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Convex envelopes for edge-concave functions

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Abstract. Deterministic global optimization algorithms frequently rely on the convex underestimation of nonconvex functions. In this paper we describe the structure of the polyhedral convex envelopes of edge-concave functions over polyhedral domains using geometric arguments. An algorithm for computing the facets of the convex envelope over hyperrectangles in \mathbb{R}^3 is described. Sufficient conditions are described under which the convex envelope of a sum of edge-concave functions may be shown to be equivalent to the sum of the convex envelopes of these functions.

1. Introduction

Convex relaxation based, branch and bound algorithms are powerful approaches for the deterministic global optimization of nonconvex nonlinear and mixed integer nonlinear programming problems. A key factor influencing the convergence rate of these algorithms is the quality of the convex relaxations. The tightest underestimator of a nonconvex function over its domain is the convex envelope. An understanding of the structure of convex envelopes over hyperrectangles is therefore important for the development of branch and bound algorithms using hyperrectangular partitioning schemes.

In this paper we consider properties and representations of *vertex polyhedral convex envelopes*. A function $f : \mathbb{R}^n \supset X \rightarrow (-\infty, \infty]$ is said to be *polyhedral* if its epigraph is a polyhedral set in \mathbb{R}^{n+1} (Bertsekas et al., 2003) and *vertex polyhedral* if, furthermore, the vertices of the epigraph coincide with the vertices of the polyhedral domain X . Several classes of functions have been shown to have *vertex polyhedral* convex envelopes on certain domains, including concave functions over polytopes, and multilinear functions over hypercubes (Rikun, 1997). The multilinear functions are of particular interest in global optimization as many nonconvex NLPs may be reformulated as NLPs with univariate and multilinear constraint functions. Rikun (1997) observed that the convex envelope of a *smooth* function over a polytope is polyhedral if and only if the preimage of the vertices of the convex envelope coincides with a subset of the vertices of the domain. In the same paper a sufficient condition for the polyhedrality of the convex envelope, based on a form of local concavity, was introduced. Recently, Tardella (2003) showed that functions with *vertex polyhedral* convex envelopes may be recognized as having a property of *edge-concavity*. Further discussion of convex envelopes for lower

semi-continous functions appears in Tawarmalani and Sahinidis (2002). In the sequel we will refer to functions which have vertex polyhedral convex envelopes as *edge-concave*.

The following is a constructive characterisation of the convex envelope of an edge-concave function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ over a polytope $X := \text{conv}\{x^1, \dots, x^m\} \subset \mathbb{R}^n$ (Horst and Tuy, 1993; Floudas, 2000),

$$\text{convenv}(f, X) \Big|_x = \begin{cases} \min_{\lambda \in \mathbb{R}^m} \sum_{i=1}^m \lambda_i f(x^i) \\ \text{subject to} \\ \sum_{i=1}^m \lambda_i x^i = x \\ \sum_{i=1}^m \lambda_i = 1 \\ \lambda_i \geq 0 \quad \text{for all } i = 1, \dots, m. \end{cases} \tag{1}$$

Here we use $\text{conv}(\cdot)$ to denote the convex hull of a set, $\text{convenv}(f, X)$ for the convex envelope of f over X and $\text{convenv}(f, X) \Big|_x$ to denote the function $\text{convenv}(f, X)$ evaluated at a point $x \in X$. Note that when X is a full dimensional hyperrectangle m equals 2^n , therefore this characterization of the convex envelope requires an exponential number of λ variables. In some cases there is a more efficient way of characterizing the convex envelope than representation (1).

A *separable* function $f : \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_t} \rightarrow \mathbb{R}$ is a sum $f := \sum_{i=1}^t f_i$ where the domains of the respective f_i 's are orthogonal subspaces, $f_i : \mathbb{R}^{n_i} \rightarrow \mathbb{R}$. The convex envelope of a separable function f over the domain $X := X_1 \times \dots \times X_t$ may be decomposed into a sum of convex envelopes (Horst and Tuy, 1993; Floudas, 2000),

$$\text{convenv}(f, X) = \sum_{i=1}^t \text{convenv}(f_i, X_i).$$

A more general case applies to summations in which $f := \sum_{i=1}^t f_i$ where the domain of each f_i is itself a Cartesian product, $f_i : X_0 \times X_i \rightarrow \mathbb{R}$, and X_0 is a simplex (Rikun, 1997),

$$\text{convenv}(f, X_0 \times \dots \times X_t) = \sum_{i=1}^t \text{convenv}(f_i, X_0 \times X_i).$$

This result has found application when X_0 is a line segment, $X_0 \subset \mathbb{R}$, (Tawarmalani et al., 2002).

An alternative means of characterizing a polyhedral convex envelope is through a system of facet defining hyperplanes. Such formulae have been developed for bilinear functions over hyperrectangles (McCormick, 1976; Al-Khayyal and Falk, 1983); bilinear functions over certain quadrilaterals (Sherali and Alameddine, 1992); special forms of multilinear functions over unit hypercubes and special discrete sets (Sherali, 1997); and for trilinear monomials over hyperrectangles (Meyer and Floudas, 2003, 2004). Although one may derive these facets by projecting the representation (1) onto X this computation is in general highly complex.

Hyperrectangles are used extensively in the domain partitioning schemes of branch and bound algorithms for global optimization. The *number of simplices* contained in the *triangulations* of hyperrectangles in \mathbb{R}^n gives us an indication of the *number of facets* defining the convex envelopes of edge-concave functions in \mathbb{R}^n . As the volume of a simplex in the unit hypercube $[0, 1]^n$ is an integral multiple of $\frac{1}{n!}$ the maximal number of simplices in a triangulation of $[0, 1]^n$ is less than $n!$, and indeed triangulations of this size may easily be determined (Haiman, 1991). Several papers have addressed issues related to the determination of *minimal* triangulations of a hypercube in \mathbb{R}^n for small n (Mara, 1976; Cottle, 1982; Sallee, 1982; Lee, 1985; Hughs, 1994; Hughes and Anderson, 1999; Smith, 2000). For n in the range 1 to 7 the exact sizes of the minimal triangulations of $[0, 1]^n$ are 1, 2, 5, 16, 67, 308, and 1493. The minimal triangulation of $[0, 1]^7$ was determined computationally by Hughes and Anderson (1999) using CPLEX to solve a large scale linear programming problem with 1, 456, 218 variables. It follows that, in general, the number of facets required to represent the convex envelope of an edge-concave function grows super-exponentially. Nevertheless, in certain instances (see Example 5), due to redundancy, only $O(n)$ facets may be required to represent the convex envelope.

The remainder of this paper is structured as follows. In Section 2, a characterization of the facets of polyhedral convex envelopes is presented using concepts from combinatorial geometry. An efficient way of generating the *facets* of the convex envelope of an edge-concave function over a box in \mathbb{R}^3 is described in Section 3. In Section 4, these insights lead us to an understanding of the properties that allow a convex envelope to be represented as a sum of convex envelopes. The paper is concluded in Section 5.

2. Geometry of facet defining hyperplanes

In this section, the geometry of facet defining hyperplanes is interpreted using concepts from combinatorial geometry. In particular, the notion of a *minimal affine dependency* is used to interpret the combinatorial structure of the graph of a function on the vertices of a polyhedron. A good introduction to these topics can be found in Ziegler (1994), Chapter 6. See the book by Björner et al. (1993) for more information on the combinatorial interpretation of polyhedra.

Let $X = \{x^1, \dots, x^n\} \subseteq \mathbb{R}^d$ be a set of n points in \mathbb{R}^d which affinely span \mathbb{R}^d . To simplify notation, X may be interpreted as a matrix composed of the columns $\{x^1, \dots, x^n\}$. The *affine dependencies* of X are the vectors $\lambda \in \mathbb{R}^n$ with $\sum_{i=1}^n \lambda_i = 0$ such that $\sum_{i=1}^n \lambda_i x^i = 0$. There is a clear geometric interpretation of affine dependencies. Let $\lambda \neq 0$ be an affine dependency and consider the positive and negative components of λ , which are denoted $P(\lambda) = \{i : \lambda_i > 0\}$ and $N(\lambda) = \{i : \lambda_i < 0\}$. Note that $\sum_{i \in P(\lambda)} \lambda_i = -\sum_{i \in N(\lambda)} \lambda_i = \Lambda$. From this we get

$$x^* := \sum_{i \in P(\lambda)} \frac{\lambda_i}{\Lambda} x^i = - \sum_{i \in N(\lambda)} \frac{\lambda_i}{\Lambda} x^i. \quad (2)$$

Observe that x^* is a point that lies within the convex hull defined by the positive coefficients as well as that defined by the negative coefficients,

$$x^* \in \text{conv}\{x_i : i \in P(\lambda)\} \cap \text{conv}\{x_i : i \in N(\lambda)\}. \tag{3}$$

Minimal affine dependencies are affine dependencies of nonempty point sets where every proper subset is affinely independent. The *support* of a vector is defined as the set of nonzero components. Minimal affine dependencies are therefore affine dependencies with inclusion-minimal supports. Geometrically the sets defined by positive and negative components of the minimal dependencies, $\text{conv}\{x^i : i \in P(\lambda)\}$ and $\text{conv}\{x^i : i \in N(\lambda)\}$, are simplices with relative interiors intersecting at a unique point x^* . These point configurations are known as *minimal Radon partitions* from Radon’s Theorem (see Ziegler (1994)) or *circuits* borrowing terminology from oriented matroid theory (Björner et al., 1993). We shall refer to points which lie in the intersection of the two simplices of a circuit as *circuit intersection points*. The set of circuit intersection points of X is denoted by $S(X)$.

Example 1. In Figure 1 the vertices of the regular pentagon are labelled $\{x^1, \dots, x^5\}$, where

$$x^i := \left(\cos\left(\frac{(0.5 - 2i)\pi}{5}\right), \sin\left(\frac{(0.5 - 2i)\pi}{5}\right) \right).$$

In this figure the set of circuit intersection points $S(X)$ is $\{y^1, \dots, y^5\}$ where

$$y^i := \lambda x^{1+i \bmod 5} + (1 - \lambda)x^{1+(i+2) \bmod 5},$$

and $\lambda := (2\cos(\frac{\pi}{5}))^{-2}$. The expression $a \bmod b$ where a and b are integers refers to the remainder upon dividing a by b . The *circuits* of $X := \{x^1, \dots, x^5\}$ are $\{x^1, x^3, x^2, x^4\}$, $\{x^2, x^4, x^3, x^5\}$, $\{x^3, x^5, x^4, x^1\}$, $\{x^4, x^1, x^5, x^2\}$, and $\{x^5, x^2, x^1, x^3\}$.

The following result (Ziegler, 1994, Lemma 6.7.), follows from Carathéodory’s Theorem.

Lemma 1. *Let $U \subseteq \mathbb{R}^n$ be a vector subspace of dimension r . Any vector $u \in U$ can be written as a finite sum $u = u' + u'' + \dots + u^k$ of $k \leq r$ vectors $u^i \in U$, where each u^i has a minimal nonempty support in U , and the j th component u^i_j is either zero or has the same sign as u_j .*

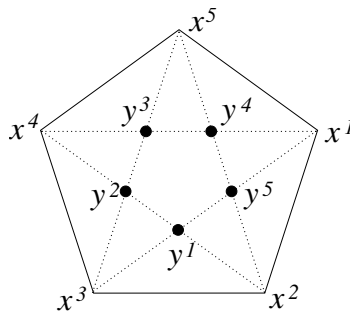


Fig. 1. Circuit intersection points of the regular pentagon

As a consequence of this lemma any affine dependency may be written as a sum of sign consistent *minimal* affine dependencies.

A d -simplex is the convex hull of any $d + 1$ affinely independent points in some \mathbb{R}^n ($n \geq d$). A 1-simplex is therefore a line, a 2-simplex is a triangle and so on. The following lemma asserts that a vertex of the intersection of two simplices with vertices in convex position is either a circuit intersection point or a vertex common to both simplices.

Lemma 2. *Let $\Delta^k := \{v_1^k, \dots, v_{d+1}^k\} \subset \mathbb{R}^d$ be a set of points spanning \mathbb{R}^d so that the convex hull $\text{conv}(\Delta^k)$ is a d -simplex. The intersection of two simplices is equivalent to the convex hull of the circuit intersection points:*

$$\text{conv}(\Delta^1) \cap \text{conv}(\Delta^2) = \text{conv}(S(\Delta^1 \cup \Delta^2)),$$

where $S(\Delta^1 \cup \Delta^2)$ is the set of circuit intersection points of $\Delta^1 \cup \Delta^2$.

Proof. There is a one-to-one mapping between the points in $\text{conv}(\Delta^1) \cap \text{conv}(\Delta^2)$ and the affine dependencies of $\Delta^1 \cup \Delta^2$. These affine dependencies may, in turn, be expressed as sums of minimal affine dependencies. See Meyer (2004) for further details.

A *triangulation* of the point configuration X is a set of d -simplices $\{\Delta^1, \dots, \Delta^m\}$ with the following properties:

1. the vertices of $\text{conv}(\Delta^i)$ are vertices of X ,
2. two simplices $\text{conv}(\Delta^i)$ and $\text{conv}(\Delta^j)$, $i \neq j$, have no interior point in common,
3. the union of simplices, $\text{conv}(\Delta^1) \cup \dots \cup \text{conv}(\Delta^m)$, equals the convex hull $\text{conv}(X)$,
4. the intersection $\text{conv}(\Delta^i) \cap \text{conv}(\Delta^j)$, $i \neq j$, is a face of both $\text{conv} \Delta^i$ and $\text{conv} \Delta^j$.

The next proposition tells us how the minimal affine dependencies of a convex polytope $\text{conv}(X)$ can be used to determine the convex envelope of an edge-concave function f over $\text{conv}(X)$ by means of a *triangulation* of X .

Proposition 1. *Let $X := \{x^1, \dots, x^n\}$ be the set of vertices of a convex polytope in \mathbb{R}^d , and let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be an edge-concave function on $\text{conv}(X)$. Let T be a triangulation of X and let $L_T : \text{conv}(X) \rightarrow \mathbb{R}$ be the following piecewise affine function defined by T :*

$$L_T(x) := \sum_{i=1}^{d+1} \lambda_i f(x^{(i)})$$

where $\lambda \in \mathbb{R}^{d+1}$

$$0 \leq \lambda_i \leq 1 \text{ for all } i = 1, \dots, d + 1, \quad \sum_{i=1}^{d+1} \lambda_i = 1$$

and $x = \sum_{i=1}^{d+1} \lambda_i x^{(i)}$, for some $\{x^{(1)}, \dots, x^{(d+1)}\} \in T$. L_T is the convex envelope $\text{convenv}(f, X)$ if and only if

$$\sum_{i \in P(\lambda)} \lambda_i f(x^i) \leq - \sum_{i \in N(\lambda)} \lambda_i f(x^i) \tag{4}$$

for all minimal affine dependencies λ where

$$\{x^i : i \in P(\lambda)\} \subseteq \Delta' \in T \tag{5}$$

and

$$\{x^i : i \in N(\lambda)\} \subseteq \Delta'' \notin T. \tag{6}$$

Proof. Assume T is such that condition (4) holds for all minimal affine dependencies for which the inclusions (5) and (6) apply. Suppose that $L_T(x)$ is not a convex function. Then from Carathéodory’s theorem and the definition of convexity there is a $\rho \in \mathbb{R}^{d+1}$, where $\rho \geq 0$, $\sum_{i=1}^{d+1} \rho_i = 1$, and a $\Delta := \{x^{(1)}, \dots, x^{(d+1)}\} \subseteq X$ such that

$$L_T \left(\sum_{i=1}^{d+1} \rho_i x^{(i)} \right) > \sum_{i=1}^{d+1} \rho_i L_T(x^{(i)})$$

Now $x^* := \sum_{i=1}^{d+1} \rho_i x^{(i)}$ lies in some simplex $\text{conv}(\Delta')$, $\Delta' \in T$ therefore $L_T(x^*)$ is a convex combination of f evaluated at the vertices of the simplex $\text{conv}(\Delta')$,

$$L_T(x^*) := \sum_{i=1}^{d+1} \lambda'_i f(x'^{(i)}).$$

The sets $\Delta' := \{x'^{(1)}, \dots, x'^{(d+1)}\}$ and $\Delta := \{x^{(1)}, \dots, x^{(d+1)}\}$ are the vertices of two simplices $\text{conv}(\Delta')$ and $\text{conv}(\Delta)$ and x^* lies in the intersection of these simplices, $x^* \in \text{conv}(\Delta) \cap \text{conv}(\Delta')$. Therefore x^* can be written as a convex combination of the vertices of $\text{conv}(\Delta) \cap \text{conv}(\Delta')$ which from Lemma 2 are also circuit intersection points. A contradiction then arises as we have assumed that condition (4) holds.

Assume L_T is the convex envelope but

$$\sum_{i \in P(\lambda)} \lambda_i f(x^i) > - \sum_{i \in N(\lambda)} \lambda_i f(x^i)$$

for some minimal affine dependency λ associated with a circuit $(\Delta' \cup \Delta'')$ where $\Delta' = \{x^i : i \in P(\lambda)\} \in T$ and $\Delta'' = \{x^i : i \in N(\lambda)\} \notin T$. From convexity we get

$$L_T \left(\sum_{i \in P(\lambda)} \lambda_i f(x^i) \right) \leq - \sum_{i \in N(\lambda)} \lambda_i f(x^i)$$

But $L_T \left(\sum_{i \in P(\lambda)} \lambda_i f(x^i) \right) = \sum_{i \in P(\lambda)} \lambda_i f(x^i)$ which leads to a contradiction and completes the proof.

Let X be a finite set of points in \mathbb{R}^d , and $f : \text{conv}(X) \rightarrow \mathbb{R}$ an edge-concave function. A set of affinely independent points $X' \subset X$ is said to be *dominated* if there exists a minimal affine dependency λ such that

$$\sum_{i \in P(\lambda)} \lambda_i f(x^i) > - \sum_{i \in N(\lambda)} \lambda_i f(x^i)$$

and $\{x^i : i \in P(\lambda)\} \subseteq X'$. If no such λ exists, X' is said to be *nondominated*. If every minimal affine dependency λ for which $\{x^i : i \in P(\lambda)\} \subseteq X'$ is such that

$$\sum_{i \in P(\lambda)} \lambda_i f(x^i) < - \sum_{i \in N(\lambda)} \lambda_i f(x^i) \quad (7)$$

then X' is a *dominant* subset of X . We will use the notation $\mathcal{D}^0(f, X)$ and $\mathcal{D}^+(f, X)$ to denote, respectively, the sets of all *nondominated* and *dominant* subsets of X . To denote the related sets of minimal affine dependencies we use the notation,

$$\begin{aligned} \hat{\mathcal{D}}^0(f, X) &:= \{\lambda \in \mathcal{A}(X) : P(\lambda) \subseteq \mathcal{D}^0(f, X)\} \\ \hat{\mathcal{D}}^+(f, X) &:= \{\lambda \in \mathcal{A}(X) : P(\lambda) \subseteq \mathcal{D}^+(f, X)\}. \end{aligned}$$

where $\mathcal{A}(X)$ is the set of all minimal affine dependencies of X . Proposition 1 describes the polyhedral convex envelope of a function in terms of a piecewise affine function with domains of linearity corresponding to simplices with maximal *nondominated* vertex sets. It is understood that these terms define properties of X relative to f not properties of X itself.

A dominance relation between signed subsets of a circuit is said to be *strict* if either $\sum_{i \in P(\lambda)} \lambda_i f(x^i) > - \sum_{i \in N(\lambda)} \lambda_i f(x^i)$ or $\sum_{i \in P(\lambda)} \lambda_i f(x^i) < - \sum_{i \in N(\lambda)} \lambda_i f(x^i)$, where λ is the minimal affine dependency associated with that circuit. When all nondominated subsets are also dominant, the triangulation defining the convex envelope of f is *unique*. When this is not the case the convex envelope defining triangulation may not be unique. Note that small perturbations ϵ^i may be added to $f(x^i)$ to ensure that all dominance relations are strict and that all nondominated subsets of X are dominant. If each ϵ^i is so small that the directions of the strict dominance relations of the original function f are unaltered then the unique triangulation T defining the convex envelope of the perturbed function also defines the convex envelope of f .

Example 2. Consider X , the vertex set of the regular pentagon in Figure 2, and let $f : \text{conv}(X) \rightarrow \mathbb{R}$ be an edge-concave function such that $f(x^i) := i$. Proposition 1 provides the necessary and sufficient conditions to define the convex envelope, $\text{conv}(f, X)$. The following inequality describes the dominance relationships in Proposition 1:

$$\begin{aligned} \lambda f(x^1) + (1 - \lambda) f(x^3) &< \lambda f(x^2) + (1 - \lambda) f(x^5) \\ \lambda f(x^3) + (1 - \lambda) f(x^1) &< \lambda f(x^2) + (1 - \lambda) f(x^4) \\ \lambda f(x^1) + (1 - \lambda) f(x^4) &< \lambda f(x^5) + (1 - \lambda) f(x^2) \\ \lambda f(x^4) + (1 - \lambda) f(x^1) &< \lambda f(x^5) + (1 - \lambda) f(x^3) \end{aligned}$$

The maximal *nondominated* subsets of $X = \{x^1, \dots, x^5\}$ are $\{x^1, x^2, x^3\}$, $\{x^1, x^3, x^4\}$, and $\{x^1, x^4, x^5\}$. $\mathcal{D}^0(f, X)$ contains these sets and all subsets thereof.

The triangulation T shown in Figure 2 satisfies the conditions in Proposition 1 and the associated piecewise affine function $L_T(x)$ is the convex envelope of the point set.

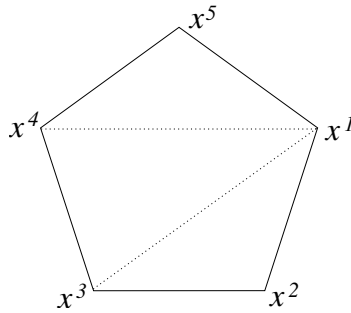


Fig. 2. A triangulation of the regular pentagon

3. Algorithm for facet determination

This section describes a procedure to determine the complete set of facets defining the convex envelope of a function $f : \text{conv}(V) \mapsto \mathbb{R}$ where f has a polyhedral convex envelope and V is the set of vertices of a hyperrectangle in \mathbb{R}^3 . In Section 2 it was shown that there is a relationship between the nondominated signed subsets of the circuits and a triangulation of the hyperrectangle. The cells of the triangulation in turn define the facets of the convex envelope of f . The procedure for determining the facets is based on these ideas and involves the following steps.

- Step 1: Calculate the function values at vertices of the hyperrectangle and determine the nondominated subsets of V .
- Step 2: Determine the triangulation type.
- Step 3: Determine the transformation from the representative triangulation to the current triangulation.
- Step 4: Calculate the facet defining hyperplanes from the cells of the current triangulation.

Each of these steps is discussed below.

3.1. Step 1: dominance relations

The function f is evaluated at each of the vertex points v^i and the dominant subsets are determined. In cases where neither signed subset of a circuit strictly dominates the other, the tie is broken in a way that is consistent with previous tie breaks. In other words the sets $\mathcal{D}^0(f, V)$ and $\mathcal{D}^+(f, V)$ are determined and if $\mathcal{D}^0(f, V) \neq \mathcal{D}^+(f, V)$ a small ϵ^i ($\epsilon^i < \min\{\sum \lambda_j f(v^j) \neq 0\}$) is added to each $f(v^i)$ to produce a perturbed function f' in such a way that $\mathcal{D}^0(f', V) = \mathcal{D}^+(f', V)$ and $\mathcal{D}^+(f, V) \subseteq \mathcal{D}^+(f', V)$.

3.2. Step 2: triangulation class

Up to reorientation the 3-cube can be triangulated in six different ways, which we will refer to as triangulation types. *Standard representatives* of these six types are depicted in Figure 3.

Cell	Vertices	Figure	Vertices	Figure
		Type A		Type B
1	1 2 3 5		1 2 4 8	
2	4 6 7 8		1 2 6 8	
3	2 3 5 7		1 5 6 8	
4	2 4 6 7		1 5 7 8	
5	2 5 6 7		1 3 7 8	
6	2 3 4 7		1 3 4 8	
		Type C		Type D
1	1 2 3 5		1 2 3 5	
2	2 3 5 4		2 3 5 7	
3	2 4 5 6		2 5 6 7	
4	4 5 6 8		2 6 7 8	
5	4 5 7 8		2 3 4 8	
6	3 4 5 7		2 3 7 8	
		Type E		Type F
1	1 2 3 5		1 2 3 8	
2	2 3 5 8		1 2 5 8	
3	2 3 4 8		1 3 5 8	
4	2 5 6 8		2 5 6 8	
5	3 5 7 8		3 5 7 8	
6			2 3 4 8	

Fig. 3. Triangulation types of the 3-cube

Figure 3 identifies the vertices of the triangulation cells in the figures. For example, the first row of Figure 3 describes cell 1 of the standard representative of triangulation type **A** as having the vertices 1, 2, 3 and 5. Notice that each of the triangulations has six cells, except Type **E**, which has five.

One way of classifying the triangulations is by counting the number *dominant diagonals* incident with each vertex. In Figure 3 the dominant diagonals are the edges of the cells which are not edges of the hyperrectangle. In triangulation **A**, for example, no dominant diagonals are incident with vertex 1, three dominant diagonals are incident with vertex 2, two dominant diagonals are incident with vertex 3, and so on. The number of dominant diagonals incident with each vertex is summarized in Table 1 for all triangulations. If we then count the number of occurrences of 0,1,2,3, and 4 in each of the rows we see that each of the triangulations can be uniquely identified in this way. For example type **A** is the only type with four 2's and type **B** is the only type with six

Type	Vertices							
	1	2	3	4	5	6	7	8
A	0	3	2	2	2	2	3	0
B	4	1	1	1	1	1	1	4
C	0	2	2	3	4	1	1	1
D	0	4	3	0	2	1	2	2
E	0	3	3	0	3	0	0	3
F	1	3	3	0	3	0	0	4

Table 1. Number of dominant diagonals incident with vertices

1’s. Step 2, therefore, involves counting the number of dominant diagonals incident with each vertex and comparing the pattern with those in Table 1.

3.3. Step 3: reorientation

Having found the triangulation type, we need to know how the *standard* triangulation of type s , T^s , is related to the triangulation T^* defining the convex envelope of f over V . That is, we wish to find a *linear transformation* mapping T^s onto T^* . To do this, a 3-tuple of linearly independent points in the standard representative T^s is identified with a 3-tuple of points in the current instance T^* .

Notice, in Figure 3 (a), for example, there are only two vertices, 2 and 7, with three incident diagonals. *Adjacent* to vertex 2 there are exactly two vertices, 4 and 6, with two incident dominant diagonals. Due to symmetry, (2, 4, 6) is equivalent to (7, 5, 3), moreover, points 2, 4, and 6 are linearly independent. For type **A** triangulations we can reorient the standard representative by matching vertices v^2, v^4 , and v^6 with \tilde{v}^1, \tilde{v}^2 and \tilde{v}^3 where \tilde{v}^1 is a vertex with three incident diagonals and \tilde{v}^2 and \tilde{v}^3 are adjacent to \tilde{v}^1 and each have two incident diagonals. The vertices used to reorient the standard triangulations are summarized in Table 2.

Columns 2 to 4 of this table identify the vertices of the standard triangulation as depicted in Figure 3. Columns 5 to 7 indicate the number of dominant diagonals incident with the matching vertices. If the vertices in columns 6 and 7 are, in addition, required to be adjacent to the vertex in column 5 this is indicated by a star. Consider Figures 4 (a) and (b) for example. The triangulation depicted in Figure 4 (a) is the standard type **A** triangulation. In Figure 4 (b) the same triangulation is represented in a different orientation. In both Figures 4 (a) and (b) the white dots are vertices with three incident diagonals and the black dots are the only vertices adjacent to the white dots with exactly two incident diagonals. Identifying vertices v^2, v^4 and v^6 in Figure 4 (a) with vertices $v^{5'}, v^{7'}$ and $v^{1'}$ in Figure 4 (b) we see that T^A may be rotated to coincide with T^* .

To determine the reorientation it is convenient to consider the mapping of the cube $C := [-1, 1]^3$ onto itself. Let the linearly independent identifying vertices of T^s be the columns of the matrix $X^s \in \mathbb{R}^{3 \times 3}$. In a similar way, let the columns of $X^* \in \mathbb{R}^{3 \times 3}$ be associated with the three identifying vertices of T^* . Let a matrix $L \in \mathbb{R}^{3 \times 3}$ relate X^s and X^* :

$$X^* = L(X^s).$$

Type	standard			identity		
A	2	4	6	3	2*	2*
B	1	2	3	4	1*	1*
C	1	2	3	0	2	2
D	6	2	5	1	4	2*
E	1	4	6	0	0	0
F	1	4	6	1	0	0

Table 2. Identifying vertices

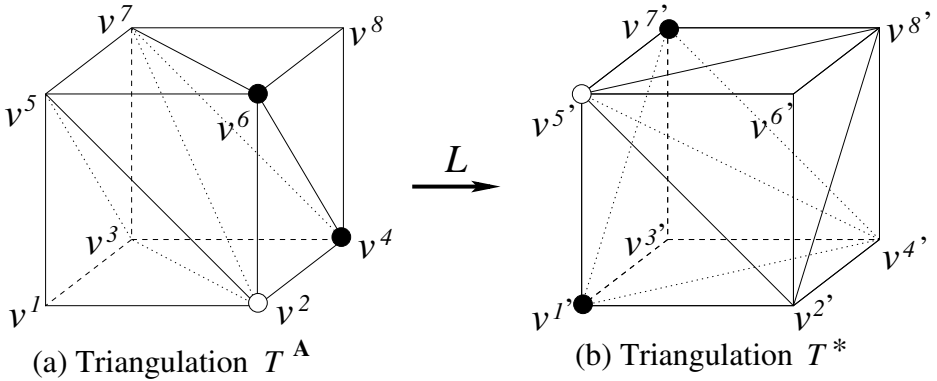


Fig. 4. Illustration of reorientation

Using L any vertex v' of C in triangulation T^s can be matched with the corresponding vertex v'' of C in triangulation T^* :

$$v'' = Lv'.$$

3.4. Step 4: compute facets

Using the transformation in step 3 each vertex in T^s is identified with a vertex in T^* . As a result, each cell of the triangulation T^s can be associated with a cell in T^* . In other words there is a one to one map,

$$T^s \ni \Delta_i^s \mapsto \Delta_i^* \in T^*.$$

The facet defining hyperplane, $w = \langle \pi^{\Delta_i^*}, x \rangle + \pi_0^{\Delta_i^*}$, associated with a cell of the current triangulation, $\Delta_i^* \in T^*$, can now be determined through the solution of a system of linear equations,

$$\begin{bmatrix} 1 & v_1^{i_1} & v_2^{i_1} & v_3^{i_1} \\ 1 & v_1^{i_2} & v_2^{i_2} & v_3^{i_2} \\ 1 & v_1^{i_3} & v_2^{i_3} & v_3^{i_3} \\ 1 & v_1^{i_4} & v_2^{i_4} & v_3^{i_4} \end{bmatrix} \begin{bmatrix} \pi_0^{\Delta_i^*} \\ \pi_1^{\Delta_i^*} \\ \pi_2^{\Delta_i^*} \\ \pi_3^{\Delta_i^*} \end{bmatrix} = \begin{bmatrix} f(v^{i_1}) \\ f(v^{i_2}) \\ f(v^{i_3}) \\ f(v^{i_4}) \end{bmatrix},$$

in which $\{v^{i_1}, v^{i_2}, v^{i_3}, v^{i_4}\} := \Delta_i^*$.

Example 3. To illustrate this process, consider the optimization problem from Sherali and Adams (1999), Chapter 7,

$$\begin{aligned} & \min f_1 + f_2 + f_3 + f_4 \\ & \text{subject to} \\ & \quad -4x_1 - 3x_2 - x_3 \geq -20 \\ & \quad \quad x_1 + 2x_2 + x_3 \geq 1 \end{aligned} \tag{8}$$

$$2 \leq x_1 \leq 5, 0 \leq x_2 \leq 10, 4 \leq x_3 \leq 8$$

where

$$\begin{aligned} f_1 &= x_1 x_2 x_3 - 2x_1 x_2 - 3x_1 x_3 + 5x_2 x_3 \\ f_2 &= -x_3^2 \\ f_3 &= x_1^2 \\ f_4 &= 5x_2 + x_3 \end{aligned}$$

In this problem f_1 is multilinear, f_2 is univariate concave, f_3 is convex and f_4 is linear. Here we focus on the construction of the convex envelope of f_1 .

Step 1

The function is evaluated at all vertices of the hyperrectangle $[2.0, 5.0] \times [0.0, 10.0] \times [4.0, 8.0]$:

$$\begin{aligned} f^1 &= f_1(\underline{x}_1, \underline{x}_2, \underline{x}_3) = -24 & f^5 &= f_1(\underline{x}_1, \underline{x}_2, \overline{x}_3) = -48 \\ f^2 &= f_1(\overline{x}_1, \underline{x}_2, \underline{x}_3) = -60 & f^6 &= f_1(\overline{x}_1, \underline{x}_2, \overline{x}_3) = -120 \\ f^3 &= f_1(\underline{x}_1, \overline{x}_2, \underline{x}_3) = 216 & f^7 &= f_1(\underline{x}_1, \overline{x}_2, \overline{x}_3) = 472 \\ f^4 &= f_1(\overline{x}_1, \overline{x}_2, \underline{x}_3) = 240 & f^8 &= f_1(\overline{x}_1, \overline{x}_2, \overline{x}_3) = 580. \end{aligned}$$

The dominance relations between the complementary sets of the circuits of X are determined. Using an overline to indicate the dominant signed subsets, the relationships between *diagonals* on the facets of the hyperrectangle are,

$$\{\overline{1, 6}, 2, 5\}, \{1, 4, \overline{2, 3}\}, \{1, 7, \overline{3, 5}\}, \{2, 8, \overline{4, 6}\}, \{3, 8, \overline{4, 7}\}, \{5, 8, \overline{6, 7}\}.$$

For example, $\lambda = (1, -1, 0, 0, -1, 1, 0, 0)$ is a minimal affine dependency between two pairs of vertices on a facet of the hyperrectangle. $f^1 + f^6 = -144$ is less than $f^2 + f^5 = -108$, therefore, the signed subset $\{1, 6\}$ dominates the subset $\{2, 5\}$. We write $\{\overline{1, 6}, 2, 5\}$ to show this relationship.

A single long diagonal dominates the others,

$$\{\overline{3, 6}, 1, 8\}, \{\overline{3, 6}, 2, 7\}, \{\overline{3, 6}, 4, 5\}.$$

The dominant long diagonal, $\{3, 6\}$, is not dominated by either of the corner slicing simplices,

$$\begin{aligned} (2f^3 + f^6) &= 312 < (f^1 + f^4 + f^7) = 688 \implies \overline{3, 6}, 1, 4, 7 \\ (f^3 + 2f^6) &= -24 < (f^2 + f^5 + f^8) = 472 \implies \overline{3, 6}, 2, 5, 8. \end{aligned}$$

Note that in this case the nondominated and dominant sets coincide and

$$\mathcal{D}^+(f, X) = \{\{1, 6\}, \{2, 3\}, \{3, 5\}, \{4, 6\}, \{4, 7\}, \{6, 7\}, \{3, 6\}\}.$$

Step 2

The number of dominant diagonals incident with each vertex can be summarized as follows:

vertex	1	2	3	4	5	6	7	8
number	1	1	3	2	1	4	2	0

One vertex has no *incident diagonals*, three vertices have one, two vertices have two, one vertex has three, and one vertex has four incident diagonals. Comparing this pattern to those in Table 1 we find that the current triangulation is of type **C**.

Step 3

Vertex 1 of the standard type **C** triangulation T^C matches the vertex of T^* with no incident diagonals, vertex 8. T^C vertex 2 matches a T^* vertex with two incident diagonals, vertex 4, and symmetrically T^C vertex 3 matches the other T^* vertex with two incident diagonals, vertex 7.

$$L = X^*(X^C)^{-1} = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \end{bmatrix}^{-1} = \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$$

Using L we find that the vertices $\{1, 2, \dots, 8\}$ of triangulation T^C map onto the vertices $\{8, 4, 7, 3, 6, 2, 5, 1\}$ of triangulation T^* .

Step 4

Now each cell Δ_i^* of triangulation T^* is the image under L of some cell Δ_i^C of the triangulation T^C . The cells of T^C may be looked up in Figure 3 and mapped onto the cells of T^* as follows,

$$\begin{aligned} \Delta_1^C &:= \{x^1, x^2, x^3, x^5\} \xrightarrow{L} \{x^8, x^4, x^7, x^6\} := \Delta_1^* \\ \Delta_2^C &:= \{x^2, x^3, x^5, x^7\} \xrightarrow{L} \{x^4, x^7, x^6, x^3\} := \Delta_2^* \\ \Delta_3^C &:= \{x^2, x^4, x^5, x^6\} \xrightarrow{L} \{x^4, x^3, x^6, x^2\} := \Delta_3^* \\ \Delta_4^C &:= \{x^4, x^5, x^6, x^8\} \xrightarrow{L} \{x^3, x^6, x^2, x^1\} := \Delta_4^* \\ \Delta_5^C &:= \{x^4, x^5, x^7, x^8\} \xrightarrow{L} \{x^3, x^6, x^5, x^1\} := \Delta_5^* \\ \Delta_6^C &:= \{x^3, x^4, x^5, x^7\} \xrightarrow{L} \{x^7, x^3, x^6, x^5\} := \Delta_6^*. \end{aligned}$$

Equations defining the facets of the convex envelope of f over X are then computed by solving a system of linear equations for each cell.

The facets associated with the cells Δ_k^* , $k = \{1, 2, \dots, 6\}$, are defined by systems of linear equations. Solving these equations we get,

$$\begin{aligned} \pi^{\Delta_1^*} &= [-980.0, 36.0, 70.0, 85.0] \\ \pi^{\Delta_2^*} &= [-672.0, 8.0, 61.6, 64.0] \\ \pi^{\Delta_3^*} &= [-40.0, 8.0, 30.0, -15.0] \\ \pi^{\Delta_4^*} &= [-60.0, -12.0, 24.0, -15.0] \\ \pi^{\Delta_5^*} &= [48.0, -24.0, 24.0, -6.0] \\ \pi^{\Delta_6^*} &= [-512.0, -24.0, 52.0, 64.0]. \end{aligned}$$

The following is a convex relaxation of Problem 8:

$$\begin{aligned} &\min w_1 + w_2 + f_3 + f_4 \\ \text{subject to} & \\ &w_1 \geq \pi^{\Delta_k^*}(1, x_1, x_2, x_3)^\top \quad \text{for all } k = 1, \dots, 6 \\ &w_2 \geq -x_3^2 + (-x_3^2 + x_3^2) \frac{x_3 - x_3}{x_3 - x_3} \\ &-4x_1 - 3x_2 - x_3 \geq -20 \\ &x_1 + 2x_2 + x_3 \geq 1 \\ &2 \leq x_1 \leq 5, 0 \leq x_2 \leq 10, 4 \leq x_3 \leq 8. \end{aligned}$$

This problem has an optimal solution of -119 which is identical to the global solution to (8). Serali and Adams (1999) report a solution of -120 for a linear convex relaxation of the problem derived by the Reformulation Linearization Technique.

4. Decompositions of convex envelopes of sums

This section describes conditions under which the convex envelope of a sum of edge-concave functions can be decomposed into the sum of convex envelopes of the summands. Consider three polytopes $X \subset \mathbb{R}^m$, $Y \subset \mathbb{R}^n$ and $Z \subset \mathbb{R}^p$. Let $g : X \times Y \rightarrow \mathbb{R}$ and $h : X \times Z \rightarrow \mathbb{R}$ be edge-concave functions and let $f : X \times Y \times Z \rightarrow \mathbb{R}$ be the sum of g and h . Here we investigate conditions under which

$$\text{convex}(f, X \times Y \times Z) = \text{convex}(g, X \times Y) + \text{convex}(h, X \times Z).$$

These conditions are based on relationships between the projections of triangulations of $X \times Y$ and $X \times Z$ onto X . It is shown that if the convex envelope defining triangulations of a pair of functions g and h project onto a common triangulation of the x -space, the convex envelope of the sum $g + h$ can be decomposed into the sum of convex envelopes of g and h .

It is well known that the convex envelope of f is equivalent to the sum of the convex envelopes of g and h when g and h are *separable*, that is when X is empty. This is also true when X is a simplex in \mathbb{R}^m (Rikun, 1997).

Lemma 3. *Let $X \subset \mathbb{R}^m$, $Y \subset \mathbb{R}^n$, and $Z \subset \mathbb{R}^p$ be vertex sets of three convex polytopes. Define the edge-concave functions $g : X \times Y \rightarrow \mathbb{R}$, $h : X \times Z \rightarrow \mathbb{R}$ and $f := g + h : X \times Y \times Z \rightarrow \mathbb{R}$. If X is a simplex the convex envelope of f can be decomposed into the sum of the convex envelopes of g and h ,*

$$\text{convex}(f, X \times Y \times Z) = \text{convex}(g, X \times Y) + \text{convex}(h, X \times Z).$$

In many applications in global optimization relaxations of convex envelopes are constructed over hyperrectangles. In Proposition 2, we address cases where X is a polytope of dimension greater than one.

Proposition 2. *Let $X \subset \mathbb{R}^m$, $Y \subset \mathbb{R}^n$ and $Z \subset \mathbb{R}^p$ be the vertex sets of three convex polytopes. Consider the edge-concave functions $f : X \times Y \rightarrow \mathbb{R}$ and $g : X \times Z \rightarrow \mathbb{R}$ with convex envelopes defined, respectively by L_R^f and L_S^g as in Proposition 1. R and S are triangulations of $\text{conv}(X \times Y)$ and $\text{conv}(X \times Z)$, respectively. Define the projection of a simplex $\Delta \in \mathbb{R}^{m+n'}$ onto the x -space as*

$$P_x(\Delta) := \{x \in \mathbb{R}^m : \exists(x, w) \in \Delta\}.$$

If there exist convex envelopes L_R^f and L_S^g and a triangulation T of X such that for each $\Delta \in R$ there is a $\Delta'' \in T$ such that $P_x(\Delta) = \Delta''$, and for each $\Delta' \in S$ there is a $\Delta'' \in T$ such that $P_x(\Delta') = \Delta''$ then the convex envelope of $f + g : X \times Y \times Z \rightarrow \mathbb{R}$ is the sum of the convex envelopes of f and g ,

$$\text{convex}(f, X \times Y \times Z) = \text{convex}(g, X \times Y) + \text{convex}(h, X \times Z).$$

Proof. We start with the following general observation: for any $f : X \rightarrow \mathbb{R}$, X and $X' \subseteq X$ the convex envelope of f over the subdomain X' is at least as tight as the convex envelope of f over X itself, $\text{convex}(f, X) \Big|_x \leq \text{convex}(f, X') \Big|_x \forall x \in X' \subseteq X$. We see from this observation that, for any $\Delta \in T$, $\text{convex}(f + g, \Delta \times Y \times Z) \Big|_{(x,y,z)} \geq \text{convex}(f + g, X \times Y \times Z) \Big|_{(x,y,z)} \forall (x, y, z) \in \Delta \times Y \times Z$. By assumption, the convex envelope defining triangulations R and S project onto the x -space as T , a triangulation of $\text{conv}(X)$. Therefore, for any $\Delta \in T$,

$$\text{convex}(f, \Delta \times Y) \Big|_{(x,y)} = \text{convex}(f, X \times Y) \Big|_{(x,y)} \quad \forall (x, y) \in \Delta \times Y$$

and

$$\text{convex}(g, \Delta \times Z) \Big|_{(x,z)} = \text{convex}(g, X \times Z) \Big|_{(x,z)} \quad \forall (x, z) \in \Delta \times Z.$$

It follows from Lemma 3 that $\text{convex}(f + g, \Delta \times Y \times Z) \Big|_{(x,y,z)} = \text{convex}(f, \Delta \times Y) \Big|_{(x,y)} + \text{convex}(g, \Delta \times Z) \Big|_{(x,z)}$ for all $(x, y, z) \in \Delta \times Y \times Z$. The required result follows immediately.

Proposition 2 extends the earlier result of Rikun (1997) and reduces to this result when $\text{conv}(X)$ is a simplex and the triangulation of the x -space is unique.

Example 4. As an illustration consider the multilinear function

$$f(x_1, x_2, y, z) = g(x_1, x_2, y) + h(x_1, x_2, z)$$

where

$$g(x_1, x_2, y) = x_1 x_2 y + 3x_1 x_2 + 2x_1 y + 1x_2 y$$

and

$$h(x_1, x_2, z) = x_1x_2z + 3x_1x_2 + 1x_1z + 2x_2z$$

over the domain $(x_1, x_2, y, z) \in [0, 1]^4$. Using the method described in Section 3 the convex envelopes of g and h can be determined. Figures 5 (a) and (b) illustrate the triangulations T and T' producing the respective convex envelopes. In Figure 5 (a) the vertices are labelled in such a way that $v^1 = (\underline{x}_1, \underline{x}_2, \underline{y})$, $v^2 = (\overline{x}_1, \underline{x}_2, \underline{y})$, $v^3 = (\underline{x}_1, \overline{x}_2, \underline{y})$, $v^4 = (\overline{x}_1, \overline{x}_2, \underline{y})$, $v^5 = (\underline{x}_1, \underline{x}_2, \overline{y})$, $v^6 = (\overline{x}_1, \underline{x}_2, \overline{y})$, $v^7 = (\underline{x}_1, \overline{x}_2, \overline{y})$, $v^8 = (\overline{x}_1, \overline{x}_2, \overline{y})$. Similarly, in Figure 5 (b) the vertices are labelled $v^{1'} = (\underline{x}_1, \underline{x}_2, \underline{z})$, $v^{2'} = (\overline{x}_1, \underline{x}_2, \underline{z})$, $v^{3'} = (\underline{x}_1, \overline{x}_2, \underline{z})$, $v^{4'} = (\overline{x}_1, \overline{x}_2, \underline{z})$, $v^{5'} = (\underline{x}_1, \underline{x}_2, \overline{z})$, $v^{6'} = (\overline{x}_1, \underline{x}_2, \overline{z})$, $v^{7'} = (\underline{x}_1, \overline{x}_2, \overline{z})$, $v^{8'} = (\overline{x}_1, \overline{x}_2, \overline{z})$. The cells of T and T' project onto the x -space in such a way as to form triangulations of the x -space as illustrated in Figures 5 (a) and (b). As these projected triangulations are the same, the conditions of Proposition 2 apply, hence the convex envelope of f is the sum of the convex envelopes of g and h ,

$$\text{convex}(f, X \times Y \times Z) = \text{convex}(g, X \times Y) + \text{convex}(h, X \times Z).$$

Again applying the algorithm of Section 3, the convex envelopes

$$\text{convex}(x_1x_2y, X \times Y) \text{ and } \text{convex}(3x_1x_2 + 2x_1y + 1x_2y, X \times Y)$$

can be determined. Triangulations defining both of these convex envelopes can be represented as the triangulation in Figure 5 (a). Using Proposition 2 we see that

$$\begin{aligned} \text{convex}(g, X \times Y) &= \text{convex}(x_1x_2y, X \times Y) \\ &+ \text{convex}(3x_1x_2 + 2x_1y + 1x_2y, X \times Y). \end{aligned}$$

Another application of the method in Section 3 shows that the triangulations defining both, $\text{convex}(x_1x_2z, X \times Z)$ and $\text{convex}(3x_1x_2 + 1x_1z + 2x_2z, X \times Z)$ may be represented as the triangulation in Figure 5 (b), therefore,

$$\begin{aligned} \text{convex}(h, X \times Z) &= \text{convex}(x_1x_2z, X \times Z) \\ &+ \text{convex}(3x_1x_2 + 1x_1z + 2x_2z, X \times Z). \end{aligned}$$

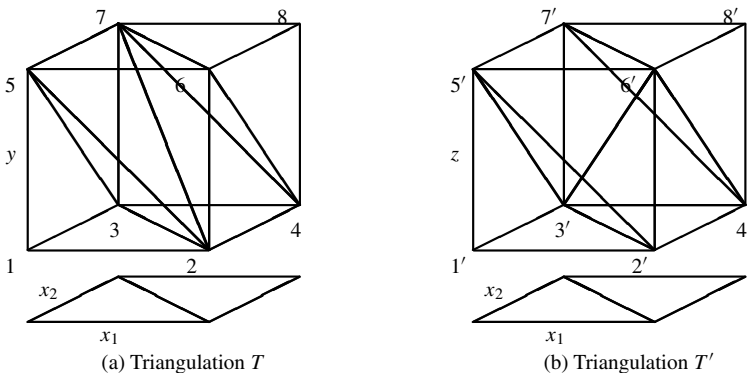


Fig. 5. Triangulations for $\text{convex}(g, X \times Y)$ and $\text{convex}(h, X \times Z)$

Example 5. The convex envelope of the multilinear function $\psi(x) = -\alpha \prod_{i=1}^n x_i$, $\alpha > 0$ over the unit hypercube can be shown to be (Crama, 1993)

$$\text{convex}(\psi, [0, 1]^n) = \max_i \{-\alpha x_i\}.$$

Observe that this convex envelope has n domains of linearity, each of which may be described as the convex hull of a the union of a facet and a vertex of the unit hypercube, $\text{conv}(\{x : x_i = 0\} \cup (1, 1, \dots, 1))$. Now consider the multilinear function $f(x) = -\sum_{i=1}^m \alpha_i \prod_{j \in Q_i} x_j$ where $\alpha_i > 0$ for all $i \in \{1, \dots, m\}$, and $Q_i \subseteq \{1, \dots, n\}$ is the set of indices defining the monomial in the i^{th} term of the function. The domains of linearity of each of the terms are such that the terms in f may be partitioned arbitrarily into functions g and h that satisfy the conditions of Proposition 2. By recursively repartitioning terms and applying Proposition 2, we may write the convex envelope of f as the sum of the convex envelopes of the individual terms

$$\text{convex}(f, [0, 1]^n) = \sum_{i=1}^m \text{convex}(-\alpha_i \prod_{j \in Q_i} x_j).$$

5. Conclusions

The facial structure of the convex envelopes of edge-concave functions was elucidated through a connection between the minimal affine dependencies of the polytopal domain vertices, triangulations of this domain and the facets of the convex envelope. An algorithm for computing the facets of the convex envelope over hyperrectangles in \mathbb{R}^3 was described. Using these analysis techniques, we derived sufficient conditions under which the convex envelope of a sum of edge-concave functions may be shown to be equivalent to the sum of the convex envelopes of these functions. We suggest two promising avenues for the extension of this work: applications to more general functional forms, and the derivation of tight yet efficient convex underestimators over domains of larger dimensionality.

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