

The Face Generated by a Point, Generalized Affine Constraints, and Quantum Theory

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We analyze faces generated by points in an arbitrary convex set and their relative algebraic interiors, which are nonempty as we shall prove. We show that by intersecting a convex set with a sublevel or level set of a generalized affine functional, the dimension of the face generated by a point may decrease by at most one. We apply the results to the set of quantum states on a separable Hilbert space. Among others, we show that every state having finite expected values of any two (not necessarily bounded) positive operators admits a decomposition into pure states with the same expected values. We discuss applications in quantum information theory.

Keywords: Face generated by a point, extreme set, relative algebraic interior, generalized affine constraint, extreme point, generalized compactness, quantum state, pure-state decomposition, minimal output entropy, operator E-norms.

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1. Introduction

Many tasks of mathematical physics and quantum communication theory require the analysis of the convex geometry of intersections of convex sets with a well-known geometry and sublevel sets of one or more generalized affine maps that take values in $\mathbb{R} \cup \{+\infty\}$. Our motivating example is the set of density operators on a separable Hilbert space with bounded expected values of one or more positive, generally, unbounded linear operators. The analysis of several important characteristics of quantum systems and channels leads to the optimization over sets of density operators of the above type, see the monographs [8, 26, 28] and the research papers [3, 5, 9, 14, 29, 30]. Therefore, our mission is to understand the convex geometry of these sets and to enable the use of analytic techniques.

We start with basics in Section 2. Relying on the *Kuratowski-Zorn lemma*, we show that the face generated by a point in a convex set has a nonempty relative algebraic interior, which contains this point. We discuss corollaries and examples and we describe the face generated by a point in the intersection of two convex sets.

In Section 3 we show that by intersecting a convex set with a sublevel set or a level set of a generalized affine map, the dimension of the face generated by a point may

decrease by at most one and cannot decrease from an infinite to a finite value. This allows us to exploit gaps in the list of dimensions of faces. For example, if the convex set has no faces of dimension $1, 2, \dots, n$, then every extreme point of the intersection of the convex set with the sublevel or level sets of up to n generalized affine maps is an extreme point of the original convex set.

Beginning with Section 4, we study the class of generalized affine maps $\mathfrak{S}(\mathcal{H}) \rightarrow [0, +\infty]$ on the set $\mathfrak{S}(\mathcal{H})$ of quantum states, defined as the expected value functionals $f_H : \rho \mapsto \text{Tr } H\rho$ of positive (not necessarily bounded) operators H on a separable Hilbert space $\mathcal{H}$. The list of dimensions of faces of $\mathfrak{S}(\mathcal{H})$ has a gap between zero (pure state) and three (Bloch ball). Hence, every extreme point of the intersection of the sublevel or level sets of the expected value functionals f_{H_1}, f_{H_2} of two positive operators H_1, H_2 is a pure state. We also show that this is not true for more than two operators nor for classical states.

In Section 5 we combine convex geometry with topology and measure theory. As the sublevel sets of f_{H_1} and f_{H_2} are closed, μ -compact, and convex sets [9, 17], we are able to write each state in their intersection as the barycenter of a probability measure supported on the set of pure states in the intersection of the same sublevel sets. Although the level sets of f_{H_1} and f_{H_2} are not closed, every state having finite expected values regarding H_1 and H_2 admits a decomposition into pure states that have the same expected values almost surely. As an example, any bipartite state with finite marginal energies can be decomposed into pure states with the same marginal energies.

The results allow us to show that the supremum of any convex function on the intersection of the sublevel or level sets of f_{H_1} and f_{H_2} can be taken only over pure states, provided that this function is lower semicontinuous or upper semicontinuous and upper bounded. This result (in case $H_2 = H_1$) simplifies essentially definitions of several characteristics used in quantum information theory and adjacent fields of mathematical physics. These applications are considered in Section 6.

2. On the face generated by a point

We explore the face of a convex set generated by a point and the relative algebraic interior of such a face. The reader may recognize the finite-dimensional counterparts to our findings, for example from [18].

We work in the setting of a real vector space V and a convex subset $K \subseteq V$. A subset $E \subseteq K$ is an *extreme set* (or an *extreme subset of K* if we wish to emphasize the set K) if whenever $x \in E$ and

$$x = (1 - \lambda)y + \lambda z$$

for some $\lambda \in (0, 1)$ and $y, z \in K$, then y and z are also in E , see [15] for this definition. A point $x \in K$ is called an *extreme point* if $\{x\}$ is an extreme set. We denote the set of extreme points of K by $\text{ext}(K)$. A *face* of K is a convex, extreme subset of K . Note that if x is an extreme point, then $\{x\}$ is a face. As the intersection of an arbitrary family of faces of K is a face of K , the smallest face $F_K(x)$ of K that contains $x \in K$ exists. We call $F_K(x)$ the *face of K generated by x* .

A *linear combination* of $n \in \mathbb{N}$ points $x_1, \dots, x_n \in V$ is a sum

$$\alpha_1 x_1 + \dots + \alpha_n x_n$$

with weights $\alpha_i \in \mathbb{R}$, $i = 1, \dots, n$. The linear combination is an *affine combination* if $\alpha_1 + \dots + \alpha_n = 1$ and a *convex combination* if $\alpha_1 + \dots + \alpha_n = 1$ and $\alpha_i \geq 0$ for all $i = 1, \dots, n$. Given a subset $X \subseteq V$, the set $\text{aff}(X)$ of all affine combinations of points from X is the *affine hull* of X . This is the smallest affine subspace of V containing X . The *translation vector space* $\text{lin}(X)$ is the set of differences between each two points from $\text{aff}(X)$.

The *algebraic interior* of the convex set K is the set of all points $x \in K$ such that for every straight line $g \subseteq V$ passing through x the point x lies in the interior of the intersection $K \cap g$. We call *relative algebraic interior* of K the set $\text{ri}(K)$ of all points $x \in K$ such that for every straight line $g \subseteq \text{aff}(K)$ passing through x the point x lies in the interior of the intersection $K \cap g$.

Lemma 2.1. *Let $C \subseteq K$ be a convex subset, $E \subseteq K$ an extreme subset, $F \subseteq K$ a face of K , and let $x \in K$ be a point. Then*

- (a) $\text{ri}(C) \cap E \neq \emptyset \implies C \subseteq E$,
- (b) $x \in F \iff F_K(x) \subseteq F$,
- (c) $x \in \text{ri}(F) \implies F = F_K(x)$.

Proof. (a) Let $x \in \text{ri}(C)$ and $y \in C$ with $y \neq x$. Then x is an interior point of the intersection $C \cap g$ of C with the line g through x and y . Hence, if x lies in the extreme set E so does y .

(b) The inclusion $F_K(x) \subseteq F$ is true as $F_K(x)$ is the minimal face containing x . The converse is obvious as $x \in F_K(x)$.

(c) The inclusion $F \subseteq F_K(x)$ follows from part (a) with $C = F$ and $E = F_K(x)$. The inclusion $F_K(x) \subseteq F$ follows from part (b). $\square$

Corollary 2.7 provides the converse to Lemma 2.1, part (c).

Lemma 2.2. *The complement $K \setminus \text{ri}(K)$ of the relative algebraic interior $\text{ri}(K)$ is an extreme subset of K and $\text{ri}(K)$ is a convex set.*

Proof. By the definition of the relative algebraic interior we have

$$K \setminus \text{ri}(K) = \{x \in K \mid \exists v \in \text{lin}(K) : x + \epsilon v \notin K \ \forall \epsilon > 0\}.$$

The right-hand side is an extreme set. Indeed, let $x, y, z \in K$, $\lambda \in (0, 1)$, and $x = (1 - \lambda)y + \lambda z$. If $y \in \text{ri}(K)$, then for all vectors $v \in \text{lin}(K)$ there is $\epsilon_{y,v} > 0$ such that $y + \epsilon_{y,v}v \in K$. Hence we have $x + (1 - \lambda)\epsilon_{y,v}v \in K$, that is to say $x \in \text{ri}(K)$. Similarly, $x \in K \setminus \text{ri}(K)$ implies $z \in K \setminus \text{ri}(K)$, which proves that $K \setminus \text{ri}(K)$ is an extreme set.

The set $\text{ri}(K)$ is convex as it is the complement of an extreme set. Indeed, it is easy to show that the complement $K \setminus S$ of a subset $S \subseteq K$ is convex if and only if $(1 - \lambda)y + \lambda z \in S$ implies that at least one of the points y or z lies in S for all $y, z \in K$ and $\lambda \in (0, 1)$, while both y and z needed to lie in S if S were an extreme set. $\square$

It is well known that nonempty convex sets may have empty relative algebraic interiors, see Section III.1.6 of [2] and the Examples 2.8 and 2.10 below. This is not the case for faces generated by points in a convex set.

Theorem 2.3. *Let x be a point in K . The affine hull of the face of K generated by x is*

$$\text{aff } F_K(x) = \{y \in V \mid \exists \epsilon > 0 : x \pm \epsilon(y - x) \in F_K(x)\}. \quad (1)$$

In particular, x lies in the relative algebraic interior of $F_K(x)$.

Proof. The second assertion follows from equation (1) and from the definition of the relative algebraic interior. We prove the equation (1). As the inclusion “ $\supseteq$ ” is clear, it suffices to prove “ $\subseteq$ ”. First, note that for all $v \in V$ the set

$$E_v = \{y \in F_K(x) \mid y + \epsilon v \notin F_K(x) \ \forall \epsilon > 0\}$$

is an extreme subset of $F_K(x)$. The proof is similar to the proof of Lemma 2.2.

The main idea is as follows. If $x + v \in \text{aff}(F_K(x))$, then it follows that E_v and E_{-v} are proper subsets of $F_K(x)$, as we detail below. If x lies in E_v , then according to the Kuratowski-Zorn lemma, there is a maximal convex subset C of E_v containing x . Below, we show that C is a face of $F_K(x)$. Since $F_K(x)$ is the minimal face containing x , this implies that x lies outside of E_v . Similarly, x lies outside of E_{-v} . This means that there are $\epsilon_1, \epsilon_2 > 0$ such that $x + \epsilon_1 v, x - \epsilon_2 v \in F_K(x)$. As $F_K(x)$ is convex, it follows that $x \pm \epsilon v \in F_K(x)$ where $\epsilon = \min(\epsilon_1, \epsilon_2)$. In other words, $x + v$ lies in the right-hand side of (1).

As promised, we show that E_v and E_{-v} are proper subsets of $F_K(x)$ if $x + v$ lies in $\text{aff}(F_K(x))$. The vector $v = \sum_{i=1}^n \alpha_i x_i$ is a linear combination of points $x_1, \dots, x_n$ from $F_K(x)$ such that $\alpha_1 + \dots + \alpha_n = 0$. We can take $M \doteq (|\alpha_1| + \dots + |\alpha_n|)/2$ to be strictly positive. Then the points

$$y = \sum_{\alpha_i > 0} \frac{\alpha_i}{M} x_i \quad \text{and} \quad z = - \sum_{\alpha_i < 0} \frac{\alpha_i}{M} x_i$$

lie in $F_K(x)$ and $y - z = \frac{1}{M}v$ holds. This proves $z \notin E_v$ and $y \notin E_{-v}$.

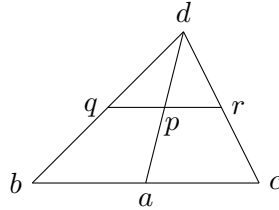


Figure 2.1: Sketch for the proof of Theorem 2.3.

We prove the claim that every maximal convex subset C of E_v is a face of $F_K(x)$. The same conclusion is true for maximal convex subsets of E_v containing x . As C is convex, it suffices to show that C is an extreme set. Let $a = (1 - \lambda)b + \lambda c$ be a point in C , where $b, c \in F_K(x)$ and $\lambda \in (0, 1)$. Since C is a maximal convex subset of E_v , the claim is confirmed by proving that E_v contains the convex hulls of $C \cup \{b\}$

and of $C \cup \{c\}$. Let $d \in C$ and let $p = (1 - \mu)a + \mu d$, $q = (1 - \mu)b + \mu d$, and $r = (1 - \mu)c + \mu d$, where $\mu \in [0, 1]$. Then $p = (1 - \lambda)q + \lambda r$ as shown in Figure 2.1. Since $p \in [a, d] \subseteq C \subseteq E_v$, and as E_v is an extreme set, it follows that $q, r \in E_v$. $\square$

The extreme set E_v in the proof of Theorem 2.3 is not convex in general. As an example, consider the square $K = [-1, 1] \times [-1, 1]$, $x = (0, 0)$, and $v = (1, 1)$. Then $F_K(x) = K$ and $E_v = \{(\eta, \xi) \in K : \eta = 1 \text{ or } \xi = 1\}$ is the nonconvex union of two perpendicular segments. See also Corollary 2.5.

Note that (because $F_K(x)$ is an extreme subset of K) equation (1) implies that the affine hull of the face of K generated by a point $x \in K$ is

$$\text{aff } F_K(x) = \{y \in V \mid \exists \epsilon > 0 : x \pm \epsilon(y - x) \in K\}. \quad (2)$$

Corollary 2.4. *Let $x \in K$. Then $F_K(x) = \bigcup_{y, z \in K, x \in (y, z)} [y, z]$. The right-hand side is the union over all closed segments in K for which x lies on the open segment. (By definition $[x, x] = (x, x) = \{x\}$.)*

Proof. The inclusion “ $\supseteq$ ” follows as $F_K(x)$ is an extreme set containing x . Conversely, let $y \in F_K(x)$. By equation (2) there is $\epsilon > 0$ such that the point $z_- = x - \epsilon(y - x)$ lies in K . Then $x = \frac{1}{1+\epsilon}z_- + \frac{\epsilon}{1+\epsilon}y$ shows that x lies in the open segment (z_-, y) . This completes the proof. $\square$

Corollary 2.4 shows that the closure of $F_K(x)$ in a topological vector space would be the *face function* of K at a point x in K , as studied in [10]. A subset E of K satisfying the property (b) of Corollary 2.5 below is called an *extreme set* in the paper [16]. The faces with nonempty relative algebraic interiors are the building blocks of extreme sets and of convex sets in the sense of Corollary 2.5, part (c), and Corollary 2.6, respectively.

Corollary 2.5. *Let $E \subseteq K$ be a subset. The following assertions are equivalent. The set E*

- (a) *is an extreme subset of K ,*
- (b) *contains the face $F_K(x)$ of K generated by any point x in E ,*
- (c) *is a union of faces of K having nonempty relative algebraic interiors,*
- (d) *is a union of faces of K .*

Proof. The implication (a) $\Rightarrow$ (b) follows from Corollary 2.4. The implication (b) $\Rightarrow$ (c) follows from Theorem 2.3 as x is a relative algebraic interior point of $F_K(x)$ for all $x \in K$. The implication (c) $\Rightarrow$ (d) is obvious and (d) $\Rightarrow$ (a) is true as every union of extreme sets is an extreme set. $\square$

Corollary 2.6. *The family of relative algebraic interiors of faces of K is a partition of K .*

Proof. The family $\{\text{ri}(F_K(x)) : x \in K\}$ covers K , as Theorem 2.3 shows $x \in \text{ri}(F_K(x))$ for all $x \in K$. Let F, G be faces of K that intersect in their relative algebraic interiors, say $x \in \text{ri}(F) \cap \text{ri}(G)$. Then part (c) of Lemma 2.1 provides $F = G = F_K(x)$. This proves the claim. $\square$

We characterize relative algebraic interiors of faces.

Corollary 2.7. *Let F be a face of K and x a point in K . Then*

$$x \in \text{ri}(F) \iff F = F_K(x).$$

In particular, if x and y are points in K , then

$$x \in \text{ri}(F_K(y)) \iff F_K(y) = F_K(x).$$

Proof. The first statement follows directly from part (c) of Lemma 2.1 and Theorem 2.3. The second statement is the special case $F = F_K(y)$ of the first statement. $\square$

Example 2.8. (Univariate polynomials) Let V be the vector space of all countably infinite sequences of real numbers such that all but finitely many terms are zero. Each nonzero element from V may be written in the form

$$v = (a_0, a_1, a_2, \dots, a_{n-1}, a_n, 0, 0, 0, \dots), \quad a_n \neq 0$$

where $a_i \in \mathbb{R}$ for all $i = 0, \dots, n$ and $n \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$. There is a one-to-one correspondence between V and the space $\mathbb{R}[x]$ of all polynomials in one variable x with real coefficients, *via* the identification of the above vector v with the nonzero polynomial

$$p = a_n x^n + a_{n-1} x^{n-1} + \dots + a_2 x^2 + a_1 x + a_0, \quad a_n \neq 0. \quad (3)$$

The *degree* of p is $n = \deg(p)$ and the *leading coefficient* is a_n .

It is well known that the convex set $K \subset \mathbb{R}[x]$ of polynomials with positive leading coefficients has an empty relative algebraic interior [2]. Below in Lemma 2.9 we show that the subsets of K consisting of polynomials of constant degrees are relative algebraic interiors of faces of K . As the family of relative algebraic interiors of all faces is a partition of K (see Corollary 2.6), we corroborate that the relative algebraic interior $\text{ri}(K)$ is empty. $\square$

Lemma 2.9. *Let $K \subset \mathbb{R}[x]$ denote the convex set of univariate polynomials with positive leading coefficients. The face of K generated by a polynomial $p \in K$ is $F_K(p) = F_{\deg(p)}$, where*

$$F_n = \{q \in K \mid \deg(q) \leq n\}, \quad n \in \mathbb{N}_0.$$

The relative algebraic interior of F_n is

$$\text{ri}(F_n) = \{q \in K \mid \deg(q) = n\}, \quad n \in \mathbb{N}_0,$$

which is an open half-space of dimension $n + 1$. Every nonempty extreme subset of K is equal to K or to one of the faces F_n , $n \in \mathbb{N}_0$.

Proof. Let $p, q \in K$ be polynomials with positive leading coefficients. Corollary 2.4 shows that q lies in $F_K(p)$ if and only if there is $\lambda < 0$ such that $(1 - \lambda)p + \lambda q \in K$, which is equivalent to $\deg(q) \leq \deg(p)$. This proves that $F_K(p) = F_{\deg(p)}$. Corollary 2.7 shows that q lies in $\text{ri}(F_K(p))$ if and only if $F_K(p) = F_K(q)$, or equivalently $\deg(p) = \deg(q)$.

We show that every nonempty extreme subset E of K equals K or F_n for some $n \in \mathbb{N}_0$. Let $I = \{\deg(p) : p \in E\}$. Then $E = \bigcup_{i \in I} F_n$ holds as $p \in E$ implies $F_{\deg(p)} = F_K(p) \subseteq E$ by Corollary 2.5. Since $F_0 \subseteq F_1 \subseteq F_2 \subseteq \dots$, this implies $E = F_n$ if $\sup(I) = n < \infty$ and $E = K$ if $\sup(I) = \infty$. $\square$

Example 2.10. (Discrete probability measures) The set of probability measures on the set of natural numbers $\mathbb{N} = \{1, 2, 3, \dots\}$ is affinely isomorphic to the set

$$\Delta_{\mathbb{N}} = \left\{ p : \mathbb{N} \rightarrow \mathbb{R} \mid p(n) \geq 0 \ \forall n \in \mathbb{N}, \text{ and } \sum_{n \in \mathbb{N}} p(n) = 1 \right\}$$

of probability densities with respect to the counting measure. The set of extreme points $\text{ext}(\Delta_{\mathbb{N}})$ consists of the densities $\delta_n(m) = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$, $m \in \mathbb{N}$, concentrated at the points $n \in \mathbb{N}$. We may think of $\Delta_{\mathbb{N}}$ as a *simplex*, or better a σ -*simplex*, as each density $p \in \Delta_{\mathbb{N}}$ can be written in a unique way as a countable convex combination $p = \sum_{n \in \mathbb{N}} \lambda_n \delta_n$ of extreme points, where $\lambda_n \geq 0$ for all $n \in \mathbb{N}$, and $\sum_{n \in \mathbb{N}} \lambda_n = 1$.

Let $\text{supp}(p) = \{n \in \mathbb{N} : p(n) > 0\}$ denote the *support* of a density $p \in \Delta_{\mathbb{N}}$ and

$$\Delta_I = \{p \in \Delta_{\mathbb{N}} \mid \text{supp}(p) \subseteq I\}$$

the set of densities supported on a subset $I \subseteq \mathbb{N}$. The convex set Δ_I is an extreme subset and hence a face of $\Delta_{\mathbb{N}}$ as

$$\text{supp}((1 - \lambda)p + \lambda q) = \text{supp}(p) \cup \text{supp}(q) \quad (4)$$

holds for all $p, q \in \Delta_{\mathbb{N}}$ and $\lambda \in (0, 1)$. Therefore, $\text{ext}(\Delta_I) = \{\delta_n \mid n \in I\}$. The convex hull

$$\text{conv}(\{\delta_n \mid n \in I\}) = \{p \in \Delta_I : |\text{supp}(p)| < \infty\}$$

is the set of densities with finite support in I . Again by equation (4), the convex set $\text{conv}(\{\delta_n \mid n \in I\})$ is an extreme subset and hence a face of $\Delta_{\mathbb{N}}$.

For finite subsets $I \subset \mathbb{N}$ we have $\text{conv}(\{\delta_n \mid n \in I\}) = \Delta_I$. Lemma 2.12 below shows $F_{\Delta_{\mathbb{N}}}(p) = \Delta_{\text{supp}(p)}$, which has relative algebraic interior

$$\text{ri}(F_{\Delta_{\mathbb{N}}}(p)) = \{q \in \Delta_{\mathbb{N}} : \text{supp}(q) = \text{supp}(p)\}$$

for all densities $p \in \Delta_{\mathbb{N}}$ of finite support.

Let $I \subseteq \mathbb{N}$ be infinite. Then the face $\text{conv}(\{\delta_n \mid n \in I\})$ has an empty relative algebraic interior. This follows from part (c) of Lemma 2.1, as $F_{\Delta_{\mathbb{N}}}(p) = \Delta_{\text{supp}(p)}$ is strictly included in $\text{conv}(\{\delta_n \mid n \in I\})$ for all densities p with finite support in I . The relative algebraic interior of the simplex Δ_I is empty, too, but for different reasons aside from the support sizes. Let us consider the interval

$$\mathcal{I}(I) = \{F \text{ is a face of } \Delta_{\mathbb{N}} \mid \text{conv}(\{\delta_n \mid n \in I\}) \subseteq F \subseteq \Delta_I\},$$

partially ordered by inclusion. Lemma 2.12 shows that the face $F_{\Delta_{\mathbb{N}}}(p)$ belongs to $\mathcal{I}(I)$ if and only if $\text{supp}(p) = I$ and that the inclusion of such faces is determined by the asymptotics of converging series.

Following an example by Hadamard [6], we define the map $p_H : \mathbb{N} \rightarrow \mathbb{R}$,

$$p_H(n) = p(n)/(\sqrt{r_n} + \sqrt{r_{n+1}}) = \sqrt{r_n} - \sqrt{r_{n+1}}, \quad n \in \mathbb{N},$$

for every density $p \in \Delta_{\mathbb{N}}$ with infinite support I and $r_n = \sum_{m \geq n} p(m)$. The map p_H is a probability density with support I , and for $n \in I$ we have

$$p(n)/p_H(n) = \sqrt{r_n} + \sqrt{r_{n+1}} \xrightarrow{n \rightarrow \infty} 0 \quad \text{and} \quad p_H(n)/p(n) \xrightarrow{n \rightarrow \infty} \infty.$$

Lemma 2.12 shows that $p \in F_{\Delta_{\mathbb{N}}}(p_H)$ and $p_H \notin F_{\Delta_{\mathbb{N}}}(p)$. Part (b) of Lemma 2.1 then implies that $\mathcal{I}(I)$ contains the infinite chain of strictly included faces

$$F_{\Delta_{\mathbb{N}}}(p) \subset F_{\Delta_{\mathbb{N}}}(p_H) \subset F_{\Delta_{\mathbb{N}}}((p_H)_H) \subset \cdots \quad (5)$$

The strict inclusions $F_{\Delta_{\mathbb{N}}}(p) \subset \Delta_I$ for all densities p with support I , the strict inclusions $F_{\Delta_{\mathbb{N}}}(q) \subseteq \Delta_J \subset \Delta_I$ for all densities q with support $J \subset I$, and part (c) of Lemma 2.1 show $\text{ri}(\Delta_I) = \emptyset$.

We close the example with a glimpse at the interval $\mathcal{I}(\mathbb{N})$. We consider the Euler-Riemann zeta function $\zeta(s) = \sum_{n \in \mathbb{N}} n^{-s}$ and the map $p_s : \mathbb{N} \rightarrow \mathbb{R}$, $n \mapsto \zeta(s)^{-1} \cdot n^{-s}$ for all $s > 1$. Lemma 2.12 shows that $p_s \in F_{\Delta_{\mathbb{N}}}(p_t)$ holds if and only if $t \leq s$ for all $s, t > 1$. Hence, part (b) of Lemma 2.1 proves

$$F_{\Delta_{\mathbb{N}}}(p_s) \subseteq F_{\Delta_{\mathbb{N}}}(p_t) \iff t \leq s, \quad s, t > 1.$$

The interval $\mathcal{I}(\mathbb{N})$ contains the uncountable chain of faces $\{F_{\Delta_{\mathbb{N}}}(p_s) : s > 1\}$. $\square$

Question 2.11. We noted in Example 2.10 that the partial ordering of the faces generated by points of the σ -simplex $\Delta_{\mathbb{N}}$ is governed by the asymptotics of converging series, a classical topic of real analysis [11, Section 41]. Could the σ -simplex $\Delta_{\mathbb{N}}$ provide a convex geometry approach to the theory of series?

We showed in Example 2.10 that the convex sets $\text{conv}(\{\delta_n \mid n \in I\})$ and Δ_I are faces of the σ -simplex $\Delta_{\mathbb{N}}$ and that they have empty relative algebraic interiors for all infinite subsets $I \subseteq \mathbb{N}$. Are there any other faces of $\Delta_{\mathbb{N}}$ that also have empty relative algebraic interiors?

Lemma 2.12. *The face of $\Delta_{\mathbb{N}}$ generated by a density $p \in \Delta_{\mathbb{N}}$ is*

$$F_{\Delta_{\mathbb{N}}}(p) = \{q \in \Delta_{\text{supp}(p)} \mid \sup_{n \in \text{supp}(p)} q(n)/p(n) < \infty\}. \quad (6)$$

The face $F_{\Delta_{\mathbb{N}}}(p)$ has the relative algebraic interior

$$\text{ri}(F_{\Delta_{\mathbb{N}}}(p)) = \{q \in F_{\Delta_{\mathbb{N}}}(p) \mid \inf_{n \in \text{supp}(p)} q(n)/p(n) > 0\}. \quad (7)$$

Proof. Corollary 2.4 shows that a density $q \in \Delta_{\mathbb{N}}$ lies in $F_{\Delta_{\mathbb{N}}}(p)$ if and only if there is $\lambda < 0$ such that $(1 - \lambda)p + \lambda q \in \Delta_{\mathbb{N}}$. If such a $\lambda < 0$ exists, $q(n) = 0$ holds for all $n \notin \text{supp}(p)$ and $\frac{q(n)}{p(n)} \leq \frac{1-\lambda}{-\lambda}$ holds for all $n \in \text{supp}(p)$. Conversely, let $q \in \Delta_{\text{supp}(p)}$ and let $\mu = \sup_{n \in \text{supp}(p)} \frac{q(n)}{p(n)} < \infty$. As q is a probability density supported on

$\text{supp}(p)$, we have $\mu \geq 1$ with equality if and only if $p = q$. As $p \in F_{\Delta_{\mathbb{N}}}(p)$, we may assume $\mu > 1$ and define $\lambda = \frac{-1}{\mu-1}$. Then

$$\frac{\mu}{\mu-1}p(n) + \frac{-1}{\mu-1}q(n) \geq \frac{\mu}{\mu-1}p(n) + \frac{-1}{\mu-1}\mu p(n) = 0 \quad \forall n \in \text{supp}(p)$$

completes the proof of equation (6).

Corollary 2.7 shows that a density function $q \in \Delta_{\mathbb{N}}$ lies in $\text{ri}(F_{\Delta_{\mathbb{N}}}(p))$ if and only if $F_{\Delta_{\mathbb{N}}}(p) = F_{\Delta_{\mathbb{N}}}(q)$. By equation (6) this is equivalent to $\text{supp}(p) = \text{supp}(q)$ and

$$\sup_{n \in \text{supp}(p)} \frac{r(n)}{p(n)} < \infty \quad \Longleftrightarrow \quad \sup_{n \in \text{supp}(p)} \frac{r(n)}{q(n)} < \infty \quad \forall r \in \Delta_{\text{supp}(p)}. \quad (8)$$

To prove the equivalence of (8) and the conditions specifying the right-hand side of (7), it suffices to assume $\text{supp}(p) = \text{supp}(q)$ and to prove that (8) is equivalent to

$$\sup_{n \in \text{supp}(p)} q(n)/p(n) < \infty \quad \text{and} \quad \sup_{n \in \text{supp}(p)} p(n)/q(n) < \infty. \quad (9)$$

If the first condition of (9) fails, then $r = q$ shows that (8) fails. Similarly, if the second condition fails then $r = p$ shows that (8) fails. Conversely, if (9) is true, then

$$\sup_{n \in \text{supp}(p)} \frac{r(n)}{p(n)} = \sup_{n \in \text{supp}(p)} \frac{r(n)}{q(n)} \cdot \frac{q(n)}{p(n)} \leq \sup_{n \in \text{supp}(p)} \frac{r(n)}{q(n)} \cdot \sup_{n \in \text{supp}(p)} \frac{q(n)}{p(n)}$$

proves the implications “ $\Leftarrow$ ” of (8). The opposite implications are proved in a similar way. $\square$

The face generated by a point in the intersection of two convex sets is easily described in terms of the individual sets.

Proposition 2.13. *Let $K, L \subseteq V$ be two convex sets and let $x \in K \cap L$. Then*

- (a) $F_{K \cap L}(x) = F_K(x) \cap F_L(x),$
- (b) $\text{ri}(F_K(x) \cap F_L(x)) = \text{ri}(F_K(x)) \cap \text{ri}(F_L(x)),$
- (c) $\text{aff}(F_K(x) \cap F_L(x)) = \text{aff}(F_K(x)) \cap \text{aff}(F_L(x)).$

Proof. Part (c). We prove the equation by demonstrating the two inclusions

$$\text{aff}(F_{K \cap L}(x)) \subseteq \text{aff}(F_K(x) \cap F_L(x)) \subseteq \text{aff}(F_K(x)) \cap \text{aff}(F_L(x)) \quad (10)$$

and the equality of the first and third terms of (10). The latter follows from equation (2), according to which for all $y \in V$ we have

$$\begin{aligned} & y \in \text{aff}(F_{K \cap L}(x)) \\ \Longleftrightarrow & \exists \epsilon > 0 : x \pm \epsilon(y - x) \in K \cap L \\ \Longleftrightarrow & (\exists \epsilon_K > 0 : x \pm \epsilon_K(y - x) \in K) \wedge (\exists \epsilon_L > 0 : x \pm \epsilon_L(y - x) \in L) \\ \Longleftrightarrow & y \in \text{aff}(F_K(x)) \cap \text{aff}(F_L(x)). \end{aligned}$$

It is clear that $F = F_K(x) \cap F_L(x)$ is a face of $K \cap L$ containing x . Hence we have $F_{K \cap L}(x) \subseteq F$, which implies the first inclusion of (10). The second inclusion follows because $\text{aff}(F)$ is the smallest affine space containing F .

Part (b). The inclusion “ $\supseteq$ ” follows from the definition of the relative algebraic interior and from $\text{aff}(F) \subseteq \text{aff}(F_K(x)) \cap \text{aff}(F_L(x))$ provided in part (c). To prove the inclusion “ $\subseteq$ ” it suffices to show $\text{ri}(F) \subseteq \text{ri}(F_K(x))$. Lemma 2.2 shows that $\text{ri}(F_K(x))$ is the complement of an extreme subset of $F_K(x)$. As F intersects $\text{ri}(F_K(x))$, namely in x , part (a) of Lemma 2.1 shows that $\text{ri}(F) \subseteq \text{ri}(F_K(x))$.

Part (a). By Theorem 2.3, the point x lies in $\text{ri} F_K(x) \cap \text{ri} F_L(x)$. This and the inclusion “ $\supseteq$ ” of part (b) imply that x lies in the relative algebraic interior of the face F of $K \cap L$. Thus, part (c) of Lemma 2.1 proves the claim. $\square$

Note that the assertions of Proposition 2.13 are simplified according to the rules $F_L(x) = L = \text{ri}(L) = \text{aff}(L)$ if L is an affine space (incident with x).

3. Convex sets under generalized affine constraints

We study sublevel sets and level sets of generalized affine maps on convex sets and we analyze the dimensions of the faces generated by their points. In addition to general convex sets, we discuss the class of pyramids.

As before, let V be a real vector space and $K \subseteq V$ a convex subset. A map $f : K \rightarrow \mathbb{R}$ is called an *affine map* if

$$f(\lambda x + \mu y) = \lambda f(x) + \mu f(y), \quad x, y \in K, \quad \lambda, \mu \geq 0, \quad \lambda + \mu = 1. \quad (11)$$

Consider the extended real line $\mathbb{R} \cup \{+\infty\}$ with the obvious ordering and arithmetics¹. We call

$$f : K \rightarrow \mathbb{R} \cup \{+\infty\}$$

a *generalized affine map on K* if f satisfies the equation (11) with the extended arithmetics. Let $\alpha \in \mathbb{R}$ and let

$$\begin{aligned} K_f &= \{x \in K : f(x) < +\infty\}, \\ K_f^{\leq} &= \{x \in K : f(x) \leq \alpha\}, & (\text{sublevel set}) \\ K_f^{\overline{}} &= \{x \in K : f(x) = \alpha\}. & (\text{level set}) \end{aligned} \quad (12)$$

If $\alpha \in \mathbb{R}$ is unspecified, we assume the sublevel set $K_f^{\leq}$ and level set $K_f^{\overline{}}$ are taken at the same value of α .

Lemma 3.1. *The set K_f is a face of K .*

Proof. Let $x, y \in K$, $\lambda \in [0, 1]$, and $z = (1 - \lambda)x + \lambda y$ throughout the proof.

To show that K_f is convex, we assume that $x, y \in K_f$. Then $f(x) < +\infty$ and $f(y) < +\infty$ gives

$$f(z) = f((1 - \lambda)x + \lambda y) = (1 - \lambda)f(x) + \lambda f(y) < +\infty,$$

¹We have $\alpha < +\infty$ for all $\alpha \in \mathbb{R}$. The addition is defined as $(+\infty) + (+\infty) = +\infty$ and $\alpha + (+\infty) = (+\infty) + \alpha = +\infty$ for all $\alpha \in \mathbb{R}$. The multiplication with non-negative scalars is defined as $0 \cdot (+\infty) = (+\infty) \cdot 0 = 0$ and $\lambda \cdot (+\infty) = (+\infty) \cdot \lambda = +\infty$ for all $\lambda > 0$.

which means $z \in K_f$. To show that K_f is an extreme set, it suffices to show that $x \notin K_f$ or $y \notin K_f$ implies $z \notin K_f$ for all $\lambda \in (0, 1)$. If $x \notin K_f$, then $f(x) = +\infty$ yields

$$f(z) = f((1 - \lambda)x + \lambda y) = (1 - \lambda)f(x) + \lambda f(y) = +\infty + \lambda f(y) = +\infty,$$

which means $z \notin K_f$. Similarly, $y \notin K_f \implies z \notin K_f$. $\square$

Lemma 3.2. *The level set K_f^- is a face of the sublevel set $K_f^{\leq}$.*

Proof. Let $\alpha \in \mathbb{R}$, let $x, y, z \in K_f^{\leq}$, let $\lambda \in [0, 1]$, and let $x = (1 - \lambda)y + \lambda z$. The level set K_f^- is convex, as $f(x) = \alpha$ holds if $f(y) = f(z) = \alpha$. The set K_f^- is an extreme subset of $K_f^{\leq}$ as

$$f(x) = (1 - \lambda)f(y) + \lambda f(z) < \alpha$$

holds for all $\lambda \in (0, 1)$ if $f(y) < \alpha$ or $f(z) < \alpha$. $\square$

Let $\mathbb{N}_0 = \{0, 1, 2, \dots\}$.

Theorem 3.3. *Let $f : K \rightarrow \mathbb{R} \cup \{+\infty\}$ be a generalized affine map. Let C denote a sublevel set $C = K_f^{\leq}$ or a level set $C = K_f^-$ and let x be a point in C . If the face $F_C(x)$ of C generated by x has dimension $m \in \mathbb{N}_0$, then the face $F_K(x)$ of K generated by x has dimension m or $m + 1$.*

Proof. The inclusion $F_K(x) \supseteq F_C(x)$ holds as $F_K(x) \cap C$ is a face of C , and provides the lower bound of $\dim F_K(x) \geq m$.

Assume that $F_K(x)$ has dimension $m + 2$ or larger. We may choose an affine subspace $A \subseteq \text{aff } F_K(x)$ of dimension $m + 2$ incident with x . As K_f is an extreme subset of K by Lemma 3.1 and as $x \in K_f$, Corollary 2.5 proves $F_K(x) \subseteq K_f$. This means that f has finite values on the convex set

$$X = A \cap F_K(x).$$

As x lies in the relative algebraic interior of $F_K(x)$ by Theorem 2.3 and as we have $x \in A \subseteq \text{aff } F_K(x)$, Proposition 2.13 shows $x \in \text{ri}(X)$ and $\text{aff}(X) = A$.

We extend the affine map $f|_X : X \rightarrow \mathbb{R}$ to an affine map $g : A \rightarrow \mathbb{R}$, and consider the linear subspace

$$L = \{v \in \text{lin}(A) : g(y + v) = g(y) \ \forall y \in A\}$$

of the translation vector space $\text{lin}(A) = \{y - x : y \in A\}$. The space L has codimension at most one, so $\dim(L) \geq m + 1$. Since $x \in \text{ri}(X)$, Lemma 2.1 shows that x generates $X = F_X(x)$ as a face of X . Then Proposition 2.13 shows

$$x \in \text{ri}(X \cap (x + L)) \quad \text{and} \quad \text{aff}(X \cap (x + L)) = x + L.$$

As $X \cap (x + L) \subseteq C$ and as $x \in \text{ri}(X \cap (x + L))$, Lemma 2.1, part (a), provides the inclusion $X \cap (x + L) \subseteq F_C(x)$. Taking affine hulls, we get $x + L \subseteq \text{aff}(F_C(x))$. This proves $\dim(F_C(x)) > m$, which completes the proof. $\square$

We study intersections of sublevel and level sets. Let $u \subset \mathbb{N}$ be a finite subset, let $f_k : K \rightarrow \mathbb{R} \cup \{+\infty\}$ be a generalized affine map, and let $\alpha_k \in \mathbb{R}$ for all $k \in u$. For any subset $s \subseteq u$ we study the intersection

$$K_u^s = \{x \in K : f_k(x) \leq \alpha_k \forall k \in u \setminus s \text{ and } f_k(x) = \alpha_k \forall k \in s\} \quad (13)$$

of $|u| - |s|$ sublevel sets and $|s|$ level sets. If $(\alpha_k)_{k \in u}$ is unspecified and $s, t \subseteq u$, we assume the intersections of sublevel and level sets K_u^s and K_u^t are taken at the same values of $(\alpha_k)_{k \in u}$.

Lemma 3.4. *If $t \subseteq s \subseteq u$, then K_u^s is a face of K_u^t .*

Proof. Let $t \subseteq u$, $k \in u \setminus t$, and $s = t \cup \{k\}$. Lemma 3.2 shows that the intersection $(C_t^t)_{f_k}^=$ of level sets is a face of $(C_t^t)_{f_k}^{\leq}$ for all convex subsets $C \subseteq K$, that is to say, C_s^s is a face of C_t^t . If C is the intersection $C = K_{u \setminus s}^\emptyset$ of sublevel sets, it follows that $(K_{u \setminus s}^\emptyset)_s^s$ is a face of $(K_{u \setminus s}^\emptyset)_s^t$. In other words, K_u^s is a face of K_u^t . The general case follows by induction as faces of faces of a convex set are faces of the convex set. $\square$

It is useful to iterate Theorem 3.3.

Corollary 3.5. *Let $\ell \in \mathbb{N}$, let $u = \{1, 2, \dots, \ell\}$, let $s \subseteq u$, and let x be a point in the intersection K_u^s of sublevel and level sets from equation (13). If the face $F_{K_u^s}(x)$ of K_u^s generated by x has dimension $m \in \mathbb{N}_0$, then the dimension of the face $F_K(x)$ of K generated by x belongs to the set $\{m, m+1, \dots, m+\ell\}$.*

Proof. This follows from Theorem 3.3 by induction. $\square$

Corollary 3.5 allows us to exploit gaps in the list of the dimensions of the faces of K .

Corollary 3.6. *Let $m, n \in \mathbb{N}_0$ such that $n > m$, let $M \doteq \{m, m+1, \dots, n\}$, and let $D \subseteq M$. Let $\ell \in \mathbb{N}$ such that $\ell \leq n - m$, let $u = \{1, 2, \dots, \ell\}$, let $s \subseteq u$, and let K_u^s be the intersection of (sub-) level sets from equation (13).*

- (a) *If K has no face with dimension in $M \setminus D$ and if the face $F_{K_u^s}(x)$ of K_u^s generated by a point $x \in K_u^s$ has dimension in $\{m, m+1, \dots, n-\ell\}$, then $\dim F_K(x) \in D$.*
- (b) *If K has no face with dimension in M , then K_u^s has no face with dimension in $\{m, m+1, \dots, n-\ell\}$.*

Proof. Part (a). Let x be a point in K_u^s and let the dimension of the face $F_{K_u^s}(x)$ belong to the set $\{m, m+1, \dots, n-\ell\}$. Corollary 3.5 shows that the dimension of the face $F_K(x)$ belongs to M , which implies $\dim F_K(x) \in D$ by the assumptions.

Part (b). Let F be a face of K_u^s and let $\dim(F) \in \{m, m+1, \dots, n-\ell\}$. As F has finite dimension $m \geq 0$, the relative algebraic interior $\text{ri}(F)$ contains a point x , see Theorem 6.2 and Theorem 11.6 of [18]. Part (c) of Lemma 2.1 proves $F = F_{K_u^s}(x)$ and part (a) of the present corollary, with $D = \emptyset$, shows $\dim F_K(x) \in \emptyset$. This is a contradiction. $\square$

Corollary 3.6, part (a), is simplified as follows if $m = 0$, $n = \ell$, and $D = \{0\}$.

Corollary 3.7. *Let $\ell \in \mathbb{N}$, let $u = \{1, \dots, \ell\}$, and let K have no face with dimension in u . Then every extreme point of the intersection K_u^s of sublevel and level sets is an extreme point of K for all $s \subseteq u$.*

Corollary 3.7 is optimal in the sense that if K (or one of its faces) has dimension ℓ , then there are affine functionals and a point $x \in K$ such that x is an extreme point of K_u^s for all $s \subseteq u$, but not an extreme point of K . For example, the origin is an extreme point of the set

$$K_u^s = \{(x_1, \dots, x_\ell) \in \mathbb{R}^\ell : x_k \leq 0 \ \forall k \in u \setminus s \text{ and } x_k = 0 \ \forall k \in s\}$$

for all subsets $s \subseteq u$, but not an extreme point of $K = \mathbb{R}^\ell$.

We apply the results to pyramids. Let $o \in V$ be a point outside of the affine hull of K . The *pyramid* with apex o over a nonempty subset $F \subseteq K$ is the union of all closed segments joining points in F with o ,

$$P(F, o) = \bigcup_{x \in F} [x, o].$$

In addition, we define $P(\emptyset, o) = \{o\}$. We frequently write $P(F)$ instead of $P(F, o)$. Note that the pyramid over a convex subset $F \subseteq K$ is the convex hull of $F \cup \{o\}$. For every $x \in P(K, o) \setminus \{o\}$ we denote by $\hat{x}$ the point of K that is incident with the line through o and x .

Lemma 3.8. *The set of faces of $P(K, o)$ is the union of the set $\mathcal{F}_1$ of faces of K and the set of pyramids $\mathcal{F}_2 = \{P(F, o) : F \in \mathcal{F}_1\}$.*

Proof. Let G be a face of $P(K)$. First, we show $o \notin G \Rightarrow G \in \mathcal{F}_1$. As G is an extreme set, $x \in G$ and $x \notin K \cup \{o\}$ imply $o, \hat{x} \in G$. On the contrapositive, if $o \notin G$ then $G \subseteq K$. As G is a face of $P(K)$ it is *a fortiori* a face of K . This shows $G \in \mathcal{F}_1$. Secondly, we show $o \in G \Rightarrow G \in \mathcal{F}_2$. It is easy to see that G is the pyramid over some subset $F \subseteq K$. Indeed, with any point $x \in K$ the convex set G contains also the segment $[x, o]$. Moreover, if G contains a point $x \notin K \cup \{o\}$, then $o, \hat{x} \in G$. This proves $G = P(F)$ for some subset $F \subseteq K$. Since $F = G \cap K$, the set F is a face of K . This shows $G \in \mathcal{F}_2$.

Each element of $\mathcal{F}_1 \cup \mathcal{F}_2$ is a face. Let p, p_1, p_2 be any three points in the pyramid $P(K)$ such that p lies in the open segment (p_1, p_2) . We may write $p = (1 - \lambda)p_1 + \lambda p_2$, where

$$p = (1 - \eta)x + \eta o \quad \text{and} \quad p_i = (1 - \mu_i)x_i + \mu_i o, \quad i = 1, 2,$$

$x, x_1, x_2 \in K$, $\eta, \mu_1, \mu_2 \in [0, 1]$, and $\lambda \in (0, 1)$. Then

$$(1 - \eta)x + \eta o = (1 - \lambda)(1 - \mu_1)x_1 + \lambda(1 - \mu_2)x_2 + ((1 - \lambda)\mu_1 + \lambda\mu_2)o. \quad (14)$$

As $x, x_1, x_2 \in \text{aff}(K)$ and $o \notin \text{aff}(K)$, equation (14) shows $\eta = (1 - \lambda)\mu_1 + \lambda\mu_2$. The convex sets K and $\{o\}$ are extreme subsets (and hence faces) of $P(K)$ as they correspond to the extreme values $\eta = 0$ and $\eta = 1$, which require $\mu_1 = \mu_2 = 0$ and $\mu_1 = \mu_2 = 1$, respectively. That K is a face of $P(K)$ implies that every face of K is a face of $P(K)$, too. Let us show that $P(F)$ is an extreme subset of $P(K)$ for all

faces F of K . Let $p \in P(F)$. We may assume $\eta < 1$ as o is an extreme point. The equation (14) simplifies then to

$$x = \frac{(1-\lambda)(1-\mu_1)}{1-\eta}x_1 + \frac{\lambda(1-\mu_2)}{1-\eta}x_2. \quad (15)$$

If $\mu_1 = 1$, then $x_2 = x$ follows and hence $p_2 \in [x, o] \subseteq P(F)$. Similarly, $\mu_2 = 1$ implies $p_1 \in P(F)$. If $\mu_1 < 1$ and $\mu_2 < 1$, then (15) shows that $x \in (x_1, x_2)$. As $x \in F$ and as F is an extreme subset of K , we obtain $x_1, x_2 \in F$, hence $p_1, p_2 \in P(F)$. This proves that $P(F)$ is a face of $P(K)$. $\square$

By Lemma 3.8, the face of the pyramid $P(K, o)$ generated by a point is

$$F_{P(K,o)}(x) = \begin{cases} \{o\} & \text{if } x = o, \\ F_K(x) & \text{if } x \in K, \\ P(F_K(\hat{x}), o) & \text{else,} \end{cases} \quad \text{for all } x \in P(K, o). \quad (16)$$

Equation (16) allows us to simplify Corollary 3.5 when applied to pyramids.

Corollary 3.9. *Let $o \in V$ be a point outside of the affine hull of K . Let $\ell \in \mathbb{N}$, let $u = \{1, \dots, \ell\}$, let $s \subseteq u$, and let x be a point in the intersection $P(K, o)_u^s$ of sublevel and level sets. If the face $F_{P(K,o)_u^s}(x)$ of $P(K, o)_u^s$ generated by x has dimension $m \in \mathbb{N}_0$, then exactly one of the following cases applies.*

- (a) *The point x is the apex o , an extreme point of $P(K, o)_u^s$ and $P(K, o)$.*
- (b) *The point x lies in K and generates the face $F_{P(K,o)}(x) = F_K(x)$ of the pyramid $P(K, o)$. The dimension of $F_K(x)$ lies in $\{m, m+1, \dots, m+\ell\}$.*
- (c) *The point x lies outside of $K \cup \{o\}$ and generates the face $P(F_K(\hat{x}), o)$ of $P(K, o)$. The dimension of the face $F_K(\hat{x})$ of K generated by $\hat{x}$ lies in $\{m-1, m, \dots, m+\ell-1\}$ if $m \geq 1$ and in $\{0, 1, \dots, \ell-1\}$ if $m = 0$.*

Proof. The claim follows from Corollary 3.5 and equation (16). If $m = 0$, then the dimension $m-1 = -1$ of $F_K(\hat{x})$ is excluded from case (c) as $F_K(\hat{x})$ is nonempty. $\square$

We discuss the pyramidal counterpart to Corollary 3.7.

Corollary 3.10. *Let $o \in V$ be a point outside of the affine hull of K . Let $\ell \in \mathbb{N}$, let $u = \{1, \dots, \ell\}$, let $s \subseteq u$, and let K have no face with dimension in u . Then every extreme point of $P(K, o)_u^s$ is a convex combination of one extreme point of K and of the apex o of the pyramid $P(K, o)$.*

Proof. The claim follows from Corollary 3.9 when $m = 0$. Let x be an extreme point of $P(K, o)_u^s$. Case (a) of Corollary 3.9 is consistent with the claim. In case (b) we have $x \in K$ and $\dim F_K(x) \in \{0, 1, \dots, \ell\}$. The assumption $\dim(F_K(x)) \notin u$ implies that x is an extreme point of K . In case (c) we have $F_{P(K,o)}(x) = P(F_K(\hat{x}), o)$ and $\dim(F_K(\hat{x})) \in \{0, \dots, \ell-1\}$. The assumption $\dim(F_K(\hat{x})) \notin u$ shows that $\hat{x}$ is an extreme point of K . Hence, x is the convex combination $x = (1-\lambda)\hat{x} + \lambda o$ for some $\lambda \in (0, 1)$. $\square$

4. Extreme points of quantum states under expected value constraints

In the remainder of the article we explore expected value functionals on the set of quantum states. These functionals are generalized affine maps. In the present section we apply the above findings to pairs of expected value functionals. We also discuss the failure of analogous assertions for triples of expected value functionals and for the set of classical states.

Let $\mathcal{H}$ be a separable Hilbert space with inner product $\langle \cdot | \cdot \rangle$. The space $\mathfrak{T}$ of trace-class operators on $\mathcal{H}$ is a Banach space with the trace norm $\|\cdot\|_1$. The real Banach space of self-adjoint trace-class operators contains the closed convex cone $\mathfrak{T}^+$ of positive trace-class operators, which contains the closed convex sets $\mathfrak{T}^1 = \mathfrak{T}^1(\mathcal{H})$ of positive trace-class operators with trace at most one and $\mathfrak{S} = \mathfrak{S}(\mathcal{H})$ of positive trace-class operators with trace equal one called quantum states or density operators. Note that $\mathfrak{T}^1 = P(\mathfrak{S}, 0)$ is the pyramid over $\mathfrak{S}$ with apex zero.

We define a constraint on $\mathfrak{T}^+$ using a (possibly unbounded) positive operator H on $\mathcal{H}$. We approximate H by the sequence HP_n of bounded operators, where $P_n = \int_0^n dE_H(\lambda)$ is the spectral projector of H corresponding to $[0, n]$ and E_H is a spectral measure on the Borel σ -algebra of $[0, \infty)$, see for example [20]. We define the functional

$$f_H : \mathfrak{T}^+ \rightarrow [0, +\infty], \quad A \mapsto \text{Tr } HA = \lim_{n \rightarrow \infty} \text{Tr}(HP_n A).$$

The number $\text{Tr } H\rho$ is the *expected value* of the observable associated to H if $\rho \in \mathfrak{S}$ is the state of the quantum system. The map f_H is lower semicontinuous as $f_H(A) = \sup_{n \in \mathbb{N}} \text{Tr}(HP_n A)$ for all $A \in \mathfrak{T}^+$. Since H is a positive operator, the map f_H is a generalized affine map in the sense of Section 3. This remains true if we replace H with a self-adjoint, lower-bounded operator on $\mathcal{H}$. Similarly, all assertions below remain valid if we replace positive operators with self-adjoint, lower-bounded operators.

We study constraints imposed by several operators using a notation similar to equation (13). Let $\ell \in \mathbb{N}$, let H_k be a positive operator on $\mathcal{H}$, and let $E_k \in \mathbb{R}$ for all $k \in u = \{1, \dots, \ell\}$. For each subset $s \subseteq u$, we define the intersections

$$\begin{aligned} \mathfrak{S}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^s & \\ &= \{\rho \in \mathfrak{S}(\mathcal{H}) : \text{Tr } H_k \rho \leq E_k \ \forall k \in u \setminus s \text{ and } \text{Tr } H_k \rho = E_k \ \forall k \in s\} \end{aligned} \quad (17)$$

and

$$\begin{aligned} (\mathfrak{T}^1)_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^s & \\ &= \{\rho \in \mathfrak{T}^1(\mathcal{H}) : \text{Tr } H_k \rho \leq E_k \ \forall k \in u \setminus s \text{ and } \text{Tr } H_k \rho = E_k \ \forall k \in s\} \end{aligned} \quad (18)$$

of $\ell - |s|$ sublevel sets and $|s|$ level sets. We simplify the notation for *sublevel sets* by writing

$$\mathfrak{S}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell} = \mathfrak{S}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^\emptyset$$

and

$$\mathfrak{T}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^1 = (\mathfrak{T}^1)_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^\emptyset.$$

The intersections $\mathfrak{S}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}$ and $\mathfrak{T}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^1$ of sublevel sets are closed sets as the map $\mathfrak{T}^+ \rightarrow [0, +\infty]$, $A \mapsto \text{Tr } H_k A$ is lower semi-continuous for all $k = 1, \dots, \ell$.

It is well known that the set of extreme points $\text{ext}(\mathfrak{S})$ of the set of quantum states $\mathfrak{S}(\mathcal{H})$ consists of the projectors of rank one, called *pure states*. The finite-dimensional faces are isometric to the sets $\mathfrak{S}(\mathbb{C}^d)$ for all $d \leq \dim(\mathcal{H})$.

Lemma 4.1. *If a face of the set of quantum states $\mathfrak{S}(\mathcal{H})$ has finite dimension $n < \infty$, then $n = d^2 - 1$ for some $d \in \mathbb{N}$.*

Proof. Theorem 4.6 in [1] proves that the finite-dimensional closed faces of $\mathfrak{S}(\mathcal{H})$ have dimensions $d^2 - 1$, $d \in \mathbb{N}$. The claim then follows from showing that every nonempty, finite-dimensional face F of $\mathfrak{S}(\mathcal{H})$ is closed. As $\dim(F) < \infty$, the closure $\overline{F}$ is included in $\text{aff}(F)$ and the relative algebraic interior $\text{ri}(F)$ contains a point x . Let $y \in \overline{F}$ be arbitrary. As $y \in \text{aff}(F)$, the definition of the relative algebraic interior shows that there is a point $z \in F$ such that x lies in the open segment (y, z) . Since $\mathfrak{S}(\mathcal{H})$ is closed, we have $y \in \mathfrak{S}(\mathcal{H})$. As F is an extreme subset of $\mathfrak{S}(\mathcal{H})$, this shows $y \in F$ and completes the proof. $\square$

Taking into account the list of dimensions from Lemma 4.1, and invoking Corollary 3.7 and Corollary 3.10, we obtain the following assertion.

Theorem 4.2. *Let H_1, H_2 be arbitrary positive operators on $\mathcal{H}$, let $E_1, E_2 \in \mathbb{R}$, and let $s \subseteq \{1, 2\}$. Then all extreme points of the set $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ are pure states. All extreme points of the set $(\mathfrak{T}^1)_{H_1, E_1, H_2, E_2}^s$ have rank at most one.*

Theorem 4.2 implies Corollary 4.3 below by taking $H_2 = H_1$ and $E_2 = E_1$. In the sequel, we will omit further mention of similar reductions from two to one operators.

Corollary 4.3. *Let H be an arbitrary positive operator on $\mathcal{H}$, let $E \in \mathbb{R}$, and let $s \subseteq \{1\}$. Then all extreme points of the set $\mathfrak{S}_{H, E}^s$ are pure states. All extreme points of the set $(\mathfrak{T}^1)_{H, E}^s$ have rank at most one.*

Let $\mathcal{H} = \mathbb{C}^d$ for some $d \in \mathbb{N}$. The set of quantum states $\mathfrak{S}(\mathbb{C}^d)$ is a compact, convex set, which is a base of the cone $\mathfrak{T}^+(\mathbb{C}^d)$ of positive semidefinite matrices. If $H \in \mathfrak{T}^+(\mathbb{C}^d)$ then

$$f_H : \mathfrak{T}^+(\mathbb{C}^d) \rightarrow [0, +\infty), \quad A \mapsto \text{Tr } HA$$

is a continuous, affine map.

Corollary 4.4. *Let $\mathcal{H} = \mathbb{C}^d$ for some $d \in \mathbb{N}$. Let $H_1, H_2 \in \mathfrak{T}^+(\mathbb{C}^d)$ be arbitrary positive semidefinite matrices, let $E_1, E_2 \in \mathbb{R}$, and let $s \subseteq \{1, 2\}$. Then the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ of sublevel and level sets is a compact, convex set. Every state $\rho \in \mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ can be represented as*

$$\rho = \sum_{i=1}^{d^2} p_i \sigma_i, \quad (19)$$

where $\{p_i\}_{i=1}^{d^2}$ is a probability distribution and $\{\sigma_i\}_{i=1}^{d^2} \subseteq \mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ is a set of pure states.

Proof. The convex set $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ is compact as the set of quantum states $\mathfrak{S}(\mathbb{C}^d)$ is compact and as

$$\mathfrak{T}^+(\mathbb{C}^d) \rightarrow [0, +\infty), \quad A \mapsto \text{Tr } H_i A, \quad i = 1, 2$$

are continuous maps. Carathéodory's theorem asserts that every point in a compact, convex subset C of $\mathbb{R}^n$ is a convex combination of at most $n + 1$ extreme points of C , see for example [19, 21]. The claim follows as the extreme points of $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ are pure states by Theorem 4.2, and as $\dim \mathfrak{S}(\mathbb{C}^d) = d^2 - 1$. $\square$

The assertion (19) of Corollary 4.4 for the level set $\mathfrak{S}_{H, E}^{\{1\}}$ is proved in [14].

Remark 4.5. If more than two positive operators are employed, the assertion analogous to Theorem 4.2 is not valid. Perhaps, the simplest example is the Hilbert space $\mathcal{H} = \mathbb{C}^2$ and positive semidefinite matrices $H_1 = \mathbb{1} + X$, $H_2 = \mathbb{1} + Y$, and $H_3 = \mathbb{1} + Z$, where $\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the identity matrix and $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are the Pauli matrices. If $E_1 = E_2 = E_3 = 1$, then for all subsets $s \subseteq u = \{1, 2, 3\}$ the set

$$\begin{aligned} \mathfrak{S}^s &= \mathfrak{S}_{H_1, 1, H_2, 1, H_3, 1}^s \\ &= \{\rho \in \mathfrak{S}(\mathbb{C}^2) : \operatorname{Tr} H_k \rho \leq E_k \ \forall k \in u \setminus s \text{ and } \operatorname{Tr} H_k \rho = E_k \ \forall k \in s\} \end{aligned}$$

is a spherical sector of the Bloch ball $\mathfrak{S}(\mathbb{C}^2)$. Theorem 4.2 fails as the trace state $\frac{1}{2}\mathbb{1}$ is an extreme point of $\mathfrak{S}^s$ of rank two.

Theorem 6.1 below allows us to express the suprema of certain functions as suprema over pure states. However, this is not possible for more than two positive operators. Consider the map

$$f : \mathfrak{S}^s \rightarrow \mathbb{R}, \quad \rho \mapsto \operatorname{Tr}(X + Y + Z)\rho.$$

The domain $\mathfrak{S}^s$ is the intersection of $t = 3 - |s|$ sublevel sets and $|s|$ level sets. The image $f(\mathfrak{S}^s)$ is the interval $[-\sqrt{t}, 0]$. The image of the set of pure states in $\mathfrak{S}^s$ under f is the interval $[-\sqrt{t}, -1]$ if $t \geq 1$ and is empty if $t = 0$. If $t \geq 1$, then the maximum on the set of pure states is attained at t of the pure states

$$\frac{1}{2}(\mathbb{1} - X), \quad \frac{1}{2}(\mathbb{1} - Y), \quad \text{and} \quad \frac{1}{2}(\mathbb{1} - Z).$$

In any case, the maximum $f(\frac{1}{2}\mathbb{1}) = 0 > -1$ of f is neither equal to nor approximated by the values of f at pure states in $\mathfrak{S}^s$. Similarly, it is easy to check that for all $s \subseteq u$

$$\operatorname{conv}\{\rho \in \mathfrak{S}^s : \rho \text{ is a pure state}\} = \{\rho \in \mathfrak{S}^s : f(\rho) \leq -1\}.$$

No state $\rho \in \mathfrak{S}^s$ with $f(\rho) > -1$ can be the barycenter of a probability measure supported on the set of pure states in $\mathfrak{S}^s$. This shows that Theorem 5.1 and Corollary 5.3 below fail for more than two positive operators. $\square$

The classical analogues of our results fail as the set of classical states has one-dimension faces.

Remark 4.6. (Classical states) The set of classical states on the Hilbert space $\mathbb{C}^3$ with respect to an orthonormal basis e_1, e_2, e_3 of $\mathbb{C}^3$ is

$$\mathfrak{P}_3 = \{p(1)\sigma_1 + p(2)\sigma_2 + p(3)\sigma_3 : p \in \Delta_{\{1,2,3\}}\}.$$

Here, $\Delta_{\{1,2,3\}}$ is the simplex of probability densities introduced in Example 2.10 and σ_n is the projector onto the line spanned by e_n for all $n = 1, 2, 3$. The set $\mathfrak{P}_3$ is a triangle with extreme points $\sigma_1, \sigma_2, \sigma_3$.

The sublevel and level set of

$$f : \mathfrak{P}_3 \rightarrow \mathbb{R}, \quad \rho \mapsto \text{Tr}(\sigma_3 \rho) = \langle e_3 | \rho e_3 \rangle$$

at $\alpha = \frac{1}{2}$ is denoted in equation (12), respectively, as

$$(\mathfrak{P}_3)_{\bar{f}}^{\leq} = \{\rho \in \mathfrak{P}_3 : f(\rho) \leq \tfrac{1}{2}\} \quad \text{and} \quad (\mathfrak{P}_3)_{\bar{f}}^{\bar{}} = \{\rho \in \mathfrak{P}_3 : f(\rho) = \tfrac{1}{2}\}.$$

The level set $(\mathfrak{P}_3)_{\bar{f}}^{\bar{}}$ is the segment $[\rho_1, \rho_2]$ and has the extreme points $\rho_i = \frac{1}{2}(\sigma_i + \sigma_3)$, $i = 1, 2$. By Lemma 3.2, the points ρ_1, ρ_2 are also extreme points of the sublevel set $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$. The analogue of Corollary 4.3 fails for classical states as the points ρ_1, ρ_2 have rank two despite the fact that they are extreme points of $(\mathfrak{P}_3)_{\bar{f}}^{\bar{}}$ and $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$.

The sublevel set $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$ contains only two pure states, namely σ_1 and σ_2 . Hence, only the states on the segment $[\sigma_1, \sigma_2]$ can be represented as convex combinations of pure states from $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$. In particular, the analogue of Corollary 5.4 fails: It is impossible to represent any state from $(\mathfrak{P}_3)_{\bar{f}}^{\bar{}}$ as the barycenter of pure states from $(\mathfrak{P}_3)_{\bar{f}}^{\bar{}}$. Similarly, the analogue of Theorem 6.1 fails: The supremum $f(\rho_1) = 1/2$ of f on $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$ is not attained (neither approximated) by pure states as $f(\sigma_1) = f(\sigma_2) = 0$ holds for the sole pure states in $(\mathfrak{P}_3)_{\bar{f}}^{\leq}$. $\square$

5. Pure-state decomposition theorem

Let H_1 and H_2 be positive operators on a separable Hilbert space $\mathcal{H}$. If $\dim(\mathcal{H}) < \infty$, then Corollary 4.4 above provides a pure-state decomposition for the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ of sublevel and level sets for all $s \subseteq \{1, 2\}$, see (17) for the notation. If $\dim(\mathcal{H}) = \infty$, we need to differentiate between sublevel and level sets. The sublevel sets are closed, as the expected value functionals are lower semicontinuous. The level sets are not closed. We prove pure-state decompositions for both, the sublevel and level sets.

We begin with sublevel sets. If H_1 (or H_2) is a positive operator with a discrete spectrum of finite multiplicity, then the intersections $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ and $\mathfrak{T}_{H_1, E_1, H_2, E_2}^1$ of sublevel sets are compact. Indeed, it has been shown in [7] that $\mathfrak{S}_{H_1, E_1}$ is compact². It follows that $\mathfrak{S}_{H_1, E_1, H_2, E_2} = \mathfrak{S}_{H_1, E_1} \cap \mathfrak{S}_{H_2, E_2}$ is compact as $\mathfrak{S}_{H_2, E_2}$ is closed. Similarly, one can show that $\mathfrak{T}_{H_1, E_1, H_2, E_2}^1$ is compact by using Proposition 11 in [24, Appendix].

If H_1 and H_2 are arbitrary positive operators, the sets $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ and $\mathfrak{T}_{H_1, E_1, H_2, E_2}^1$ are closed but not *compact*. Yet, they are μ -compact by Proposition 2 in [9] and Proposition 4 in [17], respectively. Proposition 5 in [17] provides generalized assertions of Krein-Milman's theorem and of Choquet's theorem for μ -compact sets. We employ Theorem 4.2 to make these assertions more explicit.

²Recall that if a positive operator H on an infinite dimensional Hilbert space $\mathcal{H}$ has a discrete spectrum of finite multiplicity, then there is sequence of non-negative numbers $(\lambda_n)_{n \in \mathbb{N}}$ and an orthonormal basis $\{e_n : n \in \mathbb{N}\}$ of $\mathcal{H}$ such that $\lim_{n \rightarrow \infty} \lambda_n = \infty$ and $H e_n = \lambda_n e_n$ for all $n \in \mathbb{N}$. See for example [20], Corollary 5.11 and Proposition 5.12.

Theorem 5.1. *Let H_1, H_2 be arbitrary positive operators on $\mathcal{H}$ and E_1, E_2 nonnegative numbers such that the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ of sublevel sets is nonempty. Then the set $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ of extreme points is equal to the set of pure states $\mathfrak{S}_{H_1, E_1, H_2, E_2} \cap \text{ext } \mathfrak{S}(\mathcal{H})$, which is nonempty and closed.*

- (A) *(Krein-Milman's theorem) The set $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ is the closure of the convex hull of $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$.*
- (B) *(Choquet's theorem) Any state $\rho \in \mathfrak{S}_{H_1, E_1, H_2, E_2}$ can be represented as the barycenter $\rho = \int \sigma \mu(d\sigma)$ of some Borel probability measure μ supported by $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$.*

Proof. Theorem 4.2 shows that the set of extreme points $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ is the intersection of $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ and the set of pure states $\text{ext } \mathfrak{S}(\mathcal{H})$. As both sets are closed, their intersection is closed.

The remaining assertions follow from Proposition 5 in [17] as $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ is μ -compact and since $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ is closed. $\square$

Note that the closedness of the set $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ is not obvious even in the case when both operators H_1 and H_2 have discrete spectrum or in the case of $\dim(\mathcal{H}) < \infty$. The closedness of the set of extreme points is necessary for the stability [16, 17] of $\mathfrak{S}_{H_1, E_1, H_2, E_2}$.

Question 5.2. Under which conditions on the operators H_1 and H_2 can part B of Theorem 5.1 be strengthened to the statement that any state in $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ is a *countable* convex combination of pure states in $\mathfrak{S}_{H_1, E_1, H_2, E_2}$? This and the arguments of Corollary 5.4 below would imply that any state with finite expected values of H_1 and H_2 is a *countable* convex combination of pure states with the same expected values.

Pure-state decompositions are more subtle for level than sublevel sets.

Corollary 5.3. *Let H_1, H_2 be arbitrary positive operators on $\mathcal{H}$, let E_1, E_2 be real numbers, let $s \subseteq \{1, 2\}$, and let ρ lie in the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ of sublevel and level sets. Then ρ can be represented as the barycenter*

$$\rho = \int \sigma \mu(d\sigma) \quad (20)$$

of some Borel probability measure μ supported by $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ such that we have $\mu(\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}^s) = 1$.

Proof. The assertion B of Theorem 5.1 implies that equation (20) holds for some probability measure μ supported by the set $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$. Since the function $\mathfrak{S}_{H_1, E_1, H_2, E_2} \rightarrow [0, +\infty]$, $\sigma \mapsto \text{Tr } H_k \sigma$ is affine and lower semicontinuous, and since the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ of sublevel sets is closed, bounded, and convex, we have (see, f.i., [22, the Appendix])

$$\int \text{Tr}(H_k \sigma) \mu(d\sigma) = \text{Tr } H_k \rho, \quad k = 1, 2. \quad (21)$$

If $\text{Tr } H_k \rho = E_k$ holds for $k \in \{1, 2\}$, then equation (21) implies $\text{Tr } H_k \sigma = E_k$ for μ -almost all σ as $\text{Tr } H_k \sigma \leq E_k$ holds for all σ in the support of μ . $\square$

Corollary 5.4. *Let H_1 and H_2 be arbitrary positive operators on $\mathcal{H}$. Any state ρ such that $\text{Tr } H_k \rho = E_k < +\infty$, $k = 1, 2$, can be represented as*

$$\rho = \int \sigma \mu(d\sigma), \quad (22)$$

where μ is a Borel probability measure supported by pure states such that $\text{Tr } H_k \sigma = E_k$, $k = 1, 2$, for μ -almost all σ .

Proof. Corollary 5.4 is the case $s = \{1, 2\}$ of Corollary 5.3. $\square$

Theorem 5.1 and its Corollaries 5.3 and 5.4 are not valid for more than two operators, as the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2, \dots, H_\ell, E_\ell}^s$ of sublevel and level sets may have extreme points that are no pure states if $\ell \geq 3$. See Remark 4.5 for an example.

A Borel probability measure supported on pure states is known as a *generalized ensemble* of pure states [9], and its barycenter as a *continuous convex combination* of pure states. The probability measure μ in part B of Theorem 5.1 is a generalized ensemble of pure states with bounded expected values. In the strict sense, the probability measure μ in Corollary 5.4 is not a generalized ensemble of pure states with fixed expected values, as the support of μ may contain a set of μ -measure zero where one of the expected values could be smaller than the fixed value.

Example 5.5. (On pure-state decomposition of bipartite states) If quantum systems A and B are described by Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, then the bipartite system AB is described by the tensor product of these spaces, i.e. $\mathcal{H}_{AB} \doteq \mathcal{H}_A \otimes \mathcal{H}_B$. A state in $\mathfrak{S}(\mathcal{H}_{AB})$ is denoted by ρ_{AB} , its marginal states³ $\text{Tr}_{\mathcal{H}_B} \rho_{AB}$ and $\text{Tr}_{\mathcal{H}_A} \rho_{AB}$ are denoted, respectively, by ρ_A and ρ_B . See for example [8, 28]. $\square$

Corollary 5.4 implies the following.

Corollary 5.6. *Let H_A and H_B be arbitrary positive operators on $\mathcal{H}_A$ and $\mathcal{H}_B$ correspondingly. Any state ρ_{AB} such that $\text{Tr } H_A \rho_A = E_A < +\infty$ and $\text{Tr } H_B \rho_B = E_B < +\infty$ can be represented as*

$$\rho_{AB} = \int \sigma_{AB} \mu(d\sigma_{AB}),$$

where μ is a Borel probability measure supported by pure states in $\mathfrak{S}(\mathcal{H}_{AB})$ such that $\text{Tr } H_A \sigma_A = E_A$ and $\text{Tr } H_B \sigma_B = E_B$ for μ -almost all σ_{AB} .

If $\dim \mathcal{H}_A = d_A < +\infty$ and $\dim \mathcal{H}_B = d_B < +\infty$ then the state ρ_{AB} can be represented as

$$\rho_{AB} = \sum_{k=1}^{d_A d_B} p_k \sigma_{AB}^k,$$

where $\{p_k\}$ is a probability distribution and $\{\sigma_{AB}^k\}$ is a set of pure states such that $\text{Tr } H_A \sigma_A^k = E_A$ and $\text{Tr } H_B \sigma_B^k = E_B$ for all k .

Question 5.7. If H_A and H_B are Hamiltonians of systems A and B , then Corollary 5.6 states that any bipartite state with finite marginal energies can be decomposed into pure states with the same marginal energies. An interesting open question is the possibility of a similar decomposition of a state of a composite quantum system consisting of more than two subsystems.

³Here $\text{Tr}_{\mathcal{H}_X}$ denotes the partial trace over the space $\mathcal{H}_X$.

6. Applications to quantum information theory

In this section we consider some applications of our main results in quantum information theory and mathematical physics. These applications are based on the following observation.

Theorem 6.1. *Let H_1, H_2 be arbitrary positive operators, let $E_1, E_2 \in \mathbb{R}$, let $s \subseteq \{1, 2\}$, and let $f : \mathfrak{S}_{H_1, E_1, H_2, E_2}^s \rightarrow [-\infty, \infty]$ be a convex function on the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ of sublevel and levels sets. If f is either lower semicontinuous or upper semicontinuous and upper bounded, then*

$$\sup\{f(\rho) : \rho \in \mathfrak{S}_{H_1, E_1, H_2, E_2}^s\} = \sup\{f(\rho) : \rho \in \text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}^s\}, \quad (23)$$

where $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ is the set of pure states in $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$.

If the domain of f is the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ of sublevel sets ($s = \emptyset$), if f is upper semicontinuous, and if one of the operators H_1 or H_2 has discrete spectrum of finite multiplicity, then the supremum on the right-hand side of (23) is attained at a pure state in $\mathfrak{S}_{H_1, E_1, H_2, E_2}$.

Proof. By Corollary 5.3 and Theorem 4.2, for any mixed state ρ in $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ there is a probability measure μ supported by the set of pure states in the intersection $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ of sublevel sets such that

$$\rho = \int \sigma \mu(d\sigma)$$

and such that $\mu(\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}^s) = 1$. The assumed properties of the function f guarantee (see, f.i., [22, the Appendix]) the validity of the Jensen inequality

$$f(\rho) \leq \int f(\sigma) \mu(d\sigma),$$

which implies the existence of a pure state σ in $\mathfrak{S}_{H_1, E_1, H_2, E_2}^s$ such that $f(\sigma) \geq f(\rho)$.

If one of the operators H_1 or H_2 has discrete spectrum of finite multiplicity, then the set $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ is compact. Hence, the set of extreme points $\text{ext } \mathfrak{S}_{H_1, E_1, H_2, E_2}$ is compact by Theorem 5.1. This and the above arguments imply that the first supremum in (23) is attained at a pure state in $\mathfrak{S}_{H_1, E_1, H_2, E_2}$ (provided that the function f is upper semicontinuous). $\square$

Of course, we may replace the convex function f in Theorem 6.1 by the concave function $-f$ (and supremum by infimum). This idea is motivated by potential applications, since many important characteristics of a state in quantum information theory are concave lower semicontinuous and nonnegative. See the following

Example 6.2. (The minimal output entropy of an energy-constrained quantum channel) The *von Neumann entropy* of a quantum state ρ in $\mathfrak{S}(\mathcal{H})$ is a basic characteristic of this state defined by the formula $H(\rho) = \text{Tr } \eta(\rho)$, where $\eta(x) = -x \log x$ for $x > 0$ and $\eta(0) = 0$. The function $H(\rho)$ is concave and lower semicontinuous on the set $\mathfrak{S}(\mathcal{H})$ and takes values in $[0, +\infty]$, see for example [8, 12, 27].

A quantum channel from a system A to a system B is a completely positive trace-preserving linear map $\Phi : \mathfrak{T}(\mathcal{H}) \rightarrow \mathfrak{T}(\mathcal{K})$ between the Banach spaces $\mathfrak{T}(\mathcal{H})$ and $\mathfrak{T}(\mathcal{K})$, where $\mathcal{H}$ and $\mathcal{K}$ are Hilbert spaces associated with the systems A and B ,

respectively. In the analysis of information abilities of quantum channels, the notion of the minimal output entropy of a channel is widely used [8, 4, 13, 14, 25]. It is defined as

$$H_{\min}(\Phi) = \inf_{\rho \in \mathfrak{S}(\mathcal{H})} H(\Phi(\rho)) = \inf_{\varphi \in \mathcal{H}_1} H(\Phi(|\varphi\rangle\langle\varphi|)), \quad (24)$$

where $\mathcal{H}_1$ is the unit sphere in $\mathcal{H}$, and $|\varphi\rangle\langle\varphi|$ denotes the projector of rank one onto the line spanned by $\varphi \in \mathcal{H}_1$. The second equality of (24) follows from the concavity of the function $\rho \mapsto H(\Phi(\rho))$ and from the possibility to decompose any mixed state into a convex combination of pure states.

In studies of infinite-dimensional quantum channels, it is reasonable to impose the energy-constraint on input states of these channels. So, alongside with the minimal output entropy $H_{\min}(\Phi)$, it is reasonable to consider its constrained versions (cf. [14])

$$H_{\min}(\Phi, H, E) = \inf_{\rho \in \mathfrak{S}(\mathcal{H}): \text{Tr } H\rho \leq E} H(\Phi(\rho)), \quad (25)$$

$$H_{\min}^-(\Phi, H, E) = \inf_{\rho \in \mathfrak{S}(\mathcal{H}): \text{Tr } H\rho = E} H(\Phi(\rho)), \quad (26)$$

where H is a positive operator, the *energy observable*. In contrast to the unconstrained case, it is not obvious that the infima in (25) and (26) can be taken only over pure states satisfying the conditions $\text{Tr } H\rho \leq E$ and $\text{Tr } H\rho = E$ correspondingly. In [14] it is shown that this holds in the finite-dimensional settings. The above Theorem 6.1 allows to prove the same assertion for an arbitrary infinite-dimensional channel Φ and any energy observable H . $\square$

Corollary 6.3. *Let H be an arbitrary positive operator and let E be greater than the infimum of the spectrum of H . Then both infima in (25) and (26) can be taken over pure states, i.e.*

$$H_{\min}(\Phi, H, E) = \inf_{\varphi \in \mathcal{H}_1: \langle \varphi | H | \varphi \rangle \leq E} H(\Phi(|\varphi\rangle\langle\varphi|)), \quad (27)$$

$$H_{\min}^-(\Phi, H, E) = \inf_{\varphi \in \mathcal{H}_1: \langle \varphi | H | \varphi \rangle = E} H(\Phi(|\varphi\rangle\langle\varphi|)). \quad (28)$$

If the operator H has a discrete spectrum of finite multiplicity, then the infimum in (27) is attained at a unit vector.

Proof. By Theorem 6.1, it suffices to note that the function $\rho \mapsto H(\Phi(\rho))$ is concave nonnegative and lower semicontinuous (as a composition of a continuous and a lower semicontinuous function). $\square$

The definitions of the quantities $H_{\min}(\Phi, H, E)$ and $H_{\min}^-(\Phi, H, E)$ are significantly simplified by Corollary 6.3. It also shows that

$$H_{\min}(\widehat{\Phi}, H, E) = H_{\min}(\Phi, H, E) \quad \text{and} \quad H_{\min}^-(\widehat{\Phi}, H, E) = H_{\min}^-(\Phi, H, E),$$

where $\widehat{\Phi}$ is a complementary channel to the channel Φ , since for any pure state ρ we have $H(\widehat{\Phi}(\rho)) = H(\Phi(\rho))$, see Section 8.3 of [8].

Example 6.4. (On the definition of the operator E-norms) On the algebra $\mathfrak{B}(\mathcal{H})$ of all bounded operators one can consider the family $\{\|A\|_E^H\}_{E>0}$ of norms induced by a positive operator H with the infimum of the spectrum equal to zero [23].

For any $E > 0$ the norm $\|A\|_E^H$ is defined as

$$\|A\|_E^H \doteq \sup_{\rho \in \mathfrak{S}(\mathcal{H}) : \text{Tr } H\rho \leq E} \sqrt{\text{Tr } A\rho A^*}. \quad (29)$$

These norms, called operator E -norms, appear as “doppelganger” of the energy-constrained Bures distance between completely positive linear maps in the generalized version of the Kretschmann-Schlingemann-Werner theorem [23, Section 4].

For any $A \in \mathfrak{B}(\mathcal{H})$ the function $E \mapsto \|A\|_E^H$ is concave and tends to $\|A\|$ (the operator norm of A) as $E \rightarrow +\infty$. All the norms $\|A\|_E^H$ are equivalent (for different E and fixed H) on $\mathfrak{B}(\mathcal{H})$ and generate a topology depending on the operator H . If H is an unbounded operator then this topology is weaker than the norm topology on $\mathfrak{B}(\mathcal{H})$, it coincides with the strong operator topology on bounded subsets of $\mathfrak{B}(\mathcal{H})$ provided that the operator H has discrete spectrum of finite multiplicity.

If we assume that the supremum in (29) can be taken only over pure states ρ such that $\text{Tr } H\rho \leq E$ then we obtain the following simpler definition

$$\|A\|_E^H \doteq \sup_{\varphi \in \mathcal{H}_1, \langle \varphi | H | \varphi \rangle \leq E} \|A\varphi\|, \quad (30)$$

which shows the sense of the norm $\|A\|_E^H$ as a constrained version of the operator norm $\|A\|$. In the preliminary version of [23] the above assumption was proved only in the case when the operator H has discrete spectrum of finite multiplicity. Theorem 6.1 (applied to the continuous affine function $f(\rho) = \text{Tr } A\rho A^*$) allows to fill this gap. $\square$

Corollary 6.5. *For an arbitrary positive operator H , the definitions (29) and (30) coincide for any $A \in \mathfrak{B}(\mathcal{H})$.*

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