2 \\
\alpha_{21}^{\pi} &= \beta_{21}^{\pi} + \alpha_{22}^{\pi} = 2 + \hat{f}[e(1,2) + e(2,1)] - \hat{f}[e(1,2) + e(2,2)] = 5.
\end{aligned}
$$

using the notation used in the proof of Theorem 3.8.

It follows that $6y_{11} + 5y_{21} + 2y_{22} + 4 \geq z$ defines a facet of the hypograph of the concave envelope of $\hat{f}$ over $\hat{G}$. □

Next, we discuss several results in the literature that are special cases of Theorem 3.8. Let $D = \{1, \ldots, \sum_{i=1}^{n} d_i\}$. For $d \in D$, let $i(d) = \min\{i \mid \sum_{i'=1}^{i} d_i \geq d\}$ and $j(d) = d - \sum_{i'=1}^{i(d)-1} d_{i'}$. For an element d of D, the pair $(i(d), j(d))$ is the index of the variable of G that would be in d^{th} position if the variables were ordered as $y_{11}, \ldots, y_{1d_1}, \ldots, y_{n1}, \ldots, y_{nd_n}$.

Corollary 3.10 (Theorem 4 and Theorem 6 in [31]) *Consider the function* $\phi_G^m(y) : G \mapsto \mathbb{R}$ *defined as* $\phi_G^m(y) = \sum_{J \subseteq D, |J|=m} \left[\prod_{d \in J} y_{i(d)j(d)}\right]$, *where* $m \leq n$ *and* G *is of the form* (8). *Define* $\phi_{vert(G)}^m(y)$ *as the restriction of* $\phi_G^m(y)$ *over the vertices of* G. *Then the concave envelope of* $\phi_{vert(G)}^m(y)$ *over* G *is given by:*

$$
\operatorname{conc}_G \phi_{vert(G)}^m(y) = \min\left\{ \sum_{k=m}^{n} \binom{k-1}{m-1} \sum_{j=1}^{d_{i_k}} y_{i_k j} \;\middle|\; \{i_m, \ldots, i_n\} \subseteq \{1, \ldots, n\} \right\}. \tag{11}
$$

Further, if $d_i = 1$ *for all* i, *then* $\operatorname{conc}_G \phi_G^m(y) = \operatorname{conc}_G \phi_{vert(G)}^m(y)$ *for* $y \in G$.

Proof Let $N = \{1, \ldots, n\}$. We may restrict the summation in $\phi_{vert(G)}^m(y)$ to those subsets J of D that are such that, for any d and d' in J, $i(d) \neq i(d')$. This is because if a certain subset J does not satisfy this condition, then $\prod_{d \in J} y_{i(d)j(d)}$ equals zero for every $y \in \text{vert}(G)$. If $d_i = 1$ for all i, this condition holds trivially.

Therefore, we may rewrite

$$
\begin{aligned}
\phi_{vert(G)}^m(y) &= \sum_{U = \{i_1, \ldots, i_m\} \subseteq N} \sum_{j_1=1}^{d_{i_1}} \sum_{j_2=1}^{d_{i_2}} \cdots \sum_{j_m=1}^{d_{i_m}} y_{i_1 j_1} y_{i_2 j_2} \ldots y_{i_m j_m} \\
&= \sum_{U \subseteq N, |U|=m} \left[\prod_{i \in U} \sum_{j=1}^{d_i} y_{ij} \right].
\end{aligned}
$$

The concave envelope of $\phi^m_{vert(G)}(y)$ is of the form (10) derived in Theorem 3.8:

$$\sum_{U\subseteq N, |U|=m} \min_{i\in U} \left(\sum_{j=1}^{d_i} y_{ij}\right) = \sum_{U\subseteq N, |U|=m} \min_{i\in U} (S_i)$$

where $S_i = \sum_{j=1}^{d_i} y_{ij}$ and $S = (S_1, \ldots, S_n)$. Let $\{\pi_1, \ldots, \pi_n\}$ be the permutation of $\{1, \ldots, n\}$ that sorts S_i in increasing order, i.e., $S_{\pi_1} \le S_{\pi_2} \le \cdots \le S_{\pi_n}$. Since S_{π_p} is the p^{th} smallest among all Ss, it will be minimum in all subsets U that do not contain $\{\pi_1, \pi_2, \ldots, \pi_{p-1}\}$. Observe that there are $\binom{n-p}{m-1}$ such sets when $1 \le p \le n-m+1$ and 0 otherwise. It follows that the concave envelope is given by

$$\min_{\pi\in\Pi_n} \sum_{p=1}^{n-m+1} \binom{n-p}{m-1} S_{\pi_p} = \min_{\pi\in\Pi_n} \sum_{k=m}^{n} \binom{k-1}{m-1} S_{\pi_{n-k+1}}, \tag{12}$$

where Π_n is the set of permutations of $\{1, \ldots, n\}$ and $k = n - p + 1$. Expression (11) follows by noticing that the underestimating affine function does not depend on the entire permutation but only on the subset $\{\pi_1, \ldots, \pi_{n-m+1}\}$. Finally, if $d_i = 1$ for all i, then $\phi^m_G(y)$ is concave-extendable from the vertices of G and therefore $\text{conc}_G\, \phi^m_G(y) = \text{conc}_G\, \phi^m_{\text{vert}(G)}(y)$ for $y \in G$. □

Note that in general, $\text{conc}_G\, \phi^m_G(y)$ and $\text{conc}_G\, \phi^m_{\text{vert}(G)}(y)$ are different when d_i is not equal to 1 for some i. For example, consider xy over $\{(x, y) \in \mathbb{R}^2 \mid x + y \le 1, x, y \ge 0\}$. The function in Corollary 3.10 can be reduced to this case by setting $n = 1, d_1 = 2$, and $m = 2$. It can be argued easily that the concave envelope is $\frac{xy}{x+y}$ if $x + y > 0$ and 0 if $(x, y) = (0, 0)$; see Example 2 in [18]. This function is non-polyhedral and not concave-extendable from vertices.

Corollary 3.11 *([22]) Let $N = \{1, \ldots, n\}$ and $\Gamma = 2^N$. The concave envelope of $\phi(x) = \sum_{T\subseteq\Gamma} a_T \prod_{i\in T} x_i$, where $a_T \ge 0$ for all $T \subseteq \Gamma$ over the unit hypercube is given by:*

$$\sum_{T\subseteq\Gamma} a_T \min_{i\in T}\{x_i\}.$$

Proof Follows directly from Theorem 3.8 by setting $d_i = 1$ for all i. □

Corollary 3.12 (Theorem 1 in [27]) *Consider the set:*

$$X = \left\{ (x, t) \in \mathbb{R}^{n+1} \;\middle|\; t \le \sum_{1\le i<j\le n} q_{ij} x_i x_j, x \in \{0, 1\}^n \right\}$$

where $q_{ij} \geq 0$ *for* $i, j = 1, \ldots, n$ *and* $q_{ij} = q_{ji}$. *Then,*

$$\mathrm{conv}(X) = \left\{ (x,t) \in \mathbb{R}^{n+1} \;\middle|\; t \leq \sum_{i=2}^{n} \sum_{j=1}^{i-1} q_{\pi(j)\pi(i)} x_{\pi(i)},\, x \in [0,1]^n \;\forall \pi \in \Pi_n \right\}$$

where Π_n *is the set of permutations of* $\{1, \ldots, n\}$.

Proof Using Corollary 3.11, we obtain that the concave envelope of $\sum_{1 \leq i < j \leq n} q_{ij} x_i x_j$ over $[0,1]^n$ is given by $\sum_{1 \leq i < j \leq n} q_{ij} \min\{x_i, x_j\}$. For any permutation $\pi \in \Pi_n$, we then write

$$\sum_{1 \leq i < j \leq n} q_{ij} \min\{x_i, x_j\} = \sum_{i=2}^{n} \sum_{j=1}^{i-1} q_{\pi(j)\pi(i)} \min\{x_{\pi(j)}, x_{\pi(i)}\} \leq \sum_{i=2}^{n} \sum_{j=1}^{i-1} q_{\pi(j)\pi(i)} x_{\pi(i)},$$

where the inequality holds since $q_{ij} \geq 0$ and $x \geq 0$. The result then follows by observing that the above inequality is satisfied at equality for any permutation π satisfying $x_{\pi(1)} \geq x_{\pi(2)} \geq \cdots \geq x_{\pi(n)}$. □

Observe that the result of Corollary 3.12 can be trivially extended to allow terms of the form $q_{ii} x_i^2$ where $q_{ii} > 0$ since $q_{ii} x_i^2$ can be replaced with $q_{ii} x_i$ before the envelope is constructed. The supermodularity of the resulting function follows directly.

Corollary 3.13 (Theorem 1 in [5]) *The concave envelope of* $m(x) = \prod_{i=1}^{n} x_i$ *over* $\prod_{i=1}^{n} [L_i, U_i]$, *where* $U_i > L_i \geq 0$ *for all i, is given by:*

$$\min_{\pi \in \Pi_n} \sum_{i=1}^{n} \left(\left(\prod_{j | \pi(j) < \pi(i)} U_j \right) \left(\prod_{j | \pi(j) > \pi(i)} L_j \right) (x_i - L_i) \right) \tag{13}$$

where Π_n *is the set of permutations of* $\{1, \ldots, n\}$.

Proof Clearly, $m(x)$ is supermodular and concave-extendable from $\prod_{i=1}^{n} \{L_i, U_i\}$. Using Transformation (1), we define $m'(x') = m(x)$ where $x' = T(x)$, i.e., $m'(x') = \prod_{i=1}^{n} \left(L_i + (U_i - L_i) x'_i \right)$. This transformation does not alter supermodularity or concave-extendability. Therefore, it follows that the concave envelope can be constructed as in Theorem 3.3. Then, following (6), the concave envelope of m' over $[0,1]^n$ is given by

$$\min_{\pi \in \Pi} \sum_{i=1}^{n} \left(\left(\prod_{j | \pi(j) \leq \pi(i)} U_j \right) \left(\prod_{j | \pi(j) > \pi(i)} L_j \right) - \left(\prod_{j | \pi(j) < \pi(i)} U_j \right) \right.$$
$$\left. \times \left(\prod_{j | \pi(j) \geq \pi(i)} L_j \right) \right) x'_i.$$

Factoring out $(\prod_{j | \pi(j) < \pi(i)} U_j)(\prod_{j | \pi(j) > \pi(i)} L_j)$ and substituting $x'_i = \frac{x_i - L_i}{U_i - L_i}$, we obtain (13). □

Linear transformations can often be used to make functions supermodular. For example, Theorem 3.8 uses a transformation that maps G to S and uses supermodularity of the corresponding transformed function. Another useful transformation, which we refer to as *switching*, involves transforming a variable from x to $1 - x$. For a given $x \in \mathbb{R}^n$ and $T \subseteq \{1, \ldots, n\}$, we denote by $x(T)$ the vector in $\mathbb{R}^n$ obtained as $x(T)_i = 1 - x_i$ if $i \in T$ and $x(T)_i = x_i$ otherwise. Further, for a function $f : \{0, 1\}^n \mapsto \mathbb{R}$ we define $f(T) : \{0, 1\}^n \mapsto \mathbb{R}$ such that $f(T)(x) = f(x(T))$. It is easy to verify that $\mathrm{conc}(f)(x) = \mathrm{conc}(f(T))(x(T))$. Let $\mathcal{S} = \{P_1, \ldots, P_k\}$ be a polyhedral subdivision of $[0, 1]^n$, where each P_i is a polyhedron. Then for each i, define $P_i(T) = \{x \mid x(T) \in P_i\}$ and let $\mathcal{S}(T) = \{P_1(T), \ldots, P_k(T)\}$ be the corresponding polyhedral subdivision of $[0, 1]^n$.

As we discussed in Sect. 1, functions of the type $f(a_0 + \sum_{i=1}^n a_i x_i)$ appear commonly as an intermediate step in the construction of relaxations of factorable programs. Typically, the weakening step of substituting $a_0 + \sum_{i=1}^n a_i x_i$ with a new variable y is performed before the actual relaxation is obtained. In the following corollary, we show that such a step is unnecessary by deriving the concave envelope of $f(a_0 + \sum_{i=1}^n a_i x_i)$ over the unit hypercube. We show later in Example 3.23 that the relaxation obtained by using Corollary 3.14 has the potential to significantly improve the relaxations used in factorable programming.

Corollary 3.14 *Let $g(x) = f(L(x)) : [0, 1]^n \mapsto \mathbb{R}$ where f is convex and $L(x) = a_0 + \sum_{i=1}^n a_i x_i$. Let $T = \{i \mid a_i < 0\}$. Then, $g(T)(x)$ is concave-extendable from $\{0, 1\}^n$ and supermodular. The concave envelope of $g(x)$ is determined by $\mathcal{K}(T)$.*

Proof The convexity of g and, hence, of $g(T)$ follows from the assumptions in the corollary. Therefore, $g(T)$ is concave-extendable from $\{0, 1\}^n$. First assume that $T = \emptyset$. Let $x', x'' \in [0, 1]^n$ and assume without loss of generality that $L(x') \leq L(x'')$. Then, $L(x' \wedge x'') \leq L(x') \leq L(x'') \leq L(x' \vee x'')$. Further, $L(x') + L(x'') = L(x' \wedge x'') + L(x' \vee x'')$ since $L(\cdot)$ is affine. Using Hardy-Littlewood-Polyá/Karamata's inequality, we obtain that $f(L(x')) + f(L(x'')) \leq f(L(x' \wedge x'')) + f(L(x' \vee x''))$ since the sequence $(L(x' \wedge x''), L(x' \vee x''))$ is majorized by $(L(x'), L(x''))$ and f is convex; see Section 3.17 in [13]. The result then follows from Theorem 3.3. Now, assume that $T \neq \emptyset$. Applying the corollary to $g(T)$, we conclude that the concave envelope of $g(T)$ is defined by $\mathcal{K}$. Since $\mathrm{conc}(g)(x) = \mathrm{conc}(g(T))(x(T))$, we conclude that $\mathrm{conc}(g)(x)$ is described by the triangulation $\mathcal{K}(T)$. □

The following result is a direct consequence of Theorem 3.3 that is well-suited for certain disjunctive applications.

Corollary 3.15 *Consider a function $f(y, x) = f(y, x_1, \ldots, x_n) : \{0, 1\}^{n+1} \mapsto \mathbb{R}$ and define $f_0(x) := f(0, x)$ and $f_1(x) := f(1, x)$. Then, $f(y, x)$ is supermodular if and only if f_0 and f_1 are supermodular, and $f_1(x) - f_0(x)$ is a non-decreasing function of x. Assume f_0 and f_1 are supermodular and $f_1(x) - f_0(x)$ is monotone. Then, the concave envelope of f over $[0, 1]^{n+1}$ is described by $\mathcal{K}(T)$ where $T = \emptyset$ if $f_1(x) - f_0(x)$ is non-decreasing and $T = \{1\}$ if $f_1(x) - f_0(x)$ is non-increasing.*

Proof For the direct implication, note that f_0 and f_1 have to be supermodular if f is supermodular. Further, for any $x' \geq x$, $f(1, x) + f(0, x') \leq f(1, x') + f(0, x)$ as f

is supermodular and $x \vee x' = x'$ and $x \wedge x' = x$. This shows that $f_1(x) - f_0(x)$ is non-decreasing. For the reverse implication, consider two arbitrary points (y', x') and (y'', x'') in $\{0, 1\}^{n+1}$. If $y' = y''$, then the supermodularity of f_0 and f_1 implies that $f(y', x') + f(y'', x'') \le f((y', x') \wedge (y'', x'')) + f((y', x') \vee (y'', x''))$. Therefore, we assume without loss of generality that $y' = 0$ and $y'' = 1$. Then,

$$\begin{aligned} f(y', x') + f(y'', x'') &= f_0(x') + f_0(x'') + f_1(x'') - f_0(x'') \\ &\le f_0(x' \wedge x'') + f_0(x' \vee x'') + f_1(x' \vee x'') - f_0(x' \vee x'') \\ &= f_0(x' \wedge x'') + f_1(x' \vee x'') \\ &= f((y', x') \wedge (y'', x'')) + f((y', x') \vee (y'', x'')), \end{aligned}$$

where the first inequality holds because f_0 is supermodular and because $f_1(x) - f_0(x)$ is non-decreasing and the last equality holds because $y' \wedge y'' = 0$ and $y' \vee y'' = 1$. The rest of the result follows from Theorem 3.3 after switching y if $f_1(x) - f_0(x)$ is non-increasing. □

In the statement of Corollary 3.15, we emphasize that the polyhedral subdivision $\mathcal{K}(\{1\})$ is obtained from Kuhn's triangulation by switching the first variable of the function f, i.e., it is obtained by switching the variable y and not the variable x_1.

Corollary 3.15 also applies to certain nonlinear functions that do not intrinsically exhibit a disjunctive structure. Consider $f(y, x) = f_0(x) + y(f_1(x) - f_0(x))$. When x is fixed, the function is linear in y. Therefore, it suffices to restrict $y \in \{0, 1\}$ when building the envelope of f. Then, Corollary 3.15 yields the concave envelope of $f(y, x)$ when $f_0(\cdot)$ and $f_1(\cdot)$ are supermodular and concave-extendable from vertices and $f_1(\cdot) - f_0(\cdot)$ is non-decreasing. In fact, under such assumptions, the proof of Corollary 3.15 can be easily generalized to show that $f(y, x) = f_0(x) + y(f_1(x) - f_0(x))$ is supermodular over $[0, 1]^{n+1}$. Let (y', x') and (y'', x'') belong to $[0, 1]^{n+1}$ and assume that $0 \le y' \le y'' \le 1$. Then,

$$\begin{aligned} f(y', x') + f(y'', x'') &= f(y', x') + f(y', x'') + f(y'', x'') - f(y', x'') \\ &\le f(y', x' \vee x'') + f(y', x' \wedge x'') + (y'' - y')(f_1(x'') - f_0(x'')) \\ &\le f(y', x' \vee x'') + f(y', x' \wedge x'') + (y'' - y')(f_1(x' \vee x'') - f_0(x' \vee x'')) \\ &= f(y', x' \vee x'') + f(y', x' \wedge x'') + f(y'', x' \vee x'') - f(y', x' \vee x'') \\ &= f(y'', x' \vee x'') + f(y', x' \wedge x''), \end{aligned}$$

where the first inequality follows from the supermodularity of $f_0(x)$ and $f_1(x)$ and the definition of $f(y, x)$ while the second inequality follows since $y'' \ge y'$, $f_1(x) - f_0(x)$ is non-decreasing, and $x' \vee x'' \ge x''$. More generally, for a fixed $y' \in [0, 1]$, the concave-extendability of $f(y', x)$ follows from [36]. Therefore, given y^L and y^U such that $0 \le y^L \le y^U \le 1$, Theorem 3.3 can be used to develop the concave envelope of $f(y, x)$ over $\left[y^L, y^U\right] \times [0, 1]^n$.

In Corollary 3.16, we particularize the result of Corollary 3.15 to situations where $f(y, x) = yg(x)$. This results therefore applies to functions such as $\frac{y}{1+\sum_{i=1}^n x_i}$ and $y \log(1 + \sum_{i=1}^n x_i)$. It also applies to functions such as $\frac{y}{y+\sum_{i=1}^n x_i}$ and $y \log(y + \sum_{i=1}^n x_i)$ if one restricts their domain to those points in the unit hypercube satisfying $y + \sum_{i=1}^n x_i \ge 1$. This is a natural restriction when the variables y and x_i are binary;

see [6] for applications in consistent biclustering problems. The supermodularity of these functions for a fixed y follows from Corollary 3.14 and, therefore, Corollary 3.15 applies.

Corollary 3.16 *Consider a function $f(y,x) = f(y,x_1,\dots,x_n) : \{0,1\}^{n+1} \mapsto \mathbb{R}$, where $f(0,x) = 0$ and $f(1,x) = f_1(x)$. Assume $f_1(x)$ is non-increasing and supermodular. Then, $\operatorname{conc}_{[0,1]^{n+1}}(f)$ is described by $\mathcal{K}(\{1\})$. Further, let $W = \{(y,x) \in [0,1]^{n+1} \mid y + \sum_{i=1}^n x_i \geq 1\}$. Then, for any $(y,x) \in W$, $\operatorname{conc}_W(f)(y,x) = \operatorname{conc}_{[0,1]^{n+1}}(f)(y,x)$.*

Proof It follows from Corollary 3.15 that $\operatorname{conc}_{[0,1]^{n+1}}(f)(y,x)$ is described by $\mathcal{K}(\{1\})$. Since $W \subseteq [0,1]^{n+1}$, $\operatorname{conc}_{[0,1]^{n+1}}(f)(y,x) \geq \operatorname{conc}_W(f)(y,x)$. Observe that $\operatorname{conc}_{[0,1]^{n+1}}(f)(y,x)$ is linear over $Y = \{(y,x) \mid 0 \leq x_1,\dots,x_n \leq 1-y \leq 1\}$. However, Y is obtained as a union of simplices in $\mathcal{K}(\{1\})$. In particular, if K_π is the simplex associated with permutation π (after replacing y with $1-\bar{y}$), then $Y = \bigcup_{\pi\in\Pi'} K_\pi$, where Π' is the set of permutations of $\{1,\dots,n+1\}$ that are restricted to have 1 as the first element. Let $W' = \operatorname{cl}([0,1]^{n+1}\setminus Y)$. Because the vertices of Y are $(1,0)$ and $(0,\sum_{j\in J} e_j)$ for $J \subseteq N$, then it can be verified that $\operatorname{vert}(W) = \operatorname{vert}(W')$. Since W is convex, it follows that $W = \operatorname{conv}(W')$. Let $W'' = Y \cap \{(y,x) \mid y + \sum_{i=1}^n x_i \geq 1\}$. It is easy to see that W'' is the convex hull of $\left\{(0,x) \in [0,1]^{n+1} \mid \sum_{i=1}^n x_i \geq 1\right\}$ and $(1,0)$. Therefore, W'' has binary extreme points. It can now be easily verified that, for any $(y,x) \in W$, $\operatorname{conc}_{[0,1]^{n+1}}(f)(y,x)$ is a feasible solution to $D(y,x)$. Therefore, $\operatorname{conc}_{[0,1]^{n+1}}(f)(y,x) \leq \operatorname{conc}_W(f)(y,x)$. It follows that, for any $(y,x) \in W$, $\operatorname{conc}_W(f)(y,x) = \operatorname{conc}_{[0,1]^{n+1}}(f)(y,x)$. $\square$

Corollary 3.16 can also be derived as a consequence of Theorem 3.3 applied to $f_1(x)$ along with Theorem 4.1, which will be proven later and describes the concave envelope of $yg(x)$ under more general conditions.

Example 3.17 Let $g(z)$ be a convex non-increasing function and define $f(y,x) = yg(\sum_{i=1}^n x_i)$ where we assume that $x \in \{0,1\}^n$ and $y \in [0,1]$. It follows from its definition that g is concave-extendable from the vertices. Further, $g(\sum_{i=1}^n x_i)$ is supermodular by Corollary 3.14. By definition, it is concave-extendable from the vertices. The concave envelope is therefore given by Corollary 3.16. In particular, if Π_n is the set of permutations of $\{1,\dots,n\}$ then $\mathcal{S} = \bigcup_{\pi\in\Pi_n, 0\leq m\leq n} S(\pi,m)$ gives the polyhedral subdivision $\mathcal{K}(\{1\})$ of $[0,1]^n$ that defines the concave envelope of $f(y,x)$ where

$$S(\pi,m) = \left\{(y,x) \in \mathbb{R}^{n+1} \;\middle|\; x_{\pi(0)} \geq x_{\pi(1)} \geq \dots \geq x_{\pi(m)} \geq 1-y \geq x_{\pi(m+1)} \geq \dots \geq x_{\pi(n)} \geq x_{\pi(n+1)}\right\}$$

and we assume $x_{\pi(0)} = 1$ and $x_{\pi(n+1)} = 0$. Further, the concave envelope of $f(y,x)$ over $[0,1]^{n+1}$ is $\min_{\pi\in\Pi_n, 0\leq m\leq n} h^{S(\pi,m)}(y,x)$ where $h^{S(\pi,m)}(y,x)$ is the facet of

$\text{conc}_{[0,1]^{n+1}} f(y, x)$ that is tight over $S(\pi, m)$ and can be computed using (6) to be:

$$h^{S(\pi,m)}(y, x) = g(0) + \sum_{i=1}^{m}(g(i) - g(i-1))x_{\pi(i)} - g(m)(1 - y).$$

The restriction of the concave envelope to $W = \{(y, x) \in [0, 1]^{n+1} \mid y+\sum_{i=1}^{n} x_i \geq 1\}$ gives the concave envelope over W as proven in Corollary 3.16. As an illustration, consider $f(y, x) = \frac{y}{y+\sum_{i=1}^{n} x_i}$ where $(y, x) \in W \cap \{0, 1\}^{n+1}$. Then, the concave envelope of $f(y, x)$ over W is given by:

$$\min_{\pi\in\Pi_n, 0\leq m\leq n}\left(1 - \sum_{i=1}^{m}\frac{1}{i(i+1)}x_{\pi(i)} - \frac{1}{m+1}(1 - y)\right). \tag{14}$$

This fractional function appears in the formulation of consistent biclustering problems [6]. The standard factorable relaxation introduces $z = \frac{1}{y+\sum_{i=1}^{n} x_i}$ and $w = yz$ to represent $\frac{y}{y+\sum_{i=1}^{n} x_i}$. Let $u(x, y) = y + \sum_{i=1}^{n} x_i$. Then, $z = \frac{1}{u(x,y)}$ is relaxed over $u(x, y) \in [1, n+1]$ as $\frac{1}{u(x,y)} \leq z \leq \frac{n+2}{n+1} - \frac{u(x,y)}{n+1}$. Finally, $w \leq \min\left\{y, \frac{1}{n+1}y + z - \frac{1}{n+1}\right\}$ which, equivalently, yields $w \leq \min\left\{y, \frac{1}{n+1}y - \frac{1}{n+1}u(x, y) + 1\right\}$ as $z \leq \frac{n+2}{n+1} - \frac{u(x,y)}{n+1}$. The same relaxation is obtained if the concave envelope of $\frac{y}{u(x,y)}$ is constructed directly over $[0, 1] \times [1, n+1]$; see [38]. Clearly, the concave envelope developed in (14) is tight when $y = 1$ and $x_i = 1$ for all $i \in I$, where $\emptyset \subsetneq I \subsetneq N$ (as it evaluates to $1 - \sum_{i=1}^{|I|} \frac{1}{i(i+1)} = \frac{1}{1+|I|}$) whereas the factorable relaxation is not tight at these points (as it evaluates to $\frac{n+2}{n+1} - \frac{|I|+1}{n+1} = \frac{n+1-|I|}{n+1}$).

Corollary 3.16 exemplifies a situation where restricting attention to $y+\sum_{i=1}^{n} x_i \geq 1$ does not result in a substantial change in the triangulation. This may appear surprising when one considers that the origin is a vertex of every simplex in Kuhn's triangulation. However, a more careful observation reveals that removing the origin does not have a significant impact in Corollary 3.16 because the triangulation is given after switching y, i.e., it is $\mathcal{K}(\{1\})$ and not $\mathcal{K}$.

When the concave envelope is determined by Kuhn's triangulation, the envelope will typically change drastically if the origin is removed from the underlying region. We next describe a situation that illustrates this phenomenon. Corollary 3.14 shows that if $f(\cdot)$ is a convex function then $f\left(\sum_{i=1}^{n} x_i\right)$ is supermodular and concave-extendable from vertices and, therefore, its concave envelope is defined by Kuhn's triangulation. In various situations, it will be useful to construct the concave envelope over $\sum_{i=1}^{n} x_i \geq 1$, a situation where the origin is no longer an extreme point of the underlying polytope. Next, we study this situation by considering the slightly more general case where we seek to determine the concave envelope of $f\left(\sum_{i=1}^{n} x_i\right)$ assuming that $f(\cdot)$ is convex over $[1, n]$ but $\frac{(n-1)}{n} f(0) + \frac{1}{n} f(n) < f(1)$. In this case, f is nonconvex over $[0, n]$ because its value at 0 is below what is required for convexity.

We first introduce a polyhedral subdivision of $[0, 1]^n$ that we will prove in Theorem 3.18 yields the concave envelope of f. For $k = 0, \ldots, n$, we define Π_n^k to be the set of permutations of exactly k elements of $\{1,\ldots,n\}$. In other words, π belongs to Π_n^k if $\pi : \{1,\ldots,k\} \to \{1,\ldots,n\}$ and $\pi(i) \neq \pi(j)$ for $i \neq j$. For such a permutation, we write that $|\pi| = k$ and use the notation $i \notin \pi$ to signify that $i \notin \{\pi(1), \pi(2), \ldots, \pi(k)\}$. We also use the notation $\tilde{\Pi} = \bigcup_{k=0}^{\max(n-2,0)} \Pi_n^k$. For $\pi \in \tilde{\Pi}$, we define

$$S_\pi = \left\{ (x_1,\ldots,x_n) \in \mathbb{R}^n \;\middle|\; \begin{array}{l} 0 = x_{\pi(0)} \leq \cdots \leq x_{\pi(|\pi|)} \leq 1 \\ \sum_{i\notin\pi} x_i \geq 1 + (n-|\pi|-1)x_{\pi(|\pi|)} \\ \sum_{i\notin\pi} x_i \leq 1 + (n-|\pi|-1)x_j, \forall j \notin \pi \end{array} \right\},$$

where $\pi(i)$ is assumed to be zero if $i \leq 0$. Let $\Delta = \left\{x \in [0,1]^n \mid \sum_{i=1}^n x_i \leq 1\right\}$. Next, we define $\mathcal{K}^{-0} = \{\Delta, \bigcup_{\pi\in\tilde{\Pi}} S_\pi\}$. We will prove in Theorem 3.18 that $\mathcal{K}^{-0}$ is a polyhedral subdivision of $[0,1]^n$. Here, we argue the weaker result that $\mathcal{K}^{-0}$ covers $[0,1]^n$ by constructing, for each $x \in [0,1]^n \setminus \Delta$, a permutation $\bar{\pi} \in \tilde{\Pi}$ for which $x \in S_{\bar{\pi}}$. For an arbitrary $x \in [0,1]^n \setminus \Delta$, we first sort the components of x in increasing order, thereby obtaining a permutation π of $\{1,\ldots,n\}$ for which $0 \leq x_{\pi(1)} \leq \cdots \leq x_{\pi(n)} \leq 1$. For $j = 0,\ldots,n-1$, define $C(j) = \sum_{i=j+1}^n (x_{\pi(i)} - x_{\pi(j)}) - (1 - x_{\pi(j)})$. Clearly, $C(j)$ is decreasing in j as $C(j) - C(j-1) = (n-j)\left(x_{\pi(j-1)} - x_{\pi(j)}\right)$. Further, since $x \in [0,1]^n \setminus \Delta$, it follows that $C(0) = \sum_{i=1}^n x_{\pi(i)} - 1 > 0$ and $C(n-1) = x_{\pi(n)} - 1 \leq 0$. Define now $\bar{j} = \max\{j \mid C(j) > 0\}$. Since $C(\bar{j}) > 0$ and $C(s) \leq 0$ for $s = \bar{j}+1,\ldots,n$, it is easy to see that $x \in S_{\bar{\pi}}$ where $\bar{\pi}$ is the permutation of $\{1,\ldots,\bar{j}\}$ such that $\bar{\pi}(t) = \pi(t)$ for $t = 1,\ldots,\bar{j}$.

It can be verified that, for all $\pi \in \tilde{\Pi}$, S_π is a simplex with $\mathrm{vol}(S_\pi) = \frac{n-1-|\pi|}{n!}$. The number of simplices in this decomposition is $1 + \frac{n!}{2!} + \cdots + \frac{n!}{n!}$ which can be overestimated and also asymptotically converges to $(e-2)n! + 1$ as n becomes large. Further, the vertices of S_π are e_i for all $i \notin \pi$, $\sum_{i\notin\pi} e_i + \sum_{j=|\pi|+1-r}^{|\pi|} e_{\pi(j)}$ for $r = 0,\ldots,|\pi|$. Given a function f, we define

$$h_\Delta(x) = (f(1) - f(0)) \sum_{i=1}^n x_i + f(0),$$

to be the interpolation of f over the vertices of Δ and, for each $\pi \in \tilde{\Pi}$,

$$h_\pi(x) = \sum_{i=1}^{|\pi|} \big(f(n-i+1) - f(n-i)\big) x_{\pi(i)} + \frac{f(n-|\pi|) - f(1)}{n-|\pi|-1} \sum_{i\notin\pi} x_i + \frac{(n-|\pi|)f(1) - f(n-|\pi|)}{n-|\pi|-1}$$

to be the interpolation of f over the vertices of S_π. Observe in particular that $h_\pi(x) = f(x)$ for all extreme points x of S_π.

Theorem 3.18 *Let $g(x) = f\left(\sum_{i=1}^{n} x_i\right)$ where $f(z)$ is a convex function over $z \in [1, n]$. Assume that g is concave-extendable from $\{0, 1\}^n$ and that $(n-1)f(0) \leq nf(1) - f(n)$. Then, $\text{conc}_{[0,1]^n}(f)$ is described by the polyhedral subdivision $\mathcal{K}^{-0}$ and*

$$\operatorname*{conc}_{[0,1]^n} f(x) = \min\left\{h_\Delta(x), \min_{\pi\in\tilde{\Pi}} h_\pi(x)\right\}.$$

Proof Consider the following sets

$$W_1 = \left\{ (x_1, \dots, x_n) \;\middle|\; \begin{array}{l} x_{\pi(0)} = \cdots = x_{\pi(|\pi|)} = 0 \\ \sum_{i\notin\pi} x_i \geq 1 \\ \sum_{i\notin\pi} x_i \leq 1 + (n - |\pi| - 1) \min_{i\notin\pi} x_i \end{array} \right\}$$

and

$$W_2 = \left\{ (x_1, \dots, x_n) \;\middle|\; \begin{array}{l} 0 = x_{\pi(0)} \leq \cdots \leq x_{\pi(|\pi|-1)} \leq 1 \\ x_{\pi(|\pi|)} = 1 \\ x_i = 1 \;\forall i \notin \pi \end{array} \right\}.$$

After introducing variables $\bar{x}_i = 1 - x_i$ for $i \notin \pi$, W_1 and W_2 are orthogonal sets. It is easy to verify using Theorem 1 in [37] that $S_\pi = \text{conv}(W_1 \cup W_2)$. Further, h_π is tight at all the extreme points of W_1 and W_2. Therefore, if we prove that $h_\pi(x) \geq f(x)$, it will follow from Theorem 2.4 that h_π defines the concave envelope of $f(x)$ over S_π. First, we verify that $f(0) \leq h_\pi(0)$. Since f is convex, $\frac{(n-|\pi|)f(1) - f(n-|\pi|)}{n-|\pi|-1}$ is increasing in $|\pi|$ for $|\pi| \leq n-2$. Therefore, the minimum value is attained when $|\pi| = 0$. However, by assumption $(n-1)f(0) \leq nf(1) - f(n)$, therefore, $f(0) \leq h_\pi(0)$. Without loss of generality, we may assume that $\pi = (1, \dots, |\pi|)$. Then, by convexity of f, it follows that

$$\frac{f(n - |\pi|) - f(1)}{n - |\pi| - 1} \leq f(n - |\pi| + 1) - f(n - |\pi|) \leq \cdots \leq f(n) - f(n-1).$$

Therefore, $h_\pi(x)$ may be rewritten as: $c_0 + \sum_{i=1}^{n} c_i \sum_{j\geq i} x_j$ where $c_i \geq 0$ for all $i \in \{1, \dots, n\}$. In particular, it is easy to verify that $\min\{h_\pi(x) \mid \sum_{i=1}^{n} x_i = y\} = r(y) = c_0 + \sum_{i=1}^{n} c_i \max\{i - n + y, 0\}$, where $r(y) = f(y)$ for $y \in \{1, n-|\pi|, \dots, n\}$. Since, $r(y)$ is linear between consecutive integer values, it follows that $r(y) \geq f(y)$. In other words, $h_\pi(x) \geq f\left(\sum_{i=1}^{n} x_i\right)$. If $f(\cdot)$ is a strictly convex function for $i \in [1, n]$ and $(n-1)f(0) < nf(1) - f(n)$ then it is easy to verify that this inequality is strict when $x \in \{0, 1\}^n \setminus (\text{vert}(W_1) \cup \text{vert}(W_2))$. Therefore, it follows that $\Delta \cup \bigcup_{\pi\in\Pi} S_\pi$ is a polyhedral subdivision of $[0, 1]^n$ that defines $\text{conc}_{[0,1]^n} f$. □

Example 3.19 Consider the function $f : \{0, 1\}^5 \to \mathbb{R}$ where $f(x) = 3 - \log_2(\sum_{i=1}^{5} x_i)$ when $x \neq 0$ and $f(x) = 0$ when $x = 0$. Clearly, this function satisfies the assumptions of Theorem 3.18. We now derive two facets of $\mathrm{conc}_{[0,1]^5}(f)$. For $\pi^a \in \Pi_5^0$, we have

$$S_{\pi^a} = \Big\{x \in \mathbb{R}^5 \mid x_1 + x_2 + x_3 + x_4 + x_5 \geq 1, x_1 + x_2 + x_3 + x_4 + x_5 \leq 1 + 4x_j, \\ \forall j = 1, \ldots, 5\Big\}.$$

The corresponding facet of $\mathrm{conc}_{[0,1]^5}(f)$ is given by

$$\begin{aligned} h_{\pi^a}(x) &= \frac{f(5) - f(1)}{4} \sum_{i=1}^{5} x_i + \frac{5f(1) - f(5)}{4} \\ &= -\frac{\log_2(5)}{4}(x_1 + x_2 + x_3 + x_4 + x_5) + \frac{\log_2(5)}{4} + 3. \end{aligned}$$

For $\pi^b \in \Pi_5^2$ with $\pi^b(1) = 1, \pi^b(2) = 2$ we have

$$S_\pi = \Big\{x \in \mathbb{R}^5 \mid 0 \leq x_1 \leq x_2 \leq 1, x_3 + x_4 + x_5 \geq 1 + 2x_2, x_3 + x_4 + x_5 \leq 1 + 2x_j, \\ \forall j = 3, \ldots, 5\Big\}.$$

The corresponding facet of $\mathrm{conc}_{[0,1]^5}(f)$ is given by

$$\begin{aligned} h_{\pi^b}(x) = (f(5) - f(4))x_1 + (f(4) - f(3))x_2 + \frac{f(3) - f(1)}{2} \sum_{i=3}^{5} x_i \\ + \frac{3f(1) - f(3)}{2} = -(\log_2(5) - 2)x_1 - (2 - \log_2(3))x_2 \\ - \frac{\log_2(3)}{2}(x_3 + x_4 + x_5) + \frac{\log_2(3)}{2} + 3. \end{aligned}$$

□

Example 3.20 Let $g(x) = \frac{1}{\sum_{i=1}^n x_i}$ where $x \in W \cap \{0, 1\}^n$ and $W := \{x \in [0, 1]^n \mid \sum_{i=1}^n x_i \geq 1\}$. Define $g(0) = 0$. Since the proof of Theorem 3.18 and the preceding dicussion show that $S_\pi \subseteq W \subseteq [0, 1]^n$, it follows that $\mathrm{conc}_{S_\pi}\, g(x) \leq \mathrm{conc}_W\, g(x) \leq \mathrm{conc}_{[0,1]^n}\, g(x)$. For each $x \in W$, there exists π such that $x \in S_\pi$ and, by Theorem 3.18, $\mathrm{conc}_{S_\pi}\, g(x) = \mathrm{conc}_{[0,1]^n}\, g(x)$; see also Remark 3.5. Therefore, $\max_{\pi \in \Pi} \mathrm{conc}_{S_\pi}\, g(x) = \mathrm{conc}_W\, g(x)$. Incidentally, the same concave envelope is also obtained if $x_i \in [0, 1]$ since $g(x)$ is a convex function and, therefore, concave-extendable from the vertices. □

Although it is in general NP-Hard to identify supermodular functions [9], some special classes of functions can be easily identified to be supermodular. It is well-known, for instance, that the function

$$\sum_{J \subseteq N} a_J \prod_{j \in J} x_i + \sum_{I \subseteq N} b_I \prod_{i \in I} (1 - x_i) \tag{15}$$

is supermodular if a_J, b_I are nonnegative for all $I, J \subseteq N$; see also Lemma 3.6 and the following discussion. A multilinear function is called *unimodular* if by switching variables x_i in some subset K of N, it can be recast into the form (15). It is shown in [9] that unimodular functions can be recognized by solving a linear programming problem. This linear program yields a polynomial time recognition technique for unimodular functions. Combined with Theorem 3.3, this allows construction of concave envelopes of many multilinear functions. In certain cases, it is easy to recognize that the function is unimodular. The following result illustrates one such example.

Corollary 3.21 (Theorem 15 in [8]) *Consider* $f(x, y) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x_i y_j$ *where* $x \in [0, 1]^n$, $y \in [0, 1]^m$*, and* $a_{ij} \geq 0$ *for* $i = 1, \ldots, n$, $j = 1, \ldots, m$. *Then,*

$$\operatorname*{conc}_{[0,1]^{n+m}}(f)(x, y) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} \min\{x_i, y_j\}$$

and $\mathrm{conv}_{[0,1]^{n+m}}(f)(x, y) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} \max\{x_i + y_j - 1, 0\}$.

Proof The concave envelope follows directly from Corollary 3.11. Now, we switch the y variables to write

$$f(x, \bar{y}) = \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x_i (1 - \bar{y}_j) = \sum_{i=1}^{n} \left(\sum_{j=1}^{m} a_{ij} \right) x_i - \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} x_i \bar{y}_j.$$

Since $f(x, \bar{y})$ is submodular (negative of a supermodular function), the convex envelope of $f(x, \bar{y})$ can be obtained as $-\mathrm{conc}_{[0,1]^n}(-f)(x, \bar{y})$ which, according to Corollary 3.11, is $\sum_{i=1}^{n} (\sum_{j=1}^{m} a_{ij}) x_i - \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} \min\{x_i, \bar{y}_j\}$. $\square$

Example 3.22 Let $f(x) = \sum_{i=1}^{k} a_i \prod_{j \in J_i} f_{ij}(x_j)$ where $a_i \geq 0$, each f_{ij} is nonnegative, convex and for each i, either $f_{ij}(x_j)$ is increasing or decreasing for all $j \in J_i$. The convexity of $f_{ij}(\cdot)$ implies that $f(x)$ is concave-extendable from the vertices of the hypercube. Since the product of nonnegative increasing (decreasing) univariate functions is supermodular, the concave envelope of $f(x)$ follows from Theorem 3.3. As a concrete example, we may set $f_{ij}(x_j) = x_j^{q_{ij}}$ where $q_{ij} \geq 1$ for all j or $q_{ij} < 0$ for all j. Observe that this example extends the class of functions treated in (15) and in Corollary 3.11. $\square$

Example 3.23 Let $f(x) = \sum_{i=1}^{k} g_i \left(a_i + \sum_{j=1}^{n} a_{ij} x_j \right)$ where for each j either $a_{ij} \geq 0$ or $a_{ij} \leq 0$ for all i, and, for each i, g_i is a convex function. It follows from Corollary 3.14 that the concave envelope of $f(x)$ is given by $\mathcal{K}(T)$ where $T = \{j \mid a_{ij} \leq 0 \,\forall i\}$. As an example, let $c_i \geq 0$ for all i and set $g_i(\cdot) = -c_i \log(\cdot)$. In particular, consider `hs62` from `globallib` which was originally formulated in [15]:

$$\begin{aligned}
\min\ & -32.174\Bigg(\ 255\log\left(\tfrac{0.03+x+y+z}{0.03+0.09x+y+z}\right)+280\log\left(\tfrac{0.03+y+z}{0.03+0.07y+z}\right)\\
&\qquad\qquad +290\log\left(\tfrac{0.03+z}{0.03+0.13z}\right)\Bigg)\\
\text{s.t.}\ & x+y+z=1\\
& x,y,z\geq 0.
\end{aligned}$$

If we solve the factorable relaxation, we obtain a lower bound of -83126.9. The objective function $h(x,y,z)$ of the above problem can be written as $h(x,y,z) = -32.174(g(x,y,z)+f(x,y,z))$ where

$$\begin{aligned}
g(x,y,z) = {} & 255\log(0.03+x+y+z)+280\log(0.03+y+z)\\
& +290\log(0.03+z)
\end{aligned}$$

and

$$\begin{aligned}
f(x,y,z) = {} & 255\log\left(\frac{1}{0.03+0.09x+y+z}\right)+280\log\left(\frac{1}{0.03+0.07y+z}\right)\\
& +290\log\left(\frac{1}{0.03+0.13z}\right). \qquad (16)
\end{aligned}$$

Since $g(x,y,z)$ is concave, a convex underestimator of $h(x,y,z)$ can be obtained as $-32.174(g(x,y,z)+\mathrm{conc}_T\, f(x,y,z))$ where T is any superset of the simplex $S=\{(x,y,z)\mid x+y+z=1, x,y,z\geq 0\}$. If we choose $T=[0,1]^3$, we can compute $\mathrm{conc}_T\, f(x,y,z)$ using Corollary 3.14, which in turn, yields a lower bound of -52944.9.

If one further realizes that S can be transformed to a lattice family (in a manner similar to that of Theorem 3.8) by introducing $u=x$, $v=x+y$ and $w=x+y+z=1$, then (16) can be written as:

$$\begin{aligned}
& 255\log\left(\frac{1}{1.03-0.91u}\right)+280\log\left(\frac{1}{1.03-0.07u-0.93v}\right)\\
& +290\log\left(\frac{1}{0.16-0.13v}\right). \qquad (17)
\end{aligned}$$

The feasible region in the (u,v) space is given by $S'=\{(u,v)\mid 0\leq u\leq v\leq 1\}$. Since the coefficients of u and v are nonpositive, we introduce $\bar{u}=1-u$ and $\bar{v}=1-v$ to obtain S''. Notice that a lattice family remains a lattice family if all variables are complemented. Then, the concave envelope of (17) over S'' can be developed using Theorem 3.3 and then linearly transformed to derive the following concave envelope of (16) over S:

$$
\begin{aligned}
-f(x,y,z) \geq\ & 535\log(103) - 490\log(2) - 1650\log(5) + \big(825\log(3) - 535\log(103) \\
& -650\log(2)\big)x + \big(280\log(5) - 280\log(103) - 880\log(2) \\
& +290\log(3)\big)y.
\end{aligned}
$$

The concave envelope could have also been developed simply by realizing that (16) is convex and the feasible region is a triangle, i.e., $-f(x,y,z) \geq -f(1,0,0)x - f(0,1,0)y - f(0,0,1)z$ and replace z by $1-x-y$ to express the inequality in the above form. However, we chose to develop it in the above way to demonstrate the techniques developed in this section. With the concave envelope introduced into the formulation, the lower bound improves to -42429.2. The global minimum has an objective value of -26272.5. It is interesting to observe that the proposed relaxation leads to a 53 % improvement without recognizing the lattice family and 71.5 % improvement after recognizing the lattice family when compared to the standard factorable relaxation. □

4 Convex envelopes of disjunctive functions

As shown in Sects. 2 and 3, if the envelope of a nonlinear function is polyhedral, it can be described using polyhedral subdivisions. In this section, we show that polyhedral subdivisions also play an important role in characterizing non-polyhedral envelopes of certain functions. To this end, we consider disjunctive functions of the form $xf(y)$ where $f(\cdot)$ is convex and non-increasing. Such functions are typically not convex, even in the simple case where $f(y) = -y$. However, since $xf(y)$ is convex for any fixed x, the convex envelope can be formed over the hypercube using disjunctive programming. Disjunctive functions appear commonly in factorable programming. However, their structure is not typically exploited since traditional techniques only give the description of the convex envelope in a lifted space. In Theorem 4.1, we show that the convex envelope can be written in the original space without introducing additional variables when $f(y)$ is non-increasing and the lower bound on x is 0. In this description, we use the recession function $f0^+(y)$ of f where $f0^+(y) = \sup\{f(x+y) - f(x) \mid x \in \operatorname{dom} f\}$; see Section 8 in [26].

Theorem 4.1 *Consider a function $g(x,y) = xf(y)$ where $(x,y) \in [0,1] \times [0,1]^n$. Let $f(y)$ be a convex non-increasing function and (x',y') be a point in the domain. Let $y'' = (y''_i)_{i=1}^n$, where $y''_i = \min(y'_i, x')$. Then,*

$$
\operatorname{conv}(g)(x',y') = h(x',y') := \begin{cases} x'f\left(\frac{y''}{x'}\right) & if\, x' > 0 \\ f0^+(y'') & if\, x' = 0 \\ \infty & otherwise. \end{cases} \tag{18}
$$

Proof Since $xf(y)$ is linear in x for any fixed value of $y \in [0,1]^n$, it suffices to consider $x \in \{0,1\}$ when building the convex envelope of this function over $[0,1]^{n+1}$

For a given subset J of N define $W_0(J) = \{(0, y) \in [0, 1]^{n+1} \mid y_i = 0, \forall i \in J\}$ and $W_1(J) = \{(1, y) \in [0, 1]^{n+1} \mid y_i = 1, i \in N\backslash J\}$. First, we construct the convex envelope of $g(x, y)$ over $W' = \operatorname{conv}\big(W_0(J) \cup W_1(J)\big)$. This convex envelope is obtained by convexifying the two disjunctions

$$\left.\begin{array}{l} z = 0 \\ x = 0 \\ y_J = 0 \\ 0 \le y_{N\backslash J} \le 1 \end{array}\right| \begin{array}{l} z \ge xf\left(\frac{y}{x}\right) \\ x = 1 \\ 0 \le y_J \le 1 \\ y_{N\backslash J} = 1. \end{array}$$

Observe that the above two sets are orthogonal (after variables $y_{N\backslash J}$ are complemented) and $h(x', y')$ is a closed positively homogeneous function (see Theorem 8.2 in [26]). Therefore, by Theorem 1 in [37], it follows that the convex envelope (highest convex underestimator that is lower-semicontinuous) of $g(x, y)$ over $W' = \{(x, y) \mid 0 \le y_i \le x \le y_j \le 1 \ \forall i \in J, j \in N\backslash J\}$ has the form (18). For $y \ge 0$,

$$f0^+(y) = \lim_{\lambda \uparrow \infty} \frac{f(\lambda y) - f(0)}{\lambda} \le 0$$

where the equality follows by definition (see Corollary 8.5.2 in [26]) and the inequality because f is non-increasing and $\lambda y \ge 0$. Since, over W', the convex envelope is a function of x and y_J but not of $y_{N\backslash J}$ and since $g(x, y)$ is non-increasing in y, it follows that $\operatorname{conv}_{W'}(g)(x, y) \le g(x, y)$ for all $(x, y) \in \{0, 1\} \times [0, 1]^n$. Since $\operatorname{conv}_{W'}(g)$ is convex, $\operatorname{conv}_{W'}(g)(x, y) \le \operatorname{conv}_{[0,1]^{n+1}}(g)(x, y)$ for $(x, y) \in [0, 1]^{n+1}$. However, $W' \subseteq [0, 1]^{n+1}$. Therefore, $\operatorname{conv}_{W'}(g)(x, y) \ge \operatorname{conv}_{[0,1]^{n+1}}(g)(x, y)$ for all $(x, y) \in W'$. Combining these results, we conclude that $\operatorname{conv}_{W'}(g)(x, y) = \operatorname{conv}_{[0,1]^{n+1}}(g)(x, y)$. □

We next provide some geometrical insights into the proof of Theorem 4.1, discuss settings in which it can be generalized, and describe some applications.

The convex envelope of $xf(y)$ developed in Theorem 4.1 has a simple geometric structure. It is expressed as the maximum of a finite set of positively homogeneous functions. Each function attains the maximum over one of the polytopes in the subdivision $\bigcup_{J \subseteq N} S_J$ of $[0, 1]^{n+1}$, where $S_J = \{(x, y) \mid 0 \le y_j \le x \,\forall j \in J,\ x \le y_j \le 1 \,\forall j \in N\backslash J\}$. We illustrate this characteristic on the following example.

Example 4.2 Consider the function $g : [0, 1]^2 \mapsto \mathbb{R}$ defined as $g(x, y) = \frac{x}{1+y}$. The convex envelope of g can be obtained by convexifying its restrictions to $x = 0$ and $x = 1$, restrictions that are depicted as red thick lines in Fig. 1. The proof of Theorem 4.1 argues that the convex envelope of g can be obtained by first constructing the convex envelope of g over $S_\emptyset = \{(x, y) \,|\, 0 \le x \le y \le 1\}$, which is depicted in cyan, and gluing it to the convex envelope of g over $S_{\{1\}} = \{(x, y) \,|\, 0 \le y \le x \le 1\}$, which is depicted in gray. More precisely, applying the formulas described in Theorem 4.1 yields that $\operatorname{conv}_{[0,1]}(g)(x, y) = \frac{x^2}{x+\min\{x,y\}}$ if $x > 0$ and $\operatorname{conv}_{[0,1]}(g)(x, y) = 0$ if $x = 0$. □

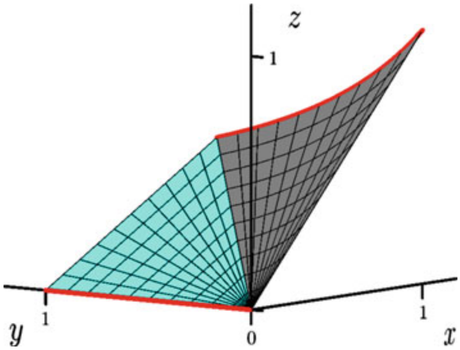

Fig. 1 Convex Envelope of $\frac{x}{1+y}$ over $[0, 1]^2$

The convex envelope derived in Example 4.2 was obtained earlier in [38] in a more general setting using disjunctive programming. We used this example solely to illustrate the polyhedral subdivision that is at the core of the proof. Observe that the proof of Theorem 4.1 relies on $g(x, y)$ being zero when x is fixed at its lower bound. However, $xf(y)$ is not zero if the lower bound is not zero. Therefore, the result does not directly yield envelopes of $xf(y)$ over general hypercubes. Nevertheless, the techniques developed here can be used to develop relaxations. For example, say $h(x, y)$ is the convex envelope of $g(x, y) - g(x^L, y)$ obtained using Theorem 4.1. Then, $g(x^L, y) + h(x, y)$ yields a relaxation. This strategy does not however yield the envelope which can be described in the higher dimensional space using the techniques of [38].

We next describe settings for which Theorem 4.1 can be adapted and/or generalized. First observe that, if $f(y)$ is non-decreasing, the convex envelope of $xf(y)$ over the unit hypercube can still be derived using Theorem 4.1 by replacing y_i with $1 - \bar{y}_i$. Second, note that if $y' > y''$ and $f(\cdot)$ is non-increasing, then $xf\left(\frac{\min(y',x)}{x}\right) \leq xf\left(\frac{\min(y'',x)}{x}\right)$. Therefore, Theorem 4.1 can be applied sequentially to convexify functions of the form $f(y)\prod_{i=1}^m x_i$. Further, the result of Theorem 4.1 also applies to more general functions $g(x, y)$ that are such that (i) $g(0, y) = 0$, (ii) $\operatorname{conv}_{[0,1]^{n+1}} g(1, y)$ is known explicitly and non-increasing, (iii) $g(x, y')$ is concave as a function of x when y is fixed at y'. Next we demonstrate applications of Theorem 4.1 in such contexts.

Corollary 4.3 *Let* $g : [0, 1]^{n+1} \mapsto \mathbb{R}$ *be defined as* $g(x, y) = \frac{x}{ax+\sum_{i=1}^n b_i y_i + c}$ *where* $a \in \mathbb{R}, b \in \mathbb{R}^n$*, and* $c \in \mathbb{R}$*. Define* $N = \{1, \ldots, n\}$, $N^+ = \{i \in N \mid b_i \geq 0\}$*, and* $N^- = N \backslash N^+$*. Assume that* $c + \sum_{i \in N^-} b_i > 0$ *and* $a \geq 0$*. Then,*

$$\operatorname*{conv}_{[0,1]^{n+1}} g(x, y) = \begin{cases} \frac{x^2}{(a+c)x + \sum_{i\in N^+} b_i \min\{x, y_i\} + \sum_{i \in N^-} b_i \max\{x + y_i - 1, 0\}} & \text{if } x > 0 \\ 0 & \text{if } x = 0. \end{cases}$$

Proof Note that $\min\{ax + \sum_{i=1}^n b_i y_i + c \mid x \in [0, 1], y \in [0, 1]^n\} = c + \sum_{i \in N^-} b_i > 0$. Therefore, the function $g(x, y)$ is well-defined over $[0, 1]^{n+1}$. Further, observe that

$$\frac{\partial^2 g(x, y)}{\partial x^2} = -\frac{2a\left(c + \sum_{i=1}^n b_i y_i\right)}{\left(ax + \sum_{i=1}^n b_i y_i + c\right)^3} \leq 0.$$

The inequality follows since $a \geq 0$, $c + \sum_{i=1}^n b_i y_i > 0$ and $ax + \sum_{i=1}^n b_i y_i + c > 0$. Therefore, $g(x, \bar{y})$ is concave in x for any fixed $\bar{y}$. The result then follows from Theorem 4.1 after complementing the variables y_i for $i \in N^-$. □

An argument similar to that of Corollary 4.3 yields the concave envelope of $g(x, y) = x \log\big(ax + \sum_{i=1}^n b_i y_i + c\big)$. In this case, using the above proof technique on $-g(x, y)$, we obtain

$$\operatorname*{conc}_{[0,1]^{n+1}} g(x, y) = \begin{cases} -x \log(x) + \\ x \log\left((a+c)x + \sum_{i \in N^+} b_i \min\{x, y_i\} \right. \\ \quad \left. + \sum_{i \in N^-} b_i \max\{x + y_i - 1, 0\} \right) & \text{if } x > 0 \\ 0 & \text{if } x = 0 \end{cases}$$

under the assumptions that $c + \sum_{i \in N^-} b_i > 0$ and $a \geq 0$. Observe that the concave envelope of $\frac{x}{ax + \sum_{i=1}^n b_i y_i + c}$ and the convex envelope of $x \log(ax + \sum_{i=1}^n b_i y_i + c)$ can also be obtained by using Corollary 3.16. Next, we show that Theorem 4.1 yields convex envelopes of many polynomial functions over the unit hypercube.

Corollary 4.4 *Consider a function* $g(x, y) = x\Big(c + \sum_{i=1}^n \sum_{j=1}^k a_{ij} y_i^{p_{ij}}\Big)$, *where* $a_{ij} \in \mathbb{R}_+$ *and* $p_{ij} - 1 \in \mathbb{R}_+$. *Then the convex envelope of* $g(x, y)$ *over* $[0, 1]^{n+1}$ *is given by:*

$$\operatorname{conv}(g)_{[0,1]^{n+1}}(x, y) = \begin{cases} cx + \sum_{i=1}^n \sum_{j=1}^k a_{ij} x^{1-p_{ij}} \max\,[x + y_i - 1, 0]^{p_{ij}} & if\ x > 0 \\ 0 & if\ x = 0. \end{cases}$$

The concave envelope of $g(x, y)$ *over* $[0, 1]^{n+1}$ *is given by:*

$$\operatorname{conc}(g)_{[0,1]^{n+1}}(x, y) = cx + \sum_{i=1}^n \left(\sum_{j=1}^k a_{ij} \right) \min\,[y_i, x]\,.$$

Proof The convex envelope is obtained using Theorem 4.1 after complementing the variables y_i. For the concave envelope, note that $g(x, y)$ is supermodular and concave-extendable from vertices. Therefore, the result follows from Theorem 3.3 and/or Corollary 3.11 as $\sum_{i=1}^n \sum_{j=1}^k a_{ij} x y_i^{p_{ij}} = \sum_{i=1}^n \sum_{j=1}^k a_{ij} x y_i$ for all $(x, y) \in \{0, 1\}^{n+1}$. □

Theorem 4.1 easily yields polyhedral subdivisions defining the convex envelope of $xf(\cdot)$ if $f(\cdot)$ has a polyhedral convex envelope. We describe next a special case of

$f(y)$ where y_i are binary-valued to illustrate the techniques involved. First, we will consider certain symmetric convex functions of binary variables and develop their convex envelopes. These functions themselves appear in nonlinear integer programming and we also discuss some of their applications. Then, we develop convex envelopes of $xf(y)$, where $f(y)$ is such a symmetric function and y are binary variables. Finally, we discuss applications of this disjunctive form and consider alterations to the polyhedral subdivision when the underlying region is restricted to a subset of the hypercube.

In order to develop the convex envelope of the symmetric function, we will need an exclusion property that helps in identifying the convex envelopes of convex functions restricted to nonconvex sets. Although, we will not need the full power of Proposition 4.5 in our subsequent development, we include it here for other potential applications.

Proposition 4.5 *Consider a closed set X and an upper-semicontinuous (lower-semicontinuous) concave (convex) function $f : \mathrm{conv}(X) \mapsto \mathbb{R}$. Let $f|_X$ be the restriction of f to X. Consider an $x \in \mathrm{conv}(X)$ and a $V \subseteq X$ such that $(x, \mathrm{conc}(f|_X)(x))$ ($(x, \mathrm{conv}(f|_X)(x))$) can be expressed as a convex combination of $(V, f(V))$. Then, it may also be assumed that $|V| = \dim(V) + 1$ and $[\mathrm{conv}(V) \setminus \mathrm{vert}(\mathrm{conv}(V))] \cap X = \emptyset$.*

Proof We denote the problem $D(x)$ with vertex set V as $D_V(x)$ and the corresponding optimal value as $z_V(x)$. The existence of V' such that $z_{V'}(x) = \mathrm{conc}(f|_X)(x)$ and $|V'| = n + 1$ follows by Carathéodory's theorem and the assumed existence of V in the statement of the result. Let V be such that $\mathrm{conv}(V)$ is the minimum volume simplex in $\mathrm{conv}(V')$ that satisfies this property. There exists a minimum since each point is chosen from a compact feasible region $\mathrm{conv}(V') \cap X$, the multipliers are chosen from a compact set, $V^\intercal\lambda$ and volume are continuous functions, and $f(V)^\intercal\lambda$ is upper-semicontinuous. If this volume is zero, first note that we can drop one point from V since any extreme solution of $D_V(x)$ will have a support at no more than $\dim(V) + 1$ points. We now reiterate to find the minimum volume simplex, where volume is now computed in $\mathrm{aff}(V)$. Therefore, we may assume that there does not exist V'' such that $\mathrm{conv}(V'') \subsetneq \mathrm{conv}(V)$ and $z_{V''}(x) = \mathrm{conc}(f)(x)$. Assume now, by contradiction, that $x' \in [\mathrm{conv}(V) \setminus \mathrm{vert}(\mathrm{conv}(V))] \cap X$. Let λ be the optimal solution of $D_V(x)$. By minimality of volume, it follows that $\lambda_i > 0$ for all i. Let λ' be a feasible solution of $D(x')$ such that $\lambda'_i > 0$ only if $v_i \in \mathrm{vert}(\mathrm{conv}(V))$. Such a point exists since $x' \in \mathrm{conv}(V)$. Define $r = \min_i\left\{\frac{\lambda_i}{\lambda'_i} \mid \lambda'_i > 0\right\}$. Further, let i' be the index that achieves this minimum. It follows that $v_{i'} \in \mathrm{vert}(\mathrm{conv}(V))$ and $0 < r$. Then,

$$\begin{aligned}\mathrm{conc}(f|_X)(x) = f(V)^\intercal\lambda = f(V)^\intercal(\lambda - r\lambda') + rf(V)^\intercal(\lambda') \le f(V)^\intercal(\lambda - r\lambda') \\ + rf(x') \le \mathrm{conc}(f|_X)(x),\end{aligned}$$

where the first inequality follows from concavity of f and the second inequality since $x' \in X$, $\lambda - r\lambda' \ge 0$, and $e^\intercal(\lambda - r\lambda') + r = 1$. Therefore, equality holds throughout. If $V'' = V\setminus\{v_{i'}\} \cup x'$, this implies that $z_{V''}(x)$ equals $\mathrm{conc}(f|_X)(x)$. Further, by construction $v_{i'} \in \mathrm{vert}(\mathrm{conv}(V))$ while $x' \notin \mathrm{vert}(\mathrm{conv}(V))$ and $x' \in \mathrm{conv}(V)$. Therefore, $v_{i'} \notin \mathrm{conv}(V'')$ and $\mathrm{conv}(V'') \subsetneq \mathrm{conv}(V)$. The existence of V'' yields a contradiction to the assumption that $\text{conv}(V)$ is a simplex of minimum volume in $\text{conv}(V')$ that yields the concave envelope at x. □

In Proposition 4.5, we assumed that there exists a V such that $z_V(x) = \text{conc}(f|_X)(x)$. Even if that is not the case, i.e., there exists a sequence V^k such that $z_{V^k}(x) \to \text{conc}(f|_X)(x)$ as $k \to +\infty$, it follows using the arguments presented in the proof that we may require that, for every k, $[\text{conv}(V^k)\setminus \text{vert}(\text{conv}(V^k))] \cap X = \emptyset$ and $|V^k| = \dim(V^k) + 1$.

In Theorem 4.6 we consider a symmetric function of binary variables, $f\left(\sum_{j=1}^n y_j\right)$, where f is a convex function, and show that its convex envelope is simple to characterize.

Theorem 4.6 *Consider a function $g(y) : [0, 1]^n \mapsto \mathbb{R}$, that is convex-extendable from vertices. Then, the polyhedral subdivision of $[0, 1]^n$ given by $\mathcal{P} = \{P_1, \dots, P_n\}$, where $P_i = \{y \in \mathbb{R}^n \mid i - 1 \le \sum_{j=1}^n y_j \le i, 0 \le y \le 1\}$ describes the convex envelope of $g(y)$ if and only if its restriction to $\{0, 1\}^n$ can be written as $f(\sum_{j=1}^n y_j)+\sum_{j=1}^n a_j y_j$ for some convex function f. The corresponding convex envelope is:*

$$\max_{i\in\{1,\dots,n\}} \Big(f(i) - f(i-1)\Big) \sum_{j=1}^n y_j + \Big(if(i-1) - (i-1)f(i)\Big) + \sum_{j=1}^n a_j y_j. \tag{19}$$

Proof ($\Leftarrow$) Define $g'(y) = f(\sum_{i=1}^n y_i)+\sum_{i=1}^n a_i y_i$ where f is the given convex function. In the proof, assume that, for any function ϕ, $\text{conv}(\cdot)$ denotes the convex envelope of ϕ over $[0, 1]^n$ unless specified otherwise. We start by assuming that $\text{conv}(g)(y) = \text{conv}(g'|_{\{0,1\}^n})(y)$, where $g'|_{\{0,1\}^n}$ denotes the restriction of g' to $\{0, 1\}^n$. Since g' is convex, $\text{conv}(g)(y) \ge g'(y)$. Consider the set $W_i = \{y \in [0, 1]^n \mid \sum_{j=1}^n y_j = i\}$. The function $g'(y)$ is linear over W_i. Since, each extreme point of W_i is also an extreme point of $[0, 1]^n$, it follows that for every $y \in W_i$, $\text{conv}(g)(y) \le g'(y)$. Combining we have, for all $y \in W_i$, that $\text{conv}(g)(y) = g'(y)$. In other words, for all $y \in [0, 1]^n$, it follows that $\text{conv}(g)(y) = \text{conv}(g'|_{\bigcup_{i=0}^n W_i})(y)$. Since $\{0, 1\}^n$ is a finite set, for all $y \in [0, 1]^n$, $\text{conv}(g)(y)$ is attained as a convex combination of function values at an appropriate subset of $\{0, 1\}^n$ which corresponds to the support of the optimal solution in $D(y)$. Then, it follows from Proposition 4.5 that $\mathcal{P}$ is the polyhedral subdivision associated with $\text{conv}(g)$.

($\Rightarrow$) For the direct implication, consider any function $g(y)$ that is convex-extendable from $\{0, 1\}^n$ and whose convex envelope is described by $\mathcal{P}$. Therefore, the restriction of $g(y)$ to $\{0, 1\}^n$ must be linear over each P_i. Let $l^i(y) = a_0^i + \sum_{j=1}^n a_j^i y_j$ equal $g(y)$ at the extreme points of P_i. Note that P_1 is a simplex. Therefore, $l^1(y)$ is uniquely defined by the extreme points of P_1. Then, since $l^i(y)$ and $l^{i+1}(y)$ match at the extreme points of W_i, it follows that they also match everywhere on $\text{aff}(W_i)$. In other words, $l^{i+1}(y)-l^i(y) = \alpha^{i+1}(\sum_{j=1}^n y_j - i)$ for $i = 1, \dots, n-1$. Further, by convexity of the envelope, $\alpha^{i+1} \ge 0$, otherwise $l^i(y)$ overestimates the function at the extreme points of W_{i+1}. In other words, $g(y) = a_0^1 + \sum_{i=1}^n a_i^1 y_i + \sum_{i=2}^n \alpha^i \max\{\sum_{j=1}^n y_j - i, 0\}$

at each point in $\{0, 1\}^n$. Since the second term is a convex function of $\sum_{j=1}^n y_j$, the result follows. $\square$

Corollary 4.7 *Consider a function $g(y) : P \mapsto \mathbb{R}$, that is convex-extendable from vertices of P, where P is a polytope and $\mathrm{vert}(P) \subseteq \{0, 1\}^n$. Assume that for each $i \in \{1, \ldots, n-1\}$, $W_i = \{y \in P \mid \sum_{j=1}^n y_j = i\}$ is integral. Then, the polyhedral subdivision $\mathcal{P} = \{P_1, \ldots, P_n\}$, where $P_i = \{y \in P \mid i-1 \le \sum_{j=1}^n y_j \le i\}$ describes the convex envelope of $g(x)$ if its restriction to $\mathrm{vert}(P)$ can be written as $f(\sum_{j=1}^n y_j) + \sum_{j=1}^n a_j y_j$ for some convex function f. The convex envelope is given by (19).*

Proof Note that W_0 and W_n are either empty or integral by definition. The remaining proof is just as that of Theorem 4.6. $\square$

We next give applications of Theorem 4.6 and Corollary 4.7 in the derivation of convex envelopes of various functions. In the following result, we use the same notation as that used in Corollary 3.10.

Corollary 4.8 (Theorem 3 and 5 in [31]) *Consider the function $\phi_G^m(y) : G \mapsto \mathbb{R}$ defined as $\phi_G^m(y) = \sum_{J \subseteq D, |J|=m} \left[\prod_{d \in J} y_{i(d)j(d)}\right]$, where $m \le n$ and G is of the form (8). Define $\phi_{\mathrm{vert}(G)}^m(y)$ as the restriction of $\phi_G^m(y)$ to the vertices of G. Then, the convex envelope of $\phi_{\mathrm{vert}(G)}^m(y)$ over G is given by:*

$$\operatorname*{conv}_G \phi_{\mathrm{vert}(G)}^m(y) = \max\left\{0, \binom{k}{m-1} \sum_{j=1}^{n} \sum_{r=1}^{d_j} y_{rj} - (m-1)\binom{k+1}{m} \;\middle|\; k = m-1, \ldots, n-1\right\}. \tag{20}$$

Further, if $d_i = 1$ for all i, then $\mathrm{conv}_G\, \phi_G^m(y) = \mathrm{conv}_G\, \phi_{\mathrm{vert}(G)}^m(y)$ for $y \in G$.

Proof As in the proof of Corollary 3.10, we may restrict attention to J such that if d and d' belong to J, then $i(d) \ne i(d')$. Note that G and $W_i = \{y \mid \sum_{j=1}^n \sum_{r=1}^{d_j} y_{jr} = i, \sum_{r=1}^{d_j} y_{jr} \le 1 \forall j\}$ are integral polytopes since the corresponding matrices are totally unimodular (see for example, Corollary 2.8, Part III in [23]). Note that $\phi_{\mathrm{vert}(G)}^m(y)$ is supermodular (see Lemma 3.6 and the following discussion). Further, over the vertices of G, $\phi_{\mathrm{vert}(G)}^m(y)$ can be expressed as $\binom{\sum_{j=1}^n \sum_{r=1}^{d_j} y_{jr}}{m}$ where $\binom{u}{m}$ is defined as zero if $u < m$. The convexity of $\phi_{\mathrm{vert}(G)}^m$ as a function of $\sum_{j=1}^n \sum_{r=1}^{d_j} y_{jr}$ then follows from Proposition 5.1 in [20], which states that, given a set S, a function, $h : 2^S \mapsto \mathbb{R}$ of the form $h(X) = g(|X|)$, where $X \subseteq S$ and $|X|$ is the cardinality of X, is supermodular if and only if g is convex. The convexity of $\binom{i}{m}$ over the nonnegative integers can also be verified directly since $\binom{i}{m} - \binom{i-1}{m} = \binom{i-1}{m-1}$ which is a non-decreasing function of i. The convex envelope then follows from Corollary 4.7. Substituting $f(i) = \binom{i}{m}$ in (19), we obtain (20) after setting $k = i-1$ and removing all terms with zero coefficients. The last statement follows just as in Corollary 3.10. $\square$

Example 4.9 Consider the function $f(y) = \frac{1}{\sum_{i=1}^n y_i}$, where $y_i \in \{0, 1\}$, and let $P = \{y \in [0, 1]^n \mid \sum_{i=1}^n y_i \geq 1\}$. The standard factorable programming relaxation uses the function itself as the convex underestimator. The function, $f(y)$, appears in the formulation of the consistent biclustering problem [6], where the authors relax $f(y)$ over P by cross-multiplying with the denominator and then relaxing $y_i f(y)$ over $[0, 1] \times \left[\frac{1}{n}, 1\right]$. Since this relaxation is valid even when $y_i \in [0, 1]$ and since it is polyhedral, it is weaker than the factorable relaxation discussed above. Further, note that $f(y)$ is convex and $W_i = \{y \in P \mid \sum_{j=1}^n y_j = i\}$ are clearly integral. Therefore, Corollary 4.7 applies and provides a description of the convex envelope of $f(y)$ over P. Observe that the factorable programming relaxation, which is non-polyhedral, is weaker than the polyhedral relaxation obtained from Corollary 4.7 when $\sum_{i=1}^n y_i \notin \mathbb{Z}$. It may be noted that the concave envelope of $f(y)$ was previously described in Example 3.20.

As mentioned before, Theorem 4.1 also provides a constructive derivation of the polyhedral subdivision describing the convex envelope of $xf(y)$ when $f(y)$ has a polyhedral envelope. We next illustrate the constructions involved for the case where the function $f(y)$ is of the form $f(\sum_{i=1}^n y_i)$, where $y \in \{0, 1\}^n$.

Corollary 4.10 *Consider $g(x, y) = xf(\sum_{i=1}^n y_i)$. Let f be a non-increasing convex function and $y \in \{0, 1\}^n$. For $I \subseteq N$ and $1 \leq l \leq |I|$, let*

$$S(I, l) = \left\{ (x, y) \;\middle|\; 0 \leq y_i \leq x \leq y_j \leq 1,\ \forall i \in I, \forall j \in N \setminus I,\ (l-1)x \leq \sum_{i \in I} y_i \leq lx \right\}.$$

Then, the polyhedral subdivision $\{S(I, l)\}_{\substack{I \subseteq N \\ 1 \leq l \leq |I|}}$ defines the convex envelope of $g(x, y)$ over $[0, 1]^{n+1}$. In particular, the convex envelope of $g(x, y)$ over $S(I, l)$ is given by:

$$\Big(f(l + |I^c|) - f(l - 1 + |I^c|)\Big) \sum_{i \in I} y_i + \Big(lf(l - 1 + |I^c|) - (l - 1)f(l + |I^c|)\Big)x \tag{21}$$

where $I^c = N \setminus I$.

Proof First note that when $x = 1$, the function $f(y)$ satisfies the conditions of Theorem 4.6. Therefore, the polyhedral subdivision is given by $\{W_1', \ldots, W_n'\}$, where $W_i' = \{y \in [0, 1]^n \mid i - 1 \leq \sum_{i=1}^n y_i \leq i\}$. In particular, over W_i'

$$\operatorname*{conv}_{[0,1]^n}(f)(y) = h(y) := \Big(f(i) - f(i - 1)\Big) \sum_{j=1}^n y_j + \Big(if(i - 1) - (i - 1)f(i)\Big). \tag{22}$$

Clearly, $\text{conv}_{[0,1]^{n+1}}(xf(y)) = \text{conv}_{[0,1]^{n+1}}(xh(y))$. Now, the situation fits the setting of Theorem 4.1. Therefore, the convex envelope over $S(I, l)$ is given by $xh(\frac{y'}{x})$, where $y_i' = \min(y_i, x)$. By definition of $S(I, l)$, $y_i' = y_i$ for $i \in I$ and $y_i' = x$ for $i \in I^c$. Expanding using (22) one obtains (21) where $i - |I^c| = l$. It follows by choosing $f(y)$ to be a strictly convex and decreasing function (such as $\frac{1}{1+y_1+\ldots+y_n}$) that the convex envelope of $g(x, y)$ is only tight at the binary points that belong to $\mathrm{vert}(S(I, l))$. Therefore, $\bigcup_{\substack{I \subseteq N \\ 0<l\leq|I|}} S(I, l)$ gives a polyhedral subdivision of $[0, 1]^{n+1}$. □

In Sect. 3, we discussed a situation where removing the origin from the underlying polytope changed the associated polyhedral subdivision completely. As we mentioned, this was because each simplex in the triangulation contained the origin as a vertex. For the function studied in Corollary 4.10, it can be easily verified that the origin is still a vertex of each polyhedron in the subdivision. However, in this case the structure of the convex envelope is not completely altered when the origin is removed from the underlying region. This result can be intuitively understood when one observes that the polytopes that form the subdivision described in Corollary 4.10 are not simplices. Therefore, even if the origin is removed from a polytope, it may still have sufficient points to describe the convex envelope over a subregion. Theorem 4.11 gives an illustration of this phenomenon. We discuss an application of this result in Example 4.12.

Theorem 4.11 *Consider $g(x, y) = xf(\sum_{i=1}^n y_i)$, where $f(z) : \mathbb{R} \mapsto \mathbb{R}$ is a convex non-increasing function. Assume that $(x, y) \in \{0, 1\}^{n+1}$ and $(x, y) \neq (0, 0)$. Let $W = \left\{(x, y) \in [0, 1]^{n+1} \mid x + \sum_{i=1}^n y_i \geq 1\right\}$. Then, the polyhedral subdivision $\mathcal{S} = \{S(i)\}_{i=0}^{n-1} \cup \{T(I, k)\}_{\substack{I\subseteq N \\ 0\leq k\leq |I|-1}}$ describes the convex envelope of $g(x, y)$ over W where*

$$S(i) = \left\{ (x, y) \;\middle|\; \begin{array}{l} 0 \leq y \leq 1 \\ 0 \leq x \leq 1 \\ 1 + (i-1)x \leq \displaystyle\sum_{j=1}^n y_j \leq 1 + ix \\ \displaystyle\sum_{j\in C} y_j \leq 1 + (|C| - 1)x \ \forall C \subseteq N \end{array} \right\}$$

and

$$T(I, k) = \left\{ (x, y) \;\middle|\; \begin{array}{l} 0 \leq y_i \leq x \,\forall i \in I \\ x \leq y_j \leq 1 \,\forall j \in I^c \\ kx \leq \displaystyle\sum_{j\in I} y_j \leq (k+1)x \\ \displaystyle\sum_{j\in I^c} y_j \geq 1 + (|I^c| - 1)x \end{array} \right\}.$$

In particular,

$$\operatorname*{conv}_W(g(x, y)) = \max\left\{ \max_{0\leq i\leq n-1} h^{S(i)}(x, y),\ \max_{\substack{I\subseteq N \\ 0\leq k\leq |I|-1}} h^{T(I,k)}(x) \right\},$$

where

$$h^{S(i)}(x, y) = \Big(if(i) - (i-1)f(i+1)\Big)x - \Big(f(i+1) - f(i)\Big)\left(1 - \sum_{j=1}^{n} y_j\right)$$

and

$$h^{T(I,k)}(x, y) = \Big(f(|I^c| + k + 1) - f(|I^c| + k)\Big)\sum_{j\in I} y_j$$
$$+\Big((k+1)f(|I^c| + k) - kf(k + 1 + |I^c|)\Big)x.$$

Proof We first show that $\mathcal{S}$ covers the unit hypercube. Consider $(x', y') \in W$. There are two cases. First assume that $\sum_{j\in C} y'_j \le 1 + (|C| - 1)x'$ for all $C \subseteq N$. Since this inequality holds for $C = N$, we have that $\sum_{j=1}^{n} y'_j \le 1 + (n-1)x'$. Further, since $(x', y') \in W$, we have that $\sum_{j=1}^{n} y'_j \ge 1 - x'$. It follows that $(x', y') \in S(i)$ for some $i \in \{0, \dots, n-1\}$. Second, assume that there exists $J \subseteq N$ such that $\sum_{j\in J^c} y'_j > 1 + (|J^c| - 1)x'$. Define $I = [J\backslash\{j \in J \mid y'_j \ge x'\}] \cup \{j \in J^c \mid y'_j < x'\}$. It is easily verified that $y'_j \le x'$ for $j \in I$, $y'_j \ge x'$ for $j \in I^c$, and that $\sum_{j\in I^c} y'_j > 1 + (|I^c| - 1)x'$. Further, by construction of I, we have that $\sum_{j\in I} y_j \le |I|x'$. It follows that $(x', y') \in T(I, k)$ where $k \in \{0, \dots, |I| - 1\}$.

Next, we show that $S(i)$ has 0-1 extreme points. In fact, we will show that $S(i) = \text{conv}(W_1(i) \cup W_2(i))$ where $W_1(i) = \{(0, y) \mid 0 \le y \le 1, \sum_{j=1}^{n} y_j = 1\}$ and $W_2(i) = \{(1, y) \mid i \le \sum_{j=1}^{n} y_j \le i + 1\}$. To this end, we will show that, independent of the choice of objective coefficients b and c, the following linear program

$$\begin{array}{llll} P(S): \min & bx + cy & & \\ \text{s.t.} & 0 \le y_j \le 1 & j = 1, \dots, n & (\alpha_j) \\ & 0 \le x \le 1 & & (\beta) \\ & 1 + (i-1)x \le \sum_{j=1}^{n} y_j \le 1 + ix & & (\delta) \\ & \sum_{j\in C} y_j \le 1 + (|C| - 1)x & \forall C \subseteq N & (\gamma_C) \end{array}$$

has an integer optimal solution. In the linear program $P(S)$, α, β, δ, and γ are the dual variables corresponding to the constraints. Each of the variables α_j, β, and δ corresponds to two constraints. Among these, the appropriate constraint depends on the sign of the associated dual variable.

We assume without loss of generality that $c_1 \le \cdots \le c_n$. Let $N(t) = \{1, \dots, t\}$. There are two cases. Assume first that $c_{i+1} \ge 0$. Define $\delta = \max\{0, c_i\} \ge 0$, $\gamma_{N(t)} = c_t - c_{t+1} \le 0$ for $t = 1, \dots, i-1$, $\gamma_{N(i)} = \min\{0, c_i\} \le 0$, $\alpha_j = c_j - \delta \ge 0$ for $j > i$. We set all other α and γ dual variables to 0. Aggregating the constraints of

$P(S)$ using the above weights α, δ and γ, we obtain

$$\sum_{j=1}^{n} c_j y_j - x \sum_{j=2}^{i} c_j \geq c_1. \tag{23}$$

Now, compute $\beta = b + \sum_{j=2}^{i} c_j$. There are two cases. If $\beta > 0$, we add constraint $x \geq 0$ with weight β to (23) to show that $bx + cy \geq c_1$ for all feasible solutions of $P(S)$. Therefore, the integer solution $x = 0$, $y_1 = 1$, and $y_j = 0$ for $j > 1$, whose objective value is c_1, is optimal for $P(S)$. If $\beta \leq 0$, we proceed similarly by adding constraint $x \leq 1$ with weight β to (23) to show that $bx + \sum_{j=1}^{n} c_j y_j \geq b + \sum_{j=1}^{i} c_i$ for all feasible solutions of $P(S)$. Therefore, the integer solution $x = 1$, $y_j = 1$ for $j \leq i$, and $y_j = 0$ for $j > i$ is optimal for $P(S)$.

Now, assume that $c_{i+1} < 0$. Define $\delta = c_{i+1} < 0$, $\gamma_{N(t)} = c_t - c_{t+1} \leq 0$ for $t = 1, \ldots, i$, and $\alpha_j = c_j - c_{i+1} \geq 0$ for $j > i+1$. We set all remaining α and γ dual variables to zero. Aggregating the constraints of $P(S)$ using the above weights α, δ and γ, we obtain that $\sum_{j=1}^{n} c_j y_j - x \sum_{j=2}^{i+1} c_j \geq c_1$. Now, compute $\beta = b + \sum_{j=2}^{i+1} c_j$. There are two cases. If $\beta > 0$, we conclude that $bx + \sum_{j=1}^{n} c_j y_j \geq c_1$ for all feasible solutions to $P(S)$ and so the integer solution $x = 0$, $y_1 = 1$, and $y_j = 0$ for $j > 1$ is optimal for $P(S)$. If $\beta \leq 0$, we obtain similarly that $bx + \sum_{j=1}^{n} c_j y_j \geq b + \sum_{j=1}^{i+1} c_j$ and so the integer solution $x = 1$, $y_j = 1$ for $j \leq i+1$, and $y_j = 0$ for $j > i+1$ is optimal for $P(S)$. Hence, $S(i) = \text{conv}(W_1(i) \cup W_2(i))$. It follows in a manner similar to Theorem 4.1 and Corollary 4.10 by applying Theorem 1 of [37] that the extreme points of $T(I, k)$ are binary.

Clearly, $h^{S(i)}(x, y) \leq 0$ if $x = 0$ and $\sum_{j=1}^{n} y_j \geq 1$ with equality when $\sum_{j=1}^{n} y_j = 1$. Also, $h^{S(i)}(x, y) = f(i) + (i - r)(f(i) - f(i+1))$ if $x = 1$ and $\sum_{j=1}^{n} y_j = r$. Then, it follows by convexity of f that $h^{S(i)}(x, y) \leq f(r)$ with equality if $r \in \{i, i+1\}$. Therefore, by Theorem 2.4, $h^{S(i)}(x, y) \leq \text{conv}_W\, g(x, y)$, with equality over $S(i)$.

From Corollary 4.10, setting $l = k + 1$, it follows that $\text{conv}_{[0,1]^{n+1}}\, g(x, y)$ over $T(I, k)$ is given by $h^{T(I,k)}(x, y)$. Therefore, $h^{T(I,k)}(x, y) \leq g(x, y)$. Further, $\text{vert}(T(I, k)) \subseteq \text{vert}(S(I, k+1))$, where $S(I, k+1)$ is defined as in Corollary 4.10. Therefore, $h^{T(I,k)}(x, y) = g(x, y)$ for $(x, y) \in \text{vert}(T(I, k))$. It follows then from Theorem 2.4 that $h^{T(I,k)}(x, y) \leq \text{conv}_W\, g(x, y)$ with equality over $T(I, k)$.

Choosing $f(\cdot)$ to be a strictly convex and decreasing function, it can be verified that $h^{S(i)}(x, y)$ is not tight at any binary point that is not an extreme point of $S(i)$. Similarly, as in Corollary 4.10, $h^{T(I,k)}(x, y)$ is not tight at any binary point that is not an extreme point of $T(I, k)$. Therefore, $\mathcal{S}$ is a polyhedral subdivision of W. $\square$

Example 4.12 Consider $g(x, y) = \frac{x}{x + \sum_{i=1}^{n} y_i}$, where $(x, y) \in \{0, 1\}^{n+1} \cap W$ and $W = \{(x, y) \in [0, 1]^{n+1} \mid x + \sum_{i=1}^{n} y_i \geq 1\}$. This function appears along with the specified constraint in the consistent biclustering problem [6]. Observe that, over its domain of definition, $g(x, y) = \frac{x}{1 + \sum_{i=1}^{n} y_i}$. Therefore, the convex envelope for $g(x, y)$ over W is described by the polyhedral division of Theorem 4.11. In particular,

$$h^{S(i)}(x, y) = \frac{1}{(i+1)(i+2)}\left[(2i+1)x - \sum_{j=1}^{n} y_j + 1\right]$$

and

$$h^{T(I,k)}(x, y) = \frac{1}{(|I^c|+k+2)(|I^c|+k+1)}\left[(|I^c|+2k+2)x - \sum_{j\in I} y_j\right].$$

Since $\frac{1}{x+\sum_{i=1}^n y_i} \in [\frac{1}{n+1}, 1]$ for all feasible solutions, the factorable relaxation of $g(x, y) = x\frac{1}{x+\sum_{i=1}^n y_i}$ takes the form $\max\left\{\frac{1}{n+1}x, x + u(x, y) - 1\right\}$ where $u(x, y)$ is a convex underestimator of $\frac{1}{x+\sum_{i=1}^n y_i}$ over the feasible region. If this convex underestimator is obtained without using the fact that variables are binary, as is typical in global optimization software, $u(x, y)$ would be chosen equal to $\frac{1}{x+\sum_{i=1}^n y_i}$ and the resulting factorable relaxation would therefore be non-polyhedral. Such a relaxation can be verified to be weaker than the relaxations that can be obtained from Corollary 4.10 and Theorem 4.11. To illustrate the difference, consider the special case $g(x, y) = \frac{x}{x+y}$. At the point $(1, 0.5)$, the factorable relaxation obtained without using integrality of the variables evaluates to $\frac{2}{3}$ while the relaxation of Corollary 4.10 obtained by defining $g(x, y) = 0$ when $x = 0$ evaluates to $\frac{3}{4}$, a value that can be computed after selecting $I = \{1\}$ and $l = 1$. Further, at the point $(0.5, 0.5)$, the factorable relaxation obtained without using integrality evaluates to $\frac{1}{2}$. The relaxation derived using Corollary 4.10 evaluates to $\frac{1}{4}$. However, the relaxation of Theorem 4.11 (in particular, $h^{S(0)}(x, y)$) evaluates to $\frac{1}{2}$ at this point. Finally, consider $(x, y) = \left(\frac{3}{4}, \frac{1}{2}\right)$. The factorable relaxation, and the relaxations obtained using Corollary 4.10 and Theorem 4.11 evaluate to $\frac{11}{20}$, $\frac{1}{2}$, and $\frac{5}{8}$ respectively. This example illustrates that, for this type of functions, Theorem 4.11 produces a relaxation that is tighter over W than the maximum of the underestimating functions obtained via the factorable relaxation and Corollary 4.10. Also, the relaxation of Corollary 4.10 is not directly comparable to the factorable relaxation since the former exploits the fact that the variables are binary whereas the latter exploits the fact that $x + \sum_{i=1}^n y_i \geq 1$. □

5 Conclusion

We studied the problem of developing convex and concave envelopes of nonlinear functions over subsets of a hyper-rectangle. In particular, we showed that the optimal value of a primal-dual pair of linear optimization problems yields the concave envelope when it has a polyhedral structure. We then showed that existence of polynomial-time separation algorithms for the concave envelopes of a set of functions imply polynomial-time separability for the concave envelope of the maximum of these functions.

Next, we showed that a result of [20] allows construction of concave envelopes of supermodular functions over a hyper-rectangle if the function is concave-extendable from the vertices of the hyper-rectangle. We generalized this construction to consider supermodular functions over a lattice family and demonstrated that this result yields simple derivations and extensions of results in the literature [5,8,22,27,31]. As a particular application, we constructed the concave envelope of the composition of a univariate convex function with a linear function, a structure commonly encountered when deriving convex relaxations of factorable programs.

We then showed that the convex envelope of certain functions that have a disjunctive property can be developed by convexifying their restrictions over carefully selected orthogonal disjunctions. As a consequence of this result, we developed convex envelopes for a variety of fractional and polynomial expressions over the unit hypercube. We then considered a convex function restricted to a nonconvex set. We derived an exclusion property that limits the subsets that need to be considered while evaluating the convex envelope outside the nonconvex set. We used this property to identify the polyhedral subdivision that characterizes the convex envelope of a symmetric function of binary variables that depends only on the cardinality of the set of binary variables that assume a value of one. This result generalizes some earlier results discovered in [31] and has other applications; see [6]. Then, we used these symmetric functions to define disjunctive functions, for which we derived convex envelopes by combining our previous results. This construction demonstrated that polyhedral subdivisions are naturally obtained by using our convexification scheme for disjunctive functions. Finally, we discussed applications of these disjunctive functions in building relaxations for the consistent biclustering problem described in [6].

The derivation of concave envelopes for nonconcave functions f yields ways to obtain convex relaxations for constraints of the form $f(x) \geq r$. Investigating the computational advantages that these new relaxations offer over those currently used in software implementations is an important direction of future research. On the theoretical side, investigating whether stronger relaxations of $f(x) \geq r$ can be obtained in closed-form is also a potentially fruitful avenue of research.

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