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On Functional Separately Convex Hulls*

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Abstract. Let D be a set of vectors in $\mathbb{R}^d$. A function $f\colon \mathbb{R}^d \to \mathbb{R}$ is called *D-convex* if its restriction to each line parallel to a nonzero vector of D is a convex function. For a set $A \subseteq \mathbb{R}^d$, the *functional D-convex hull of A*, denoted by $\mathrm{co}^D(A)$, is the intersection of the zero sets of all nonnegative D-convex functions that are 0 on A.

We prove some results concerning the structure of functional D-convex hulls, e.g., a Krein–Milman-type theorem and a result on separation of connected components.

We give a polynomial-time algorithm for computing $\mathrm{co}^D(A)$ for a finite point set A (in any fixed dimension) in the case of D being a basis of $\mathbb{R}^d$ (the case of *separate convexity*).

This research is primarily motivated by questions concerning the so-called *rank-one convexity*, which is a particular case of D-convexity and is important in the theory of systems of nonlinear partial differential equations and in mathematical modeling of microstructures in solids. As a direct contribution to the study of rank-one convexity, we construct a configuration of 20 symmetric 2×2 matrices in a general (stable) position with a nontrivial functionally rank-one convex hull (answering a question of K. Zhang on the existence of higher-dimensional nontrivial configurations of points and matrices).

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1. Introduction

1.1. *Basic Definitions and an Example*

Throughout, we assume that X is a finite-dimensional real vector space (which can be identified with some $\mathbb{R}^d$). For $a, b \in X$, we write $[a, b]$ for the segment with endpoints a, b, i.e., $[a, b] = \{\alpha a + (1-\alpha)b \mid \alpha \in [0, 1]\}$.

Let D be a set of vectors in X.

Definition 1.1 (D-Convex Set). A set $C \subset X$ is called a *D-convex set* if for any two points $x_1, x_2 \in C$ such that the segment $[x_1, x_2]$ is parallel to some nonzero vector of D, we have $[x_1, x_2] \subseteq C$. (D-convexity is also called *directional convexity* or *restricted-orientation convexity* in the literature.)

Definition 1.2 (D-Convex Function). Let f be a real function defined on a D-convex set C. We say that f is *D-convex* if, for any $x \in C$ and any $v \in D$, the function $g(t) = f(x + tv)$ is a convex function of the real variable t. (The domain of g is an interval in $\mathbb{R}$, as C is assumed to be D-convex.)

In this paper we shall mostly consider total functions (defined on the whole X).

For the special case when D consists of d orthogonal vectors (which can be identified with the standard orthonormal basis of $\mathbb{R}^d$), we shall also use the word *separate convexity* instead of D-convexity (and similarly for other derived notions).[1]

The main object of our investigation is a suitable notion of a "D-convex hull" of a set. One can define the D-convex hull of a set A as the intersection of all D-convex sets (according to Definition 1.1) containing A; this D-convex hull will be denoted by $\mathrm{co}_D(A)$.

We shall concentrate on another kind of D-convex hull, namely, one defined by means of D-convex functions. It seems less intuitive than the one just defined, but it arises naturally in applications and it even seems to have some more pleasant properties (as our results below also indicate).

Definition 1.3 (Functional D-Convex Hull). Let $A \subseteq X$. The set $\mathrm{co}^D(A)$, called[2] the *functional D-convex hull* of A, is defined as

$$\mathrm{co}^D(A) = \left\{ x \in X \mid f(x) \le \sup_{y \in A} f(y) \text{ for all } D\text{-convex } f\colon X \to \mathbb{R} \right\}.$$

A set C is *functionally D-convex* if $A = \mathrm{co}^D(A)$.

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[1] Other names used in the literature are *rectilinear convexity* (e.g., [OSSW], [RW2], and [RW1]), and *orthoconvexity* [RW3]. *Biconvexity* [AH] sometimes refers to the case $D = (\mathbb{R}^u, 0) \cup (0, \mathbb{R}^v)$, where $u + v = \dim(X)$.

[2] The notation co_D, co^D follows a widespread notational convention in mathematics, namely, that subscripts correspond to objects of a "primal" space while superscripts are used for objects related to functions on the primal space.

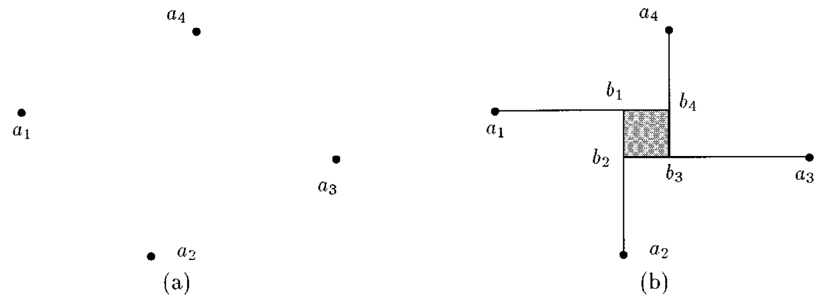

Fig. 1. A four-point configuration $\mathcal{C}_4$ with nontrivial functional separately convex hull.

Later, we shall show that this definition is equivalent to the characterization given in the abstract.

It is easy to check that the D-convex hull is always contained in the functional D-convex hull; also, if A is a closed set and $D = X$ (i.e., for the usual convexity), both these hulls of A coincide (see Section 2.1). The following (crucial) example shows that the functional D-convex hull may be much larger than the D-convex hull in general. Apparently, this example has been discovered independently by several authors (we are aware of [T] and [AH]).

Example 1.4 (A Four-Point Configuration). *Let $X = \mathbb{R}^2$, let $D = \{(0,1),(1,0)\}$ (i.e., we deal with separate convexity in the plane). Let $A = \{a_1, a_2, a_3, a_4\}$ be a configuration as in Fig.* 1(*a*). *Then $\mathrm{co}^D(A)$ consists of the four segments $a_i b_i$ and the square $b_1b_2b_3b_4$ depicted in Fig.* 1(*b*). *We shall refer to this configuration as $\mathcal{C}_4$ (meaning four points whose x-coordinates and y-coordinates are ordered as those of the points depicted, or of the mirror image of this configuration).*

Proof Sketch. For completeness, we outline a proof of the (more interesting) inclusion $C \subseteq \mathrm{co}^D(A)$, where C is the set in Fig. 1(b) (another proof will be obtained as a special case of our results later). It suffices to prove that $B = \{b_1, b_2, b_3, b_4\} \subset \mathrm{co}^D(A)$. Once we know this, we have $C = \mathrm{co}_D(A \cup B) \subseteq \mathrm{co}^D(A \cup B) = \mathrm{co}^D(A)$. Thus, let f be a D-convex function, let $M = \max_i f(a_i)$, and $M' = \max_i f(b_i)$. We need to show $M' \leq M$. However, if $M' > M$, let i be such that $f(b_i) = M'$. Looking at the segment $a_i b_{i-1}$ (where $b_0 = b_4$), we get a contradiction to the convexity of f there, since $f(a_i) < M'$, $f(b_{i-1}) \leq M'$, but $f(b_i) \geq M'$. □

Remark. We define the functional D-convex hull using *total* D-convex functions only. As a consequence, this hull is always a closed set (see below). One could use also partial D-convex functions; this leads to various topological subtleties. Such definitions are investigated in [AH] (for the special case of biconvexity). We do not proceed in this direction, since we are interested mainly in combinatorial and computational aspects of the hulls.

1.2. *Motivation and Background*

The present investigation has been inspired by a significant problem in the calculus of variations: characterization of rank-one convex and quasi-convex functions. In this section we shall try to give a rather brief and simplified account of underlying problems and applications. For the sake of brevity we introduce only the basic concepts and we omit all technicalities or even precise explanation of some terms. The reader unfamiliar with the topic is encouraged to find further information in the quoted references.

The notion of *rank-one convexity* readily serves as a special example of D-convexity. Indeed, if $X = \mathbf{M}^{m\times n}$ represents the space of $m \times n$ matrices and

$$D = \{a \in \mathbf{M}^{m\times n};\, \operatorname{rank} a \le 1\}$$

is the cone of rank-one matrices, then D-convexity becomes rank-one convexity studied in the literature. On the other hand the notion of *quasi-convexity* introduced by Morrey [M] to characterize weakly lower semicontinuous functionals on the space of vector-valued functions is intrinsically more complicated. A function f is *quasi-convex* if it satisfies the following inequality: $\int_\Omega f(a+\nabla\varphi)\,dx \ge \int_\Omega f(a)\,dx$ for all $a \in \mathbf{M}^{m\times n}$, for any smooth function $\varphi \in C_0^\infty(\Omega, \mathbb{R}^n)$ (the space of smooth vector-valued functions with compact supports in Ω), and for any bounded domain $\Omega \subset \mathbb{R}^m$. Since quasi-convexity plays a similar role in the study of vectorial variational problems (or systems of nonlinear partial differential equations) as convexity does for scalar problems, construction of quasi-convex envelopes is an important tool for the investigation of solutions to problems that are not weakly lower semicontinuous (and hence direct methods of the calculus of variations cannot be applied). Using quasi-convex functions, we define the *quasi-convex hull* of a set A, $\mathrm{co}^{qc}(A)$, similarly as $\mathrm{co}^D(A)$ in Definition 1.3. In other words, $\mathrm{co}^{qc}(A)$ is the set of points that cannot be separated from A by a quasi-convex function. Unfortunately, no reasonable description of all quasi-convex functions is known. Any quasi-convex function is rank-one convex, and hence $\mathrm{co}^D(A) \subseteq \mathrm{co}^{qc}(A)$ holds; the functional rank-one convex hull appears as a reasonable first approximation of the quasi-convex hull.[3] However, even the computation of the functional rank-one convex hull ($\mathrm{co}^D(A)$) is a difficult task and we are not aware of any efficient and reliable algorithm (even an approximate one). The question of reasonable inner and outer approximations of $\mathrm{co}^{qc}(A)$ is one of the main goals for future work.

In this paper we focus mainly on the case of separate convexity; however, we establish also some properties for a general D. The case of separately convex functions has previously been studied in this context in [T] as an easier substitute for the more general case of rank-one convexity. As we shall show the separate convexity in $\mathbb{R}^d$, $d \ge 3$, exhibits less convenient properties than the two-dimensional case and therefore generalization of the results of [T] may not be obvious. Interesting results concerning separate convexity can be also found in [AH], where this notion has been studied in connection with the limiting behavior of bimartingales in probability theory.

At the end of this section we state an example of a particular problem where rank-one convexity appears as an approximation of quasi-convexity. Let $v^{(j)}\colon\ \Omega \subset \mathbb{R}^m \to \mathbb{R}^n$

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[3] It was even conjectured that rank-one convex functions and quasi-convex functions are the same, but this turned out to be false in general, see [Š1].

be a sequence of functions such that $|\nabla v^{(j)}| \le$ const. and $\operatorname{dist}(\nabla v^{(j)}, A) \to 0$ almost everywhere in Ω for a given compact set $A \subset \mathbf{M}^{m\times n}$. We ask under which conditions on the set A the sequence $\{v^{(j)}\}$ is compact (up to a subsequence) in L^p (see [Š2]). This question is closely related to a characterization of Young measures generated by weakly convergent subsequences of the bounded sequence $\{\nabla v^{(j)}\} \subset L^p(\Omega, \mathbb{R}^n)$. Such sequences arise, for example, as minimizing sequences of energy functionals in models of phase transformations (see [BJ], [Š3], and [BFJK]), with the stored energy $E(u) = \int_\Omega W(\nabla u)\, dx$, where $u\colon \mathbb{R}^n \to \mathbb{R}^n$ is a deformation of the body and $W\colon \mathbf{M}^{n\times n} \to \mathbb{R}$ is a given nonnegative function with a nontrivial set of global minima, for definiteness $A = \{a \in \mathbf{M}^{n\times n};\ W(a) = 0\}$.

A Young measure generated by a minimizing sequence such that $\inf E(u^{(k)}) = 0$ is supported on the set A and whenever it is trivial the sequence is compact (up to a subsequence). Characterization of sets $A \subset \mathbf{M}^{n\times n}$ that allow only trivial Young measures is known only in certain particular cases. Since any point in $\operatorname{co}^{qc}(A)\backslash A$ is a center of mass of a nontrivial Young measure, description of the set $\operatorname{co}^{qc}(A)$ can give an answer to the sequence compactness problem. We refer to [B], [Š2], [T], and [Z1] and references therein for more details.

1.3. *Summary of Results*

In Section 2.1, we discuss some easy properties, such as the continuity of (total) D-convex functions. In 2.2, we show a Krein–Milman-type result, i.e., that a compact functionally D-convex set is the functional D-convex hull of its extremal points (when extremal points are defined suitably). Then (Section 2.3) we show that for a compact functionally D-convex set with finitely many connected components, the components themselves are functionally D-convex as well.

In Section 3 we discuss separate convexity. We develop an algorithm for computing the functional separately convex hull of an n-point set in $\mathbb{R}^d$, with $O(n^d)$ worst-case running time (this can easily be improved somewhat, but currently we do not know what is the best complexity one can hope for). This algorithm is based on the above-mentioned Krein–Milman-type result and a description of the hull as a union of "boxes" formed by suitable grid points. Further, we discuss the computation of separately convex envelopes of functions (Section 3.3). Finally, we construct a three-dimensional analogue of the four-point configuration from Example 1.4; namely, we exhibit a 20-point set $A \subset \mathbb{R}^3$, such that no two points of A lie in a common plane perpendicular to a coordinate axis, and with a nontrivial functional separately convex hull (strictly larger than A). This configuration is *generic*, meaning that any sufficiently small perturbation of A still yields a configuration with a nontrivial hull. Zhang [Z2] conjectured that no such configuration in $\mathbb{R}^3$ exists. The construction can be generalized to an arbitrary dimension (to appear elsewhere). A direct consequence of the three-dimensional construction for separate convexity is the existence of 20 symmetric 2×2 matrices in a general (stable) position with a nontrivial functional rank-one convex hull.

In Section 4 we consider an alternative approach to computing functionally D-convex hulls of finite sets (or sets consisting of simple "building blocks"). This yields a fast algorithm for the functional separately convex hull in the plane (Section 5). An example shows that in dimensions 3 and higher, this approach may fail in some cases, but nevertheless we believe that it might be practically interesting in the future, as it may provide the functional D-convex hull or its good outer approximation in many cases.

As a by-product of our treatment of the planar case, we also prove that the Carathéodory number for the functional separately convex hull in the plane is finite, i.e., any point belonging to the hull of a (compact) set A also belongs to the hull of some its 5-point subset (this contrasts with the separately convex hull in the plane, where the Carathéodory number is infinite). On the other hand, we construct a set D in $\mathbb{R}^3$ such that the Carathéodory number for the functional D-convexity is infinite.

2. Properties of the Functional *D*-Convex Hulls

2.1. *Basics*

Here we collect a few easy (and probably mostly known) facts about D-convexity. First we note an alternative description of $\mathrm{co}_D(A)$.

Observation 2.1. *Let us define a sequence of sets $A_0 = A$, A_1, $A_2, \ldots$ by*

$$A_{i+1} = \bigcup \{[x_1, x_2] | x_1, x_2 \in A_i,\ [x_1, x_2] \textit{ is parallel to a vector } v \in D\}\,. \tag{1}$$

Then

$$\mathrm{co}_D(A) = \bigcup_{i=1}^{\infty} A_i\,.$$

Proof. Clearly, $\bigcup A_i$ is D-convex. On the other hand, it is easy to see that $A_i \subseteq \mathrm{co}_D(A)$ for all i, by induction on i. □

Observation 2.2. *For any D and any A, we have* $\mathrm{co}_D(A) \subseteq \mathrm{co}^D(A)$.

Proof. Let $x \in \mathrm{co}_D(A)$. Then, by Observation 2.1, there is a finite sequence $x_1, x_2, \ldots,$ $x_n = x$, where each x_i is either an element of A or $x_i \in [x_j, x_k]$ for some $j, k < i$ with $[x_j, x_k]$ parallel to a vector of D. We prove by induction on i that $f(x_i) \leq \sup_{y \in A} f(y)$, for any D-convex function f. If $x_i \in A$ this is clear and if $x_i = \alpha x_j + (1 - \alpha) x_k$ we apply Jensen's inequality since f is convex on $[x_j, x_k]$. □

Remark. It is easy to check that for $D = X$ (i.e., for the usual convexity) and A closed, $\mathrm{co}_D(A) = \mathrm{co}^D(A)$. Indeed, suppose that x is not in the convex hull of A; then by the separation theorem, there exists a linear functional $q \in X^*$ with $q(x) > \sup_{y \in A} q(y)$, and this witnesses that x is not in $\mathrm{co}^X(A)$ either.

Remark. Since D-convexity and functional D-convexity are in general different, one might wonder what happens if we defined a "functionally D-convex function" as one with a functionally D'-convex epigraph, where $D' = D \times \mathbb{R}$. However, it is not difficult to see that in this case we get the same notion as a D-convex function. (To see that the epigraph of a D-convex function $f\colon X \to \mathbb{R}$ is functionally D'-convex, consider the function $F\colon X \times \mathbb{R} \to \mathbb{R}$, defined by $F(x,t) = f(x) - t$: it is D'-convex, and the epigraph of f is $F^{-1}((-\infty, 0])$.)

Next, we consider continuity of D-convex functions (similar considerations for the two-dimensional separate convexity appear in [T]).

Observation 2.3. *If the linear span of D is the whole X, then any D-convex function defined on a D-convex set $A \subseteq X$ is continuous, and even locally Lipschitz, at every point in the interior of A.*

Proof. After a suitable linear transformation of space, we may assume that D contains the coordinate axes and thus f is separately convex. Let C be a closed axis-parallel cube contained in the interior of A; let $c = (c_1, \dots, c_d)$ be its center and let 2δ be its side length.

First we show that f is bounded from above on C. Let M be the maximum of the values of f at the vertices of C. By induction on j, we get that f is also bounded by M on each j-dimensional face of C, and hence on C itself. For instance, if $C = [0,1]^d$ and we already know that $f(y) \le M$ for all y with $y_1 \in \{0,1\}$, and if $x \in C$ is an arbitrary point, we have $f(x) \le x_1 f((0, x_2, \dots, x_d)) + (1 - x_1) f((1, x_2, \dots, x_d)) \le M$; this gives the induction step from $j = d - 1$ to $j = d$. The general step is entirely similar.

We now show that f is also bounded from below. Let $x \in C$, and let z_i denote the point $(x_1, x_2, \dots, x_i, c_{i+1}, c_{i+2}, \dots, c_d)$ $(i = 0, 1, \dots, d)$. Consider the line cz_1, and let z_1' be its intersection with the boundary of C lying on the other side of c than z_1. By the convexity of f on the line cz_1, we get that $f(z_1) \ge f(c) - (f(z_1') - f(c)) = 2f(c) - M$. Then, using the line z_1z_2, we obtain $f(z_2) \ge 2f(z_1) - M \ge 4f(c) - 3M$, and, in general, induction shows that $f(z_i) \ge 2^i f(c) - (2^i - 1)M$. Hence f is also bounded from below by $m = 2^d f(c) - (2^d - 1)M$.

Let C' be the cube of side δ centered at c. For any two points $z, z' \in C'$ differing in a single coordinate, we have

$$\frac{|f(z) - f(z')|}{\|z - z'\|_1} \le \frac{2(M - m)}{\delta}.$$

For an arbitrary pair of distinct points $x, y \in C'$, we then define the "interpolating sequence" $z_0, z_1, \dots, z_d$ similarly as above, i.e., $z_i = (y_1, y_2, \dots, y_i, x_{i+1}, x_{i+2}, \dots, x_d)$, and we get

$$\frac{|f(x) - f(y)|}{\|x - y\|_1} \le \frac{\sum_{i=1}^d |f(z_{i-1}) - f(z_i)|}{\sum_{i=1}^d \|z_{i-1} - z_i\|_1} \le \max_i \frac{|f(z_{i-1}) - f(z_i)|}{\|z_{i-1} - z_i\|_1} \le \frac{2(M - m)}{\delta}.$$

□

Corollary 2.4. *If the linear span of D is the whole X and $A \subseteq X$ is arbitrary, then* $\mathrm{co}^D(A)$ *is a closed set, and is equal to* $\mathrm{co}^D(\overline{A})$ *(where $\overline{A}$ denotes the closure of A).*

Proof. For a D-convex function f, define a set $A_f = \{x \in X \mid f(x) \le \sup_A f(y)\}$. Since f is continuous, A_f is closed, and by definition we have $\mathrm{co}^D(A) = \bigcap_f A_f$, where the intersection is over all D-convex functions f. □

The next proposition shows that the definition of a functionally D-convex set can be simplified: functionally D-convex sets are exactly the zero sets of nonnegative D-convex functions.

Proposition 2.5. *Suppose that the linear span of D is the whole X. Then for any functionally D-convex set A there exists a D-convex function $f\colon X \to [0, \infty)$ such that $A = f^{-1}(0)$.*

Proof. Let $x \notin A$; by definition of a functionally D-convex set, there exists a D-convex function $f_x\colon X \to \mathbb{R}$ with $f_x(x) > \sup_{y \in A} f_x(y)$. We may assume that $\sup_A f_x = 0$ and that f_x is nonnegative (otherwise, take the D-convex function $\max(0, f_x - \sup_{y\in A} f_x(y))$). Suppose that such a function f_x has been fixed for each $x \in X \setminus A$; define an open set $U_x = \{y \in X \mid f_x(y) > 0\}$. Choose a countable set $\{x_1, x_2, \ldots\} \subset X \setminus A$ such that $\bigcup_{i=1}^{\infty} U_{x_i} = X \setminus A$ (this is possible as X is a metric Lindelöf space), and let $f_i = f_{x_i}$.

For each i, define a number

$$C_i = 2^i \max\{f_i(y) \mid \|y\| \le i + \|x_i\|\}\,.$$

For each $y \in X$, we set $f(y) = \sum_{i=1}^{\infty} C_i^{-1} f_i(y)$. We claim that this f is as required in the proposition. For each $y \in X$, the ith summand in the definition of $f(y)$ is upper-bounded by 2^{-i} for all but at most finitely many i, thus $f(y)$ is well defined. It is also easily seen that f is nonnegative and D-convex and that $f^{-1}(0) = A$. □

2.2. *A Krein–Milman-Type Theorem*

Definition 2.6. Let $A \subseteq X$ be a set. A point $e \in A$ is called a *D-extremal* point of A if there exists no segment $s \subseteq A$ parallel to some nonzero vector $v \in D$ and containing e as its interior point.

Proposition 2.7. *Let $A, B \subseteq X$ be compact sets, and suppose that all D-extremal points of B belong to A. Then $B \subseteq \mathrm{co}^D(A)$. In particular, any compact functionally D-convex set is the functional D-convex hull of the set of all its D-extremal points.*

Proof. Suppose that there exists a point $x \in B \setminus \mathrm{co}^D(A)$. This means there is a D-convex function f with $f(x) > 0 = \sup_{y\in A} f(y)$. Put $M = \max_B f$. Among the points of $y \in B$ with $f(y) = M$, consider the one with the lexicographically largest coordinate vector, and call it y_0 (the compactness of B implies that it is determined uniquely). As $f(y_0) = M > 0$, y_0 is not D-extremal, so fix a segment $s \subseteq B$ containing y_0 as its interior point and parallel to a $v \in D$. We have $f(y) \le M$ for all $y \in s$, so f is constant on s, but then y_0, as an interior point of s, cannot be lexicographically smallest on s—a contradiction. □

2.3. *A Separation Result*

Proposition 2.8. *Let $C_1, C_2 \subseteq X$ be disjoint compact sets with $C_1 \cup C_2$ being a functionally D-convex set. Then both C_1 and C_2 are functionally D-convex as well.*

Proof. Let x_0 be a point outside C_1; it suffices to find a D-convex function f which is zero on C_1 and nonzero at x_0. As is well known, we can find disjoint, bounded, and open sets U, V with $C_1 \subseteq U$, $C_2 \subseteq V$. Moreover, we may require that $x_0 \notin U$. Using Proposition 2.5, fix a nonnegative D-convex function f_0 with $C_1 \cup C_2 = f_0^{-1}(0)$. Let us define a D-convex function f by setting $f(x) = \max(f_0(x), \|x\| - R)$, where $R > 0$ is a real number so large that the ball $B(0, R)$ contains $U \cup V$. Set $\varepsilon = \min\{f(x) | x \in X \setminus (U \cup V)\}$. Clearly this minimum is attained by f, and hence $\varepsilon > 0$.

We define a function g as follows:

$$g(x) = \begin{cases} f(x) & \text{for} \quad x \in U, \\ \max(f(x), \varepsilon) & \text{for} \quad x \in X \setminus U\,. \end{cases}$$

Clearly g is zero everywhere on C_1, and $g(x_0) > 0$. To show the functional D-convexity of C_1, it suffices to check the D-convexity of g.

Let $\ell = \{x + tv | t \in \mathbb{R}\}$ be a line parallel to some vector $v \in D$. Define $I = \{x \in \ell | f(x) < \varepsilon\} \subset U \cup V$. By the D-convexity of f, I is an open (possibly empty) interval on ℓ. We distinguish two cases.

- If $I \cap U = \emptyset$, then the restriction of g on ℓ coincides with the restriction of the D-convex function $\max(f, \varepsilon)$.
- If $I \cap U \neq \emptyset$, then necessarily $I \subset U$, and hence $f \geq \varepsilon$ on $\ell \setminus U$. Therefore g restricted on ℓ equals f restricted on ℓ.

This proves the D-convexity of g and concludes the proof. □

Corollary 2.9. *Let $A \subseteq \mathbb{R}^d$ be contained in a functionally D-convex set C, which is a disjoint union of compact sets $C_1, \ldots, C_k$. Then $\mathrm{co}^D(A) = \bigcup_{i=1}^k \mathrm{co}^D(A \cap C_i)$.*

3. Functional Separately Convex Hulls of Finite Sets

Throughout this section, we discuss separate convexity only, i.e., D is an orthogonal basis of X.

3.1. *Grid Sets and Multilinear Functions*

For a point $a \in \mathbb{R}^d$, let $x_i(a)$ denote the ith coordinate of a.

Let $A \subseteq \mathbb{R}^d$ be finite. Denote $x_i(A) = \{x_i(a) | a \in A\}$, and put $\mathrm{grid}(A) = x_1(A) \times x_2(A) \times \cdots \times x_d(A)$. By a *grid* we mean any set $\mathrm{grid}(A)$ for some finite A. If a is a point of a grid G, we let a^{i+} (resp. a^{i-}) denote the point of G whose all coordinates but the ith coincide with those of a, and whose ith coordinate is the successor (resp. predecessor) of

$x_i(a)$ in $x_i(G)$ (thus, a^{i+} or a^{i-} need not exist for "border" points of G). An *elementary box* for a grid G is a Cartesian product of the form $I_1 \times I_2 \times \cdots \times I_d$, where each I_i has either the form $\{x_i\}$ for some $x_i \in x_i(G)$, or the form $[x_i(a), x_i(a^{i+})]$ for an $a \in G$.

Proposition 3.1. *Let $G \subseteq \mathbb{R}^d$ be a grid, let $f\colon G \to \mathbb{R}$ be a function. The following statements are equivalent*:

(i) *The function f can be extended to a separately convex function $\bar{f}\colon X \to \mathbb{R}$.*
(ii) *For any $a \in G$ and any i such that both a^{i+} and a^{i-} exist, f satisfies the "convexity on the triple (a^{i-}, a, a^{i+})"*:

$$f(a) \le f(a^{i-}) \frac{x_i(a) - x_i(a^{i-})}{x_i(a^{i+}) - x_i(a^{i-})} + f(a^{i+}) \frac{x_i(a^{i+}) - x_i(a)}{x_i(a^{i+}) - x_i(a^{i-})} \tag{2}$$

(*let us call such an f a D*-convex function *on G*).

For dimension $d = 2$, a weaker form of this proposition was noted by Tartar [T].

Proof. The implication (i) ⇒ (ii) is clear. Let $f\colon G \to \mathbb{R}$ satisfy (ii). First we show that f can be extended to a separately convex function on the box B_0 spanned by the points of G.

Let B be a j-dimensional elementary box of G. We claim that there exists a unique multilinear mapping $p(x_1, \ldots, x_d)$ whose values at the 2^j corners of B (which are points of G) agree with those of f. Indeed, since $d - j$ of the coordinates have a fixed value on B, we, in fact, deal with multilinear polynomials in j variables. Such polynomials have exactly 2^j coefficients, so if we regard them as a vector space, they have dimension 2^j. Hence it suffices to show that the linear map assigning to such a j-variate multilinear polynomial the vector of its 2^j values at the corners of B has a trivial kernel. This is easy to check by induction on j, however.

We define the extension $\bar{f}$ on B as the multilinear polynomial p discussed above. It is easy to check that this definition is compatible among different elementary boxes B. We need to check the separate convexity of $\bar{f}$. Let ℓ be an axis-parallel line, say the line $\{(t, x_2, x_3, \ldots, x_d) | t \in \mathbb{R}\}$. Let $B = I_1 \times \cdots \times I_d$, $I_1 = [t_0, t_1]$, be an elementary box meeting ℓ in a segment. The function $g(t) = f(t, x_2, \ldots, x_d)$ is a linear function on $[t_0, t_1]$ of the form $g(t) = a(x_2, \ldots, x_d)t + b(x_2, \ldots, x_d)$.

Let $B' = [t_1, t_2] \times I_2 \times I_3 \times \cdots \times I_d$ be the elementary box adjacent to B on the right. For $t \in [t_1, t_2]$, $g(t)$ has the form $a'(x_2, \ldots, x_d)t + b'(x_2, \ldots, x_d)$. To show convexity of g, it is enough to prove $a(x_2, \ldots, x_d) \le a'(x_2, \ldots, x_d)$. Now both a and a' are multilinear polynomials in $x_2, \ldots, x_d$. By the conditions (2) on f, we know $a(y_2, \ldots, y_d) \le a'(y_2, \ldots, y_d)$ for any corner $y = (y_2, \ldots, y_d)$ of the $(d-1)$-dimensional box $\tilde{B} = I_2 \times \cdots \times I_d$. An easy induction on the dimension shows that the inequality on all corners implies the required inequality at all points of $\tilde{B}$. This concludes the construction of a separately convex extension of f on the box B_0 spanned by the grid G.

It remains to show that the function $\bar{f}$ thus constructed has a separately convex extension on the whole space. Let G' be a grid arising from G by adding one layer of points at each side: formally, let $S_i = x_i(G)$, $S_i' = S_i \cup \{\min(S_i) - 1, \max(S_i) + 1\}$, and put $G' = S'_1 \times \cdots \times S'_d$. We show that f can be extended to G' so that it remains separately convex on G'. Having done this, we may proceed inductively, extending f on larger and larger grids. For each such extension, we then apply the above construction to extend f on the box spanned by the corresponding grid. The domains of these extensions are nested and the extensions agree on the common parts of their domains, so we can define a total separately convex extension of f as the union of all these extensions.

It remains to consider the extension from G to G'. We note that for the newly added—border—points of G', the inequalities (2) involving some old points (with f already fixed) only give lower bounds for the values of f. Let M be the maximum of the lower bounds thus imposed on any of the new points; we define the value of f at all new points as M. Then also the inequalities involving only new points will be satisfied (with equality). □

Similarly, as we have defined D-convex functions on a grid, we may also define *separately convex subsets* of a grid, *functionally separately convex subsets* of a grid, and the corresponding hulls. Namely, if $A \subseteq G$ is a subset of a grid, it is *separately convex* (in G) if we have, for any two points $a, b \in A$ differing in a single coordinate, $[a, b] \cap G \subseteq A$. A point $x \in G$ belongs to the functional separately convex hull of A if there exists no separately convex function $f\colon G \to \mathbb{R}$ with $f(x) > \max_A f(y)$.

To describe the functional separately convex hulls of finite point sets, the following notion is useful: let G be a grid and let $B \subseteq G$ be a separately convex subset of G (in the grid sense). The *box complex* of B, denoted by $\mathcal{BC}(B)$, is the set of all elementary boxes on G whose corners all belong to B. We write $|\mathcal{BC}(B)|$ for the union of all boxes of $\mathcal{BC}(B)$. It is easily checked that $|\mathcal{BC}(B)|$ equals the separately convex hull of B.

The following is a straightforward consequence to the proof of Proposition 3.1.

Corollary 3.2. *For any finite $A \subseteq X$, we have $\mathrm{co}^D(A) = |\mathcal{BC}(C)|$, where $C \subseteq \mathrm{grid}(A)$ is the functional separately convex hull of A* (*in the grid sense*).

Proof. Clearly $C \subseteq \mathrm{co}^D(A)$ (if any point of C could be separated from A by a separately convex function f, the restriction of f on $G = \mathrm{grid}(A)$ would show that this point does not belong to the functional separately convex hull of A in the grid sense), and hence also $|\mathcal{BC}(C)| \subseteq \mathrm{co}^D(A)$. On the other hand, let x be a point not lying in any box of $\mathcal{BC}(C)$. We may assume that x lies in the relative interior of some (uniquely determined) elementary box B of G. Since this box is not in $\mathcal{BC}(C)$, it has a corner c not belonging to C. Let $f\colon G \to \mathbb{R}$ be a nonnegative separately convex function of G which is zero on C and positive at c. Then the separately convex extension, $\bar{f}$, of f constructed in the proof of Proposition 3.1 is positive on the relative interior of B, and this shows $x \notin \mathrm{co}^D(A)$. □

We conclude this section with one more definition. Let $B \subseteq \mathbb{R}^d$ be finite, and let $G = \mathrm{grid}(B)$. We call a point $e \in B$ an *extremal* point of B (in the grid sense) if for each $i = 1, 2, \ldots, d$, at least one of e^{i+}, e^{i-} either does not exist or does not belong to B.

It is straightforward to check that if B is functionally separately convex (in the grid sense), then the extremal points of B are precisely the D-extremal points of $|\mathcal{BC}(B)|$ in the sense of Definition 2.6.

3.2. *An Algorithm*

Lemma 3.3. *Let G be a grid, let $B \subseteq G$ be a functionally separately convex set* (*in the grid sense*), *and let e be an extremal point of B. Then $B \setminus \{e\}$ is functionally separately convex as well.*

Proof. Let $f\colon G \to \mathbb{R}$ be a nonnegative separately convex function vanishing on B and nonzero on $G \setminus B$. Let us see which of the conditions (2) could be violated if we increase the value of $f(e)$ from 0 to some $\varepsilon > 0$ while keeping the other values unchanged. These are only the inequalities in which $f(e)$ appears on the left-hand side. Consider an i for which both e^{i+} and e^{i-} exist. Since e is extreme, we have $f(e^{i+}) > 0$ or $f(e^{i-}) > 0$, and hence the right-hand side of (2) is a strictly positive number. If we let ε be the minimum of the right-hand sides of all the (at most d) relevant inequalities, then changing $f(e)$ from 0 to ε retains the separate convexity of f. □

The Algorithm. Let $A \subseteq \mathbb{R}^d$ be a finite set. The following algorithm computes its functional separately convex hull.

1. Let B_0 be some functionally separately convex subset of $G = \mathrm{grid}(A)$ containing A. (For instance, we may use the whole G; a more efficient procedure is probably obtained by computing the iterated quadrant hull of A—see Section 4 below—and letting B_0 be the set of its grid points.)
2. Suppose that some B_i has already been computed. If B_i has an extremal point $e \notin A$, set $B_{i+1} = B_i \setminus \{e\}$, and repeat this step. If all extremal points of B_i belong to A, then B_i is the required functional separately convex hull of A (in the grid sense; the actual hull can be reconstructed as its box complex).

The correctness of the algorithm follows from Lemma 3.3 and Proposition 2.7.

When implemented carefully (using suitable data structures to maintain the current set of extremal points), this algorithm has running time $O(|\mathrm{grid}(A)|) = O(n^d)$. It would be interesting to find a faster algorithm (which would not consider all grid points).

Remark. This algorithm shows that the functional separately convex hull only depends on the combinatorial structure of A, in other words, that it is invariant under a monotone transformation of a single coordinate. Hence we may always suppose that the point coordinates are integers not exceeding $|A|$. This does not seem to be obvious from the definition.

3.3. *Remark on Computing Separately Convex Envelopes*

Definition 3.4 (D-Convex Envelope). Let $A \subseteq X$ be a set and let $f\colon A \to \mathbb{R}$ be a real function. We define the *D-convex envelope* of f, denoted by $C_D f$, by

$$C_D f(x) = \sup\{g(x) | g : X \to \mathbb{R} \text{ is } D\text{-convex},\ g(y) \leq f(y), \forall y \in A\}.$$

This is formally a function into $\mathbb{R} \cup \{\infty\}$; we let $\mathrm{dom}\, C_D f = \{x \in X | C_D f(x) < \infty\}$.

Studying D-convex envelopes (in particular, rank-one-convex envelopes as an upper bound for quasi-convex envelopes) is equally important in applications as studying the functional D-convex hulls of sets. (On the other hand, as we point out later, the D-convex envelope of a function f can be computed as a functional D'-convex hull of the graph of f for $D' = D \times \mathbb{R}$.)

Here we consider the case of separately convex envelope of a function defined on a finite set $A \subset \mathbb{R}^d$. In this case, the domain of the envelope is easily seen to be precisely $\mathrm{co}^D(A)$. Moreover, as the proofs of Proposition 3.1 and Corollary 3.2 show, the envelope is fully determined by its values at the points of $B = \mathrm{grid}(A) \cap \mathrm{co}^D(A)$ (on each elementary box of the grid of A, the envelope is the unique multilinear extension determined by the values at the vertices of the box).

Hence, let $f\colon A \to \mathbb{R}$ be a given function on an n-point set $A \subseteq \mathbb{R}^d$; we are looking for the function $g\colon B \to \mathbb{R}$, which is separately convex in the grid sense, is upper-bounded by f at the points of A, satisfies the appropriate inequalities of the form (2), and is as large as possible (we may maximize at all points simultaneously, since the maximum of two separately convex functions is separately convex). This yields a problem of maximizing a linear function subject to a number of linear constraints, which can be solved by algorithms for linear programming (see, e.g., [C]). Explicitly, with unknowns $g(b)$ ($b \in B$), the linear program is the following:

maximize $\sum_{b\in B} g(b)$ subject to

$$\begin{array}{lll} g(a) \le f(a), & & a \in A, \\ g(b) \le \alpha_{b,i}\, g(b^{i-}) + (1-\alpha_{b,i})\, g(b^{i+}), & & b, b^{i+}, b^{i-} \in B, \end{array}$$

where $\alpha_{b,i} = (x_i(b) - x_i(b^{i-}))/(x_i(b^{i+}) - x_i(b^{i-}))$.

For an n-point set in $\mathbb{R}^d$, this linear program has at most $O(n^d)$ variables and $O(n^d)$ inequalities. For the practically important case when A is a grid, the number of variables is the same as the number of input points, and the number of constrains is about d times larger.

Remark. If A is in general position, say, this approach seems unsatisfactory, in that we need to consider many more variables than original points. For the planar case, it is not too difficult to show that for the separately convex envelope g of a function given at n points, one can decompose the domain of g into $O(n)$ rectangles, such that g is a bilinear function on each of them. Therefore, g can be fully described by giving its values at the corners of these rectangles. However, currently we do not know how to find this concise description without solving the linear program given above, with possibly quadratically many variables and constraints.

Remark. The separately convex envelopes seem to be inherently more complicated than the "usual" convex envelope, and it may be that some kind of high-dimensional linear programming approach is unavoidable for its exact computation. We give an example to support this (vague) statement.

Example 3.5.

(i) *For any natural number n, there exist a finite set $A \subset \mathbb{R}^2$, a function $f\colon A \to \mathbb{R}$, and a point $c \in \mathbb{R}^2$, such that the value of $C_D f(c)$ depends essentially on the values of f at n distinct points $a_1, \ldots, a_n \in A$, in the following sense: for each i, if we decrease the value of $f(a_i)$ and leave the values of f at the other points of A unchanged, then $C_D f(c)$ decreases.*

(ii) *There exists a set $D \subseteq \mathbb{R}^3$ such that the functional D-convexity has no finite Carathéodory number, that is, for any n there exists a set $S \subseteq \mathbb{R}^3$ and a point $x \in \mathrm{co}^D(S)$ with $x \notin \mathrm{co}^D(B)$ for any at most n-point subset $B \subseteq S$. (In contrast, the usual convexity in $\mathbb{R}^d$ has Carathéodory number $d + 1$.)*

Proof. We describe an example showing (i) for $n = 6$; the generalization to an arbitrary n is immediate. Consider Fig. 2. The set $A \subset \mathbb{R}^2$ consists of the points $o = (0, 0)$, $u_6 = (0, 6)$, $v_6 = (6, 0)$ (marked on the axes by circles), and of the points $a_1 = (6, 1)$, $a_2 = (1, 6)$, $a_3 = (5, 2), \ldots, a_6 = (3, 4)$ (all these points are drawn in the xy-plane). We set $f(o) = f(u_6) = f(v_6) = 0$, and we assume $0 < f(a_1) \ll f(a_2) \ll \cdots \ll f(a_6)$ (where $\ll$ stands for "much smaller than"). Let us follow the construction of the separately convex lower envelope, g. (Formally, we describe a construction of a function g, which is certainly no smaller than the values of the envelope function; then it is easy to check, proceeding backward, that if the input values $f(a_i)$ have the right orders of magnitude, the resulting g is indeed separately convex on the grid, and thus it is the envelope itself; we omit a formal proof.) First of all, g is linear on the line v_1a_1; this determines $g(b_1)$ in terms of $f(a_1)$. Next, we look at the line u_1a_2. Here g consists of two linear pieces with a break at b_1 (since $f(a_2)$ is much larger than $f(a_1)$), so that the value $g(b_2)$ depends essentially on both $f(a_1)$ and $f(a_2)$. The next line to look at is v_2a_3; here g also consists of two linear pieces, with a break at b_2, and therefore $g(b_3)$ depends on all of $f(a_1)$, $f(a_2)$, $f(a_3)$. Proceeding further in this manner, we finally find that the value of g on the segment b_5a_6 depends essentially on all of $f(a_i)$ (that is, if the $f(a_i)$

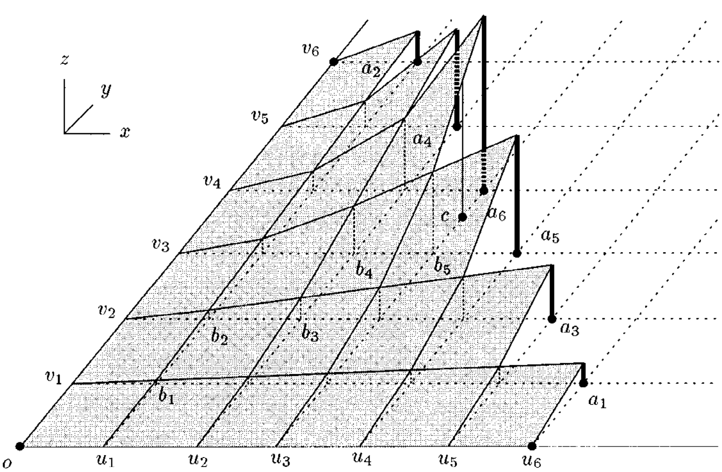

Fig. 2. An example concerning the separately convex envelope.

have right orders of magnitude, increasing any of them by an arbitrarily small amount increases the value of g at the midpoint c of the segment b_5a_6).

The above example can also be used for the proof of (ii). Indeed, let the notation be as in the example; let $S \subseteq \mathbb{R}^3$ contain the points $(x,\ f(x))$, with $x \in A$, plus the vertical semilines of the form $\{(x,t)|t \in \mathbb{R},\ t \geq M\}$ for all $x \in A$, with $M > \max f(a_i)$. Set $D = \{(0,1),(1,0)\} \times \mathbb{R}$; then one can check that the epigraph of the separately convex envelope of f is exactly the functional D-convex hull of S. Now the point $x = (c, g(c))$ belongs to this hull, but not to the hull of any set of the form $S \backslash \{(a_i,\ f(a_i))\}$. □

In Section 5.1, we show that (surprisingly) the functional separate convexity in the plane does have a finite Carathéodory number. It would be interesting to determine the Carathéodory number for some specific D, such as that for rank-one convexity or various of its specializations.

3.4. *A Nontrivial Generic Configuration in Dimension* 3

We continue discussing separate convexity, i.e., D is a basis of $\mathbb{R}^d$.

Example 3.6. *There exists a* 20*-point set* $A \subset \mathbb{R}^3$ *with* $\mathrm{co}^D(A) \neq A$ *and such that no two points of* A *lie in a common plane perpendicular to a coordinate axis.* (*Since the structure of the functional separately convex hull only depends on the ordering of coordinates, any set* A' *arising from* A *by a sufficiently small perturbation also satisfies* $\mathrm{co}^D(A') \neq A'$; *in this sense is* A *"generic."*)

Proof. We begin by choosing one four-point planar configuration as in Example 1.4. We place one copy of it in the $z = 0$ plane, and one in the $z = 1$ plane (the xy-projections are identical). Then we perturb the points a little in the z-direction, so that no two z-coordinates coincide. The resulting 8-point set and its functional separately convex hull are depicted in Fig. 3. The lower points are denoted by $a_1, \ldots, a_4$ and the corresponding upper points by $b_1, \ldots, b_4$.

This set is not generic yet, since it consists of four pairs of points on common vertical lines. For each $i = 1, \ldots, 4$, we perturb b_i a little within its horizontal plane, and we add three more points c_i, d_i, e_i, which are all located in a small cluster close to the edge a_ib_i. The heights of these clusters (i.e., ranges of z-coordinates) are chosen distinct, say close to $i/5$. Figure 4 shows a detail of this placement for $i = 1$. In this case, the order of x-coordinates is $x(c_1) < x(e_1) < x(b_1) < x(a_1) < x(d_1)$, the y-coordinates satisfy $y(c_1) < y(d_1) < y(e_1) < y(a_1) < y(b_1)$, and finally the z-coordinates satisfy $z(a_1) < z(c_1) < z(d_1) < z(e_1) < z(b_1)$. For the other i's, the configuration is rotated and lifted into an appropriate height.

In this way, we obtain a 20-point configuration A with all point coordinates distinct. It remains to show that the functional separately convex hull is nontrivial. This could be done by a computer, by running the algorithm from Section 3.2 on A. The functional separately convex hull of A is depicted in Fig. 4 (to make the picture simpler, only a part is shown). The reader need not even believe this is the complete hull; it suffices to check that the depicted set has no D-extremal points than those of A—then it must be contained in $\mathrm{co}^D(A)$ (by Proposition 2.7) and hence $\mathrm{co}^D(A) \neq A$. □

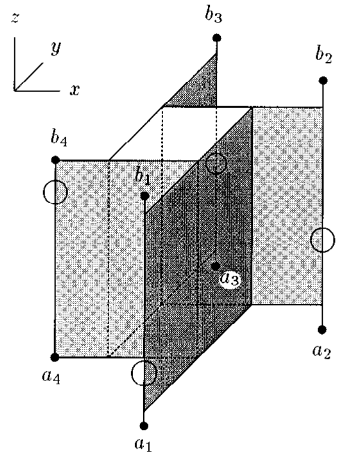

Fig. 3. The initial 8-point configuration.

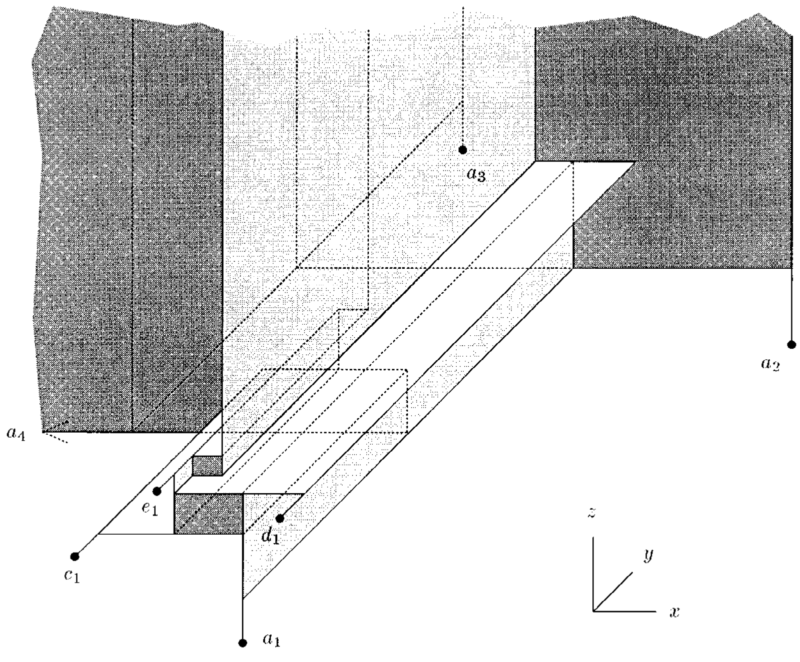

Fig. 4. A part of the 20-point configuration and its functional separately convex hull.

A Nontrivial Generic Configuration of Symmetric 2 × 2 Matrices. Let $\mathbf{S}^{2\times 2}$ denote the space of real symmetric 2 × 2 matrices. The mapping $\iota\colon \mathbb{R}^3 \to \mathbf{S}^{2\times 2}$ defined by

$$\iota\colon\ (x, y, z) \mapsto \begin{pmatrix} x+z & z \\ z & y+z \end{pmatrix}$$

is an isomorphism of the vector spaces $\mathbb{R}^3$ and $\mathbf{S}^{2\times 2}$. Each of the three vectors of $D = \{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$ is mapped to a symmetric rank-one matrix by ι, i.e., $\iota(D) \subset$ **R1**, where $\mathbf{R1} = \{a \in \mathbf{S}^{2\times 2} | \operatorname{rank} a = 1\}$. As a consequence we have, for any $A \subseteq \mathbb{R}^3$, $\iota(\mathrm{co}^D(A)) \subseteq \mathrm{co}^{\mathbf{R1}}(\iota(A))$. Hence if A is the above-constructed 20-point configuration, its ι-image is a set A' of 20 matrices with a nontrivial functional rank-one convex hull, and this property is preserved under an arbitrary sufficiently small perturbation of the matrices. Therefore we may also assume that A' contains no two rank-one connected matrices (since the set of configurations with a rank-one connection has a zero measure in the space of all configurations), and hence $\mathrm{co}_{\mathbf{R1}}(A') = A'$.

Remarks. Similarly, for any n there is a vector space isomorphism $\iota_n\colon\ \mathbb{R}^d \to \mathbf{S}^{n\times n}$ (where $d = n(n+1)/2$) such that the standard basis vectors in $\mathbb{R}^d$ are mapped to rank-one matrices. To see this, it suffices to construct a basis $\mathbf{S}^{n\times n}$ consisting of rank-one matrices. One such basis consists of the matrices $M_{k,\ell}$ for $1 \le k \le \ell \le n$, where the entry of $M_{k,\ell}$ at position (i, j) is 1 if $\{i, j\} \subseteq \{k, \ell\}$ and 0 otherwise. The construction of a basis consisting of rank-one matrices for the space $\mathbf{M}^{n\times n}$ of all $n \times n$ matrices is entirely trivial, and it gives an isomorphism of $\mathbb{R}^{n^2} \to \mathbf{M}^{n\times n}$ with similar properties. Hence nontrivial generic configurations for separate convexity in sufficiently high dimensions yield nontrivial finite generic sets for rank-one convexity. On the other hand, smaller nontrivial configurations could probably be obtained using larger sets of directions from the rank-one cone. For example, we may note that if the space of 2 × 2 matrices is identified with $\mathbb{R}^4$, then the rank-one directions contain the set $(\mathbb{R}^2, 0) \cup (0, \mathbb{R}^2)$, which corresponds to a “biconvexity” in $\mathbb{R}^4$. These are themes for further research.

4. $\mathcal{Q}$-Hulls and Iterated $\mathcal{Q}$-Hulls

Here we define yet another notion of a “generalized convex hull” (this one is usually considered in abstract convexity theory).

Definition 4.1. Let $\mathcal{Q}$ be a family of subsets of X. For a set $A \subseteq X$, we define the *$\mathcal{Q}$-hull* of A as

$$\mathcal{Q}\text{-co}(A) = \bigcap \{Q \in \mathcal{Q} | A \subseteq Q\}.$$

Clearly, if $\mathcal{Q}$ consists of functionally D-convex sets, then $\mathcal{Q}\text{-co}(A) \supseteq \mathrm{co}^D(A)$. If $\mathcal{Q}$ consisted of *all* functionally D-convex sets, then we have equality. Our intention, however, is to choose $\mathcal{Q}$ possibly “small” and consisting of “simple” sets, so that $\mathcal{Q}\text{-co}(A)$ can be computed or approximated reasonably. (For usual convexity, a suitable $\mathcal{Q}$ is of course the set of all half-spaces.) Let us define one suitable-looking $\mathcal{Q}$ for separate convexity; it is the set of complements of all translated open orthants. Formally:

Definition 4.2. For a sign vector $s \in \{-1, 1\}^d$, define

$$q_s(0) = \{x \in \mathbb{R}^d | \mathrm{sgn}(x_i) = s_i \text{ for } i = 1, 2, \ldots, d\},$$

and for $a \in \mathbb{R}^d$, let $q_s(a) = q_s(0) + a$ (for a specific orthant we write out s by writing the corresponding signs only, i.e., $q_{++}(0)$ stands for the positive open quadrant in the plane). We set $\mathcal{Q}_{sc} = \{\mathbb{R}^d \backslash q_s(a) | a \in \mathbb{R}^d,\ s \in \{-1, 1\}^d\}$. We shall refer to $\mathcal{Q}_{sc}$-co(A) as the *quadrant hull* of A. These are all points which cannot be separated from A by an open orthant (quadrant in the plane).

The sets in $\mathcal{Q}_{sc}$ are functionally separately convex. To see that, say, $\mathbb{R}^d \backslash q_s(0)$ is functionally separately convex, we may use the separately convex function

$$\varphi(x) = \begin{cases} |x_1 x_2 \ldots x_d| & \text{for } x \in q_s(0), \\ 0 & \text{otherwise.} \end{cases}$$

Remark. This substantiates the claim made in Example 1.4, namely, that the set C there is functionally convex—it is easy to check that $C = \mathcal{Q}_{sc}$-co(A). We also note that the inclusion $C \subseteq \mathrm{co}^D(A)$, which was established by a direct argument there, follows from the Krein–Milman-type statement above (Proposition 2.7): the only D-extremal points of C are those of A.

If $\mathcal{Q}$ consists of functionally convex sets, then $\mathcal{Q}$-co(A) is an outer approximation of $\mathrm{co}^D(A)$. Even for a four-point set A in the plane, however, the quadrant hull may be larger than $\mathrm{co}^D(A)$. An example is the set $A = \{(0, 0), (2, 1), (1, 2), (3, 3)\}$. Here $\mathcal{Q}_{sc}$-co(A) has three components—the points $(0, 0)$, $(3, 3)$, and the square $[1, 2]^2$. By Corollary 2.9, we get $\mathrm{co}^D(A) = \{(0, 0), (3, 3)\} \cup \mathrm{co}^D(\{(1, 2), (2, 1)\}) \subseteq \{(0, 0), (3, 3)\} \cup \mathcal{Q}_{sc}$-co $(\{(1, 2), (2, 1)\}) = A$. (Another way to see that $\mathcal{Q}_{sc}$-co$(A) \neq \mathrm{co}^D(A)$ is via Proposition 2.7).

An Iterated $\mathcal{Q}$-Hull Procedure. The preceding four-point example suggests that a better approximation of the functional D-convex hull of a set might be obtained by iterating the $\mathcal{Q}$-hull construction for components. For instance, for a finite set A, we may use the following procedure. We compute $C^{(1)} = \mathcal{Q}$-co(A), we let $C_1^{(1)}, \ldots, C_k^{(1)}$ be the partition of $C^{(1)}$ into connected components, then we compute

$$C^{(2)} = \bigcup_{i=1}^{k} \mathcal{Q}\text{-co}(A \cap C_i^{(1)}), \text{ etc.}$$

Obviously, for $j \geq |A| - 1$ we have $C^{(j)} = C^{(j+1)}$, and usually the procedure terminates much sooner.

In Section 5 we show that for separate convexity in the plane, this procedure in fact yields the functional convex hull for every finite[4] set A.

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[4] It works also for various "simple" compact sets A, such as ones with finitely many connected components; for an arbitrary compact A, it need not give the functional separately convex hull in any finite number of iterations.

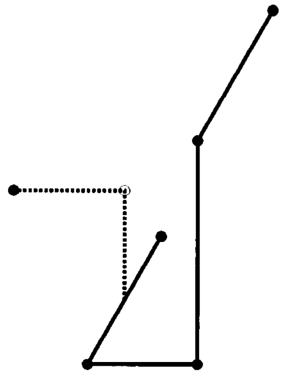

Fig. 5. A 6-point configuration whose quadrant hull is connected and larger than the functional separately convex hull.

A Counterexample. In dimension 3 and higher, the iterated quadrant hull of a finite point set can be strictly larger than the functional separately convex hull. A simple example is shown in Fig. 5 (in coordinates, the points are $(0, 1, 1)$, $(1, 0, 0)$, $(1, 2, 0)$, $(2, 0, 0)$, $(2, 0, 2)$, and $(2, 2, 2)$). The six points in $\mathbb{R}^3$ are indicated by full circles, and the functional separately convex hull is shown by full lines. The extra part of the quadrant hull is drawn by a dashed line. It is easy to see that the point marked by the empty circle cannot be separated from the other points by an octant; on the other hand, it cannot lie in the functional separately convex hull since it is extremal in the quadrant hull.

There also exist generic sets with the above property. The smallest example we could find (by a computer search) has twelve points (and a trivial functional separately convex hull). It is the following set: $A = \{(1, 7, 7), (2, 6, 3), (3, 1, 4), (4, 5, 11), (5, 4, 2), (6, 2, 8), (7, 12, 10), (8, 10, 1), (9, 9, 12), (10, 11, 6), (11, 3, 5), (12, 8, 9)\}$. A generic set for which it is easily seen that the iterated quadrant hull is larger than the functional separately convex hull is the configuration from Example 3.6. For instance, consider the point $(x(e_1), y(e_1), z(d_1))$ (look at Fig. 4). It is easy to check that this point belongs to the quadrant hull, together with the segment connecting it to e_1, say, and at the same time that it is extremal in the quadrant hull (hence it cannot belong to the functional separately convex hull). □

5. Functional Separately Convex Hulls in the Plane

Throughout this section, we consider separate convexity in the plane (i.e., $D = \{(0, 1),(0, 1)\}$). For this case, Tartar [T] has shown that a finite set $A \subset \mathbb{R}^2$ satisfies $\mathrm{co}^D(A) = A$ iff $\mathrm{co}_D(A) = A$ (i.e., no two points share an x-coordinate or a y-coordinate) and A contains no $\mathcal{C}_4$ configuration.

Here we give a description of the functional separately convex hull of compact sets in the plane (Proposition 5.1 below), which implies that the "iterated quadrant hull" procedure outlined at the end of Section 4 actually computes $\mathrm{co}^D(A)$ for finite A. Then we discuss an efficient implementation of this procedure in this particular case.

Call sets $A, B \subseteq \mathbb{R}^2$ *separated* if they lie in diagonally opposite open quadrants, i.e., there exists $a \in \mathbb{R}^2$ with either $A \subseteq q_{++}(a)$, $B \subseteq q_{--}(a)$, or with $A \subseteq q_{+-}(a)$, $B \subseteq q_{-+}(a)$. A set is *inseparable* if it cannot be partitioned into two nonempty separated subsets.

Clearly, a set with a connected quadrant hull is inseparable (since the parts in a separation would form disjoint pieces of the quadrant hull). It can be shown that also the reverse implication holds; we know of no immediate proof and we do not need this fact, so we omit its proof.

Proposition 5.1. *Let A be a compact inseparable set in the plane. Then* $\mathrm{co}^D(A) = \mathcal{Q}_{sc}\text{-}\mathrm{co}(A)$.

One proof can be given based on Proposition 2.7. We give another, slightly more technical proof, which yields an interesting extra piece of information on the Carathéodory number. We begin by a lemma.

Lemma 5.2. *Let $A \subseteq \mathbb{R}^2$ be a compact inseparable set, let u, v be points of A with $x(u) \le x(v)$, $y(u) \ge y(v)$; and let w be the point $(x(u), y(v))$ (see Fig.* 6(*a*)). *Suppose that the left top quadrant $q_{-+}(u)$ contains no point of A, and also the right bottom quadrant $q_{+-}(v)$ contains no point of A. Moreover, suppose that A', the part of A lying in the bottom-left closed quadrant $\overline{q}_{--}(w)$, is nonempty. Then there exist two points of A which together with u and v form a $\mathcal{C}_4$ configuration* (*see Example* 1.4) *such that the path $\pi = uwv$ is contained in its functional separately convex hull* (*thus also in* $\mathrm{co}^D(A)$).

Proof. Let $t \in A'$ be a point of A' with maximum y-coordinate, and let $r \in A'$ have maximum x-coordinate. Further, let ℓ be a point with the smallest x-coordinate among the points of $a \in A$ with $y(a) \ge y(v)$, and let b be a point with the smallest y-coordinate among the points of $a \in A$ with $x(a) \ge x(u)$. If $x(\ell) \le x(r)$ (as in Fig. 6(a)), then

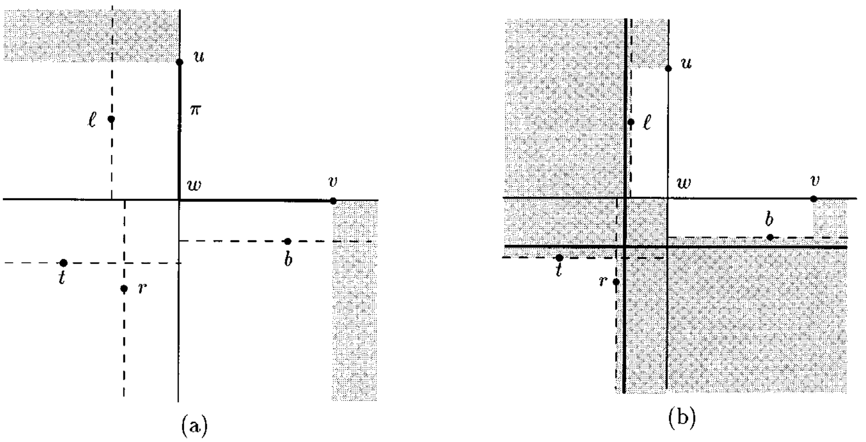

Fig. 6. Illustration for the proof of Lemma 5.2.

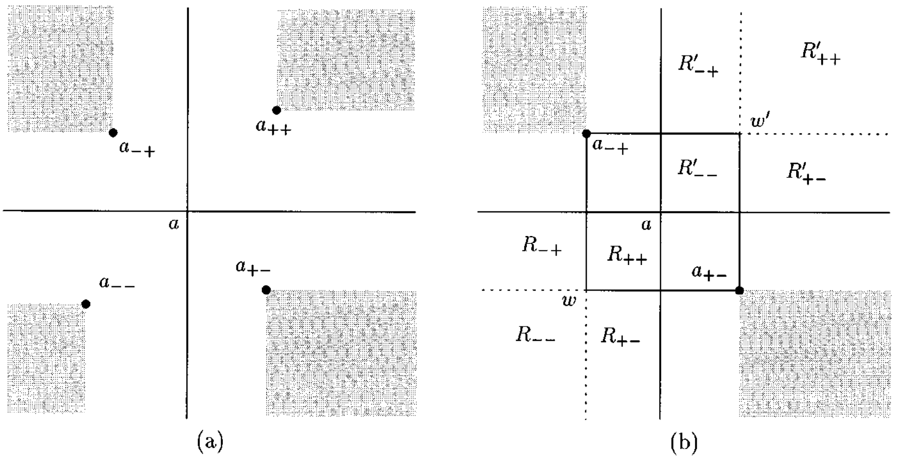

Fig. 7. Illustration for the proof of Proposition 5.1.

the points u, v, ℓ, r form a four-point configuration $\mathcal{C}_4$, and therefore (in particular) the path uwv is contained in $\mathrm{co}^D(A)$ as claimed. Similarly for $y(b) \le y(t)$, we find the configuration $\mathcal{C}_4$ as the points u, v, b, t. Finally, if both $x(\ell) > x(r)$ and $y(b) > y(t)$, we find that the quadrants with center

$$\left(\frac{x(\ell)+x(r)}{2}, \frac{y(b)+y(t)}{2}\right)$$

separate A (see Fig. 6(b); the shaded areas in the figure contain no points of A)—a contradiction. □

Proof of Proposition 5.1. Let A be inseparable and compact, and let $a \in \mathcal{Q}_{sc}\text{-co}(A)$. This means that all the four closed quadrants $\overline{q}_s(a)$ with vertices at a contain points of A. For each $s \in \{-1, 1\}^2$, choose a point $a_s \in \overline{q}_s(a) \cap A$ such that $q_s(a_s) \cap A = \emptyset$; see Fig. 7(a).

Consider the rectangle with a_{-+} and a_{+-} as its left-top and right-bottom corners, respectively, and let w, w' be its left-bottom and right-top corners, respectively; see Fig. 7(b). Draw the axis-parallel lines through w and w', and denote the resulting (closed) regions in $\overline{q}_{--}(a)$ and in $\overline{q}_{++}(a)$ as indicated in the figure.

If $R_{--} \cap A \ne \emptyset$, we may apply Lemma 5.2 with $u = a_{-+}$, $v = a_{+-}$, and we get that a four-point set $C \subseteq A$, consisting of a_{-+}, a_{+-}, and two other points of A forms a $\mathcal{C}_4$ configuration such that $\mathrm{co}^D(C)$ contains the segments $a_{-+}w$ and wa_{+-}. We now discuss possible positions of a_{++}. If $a_{++} \notin R'_{++}$, then it is easy to see that $a \in \mathrm{co}^D(C \cup \{a_{++}\})$. If $a_{++} \in R'_{++}$, a statement symmetric to Lemma 5.2 (with top and bottom reversed and left and right reversed) implies that a_{-+}, a_{+-}, and other two points of A form a $\mathcal{C}_4$ configuration C' such that $\mathrm{co}^D(C')$ contains the segments $a_{-+}w'$ and $w'a_{+-}$. Then clearly $a \in \mathrm{co}^D(C \cup C')$.

It remains to discuss the case when $R_{--} \cap A = \emptyset$. By symmetry, we may also assume that $R'_{++} \cap A = \emptyset$. Moreover, consider also the rectangle with a_{--} and a_{++}

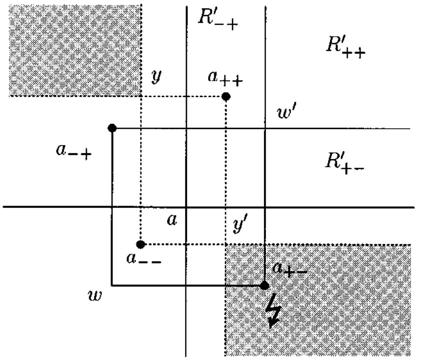

Fig. 8. A contradiction in the case $a_{--} \in R_{++}$, $a_{++} \in R'_{-+}$.

as left-bottom and right-top corners, respectively, and let y, y' be its left-top and right-bottom corners, respectively; again by symmetry, we may also assume that the regions $\overline{q}_{-+}(y)$ and $\overline{q}_{+-}(y')$ contain no points of A (note that these regions are defined using a_{--} and a_{++} analogously as R_{--} and R'_{++} were defined using a_{+-} and a_{-+}). With these assumptions, we discuss the possible positions of a_{--}. The region R_{--} was excluded. If $a_{--} \in R_{++}$, all possible positions of a_{++} lead to a contradiction to the supposed emptiness of R'_{++}, $\overline{q}_{-+}(y)$ or $\overline{q}_{+-}(y')$ (Fig. 8 illustrates this for the case $a_{++} \in R'_{-+}$, where the point a_{+-} gives a contradiction by lying in $q_{+-}(y')$). Finally, if $a_{--} \in R_{-+}$, say (the case $a_{--} \in R_{+-}$ is symmetric), the only possibility for a_{++} turns out to be $a_{++} \in R'_{+-}$, and in this case a_{+-}, a_{-+}, a_{--}, and a_{++} form a $\mathcal{C}_4$ configuration containing a in its functional D-convex hull. This proves Proposition 5.1. □

5.1. *Carathéodory Number*

The above proof in fact shows that whenever $a \in \mathrm{co}^D(A)$, there exists a subset $B \subseteq A$ of size bounded by a constant such that $a \in \mathrm{co}^D(B)$, that is, the functional separately convex hull in the plane has a bounded Carathéodory number. This is somewhat surprising, as the situation for the separately convex hull is different—for any number K one can find a set $A \subseteq \mathbb{R}^2$ and a point $a \in \mathrm{co}_D(A)$ such that $a \notin \mathrm{co}_D(B)$ for any at most K-point subset $B \subseteq A$. As an example, one may take the set

$$\left\{ \left(\frac{1}{2i-1}, 1+\frac{1}{i} \right) \middle| \, i = 1, 2, \ldots \right\} \cup \left\{ \left(\frac{1}{2i}, \frac{1}{i+1} \right) \middle| \, i = 1, 2, \ldots \right\} \cup \{(1,1)\}.$$

With a little extra effort, the Carathéodory number for the functional separately convex hull in the plane can be determined exactly.

Proposition 5.3. *Let $A \subset \mathbb{R}^2$ be compact and let $a \in \mathrm{co}^D(A)$ (where D is the union of the two coordinate axes). Then there exists an at most 5-point subset $B \subseteq A$ with $a \in \mathrm{co}^D(B)$.*

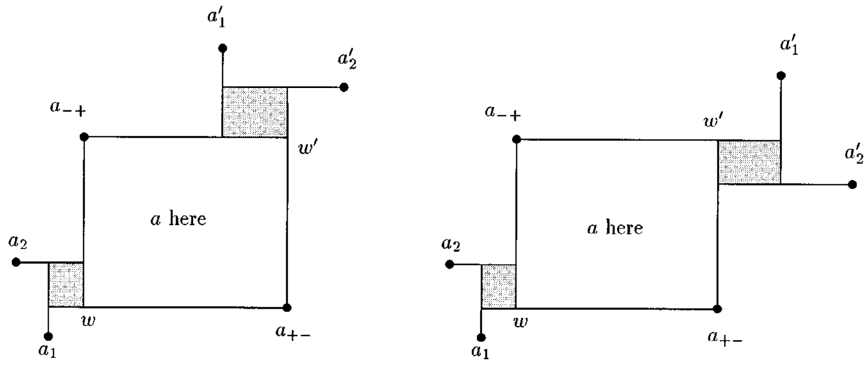

Fig. 9. Examining 6-point configurations.

Proof. We may assume A is inseparable (otherwise we may look at the inseparable piece of A whose hull contains a). By inspecting the above proof of Proposition 5.1, we find that the only situation where one needs more than five points to witness $a \in \mathrm{co}^D(A)$ is the case $a_{--} \in R_{--}$, $a_{++} \in R'_{++}$ (and the symmetric case for a_{+-} and a_{-+}). Here we have $\mathcal{C}_4$ configurations $C = \{a_{+-}, a_{-+}, a_1, a_2\}$ and $C' = \{a_{-+}, a_{+-}, a'_1, a'_2\}$. Up to symmetry, there are only two possible ways how these configurations may look, and these are depicted in Fig. 9. By an easy inspection of cases (discussing the possible position of a in the rectangle $a_{-+}wa_{+-}w'$), one can check that a always lies in the functional D-convex hull of some at most five points among $a_{-+}, a_{+-}, a_1, a_2, a'_1, a'_2$. □

5.2. *A Fast Algorithm in the Plane*

Proposition 5.4. *The functional separately convex hull of an n-point set in the plane is a disjoint union of polygons with $O(n)$ edges in total, and it can be computed in $O(n \log n)$ time.*

Proof Sketch. Based on Proposition 5.1, most of the algorithm is rather standard, so we omit various details. First we consider the case of an inseparable n-point set A. Here we need to compute the quadrant hull of A, and for this, well-known computational geometry techniques may be used, see, e.g., [PS]. For instance, we may note the following expression for the quadrant hull:

$$\mathcal{Q}_{sc}\text{-co}(A) = \bigcap_{s \in \{-1,1\}^2} U_s, \qquad \text{where} \quad U_s = \bigcup_{a \in A} \overline{q_s(a)}.$$

Indeed, a point x lies in $\mathcal{Q}_{sc}$-co(A) iff each of the closed quadrants with vertex at x contains a point of A; the union U_s is the set of all points x which contain a point of A in the closed quadrant $\overline{q_{-s}(x)}$.

Each U_s is an (unbounded) polygon bounded by a "staircase" polygonal line with at most n steps. It can be computed in $O(n \log n)$ time by an algorithm for computing the *maxima* of a planar point set, and the four sets U_s can be intersected by a plane sweep algorithm, say (see [PS] for terminology and such algorithms). To bound the number of vertices of the intersection, we note that each vertex is either a vertex of some U_s, or is an intersection of an edge of some U_s with the boundary of some $U_{s'}$ (resp. an endpoint of such an intersection if the intersection happens to be a segment). Since each edge of the boundary of U_s may only intersect the boundary of $U_{s'}$ in a single point or segment, the $O(n)$ bound on the number of vertices follows.

A slightly more interesting part of the algorithm is partitioning a finite set into inseparable pieces. Let A be the given n-point set. First we sort its points by their x-coordinates and also by their y-coordinates. Denote the points of A by $a_1, a_2, \ldots, a_n$ in such a way that $x(a_1) \le x(a_2) \le \cdots \le x(a_n)$, and let p be a permutation sorting the points in the y-direction, that is, $y(a_{p(1)}) \le \cdots \le y(a_{p(n)})$. We assume that the points of A are stored in a linear array (in the order $a_1, a_2, \ldots$), and the permutation p and its inverse p^{-1} are also stored in linear arrays.

The algorithm is easiest to describe recursively. We describe a procedure `SEPARATION` which, given the arrays storing A and p, either concludes that A is inseparable, or finds a partition $A = A_1 \dot\cup A_2$ of A into two separated sets. In the latter case, the procedure is called recursively on A_1 and on A_2. (Note that by the definition of separation, we have a sorted order for both A_1 and A_2 in both coordinates; hence in an actual implementation, the recursive call can be made with A_1 or A_2 specified as subintervals in the arrays representing A, so that we need not set up the arrays for A_1 and A_2.)

As we show below, the procedure can be implemented in such a way that it runs in $O(n)$ time on an inseparable set, or finds a separation of A into A_1, A_2 in time $O(\min(|A_1|, |A_2|))$. An easy analysis then shows that the whole recursive algorithm for decomposing A into inseparable pieces needs time $O(n \log n)$ for an n-point set A.

It remains to describe the procedure `SEPARATION`. Suppose $n > 1$. First we find out which kind of separation to look for. If $y(a_1) < y(a_n)$, then only a separation of the $--, ++$ type (i.e., all the points in the first group in the separation precede all points in the second group, for both coordinates) is possible. If $y(a_1) > y(a_n)$, we should look for a separation of the $+-, -+$ type; this case is similar to the former one and we omit its discussion.

Thus, we assume $y(a_1) < y(a_n)$. It is easy to see that the following conditions are necessary and sufficient for the sets $\{a_1, a_2, \ldots, a_i\}$ and $\{a_{i+1}, \ldots, a_n\}$ (with $1 \le i < n$) to form a separation of A of the $--, ++$ type:

$$\text{the indices } p(1), \ldots, p(i) \text{ form a permutation of } \{1, 2, \ldots, i\}, \tag{3}$$

$$x(a_i) < x(a_{i+1}) \text{ and } y(a_j) < y(a_{j'}), \quad \text{where} \quad j = p^{-1}(i),\ j' = p^{-1}(i+1). \tag{4}$$

The condition (3) can be rephrased as $\max\{p(1), p(2), \ldots, p(i)\} = i$. Thus, we start with $i = 1$ and then we increment i, maintaining a variable $cmax = \max\{p(1), \ldots, p(i)\}$, and we test for the condition $cmax = i$. Whenever this occurs, we check condition (4).

In this way, if the first set in the separation has i points, the separation is found in $O(i)$ time. In order to handle efficiently also the case when the first set in the separation is much larger than the second one, we simultaneously look for a separation "from backward." That is, at the ith step, we also consider the symmetric conditions for the sets $\{a_1, \ldots, a_{n-i}\}$ and $\{a_{n+1-i}, \ldots, a_n\}$ to be separated, i.e.,

the indices $p(n), p(n-1), \ldots, p(n-i+1)$ form a permutation of $\{n, n-1, \ldots, n-i+1\}$,

$x(a_{n+1-i}) > x(a_{n-i})$ and $y(a_j) > y(a_{j'})$, where $j = p^{-1}(n-i+1)$, $j' = p^{-1}(n-i)$.

In this way, a separation into A_1, A_2 is found in time $O(\min(|A_1|, |A_2|))$, and when i reaches $\lfloor n/2 \rfloor$ without a separation found, we know that the current input set is inseparable. □

6. Open Problems

As was indicated in Section 1.2, a long-term goal for further research is the understanding of functional rank-one convex hulls and rank-one convex envelopes of functions (and similarly for the corresponding quasi-convex notions). Below we list some immediate questions related to the current paper.

1. What is the maximum combinatorial complexity of the functional separately convex hull of n points in $\mathbb{R}^d$? ($O(n^d)$ is an easy upper bound, but perhaps it is $O(n)$ in three-dimensions etc.)? How efficiently can one compute it?
2. In particular, how efficiently can one decide whether $A = \mathrm{co}^D(A)$ for separate convexity? Are there any nice sufficient conditions? (In the plane, one has Tartar's result that $\mathrm{co}^D(A) = A$ iff $\mathrm{co}_D(A) = A$ and A has no $\mathcal{C}_4$ configuration.)
3. Is there a finite Carathéodory number for functional separate convexity in $\mathbb{R}^d$, for each d? (If yes, it has to be at least 2^d.) Is there a finite Carathéodory number for functional rank-one convexity in some dimensions?
4. What is the smallest number of points of a set $A \subset \mathbb{R}^3$ in general position with a nontrivial functional separately convex hull? (Our example gives an upper bound of 20, and an obvious lower bound is 8; a computer search revealed that no such configuration of size 8 exists.) Similarly, what is the smallest number of matrices (symmetric 2×2, say) in general position with a nontrivial functional rank-one convex hull?
5. How can our results for separate convexity be generalized to more directions in D? (The first case to look at are three directions in the plane.)
6. In particular, what do functional D-convex hulls of finite sets ("D-polytopes") look like?
7. Again, what are interesting necessary/sufficient conditions for $A = \mathrm{co}^D(A)$? In particular, what about symmetric 2×2 matrices and rank-one convexity?
8. What is a good analogue of orthants used in the definition of $\mathcal{Q}$-co for the separately convex case?
9. If we are given some "reasonable" $\mathcal{Q}$, how to compute the $\mathcal{Q}$-hull efficiently?
10. How to compute or approximate D-convex envelopes of functions efficiently?

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