Convex Analysis of Density Operators Under Affine Constraints

Research Seminar Analysis, Stochastics and Mathematical Physics
Technische Universität Chemnitz

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Speaker: Stephan Weis
(Independent Researcher, Berlin, Germany)

Joint Work with Maksim E. Shirokov
(Steklov Mathematical Institute, Moscow, Russia)

Abstract

Problems of quantum communication and mathematical physics lead to the optimization over the convex set $\mathfrak{S}(\mathcal{H})$ of density operators on a separable Hilbert space $\mathcal{H}$ under generalized affine constraints. Choquet theorem, a fundamental result in convex analysis, remained unknown in this setting until Maksim Shirokov and I proved it in the paper [3].

[3] S. Weis and M. Shirokov, *The face generated by a point, generalized affine constraints, and quantum theory*, Journal of Convex Analysis **28**:3 (2021).

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We have shown that every extreme point of the intersection of $\mathfrak{S}(\mathcal{H})$ and the (sub-) level sets of one or two generalized affine functions is a pure state [3]. This and the results of the paper [2] extend Choquet theorem to density operators under generalized affine constraints.

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Minkowski's Theorem

Extreme Points

A point x in a convex set C is an extreme point of C if whenever $x = (1 - \lambda)y + \lambda z$ for some $\lambda \in (0, 1)$ and $y, z \in C$, then $x = y = z$. Let $\text{ext}\, C$ denote the set of extreme points of C.

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Let $K \subset \mathbb{R}^n$ be a compact, convex subset and let $x \in K$. Then x is a convex combination of points $x_1, x_2, \ldots, x_{n+1} \in K$ (that is to say, $x = \lambda_1 x_1 + \lambda_2 x_2 + \cdots + \lambda_{n+1} x_{n+1}$, $\lambda_1, \lambda_2, \ldots, \lambda_{n+1} \geq 0$, $\lambda_1 + \lambda_2 + \cdots + \lambda_{n+1} = 1$).

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- If a convex function f has a maximum on a compact, convex set $K \subset \mathbb{R}^n$, then f achieves the maximum at an extreme point of K.

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Remarks.

- If a convex function f has a maximum on a compact, convex set $K \subset \mathbb{R}^n$, then f achieves the maximum at an extreme point of K.

- The projector of rank one onto the line spanned by a unit vector $\psi \in \mathbb{C}^n$ is denoted $|\psi\rangle\langle\psi|$ and called a pure state. The set of pure states is the set of extreme points of the set of density matrices $\mathfrak{S}(\mathbb{C}^n) = \{\rho \in M_n \colon \rho \succeq 0, \mathrm{Tr}(\rho) = 1\}$.

Choquet Theorem

Theorem (Choquet)

Let $K \subset B$ be a compact, convex subset of a Banach space B and let $x \in K$. Then there exists a Borel probability measure μ on B such that $\mu(\operatorname{ext} K) = 1$ and $x = \int y \, d\mu(y)$.

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Remarks.

- $\int y \, d\mu(y) \in K$ is the barycenter of the measure μ, defined as the Bochner integral of the identity function $K \to K$. We have $x = \int y \, d\mu(y)$ if and only if $f(x) = \int f(y) \, d\mu(y)$ for all $f \in B^*$, defined as Lebesgue integrals of functionals f.

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Corollary (Krein-Milman Theorem)

Let K be a compact, convex subset of a Banach space.
Then $K = \overline{\operatorname{conv}}(\operatorname{ext} K)$.

States in Quantum Information Theory

Quantum States

Quantum information theory uses density operators on a separable Hilbert space $\mathcal{H}$. The set of density operators is

$$\mathfrak{S}(\mathcal{H}) = \{\rho \in \mathfrak{T}(\mathcal{H}) \mid \rho \succeq 0, \mathrm{Tr}(\rho) = 1\},$$

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• The set $\mathfrak{S}(\mathcal{H})$ is not weak*-compact. The dual space to the space of compact operators $\mathfrak{C}(\mathcal{H})$ is $\mathfrak{T}(\mathcal{H})$, but $\mathfrak{S}(\mathcal{H})$ is not closed in $\mathfrak{T}(\mathcal{H})$. Indeed, if $(\psi_i) \subset \mathcal{H}$ is an orthonormal set, then $|\psi_i\rangle\langle\psi_i| \to 0$ in the weak*-topology, since

$$|\mathrm{Tr}\,(|\psi_i\rangle\langle\psi_i|\, T)| = |\langle\psi_i|T(\psi_i)\rangle| \leq \|\psi_i\| \cdot \|T(\psi_i)\| \overset{i\to\infty}{\longrightarrow} 0 \qquad \text{for all } T \in \mathfrak{C}(\mathcal{H}).$$

Choquet theorem cannot be applied to the non-compact set $\mathfrak{S}(\mathcal{H})$.

Non-Compact Choquet Theorem

Theorem (Edgar [1])

Let $K \subset B$ be a closed, bounded, convex, separable subset of a Banach space B and suppose that K has the Radon-Nikodym property. Then for every $x \in K$ there exists a Borel probability measure μ on B such that $\mu(\operatorname{ext} K) = 1$ and $x = \int y \, d\mu(y)$.

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- A subset X of a Banach space B has the Radon-Nikodym property if a vector-valued version of the Radon-Nikodym theorem holds.

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• Choquet proved the theorem named after himself first in the setting of compact sets of dual Banach spaces.

• Choquet theorem has been extended to locally convex spaces.

Generalized Compactness I

A non-compact Choquet-theorem for $\mathfrak{S}(\mathcal{H})$.

μ-Compactness

Let X be a closed, bounded subset of a separable Banach space and $M(X)$ the set of all Borel probability measures on X (weak topology); the barycenter of $\mu \in M(X)$ is

$$b(\mu) = \int_X x \, d\mu(x);$$

the set X is μ-compact if the pre-image of every compact subset of $\overline{\text{conv}}(X)$ under $b : M(X) \to \overline{\text{conv}}(X)$ is compact.

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Theorem 1 (Holevo and Shirokov [4])

The set of density operators $\mathfrak{S}(\mathcal{H})$ is μ-compact.

[4] A. S. Holevo and M. E. Shirokov, *Continuous ensembles and the capacity of infinite-dimensional quantum channels*, Theory of Probability & Its Applications **50**:1, 86–98 (2006).

Generalized Compactness II

Proposition 1 (Protasov and Shirokov [2])

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Theorem 2 (Krein-Milman and Choquet Theorem [2])

Let C be a closed, bounded, μ-compact, convex set, which is a separable metric space. Then

$$C = b\big(M(\overline{\text{ext}\, C}\,)\big)$$

and

$$C = \overline{\text{conv}}(\text{ext}\, C).$$

Generalized Affine Constraints on $\mathfrak{S}(\mathcal{H})$

Expected Value Functional

Let H be an arbitrary positive operator on $\mathcal{H}$. Let $P_n = \int_0^n dE_H(\lambda)$ be the spectral projector of H corresponding to $[0, n]$, where E_H is the spectral measure of H. The expected value functional of H is the map defined by

$$\mathfrak{S}(\mathcal{H}) \to [0, +\infty], \qquad \rho \mapsto \operatorname{Tr} \rho H = \lim_{n\to\infty} \operatorname{Tr}(\rho H P_n).$$

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Generalized Affine Maps

In the sequel, let V be a real vector space and $K \subseteq V$ a convex set. A generalized affine map on K is a map $f : K \to \mathbb{R} \cup \{+\infty\}$ that satisfies

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

Let $\ell \in \mathbb{N}$, let f_k be a generalized affine map on K, and let $\alpha_k \in \mathbb{R}$ for all $k \in u = \{1, \ldots, \ell\}$. For each subset $s \subseteq u$, we define the (sub-) level set

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

Generalized Affine Constraints in Mathematical Physics

Quantum Communication. A quantum channel [5] is a linear, completely positive, trace-preserving map $\Phi : \mathfrak{T}(\mathcal{H}) \to \mathfrak{T}(\mathcal{K})$. The capacity of Φ is typically infinite if $\mathcal{H}, \mathcal{K}$ are infinite-dimensional. An energy constraint on the input system $\mathcal{H}$ bounds the capacity to a finite value and leads to the optimization over the set [5–9]

$$\{\rho \in \mathfrak{S}(\mathcal{H}) \mid \mathrm{Tr}(\rho H) \leq E\},$$

where H is the energy operator and $E < \infty$ the maximal average energy.

[5] A. S. Holevo, *Quantum Systems, Channels, Information: A Mathematical Introduction*, Berlin, Boston: De Gruyter, 2019.

[6] V. Giovannetti, R. García-Patrón, N. J. Cerf, and A. S. Holevo, *Ultimate classical communication rates of quantum optical channels*, Nature Photonics **8**:10, 796–800 (2014).

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Quantum Dynamical Semigroups. [9–11]

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[10] M. E. Shirokov and A. S. Holevo, *Energy-constrained diamond norms and quantum dynamical semigroups*, Lobachevskii J. Math. **40**:10, 1569–1586 (2019).

[11] S. Becker and N. Datta, *Convergence rates for quantum evolution and entropic continuity bounds in infinite dimensions*, Commun. Math. Phys. **374**:2, 823–871 (2020).

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• The sublevel set $\mathfrak{S}(\mathcal{H})_u \doteq \mathfrak{S}(\mathcal{H})_u^{\emptyset}$ is closed, as the functionals $f_1, f_2, \ldots, f_\ell$ are lower semi-continuous. Proposition 1 and Theorem 2 above show that any state $\rho \in \mathfrak{S}(\mathcal{H})_u$ can be represented as the barycenter $\rho = \int \sigma \mu(d\sigma)$ of some Borel probability measure μ supported by $\overline{\mathrm{ext}(\mathfrak{S}(\mathcal{H})_u)}$. The problem is to tell what the extreme points of $\mathfrak{S}(\mathcal{H})_u$ are.

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• If the extreme points of $\mathfrak{S}(\mathcal{H})_u$ were pure states, then any state $\rho \in \mathfrak{S}(\mathcal{H})_u$ could be represented as the barycenter $\rho = \int \sigma \mu(d\sigma)$ of some Borel probability measure μ supported by the closed set of pure states

$$\mathrm{ext}(\mathfrak{S}(\mathcal{H})_u) = \mathfrak{S}(\mathcal{H})_u \cap \mathrm{ext}\, \mathfrak{S}(\mathcal{H}).$$

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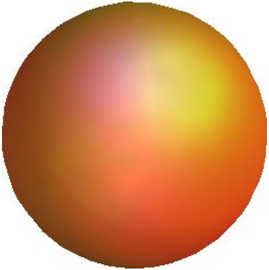
? Question

Under which conditions is every extreme point of $\mathfrak{S}(\mathcal{H})_u$ a pure state?

Affine Constraints on the Bloch Ball $\mathfrak{S}(\mathbb{C}^2)$



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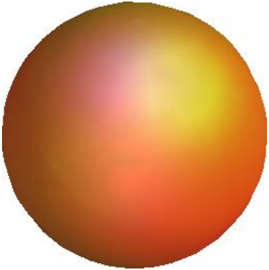

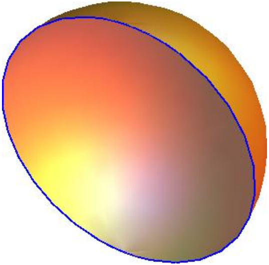

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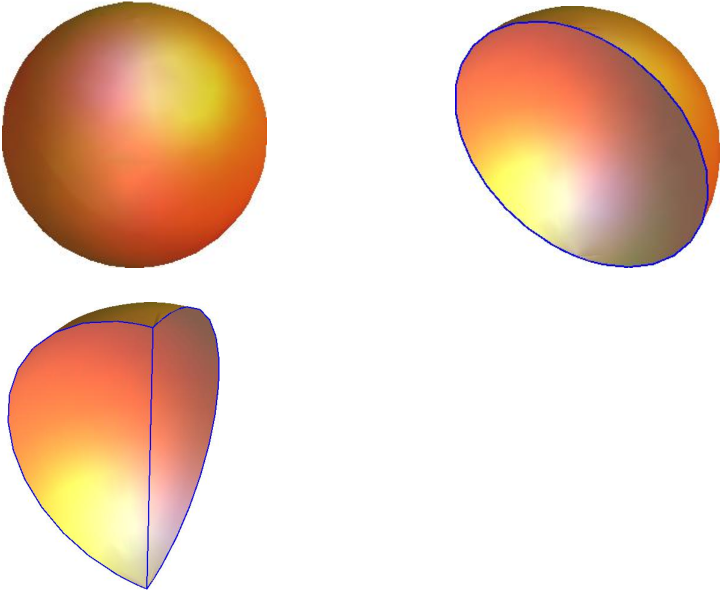

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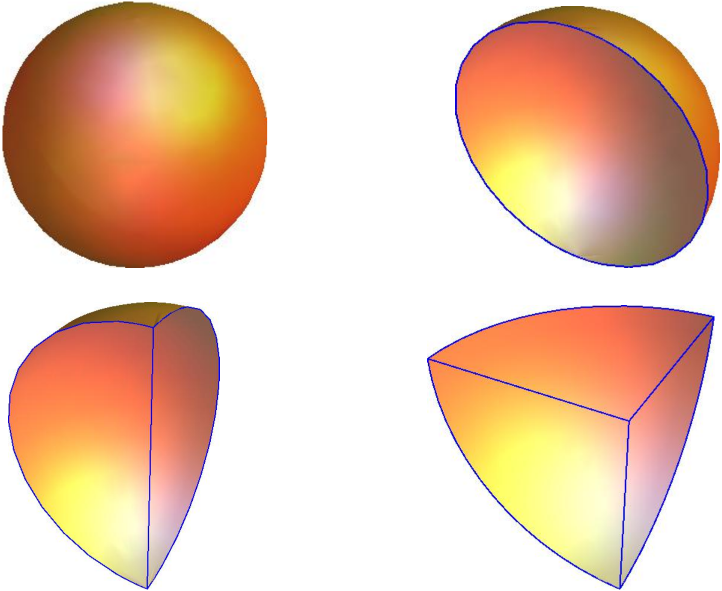

Studying Extreme Points

If $\dim(K) < \infty$, then the extreme points of a (sub-) level set K_u^s can be analyzed using relative algebraic interiors of faces of K. A careful analysis allows us to proceed in the same way if $\dim(K) = \infty$.

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Relative Algebraic Interior

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

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Example. The convex set K of polynomials in one variable with positive leading coefficients has an empty relative algebraic interior [12].

[12] A. Barvinok, *A Course in Convexity*, Providence, R.I: AMS, 2002.

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

Example. The convex set K of polynomials in one variable with positive leading coefficients has an empty relative algebraic interior [12].

- The affine hull $\mathrm{aff}(K)$ is the set of all polynomials: $\mathrm{aff}(K)$ is a linear space as $0 = 2 \cdot 1 + (-1) \cdot 2 \in \mathrm{aff}\, K$. Then $\mathrm{aff}\, K = K \cup (-K) \cup \{0\}$ contains all polynomials.

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• Let $p \in K$. If $q \in K$ such that $\deg(q) > \deg(p)$ then $p - \epsilon q \in \mathrm{aff}\, K$ but $p - \epsilon q \notin K$ for all $\epsilon > 0$. This shows $p \notin \mathrm{ri}(K)$.

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Theorem 3 (SW and Shirokov [3])

Let V be a real vector space, $K \subseteq V$ a convex subset, and $x \in K$. Then

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

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

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Proof. "$\supseteq$" as $y = \frac{\epsilon-1}{\epsilon}x + \frac{1}{\epsilon}(x + \epsilon(y-x))$. "$\subseteq$" follows from the Kuratowski-Zorn lemma and from analyzing certain extreme subsets of $F_K(x)$.

Corollaries to Theorem 3

a) Let $x \in K$. Then $F_K(x) = \bigcup_{y,z \in K, x \in (y,z)} [y, z]$.

b) Let $E \subseteq K$ be a subset. The set E is an extreme subset of K if and only if the set E is a union of faces of K.

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Proposition 2

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

- $F_{K \cap L}(x) = F_K(x) \cap F_L(x)$
- $\mathrm{ri}\left(F_K(x) \cap F_L(x)\right) = \mathrm{ri}\left(F_K(x)\right) \cap \mathrm{ri}\left(F_L(x)\right)$
- $\mathrm{aff}\left(F_K(x) \cap F_L(x)\right) = \mathrm{aff}\left(F_K(x)\right) \cap \mathrm{aff}\left(F_L(x)\right)$.

Example: Probability Distributions on $\mathbb{N}$

The convex set $\Delta_{\mathbb{N}} = \left\{ p : \mathbb{N} \to \mathbb{R} \mid p(n) \geq 0 \; \forall n \in \mathbb{N}, \text{ and } \sum_{n \in \mathbb{N}} p(n) = 1 \right\}$ has an intriguing facial structure.

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- Using Corollary a) and writing $\Delta_I \doteq \{q \in \Delta_{\mathbb{N}} \mid \mathrm{supp}(q) \subseteq I\}$ for $I \subset \mathbb{N}$, we get

$$F_{\Delta_{\mathbb{N}}}(p) = \{q \in \Delta_{\mathrm{supp}(p)} \mid \sup_{n\in\mathrm{supp}(p)} q(n)/p(n) < \infty\}$$
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• The set $\Delta_{\mathbb{N}}$ has a continuous chain of faces: The curve of probability distributions $p_s(n) = \zeta(s)^{-1} \cdot n^{-s}$, $s > 1$, generates a chain of faces of $\Delta_{\mathbb{N}}$ that obey the reverse inclusion ordering $F_{\Delta_{\mathbb{N}}}(p_s) \subseteq F_{\Delta_{\mathbb{N}}}(p_t) \iff s \geq t$ for all $s, t > 1$. Here, $\zeta(s) = \sum_{n\in\mathbb{N}} n^{-s}$ is the Euler-Riemann zeta function, $s > 1$.

Face Dimensions of (Sub-) Level Sets

If we replace the convex set K with the sublevel set $K^{\emptyset}_{\{1\}}$ or level set $K^{\{1\}}_{\{1\}}$ of a generalized affine functional, then the dimension of the face generated by a point may decrease at most by one (follows directly from Proposition 2).

Theorem 4 (SW and Shirokov [3])

Let $C = K^{s}_{\{1\}}$, $s \subset \{1\}$, and let x be a point in C. If the face $F_C(x)$ of C generated by x has dimension $m \in \mathbb{N}_0 = \{0, 1, 2, \ldots\}$, then the face $F_K(x)$ of K generated by x has dimension m or $m + 1$.

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Iterating Theorem 4, we can exploit gaps in the face dimensions of K.

Corollary 1

Let K have no face with dimension in $u = \{1, \ldots, \ell\}$. Then every extreme point of the (sub-) level set K_u^s is an extreme point of K for all $s \subseteq u$.

Theorems for two Expected Value Constraints I

Face Dimensions

Every face of the set $\mathfrak{S}(\mathcal{H})$ of density operators has its dimension from the list $0, 3, 8, \ldots, n^2 - 1, \ldots, \infty$.

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In the sequel, we consider two arbitrary positive operators H_1, H_2 on $\mathcal{H}$, their expected value functionals $\rho \mapsto \operatorname{Tr} \rho H_k$, $k = 1, 2$, on $\mathfrak{S}(\mathcal{H})$, and two arbitrary numbers $E_1, E_2 \in \mathbb{R}$. We study the (sub-) level set

$$\mathfrak{S}(\mathcal{H})^s_{\{1,2\}} = \{\rho \in \mathfrak{S}(\mathcal{H}) \mid \operatorname{Tr}(\rho H_k) \leq E_k \ \forall k \in u \setminus s \text{ and } \operatorname{Tr}(\rho H_k) = E_k \ \forall k \in s\}$$

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Theorem 5 (SW and Shirokov [3])

Every extreme point of the (sub-) level set $\mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$ is a pure state for all $s \subseteq \{1, 2\}$.

Theorems for two Expected Value Constraints II

Krein-Milman and Choquet Theorem [3]

Assume the sublevel set $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$ is nonempty. Then the set of extreme points $\mathrm{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$ is nonempty and closed and is equal to the set of pure states $\mathfrak{S}(\mathcal{H})_{\{1,2\}} \cap \mathrm{ext}\,\mathfrak{S}(\mathcal{H})$.

- The set $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$ is the closure of the convex hull of $\mathrm{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$.

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Proof. • Theorem 5 shows that the set of extreme points $\text{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$ is the intersection of $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$ and the set of pure states $\text{ext}\,\mathfrak{S}(\mathcal{H})$. As both sets are closed, their intersection is closed.

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• The remaining assertions follow from Theorem 2 as $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$ is μ-compact and since $\mathrm{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$ is closed.

Theorems for two Expected Value Constraints III

Unlike the sublevel set $\mathfrak{S}(\mathcal{H})_{\{1,2\}} = \mathfrak{S}(\mathcal{H})^{\emptyset}_{\{1,2\}}$, the (sub-) level set $\mathfrak{S}(\mathcal{H})^{s}_{\{1,2\}}$ many not be closed if $s \neq \emptyset$.

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Choquet Theorem for (Sub-) Level Sets [3]

Every state ρ in the (sub-) level set $\mathfrak{S}(\mathcal{H})^{s}_{\{1,2\}}$ can be represented as the barycenter

$$\rho = \int \sigma \mu(d\sigma) \tag{1}$$

of some Borel probability measure μ supported by $\mathrm{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$ such that $\mu(\mathrm{ext}(\mathfrak{S}(\mathcal{H})^{s}_{\{1,2\}}) = 1$ for all $s \subseteq \{1,2\}$.

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Proof. By the preceding theorem, equation (1) holds for a probability measure μ supported by the set $\operatorname{ext}(\mathfrak{S}(\mathcal{H})_{\{1,2\}})$, which implies $\operatorname{Tr} \rho H_k = \int \operatorname{Tr}(\sigma H_k)\, \mu(d\sigma)$, $k = 1, 2$ [13]. If $\operatorname{Tr} \rho H_k = E_k$ holds for $k \in \{1, 2\}$, then $\operatorname{Tr} \sigma H_k = E_k$ for μ-almost all σ as $\operatorname{Tr} \sigma H_k \leq E_k$ holds for all σ in the support of μ.

[13] M. E. Shirokov, *On properties of the space of quantum states and their application to the construction of entanglement monotones*, Izvestiya: Mathematics **74**:4, 849–882 (2010).

Theorems for two Expected Value Constraints IV

Theorem 6 [3] (Maximizing Convex Functions)

• Let $s \subseteq \{1, 2\}$ and let $f : \mathfrak{S}(\mathcal{H})^s_{\{1,2\}} \to [-\infty, \infty]$ be a convex function on the (sub-) level set. If f is either lower semicontinuous or upper semicontinuous and upper bounded, then

$$\sup\{f(\rho) : \rho \in \mathfrak{S}(\mathcal{H})^s_{\{1,2\}}\} = \sup\{f(\rho) : \rho \in \operatorname{ext} \mathfrak{S}(\mathcal{H})^s_{\{1,2\}}\}, \quad (2)$$

where $\operatorname{ext} \mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$ is the set of pure states in $\mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$.

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where $\operatorname{ext} \mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$ is the set of pure states in $\mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$.

• If the domain of f is the sublevel set $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$, if f is upper semicontinuous, and if one of the operators H_1 or H_2 has discrete spectrum of finite multiplicity (whence $\mathfrak{S}(\mathcal{H})_{\{1,2\}}$ is compact), then the supremum on the right-hand side of (2) is attained at a pure state in $\mathfrak{S}(\mathcal{H})^s_{\{1,2\}}$.

Application: Minimal Output Entropy I

Entropy

The von Neumann entropy of a quantum state ρ in $\mathfrak{S}(\mathcal{H})$ is defined by the formula $H(\rho) = \operatorname{Tr} \eta(\rho)$, where $\eta(x) = -x \log x$ for $x > 0$ and $\eta(0) = 0$.

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The von Neumann entropy is a basic characteristic of states. The function $H(\rho)$ is concave and lower semicontinuous on the set $\mathfrak{S}(\mathcal{H})$ and takes values in $[0, +\infty]$.

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In the analysis of information abilities of a quantum channel $\Phi : \mathfrak{T}(\mathcal{H}) \to \mathfrak{T}(\mathcal{K})$, the notion of the minimal output entropy is widely used [5]. It is defined as

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

where $\mathcal{H}_1$ is the unit sphere in $\mathcal{H}$.

Application: Minimal Output Entropy II

In studies of infinite-dimensional quantum channels, it is reasonable to consider the constrained minimal output entropies [14]

$$H_{\min}(\Phi, H, E) = \inf_{\rho \in \mathfrak{S}(\mathcal{H}) : \mathrm{Tr}\, H\rho \leq E} H(\Phi(\rho)), \tag{3}$$

$$H_{\min}^{=}(\Phi, H, E) = \inf_{\rho \in \mathfrak{S}(\mathcal{H}) : \mathrm{Tr}\, H\rho = E} H(\Phi(\rho)), \tag{4}$$

where H is a positive operator, the energy observable.

[14] L. Memarzadeh and S. Mancini, *Minimum output entropy of a non-Gaussian quantum channel*, Phys. Rev. A **94**:2, 022341 (2016).

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In contrast to the unconstrained case, it is not obvious that the infima in (3) and (4) can be taken only over pure states satisfying the conditions $\operatorname{Tr} H\rho \leq E$ and $\operatorname{Tr} H\rho = E$ correspondingly. In [14] it is shown that this holds in the finite-dimensional settings. The above Theorem 6 allows us to prove the same assertion for an arbitrary infinite-dimensional channel Φ and any energy observable H.

[14] L. Memarzadeh and S. Mancini, *Minimum output entropy of a non-Gaussian quantum channel*, Phys. Rev. A **94**:2, 022341 (2016).

Thank you for your attention!

These slides were created with LaTeX (beamer class and bclogo-package). The graphics were drawn with `Wolfram Mathematica`.