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Applications of cut polyhedra — II

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Abstract

This is the continuation of Part I (this issue). In this second part, we present the following applications of cut polyhedra: the max-cut problem, the Boole problem and the multicommodity flow problems in combinatorial optimization, lattice holes in geometry of numbers, density matrices of many-fermions systems in quantum mechanics, as well as some other applications, in probability theory, statistical data analysis and design theory.

As we shall frequently use results, definitions and notation from Part I, the sections in this second part are numbered consecutively.

Keywords: Cut; Polyhedron; \ell_1-metric; Hypermetric; Delaunay polytope; Probability; Boole problem; Combinatorial optimization; Max-cut problem; Multicommodity flow; Quantum mechanics; Design

We refer to the first part [31] for a general introduction, including also the topics treated here.

5. Applications in combinatorial optimization

5.1. The maximum-cut problem

Given a graph $G = (V, E)$ and nonnegative weights $w_e, e \in E$, assigned to its edges, the max-cut problem consists of finding a cut $\delta(S)$ whose weight $\sum_{e \in \delta(S)} w_e$ is as large as possible. The max-cut problem is a notorious NP-hard problem [48]. If we replace “as large” by “as small”, then we obtain the min-cut problem which can be solved using network flow techniques [46]. Several classes of graphs are known for which the max-cut problem can be solved in polynomial time. This is the case, for instance, for planar graphs [53], for graphs not contractible to $K_5$ [6], for weakly bipartite graphs, i.e., the graphs $G$ for which the polytope $\{x \in \mathbb{R}_+^E : x(C) \leq |C| - 1 \}$ for all odd cycles

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C of $G$ has all its vertices integral [52]. In fact, the class of weakly bipartite graphs includes the graphs not contractible to $K_5$ ([45] or [80]).

For definitions of the terms used in this section, see, e.g., [51, 86].

The max-cut problem can be reformulated as a linear programming problem over the cut polytope, namely, as

$$\max w^T x$$
subject to $x \in \text{CUTP}(G)$.

This is the polyhedral approach, classical in combinatorial optimization, which leads to the study of the facets of $\text{CUTP}(G)$. This approach has been used in practice for solving large instances of the max-cut problem (see, e.g., [7, 8]). Its success depends, of course, on the degree of knowledge about the facets needed for the problem at hand and of their tractability, i.e., whether they can be separated in polynomial time or, at least, whether a good separation heuristic is available.

For instance, $\text{CUTP}(G) = \text{MET}(G)$, i.e., the inequalities

$$x(F) - x(C - F) \leq |F| - 1 \quad \text{for } F \subseteq C \text{ cycle with } |F| \text{ odd}$$

are sufficient for describing $\text{CUTP}(G)$ if and only if $G$ is not contractible to $K_5$ [9]. Moreover, the above inequalities can be separated in polynomial time, implying that the max-cut problem in graphs not contractible to $K_5$ is polynomially solvable [9].

The max-cut problem in an arbitrary graph $G$ on $n$ nodes can always be formulated as

$$\max w^T x$$
subject to $x \in \text{CUTP}_n$

after setting $w_e = 0$ if $e$ is not an edge of $G$. This permits to exploit fully the symmetry of the complete graph.

The max-cut problem has many applications in various fields. For instance, the problem of determining ground states of spin glasses with an exterior magnetic field, or the problem of minimizing the number of vias (holes on a printed circuit board) subject to pin assignment and layer preferences, can both be formulated as instances of the max-cut problem; they arise, respectively, in statistical physics and VLSI circuit design. We refer to [7] for a detailed description of these two applications, together with a computational treatment. In fact, the spin glass problem was already mentioned in [72] as an optimization problem over the boolean quadric polytope. Other applications can be found in [12].

Another application is to unconstrained quadratic 0–1 programming, which consists of solving

$$\max \sum_{1 \leq i < j \leq n} c_{ij} x_i x_j$$
subject to $x \in \{0, 1\}^n$,

where $c_{ij} \in \mathbb{R}$. If we set $p_{ij} = x_i x_j$ for $1 \leq i \leq j \leq n$, this problem can be equivalently formulated as a linear programming problem over the boolean quadric polytope

$$\max c^T p$$
subject to $p \in \text{BQP}_n$. 
Just as the points of the boolean quadric polytope and of the cut polytope are in one-to-one correspondence (via the covariance map; see [31, Section 2.4]), the max-cut problem and the unconstrained quadratic programming problem are equivalent.

Other approaches, besides the polyhedral approach, have been proposed for attacking the max-cut problem. In particular, an approach based on eigenvalue methods is investigated in [23, 81, 82]. We mention briefly some facts, permitting to connect it with polyhedral aspects.

The Laplacian matrix $L$ of the graph $G$ is the $n \times n$ matrix defined by

$$
L_{ii} = \deg_G(i) \quad \text{for } i \in V, \\
L_{ij} = -a_{ij} \quad \text{for } i \neq j \in V,
$$

where $A(a_{ij})_{1 \leq i, j \leq n}$ is the adjacency matrix of $G$. Set

$$
\varphi(G) = \frac{1}{2} n \min \left( \lambda_{\max}(L + \text{diag}(u)) : u \in \mathbb{R}^n, \sum_{1 \leq i \leq n} u_i = 0 \right),
$$

where $\text{diag}(u)$ is the diagonal matrix with diagonal entries $u_1, \ldots, u_n$ and $\lambda_{\max}(L + \text{diag}(u))$ is the largest eigenvalue of the matrix $L + \text{diag}(u)$. Set

$$
\psi(G) = \max \left( \frac{1}{2} \text{Trace}(AX) : X \text{ is positive semidefinite and } A = Y, \right)
$$

where $J$ is the $n \times n$ matrix with all entries equal to 1. Let $mc(G)$ denote the maximum cardinality of a cut in $G$. Then,

(i) $mc(G) \leq \varphi(G)$ [23],

(ii) $mc(G) \leq \psi(G)$ [87].

The quantity $\psi(G)$ can be easily reformulated as

$$
\psi(G) = \max \left( \sum_{1 \leq i \leq j \leq n} a_{ij} x_{ij} : x \text{ satisfies the inequalities (19) for all integers } b_1, \ldots, b_n \right),
$$

$$
\sum_{1 \leq i \leq j \leq n} b_i b_j x_{ij} \leq \frac{1}{4} \left( \sum_{1 \leq i \leq n} b_i \right)^2. \quad (19)
$$

Inequalities (19) are clearly valid for the cut polytope $\text{CUTP}_n$, but they are never facet defining since they are dominated by the gap inequalities (5) (defined in [31, Section 2.2]); however, inequalities (19) can be separated in polynomial time while the separation problem for the gap inequalities is probably hard.

In fact, using general duality theory, it is shown that $\varphi(G) - \psi(G)$ holds [82]. Recently, it has been shown in [49] that the quantity $\psi(G)$ provides a good approximation for the max-cut problem, namely,

$$
\frac{\psi(G)}{mc(G)} \leq 1.138.
$$

5.2. Multicommodity flows

An instance of the multicommodity flow problem consists of two graphs: the supply graph $G = (V_n, E)$ together with a capacity function $c : E \to \mathbb{R}_+$, and the demand graph $H = (T, U)$ together with a demand function $r : U \to \mathbb{R}_+$, where $T \subseteq V_n$ is the set of nodes spanned by $U$. Given
A pair of nodes \((s, t)\), \(P_{st}\) denotes the set of \(st\)-paths in \(G\) and we set \(P = \bigcup_{(s, t) \in U} P_{st}\). A multiflow is a function \(f: P \to \mathbb{R}_+\). The instance \((G, H, c, r)\) is said to be feasible if there exists a feasible multiflow, i.e., a multiflow \(f: P \to \mathbb{R}_+\) satisfying the following capacity and demand requirements:

\[
\sum_{P \in P, e \in P} f_P \leq c_e \quad \text{for } e \in E, \quad \sum_{P \in P_{st}} f_P \geq r_{st} \quad \text{for } (s, t) \in U.
\]

Using the Farkas lemma, it can be checked that the following holds.

**Proposition 5.1.** The problem \((G, H, c, r)\) is feasible if and only if \(c^y - r^z \geq 0\) for all \((y, z) \in C(G, H)\), where \(C(G, H)\) is the cone defined by

\[
C(G, H) = \left\{ (y, z) \in \mathbb{R}_+^E \times \mathbb{R}_+^U : \sum_{e \in P} y_e - z_{st} \geq 0 \quad \text{for } P \in P_{st} \text{ and } (s, t) \in U \right\}.
\]

The cone \(C(G, H)\) is studied in detail in [61] and, in particular, the fractionality of its extreme rays.

Without loss of generality, we can suppose that \(G\) is the complete graph \(K_n\); then, \(r\) is extended to \(K_n\) by setting \(r_e = 0\) for the edges \(e \notin U\) and \(U = \{e: r_e > 0\}\) is called the support of \(r\) and we simply say that the pair \((c, r)\) is feasible. An alternative characterization for feasible multiflows is given by the following so-called Japanese theorem (from [56, 75], restated in [68, 69]).

**Theorem 5.2.** The pair \((c, r)\) is feasible if and only if

\[
(c - r)^T d \geq 0 \quad \text{for all } d \in \text{MET}_n.
\]

Therefore, the metric cone \(\text{MET}_n\) is the dual cone to the cone of feasible multiflows.

An obvious way for testing feasibility of the pair \((c, r)\) is to solve the linear program

\[
\min((c - r)^T d : d \in \text{MET}_n)
\]

which has \(\binom{n}{2}\) variables and \(3\binom{n}{3}\) constraints (the triangle inequalities (1) in [31]). An alternative way is to check the condition (20) for all extreme rays \(d\) of \(\text{MET}_n\). This approach leads to the study of extreme rays of the metric cone \(\text{MET}_n\) (see references on it in [31, Section 2.4]).

There are other variants of the Japanese theorem, in particular, in the more general setting of binary matroids (see [89]). In particular, the metric cone \(\text{MET}(G)\) (defined in [31, relation (11)]) arises naturally when studying multicommodity flows. It is shown in [89] that all extreme rays of \(\text{MET}(G)\) are 0-, 1-valued (i.e., \(\text{MET}(G) = \text{CUT}(G)\)) if and only if \(G\) is not contractible to \(K_5\). The graphs for which all extreme rays of \(\text{MET}(G)\) are 0-, 1-, 2-valued are characterized in [88]. The graphs for which all the vertices of the metric polytope \(\text{METP}(G)\) (defined in [31, relation (12)]) are \(\frac{1}{2}\)-integral are studied in [66] (\(x\) is said to be \(\frac{1}{2}\)-integral if \(3x\) is integral).

Since the cut cone \(\text{CUT}_n\) is contained in the metric cone \(\text{MET}_n\), a necessary condition for the existence of a feasible multiflow is the following cut condition:

\[
\sum_{e \in \delta(S)} (c_e - r_e) \geq 0 \quad \text{for all } S \subseteq V_n.
\]

The well-known Ford–Fulkerson theorem [46] states that the cut condition is, in fact, also sufficient for feasibility in the case of single commodity flows, i.e., when \(|U| = 1\). We give below some other results of this type. An integral multiflow is a multiflow \(f\) with integral values.
Theorem 5.3. Assume that the support of the demand function \( r \) is \( K_4, C_5, \) or the union of two stars (i.e., all edges are covered by two nodes). Then, the pair \( (c, r) \) is feasible if and only if the cut condition (21) holds \([76]\). Moreover, if \( c, r \) are integral, \( (c - r)^T \delta(S) \) is even for all cuts and (21) holds, then there exists an integral multijlow (see \([69]\) and references therein).

Theorem 5.4 (Karzanov \([60,62]\)). If the support graph of the demand function \( r \) is a subgraph of \( K_5 \) (including \( K_5 \)), \( c, r \) are integral and \( (c - r)^T \delta(S) \) is even for all cuts, then there exists an integral multijlow if and only if (20) holds or, equivalently, if and only if (21) holds and \( (c - r)^T d \geq 0 \) holds for all \( 0 \)-extensions of the path metrics of \( K_{2,3} \).

There is a close connection between these results and \( L_1 \)-embeddability, as noted in \([4]\). Given a semimetric \( d \) on \( V_n \), an extremal graph \([68,69]\) for \( d \) is a minimal graph \( K = (V_0, W) \) such that, for each \( x, y \in V_n \), there exists \( (s, t) \in W \) satisfying \( d_{sx} + d_{xy} + d_{yt} = d_{xt} \), and \( V_0 \) is the set of nodes covered by \( W \). The extremal graph is unique if \( d_{ij} > 0 \) for all \( i, j \in V_n \). The notion of extremal graph is a key notion for testing feasibility of multijflows.

Proposition 5.5 (Lomonossov \([68,69]\)). The pair \( (c, r) \) is feasible if and only if \( (c - r)^T d \geq 0 \) holds for all \( d \in \text{MET}_n \) having an extremal graph \( K = (V_0, W) \) such that \( W \) is a subset of the support of the demand function \( r \).

Theorem 5.6 (Karzanov \([59]\)). If \( d \in \text{MET}_n \) has an extremal graph which is \( K_4, C_5, \) or a union of two stars, then \( d \in \text{CUT}_n \). Moreover, if \( d \) satisfies the parity condition \([31, (16)]\), then \( d \) is a non-negative integer sum of cuts, i.e., \( d \) is h-embeddable.

Note that the latter two results imply the first part of Theorem 5.3.

We conclude with some additional related results.

Given a supply graph \( G \), a capacity function \( c \) and a demand graph \( H \), the maximum multijflow problem consists of finding a multijlow \( f \) not exceeding the capacity constraints whose value \( \sum_{P \in \mathcal{P}} f_P \) is as large as possible. By linear programming duality, this problem is equivalent to the linear programming problem

\[
\min (c^T y : y \in \mathbb{R}^E_+, y(P) \geq 1 \text{ for all } P \in \mathcal{P}).
\]

This leads to the study of the polytope \( P(G, H) = \{ y \in \mathbb{R}^E_+ : y(P) \geq 1 \text{ for all } P \in \mathcal{P} \} \). The fractionality of the vertices of \( P(G, H) \) is studied in detail in \([61]\); in particular, the demand graphs \( H \) for which all vertices of \( P(G, H) \) are \( \frac{1}{2} \)-integral for an arbitrary demand graph \( G \) with \( V(H) \subseteq V(G) \) are characterized.

5.3. The Boole problem

Let \( (\Omega, \mathcal{A}, \mu) \) be a probability space and let \( A_1, \ldots, A_n \) be \( n \) events of \( \mathcal{A} \). A classical question, which goes back to Boole \([11]\), is the following:

Suppose we are given the values \( p_i = \mu(A_i) \) for \( 1 \leq i \leq n \), what is the best estimation of \( \mu(A_1 \cup \cdots \cup A_n) \)?
It is easy to see that the answer is
\[ \max(p_1, \ldots, p_n) \leq \mu(A_1 \cup \cdots \cup A_n) \leq \min \left( 1, \sum_{1 \leq i \leq n} p_i \right). \]

More generally, let \( \mathcal{F} \) be a collection of subsets of \{1, \ldots, n\}. Suppose we are given the values of the joint probabilities \( p_I = \mu(\bigcap_{i \in I} A_i) \) for all \( I \in \mathcal{F} \). What is the best estimation of \( \mu(A_1 \cup \cdots \cup A_n) \) in terms of the \( p_I \)'s?

In fact, the answer to this problem is given by the facet defining inequalities for the polytope \( \text{BQP}_n^{\mathcal{F}} \) (defined in [31, Section 2.4]). Namely,
\[ \mu(A_1 \cup \cdots \cup A_n) \geq \max(w^T p: w^T z \leq 1 \text{ is facet defining for } \text{BQP}_n^{\mathcal{F}}) \]
(see Proposition 5.8 and relation (26)). In particular, when \( \mathcal{F} \) consists of all pairs and singletons, then the lower bound for \( \mu(A_1 \cup \cdots \cup A_n) \) is in terms of the facets of the boolean quadric polytope \( \text{BQP}_n \).

**Estimations for \( \mu(A_1 \cup \cdots \cup A_n) \) via linear programming**

First, we observe that [31, Theorem 3.21 remains valid for the polytope \( \text{BQP}_n^{\mathcal{F}} \) for an arbitrary nonempty set family \( \mathcal{F} \).

**Theorem 5.7.** Let \( \mathcal{F} \) be a nonempty collection of subsets of \{1, \ldots, n\} and let \( p = (p_I)_{I \in \mathcal{F}} \in \mathbb{R}^\mathcal{F} \). The following assertions are equivalent.

(i) \( p \in \text{BQ}_n^{\mathcal{F}} \) (resp. \( p \in \text{BQP}_n^{\mathcal{F}} \)).

(ii) There exist a nonnegative measure space (resp. a probability space) \((\Omega, \mathcal{A}, \mu)\) and \( A_1, \ldots, A_n \in \mathcal{A} \) such that \( p_I = \mu(\bigcap_{i \in I} A_i) \) for all \( I \in \mathcal{F} \).

**Proof.** It is identical to that of [31, Theorem 3.2]. \( \square \)

Given \( p \in \text{BQ}_n^{\mathcal{F}} \), consider the following two linear programming problems:

\[
\begin{align*}
\text{minimize} \quad & \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S \\
\text{subject to} \quad & \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S \pi^{\mathcal{F}}(S) = p, \\
& \lambda_S \geq 0 \quad \text{for } \emptyset \neq S \subseteq \{1, \ldots, n\}. \\
\end{align*}
\]

(22)

\[
\begin{align*}
\text{maximize} \quad & \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S \\
\text{subject to} \quad & \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S \pi^{\mathcal{F}}(S) = p, \\
& \lambda_S \geq 0 \quad \text{for } \emptyset \neq S \subseteq \{1, \ldots, n\}. \\
\end{align*}
\]

(23)

Let \( z_{\min} \) (resp. \( z_{\max} \)) denote the optimum value of the program (22) (resp. (23)).

So, the program (22) (resp. (23)) is evaluating the minimum value (resp. the maximum value) of \( \sum_S \lambda_S \) for a decomposition \( p = \sum_S \lambda_S \pi^{\mathcal{F}}(S), \lambda_S \geq 0, \) of \( p \in \text{BQ}_n^{\mathcal{F}} \). In particular, in the case \( \mathcal{F} = \mathcal{F}_{\leq 2} \), if
we set \( d = \varphi_{\text{opt}}^{-1}(p) \), then \( d \in \text{CUT}_{n+1} \) and \( z_{\text{min}} \) coincides with the minimum size \( s(d) \) (defined in [31, Section 2.5]). This approach, in the case of \( \mathcal{I}_{\leq 2} \), is considered in [63, 79].

**Proposition 5.8.** \( z_{\text{min}} \leq \mu(A_1 \cup \cdots \cup A_n) \leq z_{\text{max}} \).

**Proof.** For \( S \subseteq \{1, \ldots, n\} \), set \( A^S = \bigcap_{i \in S} A_i \cap \bigcap_{i \notin S} (\Omega \setminus A_i) \). Then, \( \bigcap_{I \in \mathcal{I}} A_i = \bigcup_{S \subseteq \{1, \ldots, n\}} A^S \), \( \Omega = \bigcup_{S} A^S \) and \( A_1 \cup \cdots \cup A_n = \bigcup_{S \neq \emptyset} A^S \). We have \( p_I = \mu(\bigcap_{i \in I} A_i) \) for each \( I \in \mathcal{I} \). Therefore, \( p = \sum_{S \neq \emptyset} \mu(A^S) \pi^S(S) \) holds, with \( \mu(A^S) \geq 0 \). Hence \( (\mu(A^S); \emptyset \neq S \subseteq \{1, \ldots, n\}) \) is a feasible solution to the program (22), or (23), with objective value \( \mu(A_1 \cup \cdots \cup A_n) \). This proves the result.

The dual programs to (22) and (23) are the following programs (24) and (25), respectively:

\[
\begin{align*}
\text{maximize} & \quad w^T p \\
\text{subject to} & \quad w^T \pi^S(S) \leq 1 \text{ for } \emptyset \neq S \subseteq \{1, \ldots, n\}.
\end{align*}
\]

(24)

\[
\begin{align*}
\text{minimize} & \quad w^T p \\
\text{subject to} & \quad w^T \pi^S(S) \geq 1 \text{ for } \emptyset \neq S \subseteq \{1, \ldots, n\}.
\end{align*}
\]

(25)

By linear programming duality, we have

\[
z_{\text{min}} = \max(w^T p: w^T z \leq 1 \text{ is a valid inequality for BQP}^n) \quad (26)
\]

and it is easily verified that, in relation (26), it is sufficient to consider facet defining inequalities. Similarly,

\[
z_{\text{max}} = \min(w^T p: w^T z \geq 1 \text{ is facet defining for the polytope Conv(} \pi^S(S): \emptyset \neq S \subseteq V_n)) \quad (27)
\]

(The latter polytope is distinct from BQP^n since it does not contain the origin.)

Therefore, by (26), every valid inequality for BQP^n yields a lower bound for \( \mu(A_1 \cup \cdots \cup A_n) \) in terms of the joint probabilities \( p_I = \mu(\bigcap_{i \in I} A_i) \) for \( I \in \mathcal{I} \). Examples of such lower bounds are exposed below (after Proposition 5.9).

The case when the collection \( \mathcal{I} \) of index sets is \( \mathcal{I}_{\leq m} \) is considered in [13]. The following estimations for \( \mu(A_1 \cup \cdots \cup A_n) \) are given there:

\[
y_{\text{min}} \leq \mu(A_1 \cup \cdots \cup A_n) \leq y_{\text{max}},
\]

(27)

where \( y_{\text{min}} \) is the optimum value of the linear program (28) below and \( y_{\text{max}} \) is the optimum value of (29) below, setting

\[
S_k = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} \mu(A_{i_1} \cap A_{i_2} \cap \cdots \cap A_{i_k}) \quad \text{for } 1 \leq k \leq n.
\]

minimize \( \sum_{1 \leq i \leq n} v_i \)

subject to \( \sum_{1 \leq i \leq n} \binom{i}{k} v_i = S_k \) for \( 1 \leq k \leq m \),

\[
v_i \geq 0 \quad \text{for } 1 \leq i \leq n,
\]

(28)
maximize \[ \sum_{1 \leq i \leq n} v_i \]

subject to \[ \sum_{1 \leq i \leq n} \binom{i}{k} v_i = S_k \] for \( 1 \leq k \leq m, \)
\[ v_i \geq 0 \] for \( 1 \leq i \leq n. \) \[ (29) \]

In fact, the programs (22), (23) give sharper bounds than the programs (28), (29), respectively. Namely, we have the following proposition.

**Proposition 5.9.** In the case \( \mathcal{F} = \mathcal{F}_{\leq m} \) for some integer \( m, \) \( 1 \leq m \leq n, \) we have \( y_{\min} \leq z_{\min} \leq \mu(A_1 \cup \cdots \cup A_n) \leq z_{\max} \leq y_{\max}. \)

**Proof.** Indeed, every feasible solution for (22) yields a feasible solution for (28) with the same objective value. Namely, let \( (\lambda_S, \emptyset \neq S \subseteq \{1, \ldots, n\}) \) be a feasible solution for (22), i.e., \( \lambda_S \geq 0 \) and \( p = \sum_S \lambda_S \pi_{\leq m}(S). \) Set \( v_i = \sum_{|S|=i} \lambda_S \) for \( 1 \leq i \leq n. \) Then,

\[
\sum_{1 \leq i \leq n} \binom{i}{k} v_i = \sum_{1 \leq i \leq n} \binom{i}{k} \sum_{|S|=i} \lambda_S \\
= \sum_{1 \leq i_1 < \cdots < i_k \leq n} \sum_{S: i_1, \ldots, i_k \in S} \lambda_S \\
= \sum_{1 \leq i_1 < \cdots < i_k \leq n} p_{(i_1, \ldots, i_k)} \\
= \sum_{1 \leq i_1 < \cdots < i_k \leq n} \mu(A_{i_1} \cap \cdots \cap A_{i_k}) \\
= S_k.
\]

Therefore, \((v_1, \ldots, v_n)\) is a feasible solution for (28) with \( \sum_{1 \leq i \leq n} v_i - \sum_S \lambda_S. \) This shows that \( y_{\min} \leq z_{\min}. \) The inequality \( z_{\max} \leq y_{\max} \) follows from the same argument. \( \square \)

**Examples of bounds for \( \mu(A_1 \cup \cdots \cup A_n) \)**

The best lower bound for \( \mu(A_1 \cup \cdots \cup A_n) \) is given by \( z_{\min}, \) defined by relation (26), whose evaluation relies on the knowledge of the facets of the polytope \( \text{BQP}_n^{\mathcal{F}}. \) In the case \( \mathcal{F} = \mathcal{F}_{\leq 2}, \) the facet structure of the boolean quadric polytope \( \text{BQP}_n \) has been extensively studied (directly or indirectly, via the covariance map, through the cut polytope). We describe below several examples of valid inequalities for \( \text{BQP}_n, \) together with the lower bounds they yield for \( \mu(A_1 \cup \cdots \cup A_n). \)

First, note that, if \( p = \sum_S \lambda_S \pi(S) \) with \( \lambda_S \geq 0, \) then \( n \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij} = \sum_S \lambda_S |S| (n + 1 - |S|), \) where \( n \leq |S| (n + 1 - |S|) \leq \left[ \frac{1}{2} (n + 1) \right] \left[ \frac{1}{2} (n + 1) - 1 \right] \) if \( S \neq \emptyset. \) Hence, we have:

\[
\frac{n \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{\left[ \frac{1}{2} (n + 1) \right] \left[ \frac{1}{2} (n + 1) - 1 \right]} \leq \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S,
\]

\[
\frac{n \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{n} \geq \sum_{\emptyset \neq S \subseteq \{1, \ldots, n\}} \lambda_S.
\]

(30)
and, therefore, from the definition of $z_{\text{min}}, z_{\text{max}}$ and from Proposition 5.8,

$$\frac{n \sum_{1 \leq i < n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{\left\lfloor \frac{1}{2} (n + 1) \right\rfloor \left\lfloor \frac{1}{2} (n + 1) \right\rfloor} \leq \mu(A_1 \cup \cdots \cup A_n),$$

$$\frac{n \sum_{1 \leq i < n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{n} \geq \mu(A_1 \cup \cdots \cup A_n).$$

(31)

Note that the inequalities equivalent to (30) in the context of the cut cone are the bounds on the minimum size of $d \in \text{CUT}_{n+1}$ given in [31, relation (13)].

The inequality

$$2k \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij} \leq k(k + 1)$$

(32)

is valid for the boolean quadric polytope $\text{BQP}_n$ for $1 \leq k \leq n - 1$; it is facet defining if $1 \leq k \leq n - 2$ and $n \geq 4$. Setting $b_0 = 2k + 1 - n$ and $b_1 = \cdots = b_n = 1$, inequality (32) corresponds (via the covariance map) to the inequality

$$\sum_{0 \leq i < j \leq n} b_i b_j x_{ij} \leq k(k + 1),$$

(33)

which is valid for the cut polytope $\text{CUTP}_{n+1}$; (33) is a switching of the hypermetric inequality $\text{Hyp}_{n+1}(2k + 1 - n, 1, \ldots, 1, -1, \ldots, -1)$ (with $n - k$ coefficients $+1$ and $k$ coefficients $-1$). (See, e.g., [29].) Therefore, we have the following lower bound for $\mu(A_1 \cup \cdots \cup A_n)$:

$$\frac{2}{k + 1} \sum_{1 \leq i \leq n} p_i - 2 \frac{1}{k(k + 1)} \sum_{1 \leq i < j \leq n} p_{ij} \leq \mu(A_1 \cup \cdots \cup A_n)$$

(34)

for each $k, 1 \leq k \leq n - 1$; it was found independently by several authors, including [16, 22, 47]. Note that (34) coincides with the lower bound of (31) in the case $n = 2k$.

More generally, given integers $b_1, \ldots, b_n$ and $k \geq 0$, the inequality

$$\sum_{1 \leq i \leq n} b_i (2k + 1 - b_i) p_i - 2 \sum_{1 \leq i < j \leq n} b_i b_j p_{ij} \leq k(k + 1)$$

(35)

is valid for $\text{BQP}_n$. This yields the bound

$$\frac{1}{k(k + 1)} \left( \sum_{1 \leq i \leq n} p_i b_i (2k + 1 - b_i) - 2 \sum_{1 \leq i < j \leq n} b_i b_j p_{ij} \right) \leq \mu(A_1 \cup \cdots \cup A_n).$$

The programs (28), (29) provide weaker bounds than the programs (22), (23), but they present the advantage of being easier to handle, especially for small values of $m$. Exploiting their special structure, the bounds $y_{\text{min}}$ and $y_{\text{max}}$ were explicitly described in [13] in terms of the $S_k$'s (defined in relation (27)), as we recall briefly.

Let $M$ denote the matrix corresponding to the program (22) or (23). Its columns are the $n$ vectors $a_i$, where $a_i = \left( i \choose 1, i \choose 2, \ldots, i \choose n \right)$ for $1 \leq i \leq n$. Set $h = (S_1, \ldots, S_m)$. The matrix $M$ is full rank, hence a basis $B$ consists of a set of $m$ linearly independent vectors among $a_1, \ldots, a_n$. The basis $B$ is called dual feasible if the vector $y = M_B^{-1} \cdot 1$ is feasible for the dual program of (28), i.e. $y^T a_i \leq 1$ for
\( i \in \{1, \ldots, n\} - B \), since equality holds for the indices \( i \in B \) (\( M_B \) is the submatrix of \( M \) whose columns are those vectors \( a_i \) belonging to the basis \( B \); \( 1_m \) has \( m \) coordinates equal to 1). If \( M \) is dual feasible, then the inequality \( 1_B^T M_B^{-1} b \leq \mu(A_1 \cup \cdots \cup A_n) \) holds. The dual feasible bases are explicitly described in [13] together with the corresponding bounds for \( \mu(A_1 \cup \cdots \cup A_n) \).

For example, for \( m \) even, \( \{a_1, a_2, \ldots, a_m\} \) is a dual feasible basis, yielding the bound

\[
\mu(A_1 \cup \cdots \cup A_n) \geq S_1 - S_2 + S_3 - S_4 \cdots + (-1)^{m-1} S_m,
\]

which was first given in [10]. For \( m = 2 \), this is the special case \( k = 1 \) of the bound (34); another choice of basis yields the general bound (34).

In fact, the method from [13] also works for finding estimates of the probabilities \( \mu(\{v \geq r\}) \) and \( \mu(\{v = r\}) \), where \( v \) denotes the random variable counting the number of events that occur among \( A_1, \ldots, A_n \).

Inequality (35) can alternatively be written as

\[
\left( \sum_{1 \leq i < n} b_i p_i - k \right) \left( \sum_{1 \leq i < n} b_i p_i - k - 1 \right) \geq 0
\]

with the convention that, when developing the product, the expression \( p_i p_j \) is replaced by the variable \( p_{ij} \) (setting \( p_{ii} = p_i \)). This inequality (or special cases of it) was considered in this form by many authors (e.g., [40, 63, 72, 79, 94]). This suggests naturally the following generalization of inequality (36) in the case \( \mathcal{F}_{\leq m} \), when \( m \) is an even integer. Given integers \( b_1, \ldots, b_n \) and \( k_1, \ldots, k_m \geq 0 \), the inequality

\[
\prod_{1 \leq i < m} \left( \sum_{1 \leq i < n} b_i p_i - k_i \right) \left( \sum_{1 \leq i < n} b_i p_i - k - 1 \right) \geq 0
\]

is clearly valid for the polytope \( BQP_{n \leq m}^d \). Thus arises the question of determining the parameters \( b_1, \ldots, b_n, k_1, \ldots, k_m \) for which (37) defines a facet of \( BQP_{n \leq m}^d \). This problem is, however, already difficult for the case \( m = 1 \) of the boolean quadric polytope.

### 6. Hypermetrics and geometry of numbers

#### 6.1. L-polytopes

We recall here some definitions about lattices and L-polytopes. A detailed treatment can be found in [20, 27].

Given \( x, y \in \mathbb{R}^k \), we set \( d_0(x, y) = (\|x - y\|_2)^2 \) (the square of the euclidean distance). Recall that the hypermetric cone \( HYP_n \) is defined by the hypermetric inequalities:

\[
\sum_{1 \leq i < j \leq n} b_{ij} x_{ij} \leq 0 \quad \text{for } b_1, \ldots, b_n \text{ integers with } \sum_{1 \leq i \leq n} b_i = 1.
\]

For \( d \in HYP_n \), \( (V_n = \{1, \ldots, n\}, d) \) is called a hypermetric space. It is convenient to work with the hypermetric cone \( HYP_{n+1} \) defined on the \( n + 1 \) points \( 0, 1, 2, \ldots, n \).
A subset \( L \subseteq \mathbb{R}^k \) is a lattice if, up to translation, \( L \) is a discrete subgroup of \( \mathbb{R}^k \). So, the notion of lattice considered in this section is distinct from the notion of lattice (as partially ordered set) used in [31, Section 4.41. A subset \( B = \{v_0, v_1, \ldots, v_m\} \subseteq L \) is generating for \( L \) if, for each \( v \in L \), there exist integers \( z_0, z_1, \ldots, z_m \) such that \( \sum_{0 \leq i \leq m} z_i = 1 \) and \( v = \sum_{0 \leq i \leq m} z_i v_i \). If, moreover, there is unicity of the integers \( z_i \), then \( B \) is an (affine) basis of \( L \); in this case, \( m = |B| - 1 \) is called the dimension of \( L \).

Let \( L \) be a \( k \)-dimensional lattice in \( \mathbb{R}^k \). Let \( S = S(c, r) \) denote the sphere with center \( c \) and radius \( r \). The sphere \( S \) is called an empty sphere (in Russian literature), or hole (in English literature), in \( L \) if the following two conditions hold:

1. \( \|v - c\|_2 > r \) holds for all \( v \in L \),
2. \( S \cap L \) has affine rank \( k + 1 \).

Then, the polytope \( P \) defined as the convex hull of \( S \cap L \) is called an \( L \)-polytope (or Delaunay polytope, or constellation); \( S \) is its circumscribed sphere and \( c \) is its center. The \( L \)-polytope \( P \) is generating if its set of vertices \( V(P) \) generates \( L \), and basic if \( V(P) \) contains an affine basis of \( L \). Actually all known generating \( L \)-polytopes are basic.

For \( v \in S \), let \( v^* = 2c - v \) denote its antipode on \( S \). Every \( L \)-polytope \( P \) is either asymmetric, i.e., \( v^* \notin V(P) \) for each vertex \( v \in V(P) \), or centrally symmetric, i.e., \( v^* \in V(P) \) for each \( v \in V(P) \).

Two \( L \)-polytopes \( P, P' \) have the same type if they are affinely equivalent, i.e., \( P' = T(P) \) for some affine bijective map \( T \).

Examples of \( L \)-polytopes include the \( n \)-dimensional simplex \( \alpha_n \), hypercube \( \gamma_n \), cross polytope \( \beta_n := \text{Conv}(\pm e_i: 1 \leq i \leq n) \) (where \( e_1, \ldots, e_n \) are the unit vectors in \( \mathbb{R}^n \)). Both \( \beta_n \) and \( \gamma_n \) are centrally symmetric, \( \alpha_n \) is asymmetric. All types of \( L \)-polytopes in dimension \( k \leq 4 \) have been classified in [42]:

- For \( k = 1 \), there is only \( \alpha_1 = \beta_1 = \gamma_1 \);
- For \( k = 2 \), they are \( \alpha_2 \) and \( \beta_2 = \gamma_2 \);
- For \( k = 3 \), they are \( \alpha_3, \beta_3, \gamma_3 \), the prism (with triangular base) and the pyramid (with square base);
- For \( k = 4 \), there are 19 polytopes.

Remark that the polytopes \( \alpha_n, \beta_n, \gamma_n \) are \( L \)-polytopes for any \( n \).

The following polytope \( P_{p,q} \) was studied and named repartitioning polytope by Voronoi (see also [5]). Let \( P \) be a polytope and let \( v \) be a point which does not lie in the affine space spanned by \( P \); the convex hull of \( P \) and \( v \) is called the pyramid with base \( P \) and apex \( v \) and is denoted by \( \text{Pyr}(P) \). We define iteratively \( \text{Pyr}_m(P) \) as \( \text{Pyr}(\text{Pyr}_{m-1}(P)) \), setting \( \text{Pyr}_0(P) = P \). Let \( S_p, S_q \) be two simplices of respective dimensions \( p, q \) and lying in affine spaces which intersect in one point. Then, \( P_{p,q} := \text{Pyr}_m(\text{Conv}(S_p \cup S_q)) \) is called a repartitioning polytope; it has dimension \( m + p + q \) and \( m + p + q + 2 \) vertices. In fact, \( P_{p,q} \) does not denote a concrete polytope, but corresponds to a class of affinely equivalent polytopes of the same type.

A construction of symmetric \( L \)-polytopes is given in [25]. Let \( L \) be an integral lattice (i.e. \( u^T v \) integer for all \( u, v \in L \)) and set \( m = \min(u^T u: u \in L, u \neq 0) \). For \( c \in L, c \neq 0 \), set \( P_c = \text{Conv}\{u \in L: u^T u = m \text{ and } 2u^T c = (\|c\|_2^2)\} \). Then, \( P_c \) is a symmetric \( L \)-polytope. Moreover, under some condition, the set of diagonals of \( P \) is a set of equiangular lines. (See Section 6.4.)

Finally, we mention the connection between \( L \)-polytopes and Voronoi polytopes. Given \( v_0 \in L \), the Voronoi polytope \( P_v(v_0) \) is the set \( \{x \in \mathbb{R}^d: \|x - v_0\|_2 \leq \|x - v\|_2 \text{ for all } v \in L\} \). The vertices of \( P_v(v_0) \) are exactly the centers of the \( L \)-polytopes in \( L \) which contain \( v_0 \).
6.2. Hypermetrics and L-polytopes

We state here the beautiful connection existing between hypermetrics and L-polytopes.

**Theorem 6.1** (Assouad [3]). (i) Let P be an L-polytope with set of vertices V(P). Then, (V(P), d₀) is a hypermetric space.

(ii) Let d ∈ HYPₙ₊₁. Then, there exist a lattice Lₙ ⊆ ℝᵏ of dimension k ≤ n, an L-polytope Pₙ in Lₙ and a map fₙ: [0, 1, ..., n] → V(Pₙ), fₙ(i) = vᵢ for 0 ≤ i ≤ n, such that

- {v₀, v₁, ..., vₙ} generates Lₙ,
- dᵢⱼ = d₀(vᵢ, vⱼ) = (∥vᵢ - vⱼ∥₂)² for 0 ≤ i < j ≤ n.

Moreover, the triple (Lₙ, Pₙ, fₙ) is unique, up to translation and orthogonal transformation.

Therefore, hypermetrics on n + 1 points correspond to generating L-polytopes of dimension k ≤ n.

**Proof.** (i) Let S(c, r) denote the empty sphere circumscribed to P. Let bᵥ, v ∈ V(P), be integers with ∑ᵥ∈V(P) bᵥ = 1. Then,

\[ \sum_{u, v ∈ V(P)} b_u b_v d_0(u, v) = \sum_{u, v ∈ V(P)} b_u b_v (∥u - c∥ + (c - v)∥₂)² \]

\[ = \sum_{u, v ∈ V(P)} b_u b_v (2r² + 2(u - c)²(v - c)) \]

\[ = 2r² - 2 \left( \left\| \sum_{u ∈ V(P)} b_u u - c \right\|₂² \right) ≤ 0, \]

because ∑ᵥ∈V(P) bᵥu ∈ L.

We now give a sketch of the proof of (ii). One of the basic tools used in the proof is the covariance map Φ. Define p = Φ₁₀(d), p = (pᵢⱼ)₁≤i,j≤n. By [31, relation (8)], d ∈ HYPₙ₊₁ if and only if

\[ \sum_{1 ≤ i,j ≤ n} b_i b_j p_{i,j} - \sum_{1 ≤ i,j ≤ n} b_i b_j > 0 \]

for all integers b₁, ..., bₙ. Therefore, if d ∈ HYPₙ₊₁, then the symmetric matrix (pᵢⱼ)₁≤i,j≤n is positive semidefinite and, thus, pᵢⱼ = vᵢᵀvⱼ, 1 ≤ i ≤ j ≤ n, for some vectors v₁, ..., vₙ ∈ ℝⁿ, where k is the rank of the matrix (pᵢⱼ)₁≤i,j≤n, k ≤ n.

Moreover, one can show the existence of c ∈ ℝᵏ such that 2cᵀvᵢ = (∥vᵢ∥₂)² for 1 ≤ i ≤ n. Therefore, v₀ = 0, v₁, ..., vₙ lie on the sphere S(c, r := ∥c∥₂). Remains only to show that {v₁, ..., vₙ} generates a lattice L and that the sphere S is empty in L.

**Proposition 6.2** (Deza et al. [27]). Let P be an L-polytope and let V be a subset of its set of vertices V(P). Let P' be the L-polytope associated with the hypermetric space (V, d₀). Then, V(P') ⊆ V(P) with equality if and only if V is a generating subset of V(P).

In particular, every face of an L-polytope is an L-polytope.

We summarize in Table 2 the correspondences between some special hypermetrics and their associated L-polytopes. Given d ∈ HYPₙ₊₁, F(d) denotes the smallest face of HYPₙ₊₁ containing d.
Table 2

<table>
<thead>
<tr>
<th>Hypermetric $d$</th>
<th>Associated $L$-polytope $P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$ is an $\ell_1$-metric</td>
<td>[3] Vertices of a parallelepiped</td>
</tr>
<tr>
<td>$d$ is a cut</td>
<td>$P = x_1$</td>
</tr>
<tr>
<td>$F(d) = \text{HYP}_{n+1}$</td>
<td>$P = x_n$</td>
</tr>
<tr>
<td>$F(d)$ is a facet</td>
<td>[5]</td>
</tr>
<tr>
<td>$F(d)$ is an extreme ray</td>
<td>[27]</td>
</tr>
<tr>
<td>$F(d) = F(d')$</td>
<td>$P, P'$ are affinely equivalent</td>
</tr>
</tbody>
</table>

The hypermetric cone is defined by an infinite list of inequalities. Thus arises naturally the question of deciding whether it is a polyhedral cone, i.e., whether among the infinite list of inequalities (38) only a finite number is nonredundant. The answer is yes, as stated in the following result.

**Theorem 6.3** (Deza et al. [28]). *The hypermetric cone $\text{HYP}_n$ is polyhedral.*

The proof given in [28] is based on the following two facts:

- the correspondence between the hypermetrics of $\text{HYP}_{n+1}$ and the $L$-polytopes of dimension $k \leq n$,
- the fact that, in given dimension, the number of types of $L$-polytopes is finite [93] (a direct proof is given in [28]).

Let $b_{\text{max}}^{\text{a}}$ denote the largest value of $\max_i |b_i|$ for which inequality (38) defines a facet of $\text{HYP}_n$. Then, $b_{\text{max}}^{\text{a}} < (2^{n-2}(n-1)!)/(n+1)$ is shown in [5].

6.3. Rank of an $L$-polytope

Let $d \in \text{HYP}_{n+1}$ and let $F(d)$ denote the smallest face of $\text{HYP}_{n+1}$ containing $d$. The dimension of $F(d)$ is called the rank of $d$ and is denoted as $r(d)$, or $r(V_{n+1}, d)$. Hence, $r(d) = 1$ if $d$ lies on an extreme ray of $\text{HYP}_{n+1}$, $r(d) = \binom{n+1}{2}$ if $d$ lies in the interior of $\text{HYP}_{n+1}$ and $r(d) = \binom{n+1}{2} - 1$ if $F(d)$ is a facet of $\text{HYP}_{n+1}$.

Let $P$ be an $L$-polytope. The rank $r(P)$ of $P$ is defined as the rank of the hypermetric space $(V(P), d_0)$. In fact, the rank of a hypermetric $d$ is an invariant of the associated $L$-polytope $P_d$, namely, $r(d) = r(P_d)$.

**Proposition 6.4** [27]. *Let $P$ be an $L$-polytope and let $V \subseteq V(P)$ be a generating subset. Then, $r(V, d_0) = r(V(P), d_0) = r(P)$ holds.*
Proposition 6.5 [27]. Let $P$ be an $L$-polytope. Then, $r(P) = 1$ if and only if the only affine bijective transformations $T$ (up to translation and orthogonal transformation) for which $T(P)$ is an $L$-polytope are the homotheties.

The extreme $L$-polytopes, i.e., those having rank 1, are of special importance since they correspond to the extreme rays of the hypermetric cone. For $n \leq 5$, $\text{HYP}_{n+1} = \text{CUT}_{n+1}$, i.e., the only extreme rays are the cut vectors. Therefore, the only extreme $L$-polytope of dimension $k \leq 5$ is $\alpha_k$.

Proposition 6.6 [27]. Let $P_i$, $i = 1, 2$, be an $L$-polytope in $\mathbb{R}^{k_i}$. Then, $P_1 \times P_2$ is an $L$-polytope in $\mathbb{R}^{k_1 + k_2}$ with rank $r(P_1 \times P_2) = r(P_1) + r(P_2)$.

For instance, $r(\gamma_k) = kr(\gamma_1) = k$. An important consequence of Proposition 6.6 is that, if $P$ is an extreme $L$-polytope in a lattice $L$, then $L$ must be irreducible.

Proposition 6.7 [27]. Let $P$ be a basic $L$-polytope of dimension $k$. Then,

(i) $\left(\frac{k+2}{2}\right) \leq r(P) \leq \left(\frac{k+2}{2}\right) - |V(P)|,

(ii) for $P$ centrally symmetric,

$$
 r(P) \geq \left(\frac{k + 1}{2}\right) - \frac{1}{2}|V(P)| + 1.
$$

For instance, for $\alpha_k$, $r(\alpha_k) = k + 1$, yielding equality in both inequalities of (i); for $\beta_k$, $r(\beta_k) = \left(\frac{k+1}{2}\right) - k + 1$ yielding equality in (ii).

6.4. Extreme $L$-polytopes

A direct application of Proposition 6.7 yields the following bounds for an extreme basic $L$-polytope of dimension $k$:

$$
|V(P)| \geq \frac{1}{2}k(k + 3), \tag{39}
$$

$$
|V(P)| \geq k(k + 1) \quad \text{if $P$ is centrally symmetric.} \tag{40}
$$

There is a striking analogy between the bounds (39) and (40) and some known upper bounds (see [67]) for the number $N_p$ of points in a spherical two-distance set of dimension $k$ and the number $N_i$ of lines in a set of equiangular lines of dimension $k$, namely,

$$
N_p \leq \frac{1}{2}k(k + 3) \quad \text{and} \quad N_i \leq \frac{1}{4}k(k + 1).
$$

Moreover, if $N_i = \frac{1}{4}k(k + 1)$, then $k + 2 = 4, 5$, or $k + 2 = q^2$ for some odd integer $q \geq 3$ (see [67]). The first case of equality is for $q = 3$, $k = 7$, $N_i = 28$; it corresponds to the set of 28 equiangular lines defined by the diagonals of the Gosset polytope $3_{21}$. The next case of equality is
for $q = 5$, $k = 23$, $N_l = 276$; it corresponds to the set of 276 equiangular lines defined by the diagonals of the extreme $L$-polytope $P_{23}$ constructed from the Leech lattice (see below). For $q = 7$, $k = 47$, $N_l = 1128$, it is not known whether such a set of equiangular lines exists.

However, there are examples of extreme $L$-polytopes realizing equality in the bounds (39) or (40), but not arising from some spherical two-distance set or from some equiangular set of lines; this is the case for the polytopes $P_8^5$, $P_1^6$ constructed from the Barnes–Wall lattice (see below). There are also examples of extreme $L$-polytopes not realizing equality in the bounds (39) or (40).

We have given in [27] several examples of extreme $L$-polytopes achieving or not equality in the bounds (39) or (40). We refer to [27] for a detailed account and to [20] for details on lattices.

**Extreme $L$-polytopes in root lattices**

All the extreme $L$-polytopes in root lattices are classified. Indeed, by Witt's theorem, the only irreducible root lattices are $A_n$ ($n \geq 0$), $D_n$ ($n \geq 4$) and $E_n$ ($n = 6, 7, 8$). All types of $L$-polytopes in a root lattice are given in [90] or [41]. They are the half-cube $h_v$, the cross polytope $f_v$, the simplex $x_v$, the Gosset polytope $3_21$, and the Schlafli polytope $2_21$ (whose 1-skeletons are, respectively, the half-cube graph $\frac{1}{2}H(n, 2)$, the cocktail party graph $K_n$, the complete graph $K_{n+1}$, the Gosset graph $G_{8,6}$ and the Schlafli graph $G_{3,2}$). Among them, the extreme polytopes are: the segment $x_1$, the Schlafli polytope $2_21$ and the Gosset polytope $3_21$, of respective dimensions 1, 6, 7. The polytope $2_21$ is asymmetric with 27 vertices, realizing equality in the bound (39). The polytope $3_21$ is centrally symmetric with 56 vertices, realizing equality in the bound (40). Both are basic. We do not know any other extreme $L$-polytope of dimension $k \leq 7$ besides $x_1$, $2_21$, $3_21$.

**Extreme $L$-polytopes in sections of the Leech lattice $A_{24}$**

The Leech lattice $A_{24}$ is a lattice of dimension 24. By taking suitable sections of the sphere of minimal vectors of $A_{24}$, two extreme $L$-polytopes are constructed in [27]:

- $P_{23}$, centrally symmetric, with 552 vertices, dimension 23, realizing equality in the bound (40),
- $P_{22}$, asymmetric, with 275 vertices, dimension 22, realizing equality in the bound (39).

**Extreme $L$-polytopes in sections of the Barnes–Wall lattice $A_{16}$**

The Barnes–Wall lattice $A_{16}$ is a lattice of dimension 16. Several examples of extreme $L$-polytopes are constructed from $A_{16}$ in [27]:

- $P$, centrally symmetric (constructed from a deep hole of $A_{16}$), with 512 vertices, dimension 16 (equality does not hold in (40)),
- $Q$, centrally symmetric, with 272 vertices, dimension 16, realizing equality in the bound (40),
- $P^8$, $P^{16}$, asymmetric, with 135 vertices, dimension 15, realizing equality in the bound (39),
- $Q'$, asymmetric, with 1080 vertices, dimension 15 (equality does not hold in (39)).

**Extreme hypermetric graphs**

Let $G$ be a hypermetric graph on $n$ nodes, i.e., whose path metric $d_G$ is hypermetric, and let $P_G$ denote the $L$-polytope associated with $d_G$. It is shown in [26] that, if $G$ is an extreme hypermetric graph, i.e., if $d_G$ lies on an extreme ray of the hypermetric cone $HYP_n$ and if $G \neq K_2$, then $G$ is of one of the following two types:

- **Type I**: $P_G = 3_21$, implying that $8 \leq n \leq 56$ and $G$ has diameter 2 or 3.
- **Type II**: $P_G = 2_21$, implying that $7 \leq n \leq 27$ and $G$ has diameter 2.
Moreover, for $G$ of diameter 2, $G$ is extreme of type II if and only if its suspension $VG$ is extreme of type I (recall that $VG$ is obtained from $G$ by adding a new node adjacent to all nodes of $G$).

In particular, the number of extreme hypermetric graphs is finite.

More details can be found in [26]; for instance, all regular extreme hypermetric graphs belong to the list from [14] of 187 regular graphs which have smallest eigenvalue $-2$ and are not line graphs; in particular, all nine maximal graphs of this list are extreme hypermetrics.

7. Applications in quantum mechanics

7.1. Preliminaries on quantum mechanics

The object of (nonrelativistic) quantum mechanics is to study microscopic objects, e.g., molecules, atoms, or any elementary particles. One of the fundamental differences with classical (Newtonian) mechanics is that many physical quantities can take only discrete values at the microscopic level and that the state of microscopic objects is disturbed by observations. Moreover, identical particles, i.e., with the same physical characteristics as mass, size, charge, etc., can be distinguished in classical mechanics (for instance, by following their trajectories) but they are undistinguishable within quantum mechanics. Von Neumann [92] laid the foundations for a rigorous mathematical account of quantum mechanics. We recall below some basic definitions and facts from quantum mechanics needed for our treatment. Useful references containing a detailed account of these facts include [43, 50, 70, 72, 94].

Consider a system of $N \geq 2$ identical particles. Each particle is represented by a vector $x = (r, s)$ composed by a space coordinate $r \in \mathbb{R}^3$ and a spin coordinate $s \in \mathbb{Z}_2$; $X = \mathbb{R}^3 \times \mathbb{Z}_2$ denotes the space of the coordinates. The physical state of the system is represented by a normalizable complex valued function $\psi$ defined on $X^N$, called the wavefunction. Using the fact that no physical observation can be made that permits to distinguish the particles, it can be shown that either all wavefunctions are symmetric, or all of them are antisymmetric. In the symmetric case, the particles are called bosons, and in the antisymmetric case, they are called fermions. We consider here the case of a system of $N$ fermions, i.e., the wavefunctions are antisymmetric.

Let $H(N)$ denote the set of the measurable complex-valued antisymmetric functions defined on $X^N$; $H(N)$ is a Hilbert space, called the Fock space, with inner product

$$\langle \psi_1, \psi_2 \rangle = \int_{x \in X^N} \psi_1^*(x) \psi_2(x) \, dx$$

for $\psi_1, \psi_2 \in H(N)$. Hence, the physical states of a system of fermions are represented by functions $\psi \in H(N)$ with $\langle \psi, \psi \rangle = 1$. In fact, the case of bosons can be treated in a similar way if the antisymmetry condition is replaced by the symmetry condition and the determinants by permanents in the Slater determinants (defined below).

A physical quantity of the system, or observable, is represented by a Hermitian operator $A$ of the space $H(N)$ and the expected value of $A$ in the state $\psi$ is given by

$$\langle A \rangle_\psi := \langle \psi, A \psi \rangle = \int \psi^*(x) A \psi(x) \, dx.$$
Among the observables of the system, the simplest ones are those that the system may have (then the expected value of the observable is equal to one), or lack (then the expected value is zero). Such observables are represented by orthogonal projections on subspaces of $H(N)$.

Every observable $A$ being a Hermitian operator admits a spectral decomposition. For simplicity, we assume that $A$ can be decomposed as $A = \sum_{i} \lambda_{i} E_{i}$, where the $\lambda_{i}$'s are the eigenvalues of $A$ and $E_{i}$ denotes the projection on the eigenspace associated with the eigenvalue $\lambda_{i}$. So, the projection $E_{i}$ corresponds to the property “The observable $A$ has value $\lambda_{i}$”. If the system is in the state $\psi$, then it has the property associated with $E_{i}$ if $\langle E_{i}\psi \rangle = 1$, i.e., if $A\psi = \lambda_{i}\psi$, that is, $\psi$ is an eigenvector of $A$ corresponding to the eigenvalue $\lambda_{i}$.

The standard deviation of the observable $A$ in the state $\psi$ is given by

$$\Delta_{\psi}(A) = |\langle A^2 \rangle_{\psi} - (\langle A \rangle_{\psi})^2|^{1/2}.$$

Heisenberg’s uncertainty principle states that, if $A$, $B$ are two observables of the system in the state $\psi$, then $\Delta_{\psi}(A)\Delta_{\psi}(B) \geq \frac{1}{2}|\langle [A,B]_{\psi} \rangle|$, i.e., $A$, $B$ cannot be simultaneously measured with precision if they do not commute.

An important observable of the system is its energy, represented by the Hamiltonian operator and denoted by $\Omega$. The average energy of the system in the state $\psi$ is given by $\langle \Omega \rangle_{\psi}$. A fundamental problem in quantum mechanics is to derive bounds on the average energy of the system without knowing explicitly the state $\psi$ of the system. In fact, as we shall explain below, this problem has some tight connections with the problem of finding the linear description of the boolean quadric polytope.

The density matrix of order $p$ of $\psi \in H(N)$ is the complex-valued function $\Gamma_{\psi}^{(p)}$ defined on $X^p \times X^p$ by:

$$\Gamma_{\psi}^{(p)}(x_1 \ldots x_p | x_1 \ldots x_p) = \left( \frac{N}{p} \right) \int_{y \in X^p} \psi^{*}(x_1, \ldots, x_p, y)\psi(x_1, \ldots, x_p, y) \, dy. \quad (41)$$

Density matrices were introduced in [55, 70]; Dirac [32] already considered density matrices of order $p = 1$. Density matrices have a simpler and more direct physical meaning than the wavefunction itself, in particular, the diagonal elements $\Gamma_{\psi}^{(p)}(x_1 \ldots x_p | x_1 \ldots x_p)$ which are of special importance. Indeed, $N^{-1} \Gamma_{\psi}^{(1)}(x_1 | x_1) \, dv_1$ is the probability of finding a particle with spin $s_1$ within the volume $dv_1$ around the point $r_1$, when all other particles have arbitrary positions and spins. Similarly, $(\frac{N}{p})^{-1} \Gamma_{\psi}^{(2)}(x_1 x_2 | x_1 x_2) \, dv_1 \, dv_2$ is the probability of finding a particle with spin $s_1$ within the volume $dv_1$ around the point $r_1$, and another particle with spin $s_2$ within the volume $dv_2$ around the point $r_2$, when all other particles have arbitrary spins and positions, etc.

From the antisymmetry of the wavefunction $\psi$, $\Gamma_{\psi}^{(p)}(x_1 \ldots x_p | x_1 \ldots x_p) = 0$ if $x_i = x_j$ for distinct $i, j$. In other words, particles with parallel spins are kept apart. This phenomenon is a consequence of the Pauli principle.

Density matrices have been widely studied. In particular, they were the central topic of several conferences held at Queen’s University, Kingston, Canada, yielding three volumes of proceedings [19, 39, 43].

Every Hermitian operator $A$ of $H(N)$ can be expanded as

$$A = A_0 + \sum_{i \leq N} A_i + \frac{1}{2!} \sum_{1 \leq i \neq j \leq N} A_{ij} + \cdots. \quad (42)$$
where the $n$th term is an $(n - 1)$-particle operator. Therefore, the expected value of $A$ in the state $\psi$ can be expressed, in terms of the density matrices, as follows:

$$
\langle A \rangle_\psi = A_0 + \int \{ A_1 \Gamma_\psi^{(1)}(x'_1 \mid x_1) \} x_i = x_i \, dx_1
$$

$$
+ \int \{ A_{12} \Gamma_\psi^{(2)}(x'_1 x'_2 \mid x_1 x_2) \} x_i = x_i, x'_i = x'_i \, dx_1 \, dx_2 + \ldots
$$

(43)

with the following convention for the notation $\{ A_1 \Gamma_\psi^{(1)}(x'_i \mid x_i) \} x_i = x_i$: $A_1$ operates only on the unprimed coordinate $x_1$, not on $x'_i$, but after the action of $A_1$ has been carried out, one sets again $x'_i = x_i$. The same convention applies to the other terms.

By the Hartree–Fock approximation (see [50]), one can assume that the expansion of the Hamiltonian $\Omega$ in relation (42) has only terms involving two particles at most, i.e., $\Omega = \Omega_0 + \sum_{1 \leq i < j \leq N} \Omega_{ij} + \frac{3}{2} \sum_{i \neq j} \Omega_{ij}$. In other words, one takes only into account pairwise interactions between the particles and the interaction of each particle with an exterior potential. Observe that $C_\psi$ can then be expressed as $C_\psi = \int \Sigma_{i \neq j} G_{ij}$, where $G_{ij} = \Omega_{ij} + \frac{1}{N-1} (\Omega_i + \Omega_j) + \frac{2}{N(N-1)} \Omega_0$.

Therefore, from relation (43), the average energy depends only on the second-order density matrices $\Gamma_\psi^{(2)}$. Hence, the question of finding bounds on the average energy reduces to the question of finding the boundary conditions on the second-order density matrices. In fact, the density matrices of first and second order contain already most of the useful information about the physical state of the system accessible to physicists.

Let $\Phi_k$, $k \geq 1$, be an orthonormal set (assumed to be discrete for the sake of simplicity) of functions of $H(1)$ such that each function $f \in H(1)$ can be expanded as

$$
f = \sum_{k \geq 1} \langle \Phi_k, f \rangle \Phi_k.
$$

(44)

The functions $\Phi_k$ are called the spin-orbitals. Given a set $K = \{k_1, \ldots, k_N\}$, with $1 \leq k_1 < \ldots < k_N$, the Slater determinant $\Phi_K$ is defined by

$$
\Phi_K(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det(\Phi_{k_1}(x), \ldots, \Phi_{k_N}(x))
$$

(45)

where $\Phi_k(x)$ denotes the vector $(\Phi_k(x_1), \ldots, \Phi_k(x_N))$. Equivalently,

$$
\Phi_K(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \text{Sym}(N)} \text{sign}(\sigma) \Phi_{k_{\sigma(1)}}(x_1) \ldots \Phi_{k_{\sigma(N)}}(x_N).
$$

(46)

Then, each wavefunction $\psi \in H(N)$ can be expanded as

$$
\psi(x_1, \ldots, x_N) = \sum_{K = \{k_1, \ldots, k_N\}, 1 \leq k_1 < \ldots < k_N} C_K \Phi_K,
$$

(47)
where

\[ C_K = \langle \Phi_K, \psi \rangle = \sqrt{N!} \int \psi(x_1, \ldots, x_N) \Phi_{K_1}^*(x_1) \cdots \Phi_{K_n}^*(x_N) \, dx_1 \cdots dx_N \]  

(48)

with \( \sum_K |C_K|^2 = \langle \psi, \psi \rangle = 1 \).

A usual assumption consists in selecting a finite set of \( n \) spin-orbitals \( \{ \Phi_1, \ldots, \Phi_n \} \) so that the finite sum

\[ \sum_{K \subseteq \{1, \ldots, n\}, |K| = N} C_K \Phi_K \]  

(49)

constitutes a good approximation of the wavefunction \( \psi \). From now on, we assume that \( \psi \) is, in fact, equal to the finite sum in (49). It can be shown [70] that the second-order density matrix \( \Gamma^{(2)}_\psi \) can also be expanded in terms of the Slater determinants. Namely, if \( \psi \) is given by (49) where the coefficients \( C_K \) are given by (48), then

\[ \Gamma^{(2)}_\psi(x_1'x_2' | x_1x_2) = \sum_{1 \leq i < j \leq n, 1 \leq h < k \leq n} \gamma_\psi(ij | hk) \Phi_{\{i,j\}}^*(x_1', x_2') \Phi_{\{h,k\}}(x_1, x_2). \]  

(50)

The coefficients \( \gamma_\psi(ij | hk) \) are given by

\[ \gamma_\psi(ij | hk) = \sum C_I^* C_K \delta_{i,j,I - \{i,j\}} \delta_{\{h,k\}, K - \{h,k\}}, \]  

(51)

where the sum is over all subsets \( I, K \subseteq \{1, \ldots, n\} \) of cardinality \( N \) such that \( i, j \in I, h, k \in K \) and \( I - \{i,j\} = K - \{h,k\} \), and we set \( \delta_{i,j,I} = \text{sign}(\sigma) \) if there is a permutation \( \sigma \) mapping \( i \) on \( j \), \( 1, \ldots, i \) on \( j, 1, \ldots, i \), and \( \delta_{i,j,I} = 0 \) otherwise. In particular, the diagonal terms are given by

\[ \gamma_\psi(ij | ij) = \sum_{i,j \in K \subseteq \{1, \ldots, n\}, |K| = N} |C_K|^2. \]  

(52)

They have the following physical meaning: \( (N)^{-1} \gamma_\psi(ij | ij) \) is the probability of finding a particle in the \( i \)th spin-orbital and another one in the \( j \)th spin-orbital while all other particles occupy arbitrary spin-orbitals.

7.2. The \( N \)-representability problem

Given a complex-valued function \( \Gamma \) defined on \( X^2 \times X^2 \), \( \Gamma \) is said to be \( N \)-representable if there exists a wavefunction \( \psi \in H(N) \) such that \( \Gamma = \Gamma^{(2)}_\psi \). The pure state representability problem consists of finding the conditions that \( \Gamma \) must satisfy in order to be \( N \)-representable. This problem can be relaxed to the ensemble representability problem as follows. Instead of asking whether \( \Gamma \) is the second-order density matrix of a single wavefunction \( \psi \), one may ask whether there exists a convex combination \( \sum w_\psi \psi \) (\( w_\psi \geq 0, \sum w_\psi = 1 \)) of wavefunctions such that \( \Gamma = \sum w_\psi \Gamma^{(2)}_\psi \) is the convex combination of their second-order density matrices.

Note that, from the point of view of finding a state of minimum energy, it is equivalent to consider pure states or ensembles (mixtures) of states. Indeed, both \( \langle \Omega \rangle_\psi \) and \( \sum w_\psi \langle \Omega \rangle_\psi \) have the same minimum (equal to the minimum eigenvalue of the Hamiltonian \( \Omega \) and attained at a corresponding eigenvector).
Let $\mathcal{P}_N^{(2)}$ denote the convex set consisting of the convex combinations $\sum_\psi w_\psi \Gamma_\psi^{(2)}$ ($w_\psi \geq 0$, $\sum_\psi w_\psi = 1$) of second-order density matrices of normalized wavefunctions $\psi \in H(N)$. The question of finding a characterization of $\mathcal{P}_N^{(2)}$ was formulated in [17] as the ensemble $N$-representability problem. The convex structure of $\mathcal{P}_N^{(2)}$ was studied, e.g., in [18,21,37].

The $N$-representability problem can be formulated similarly for density matrices of any order $p \geq 1$. The ensemble $N$-representability problem for density matrices of order $p = 1$ was solved in [17] (see also [64]). Namely, a matrix $I(x_1 | x_1)$ is of the form $\sum_\psi w_\psi \Gamma_\psi^{(1)}(x_1 | x_1)$ for $w_\psi \geq 0$, $\sum_\psi w_\psi = 1$, $\langle \psi, \psi \rangle = 1$ and $\psi \in H(N)$ if and only if $\text{Tr}(\Gamma) = \int I(x_1 | x_1) dx_1 = N$ and the eigenvalues of $\Gamma$ satisfy $0 \leq \lambda \leq 1$. However, the ensemble $N$-representability problem is already difficult for density matrices of order $p = 2$. In fact, as stated in Theorem 7.1, the representability problem for their diagonal elements is equivalent to the membership problem in the boolean quadric polytope and hence it is NP-hard. For $p \geq 2$, the representability problem involves not only conditions on the eigenvalues but also on the interrelations of the eigenvectors. On the other hand, no satisfactory solution exists for the pure $N$-representability problem even for the case $p = 1$.

Let $\text{BQP}_n^{f=2(N)}$ denote the polytope defined as the convex hull of the vectors $\pi^{f=2(K)}$ for $K \subseteq \{1, \ldots, n\}$ of cardinality $N$. From relation (52), if $\psi = \Phi_K$ is a Slater determinant, then $\gamma_\psi(ij | hk) = 0$ except if $(i,j) = (h,k)$ and $i,j \in K$ in which case $\gamma_\psi(ij | ij) = 1$. Therefore, the diagonal terms of $\gamma_\Phi$ coincide with the vector $\pi^{f=2}(K)$. For that reason, the polytope $\text{BQP}_n^{f=2(N)}$ is sometimes called the $N$-Slater hull (e.g., in [38,40]).

From (50), the $N$-representability problem amounts to finding the boundary conditions on the coefficients $\gamma_\psi(ij | hk)$. In fact, the boundary conditions for the diagonal terms $\gamma_\psi(ij | ij)$ are precisely the valid inequalities for the $N$-Slater hull $\text{BQP}_n^{f=2(N)}$.

**Theorem 7.1.** Given $\gamma = (\gamma_{ij})_{1 \leq i < j \leq n}$, the following assertions are equivalent.

(i) There exists a normalized wavefunction $\psi \in H(N)$ such that $\gamma_{ij} = \gamma_\psi(ij | ij)$ for all $1 \leq i < j \leq n$.

(ii) There exists a convex combination $\sum_\psi w_\psi \psi$ ($w_\psi \geq 0$, $\sum_\psi w_\psi = 1$) of normalized wavefunctions $\psi \in H(N)$ such that $\gamma_{ij} = \sum_\psi w_\psi \gamma_\psi(ij | ij)$ for $1 \leq i < j \leq n$.

(iii) The vector $\gamma$ belongs to $\text{BQP}_n^{f=2(N)}$.

**Proof.** (i) $\Rightarrow$ (ii) is clear.

(ii) $\Rightarrow$ (i): Suppose first that $\gamma_{ij} = \gamma_\psi(ij | ij)$ for some normalized $\psi \in H(N)$ given by (49). Then, from (52), $\gamma = \sum_{K \subseteq \{1, \ldots, n\}} |K| = N \sum_{K \subseteq \{1, \ldots, n\}} |C_K|^2 \pi^{f=2}(K)$ with $\sum |C_K|^2 = \langle \psi, \psi \rangle = 1$. Hence $\gamma \in \text{BQP}_n^{f=2(N)}$.

Suppose now that $\gamma_{ij} = \sum_\psi w_\psi \gamma_\psi(ij | ij)$ with $w_\psi \geq 0$, $\sum_\psi w_\psi = 1$, $\psi \in H(N)$ and $\langle \psi, \psi \rangle = 1$. Then, $\gamma = \sum_{K \subseteq \{1, \ldots, n\}} t_K \pi^{f=2}(K)$, where $t_K = \sum_{\psi} w_\psi |C_K|^2 \geq 0$ and $\sum_K t_K = 1$. Therefore, $\gamma \in \text{BQP}_n^{f=2(N)}$.

(iii) $\Rightarrow$ (i): Assume $\gamma = \sum_{K \subseteq \{1, \ldots, n\}} t_K \pi^{f=2}(K)$ for $t_K \geq 0$ and $\sum_K t_K = 1$. Set $C_K = \sqrt{t_K}$ and $\psi = \sum_K C_K \Phi_K$. Then, $\gamma = \gamma_\psi$ holds. $\square$

Therefore, the pure and ensemble representability problems are the same when restricted to the diagonal terms. However, in their general form, they are distinct problems. For instance, $\mathcal{P}_N^{(2)}$ has additional extreme points besides the second-order density matrices of the Slater determinants.
(even though those are the only extreme points when restricted to the diagonal terms). Other extreme points for \( \mathcal{B}^{(2)}_n \) are given in [18,37].

We conclude with some additional remarks.

(1) The \( N \)-representability problem for variable \( N \) leads to the study of the boolean quadric polytope \( \text{BQP}_n \).

(2) The polytopes \( \text{BQP}_n^{d-2}(N) \) and \( \text{BQP}_n(N) = \text{BQP}_n^{d-2}(N) \), lying respectively in \( \mathbb{R}^{(2)} \) and \( \mathbb{R}^{(2)} \), are in one-to-one correspondence. Indeed, each point \( x \in \text{BQP}_n(N) \) satisfies the equations:

\[
\sum_{1 \leq i < j \leq n} x_{ij} = \binom{N}{2},
\]

\[
\sum_{1 \leq j \leq n, j \neq i} x_{ij} = (N - 1)x_{ii} \quad \text{for } 1 \leq i \leq n.
\]

Hence both polytopes have the dimension \( \binom{n}{2} - 1 \).

(3) The combinatorial interpretation of the \( N \)-representability problem from Theorem 7.1 was given in [95]. Actually, this paper treats the general problem of \( N \)-representability for density matrices of arbitrary order \( p \geq 1 \). We have exposed only the case \( p = 2 \) for the sake of simplicity and because this is the case directly relevant to our problem of cuts. For arbitrary \( p \geq 2 \), the analogue of Theorem 7.1 leads to the study of the polytope \( \text{BQP}_n^{d-2}(N) \) in \( \mathbb{R}^{(p)} \), defined as the convex hull of the \( \mathcal{F}_\pi^{-}\)-intersection vectors \( \pi^{d-2}(K) \), for \( K \subseteq \{1, \ldots, n\} \), \( |K| = N \).

The facial structure of the polytope \( \text{BQP}_n^{d-2}(N) \) is studied in [94]; in particular, the full description of its facets in the cases: \( p = 2, N = 3, n = 6,7 \) and partial results in the case: \( p = 2, N = 3, n = 8 \) are given there.

(4) An additional alternative interpretation of the boolean quadric polytope \( \text{BQP}_n \) is given in [40], in terms of positive semidefinite two-body operators.

Let \( a_i \) denote the annihilation operator of the Fock space \( \bigcup\mathbb{N}_{\geq 1}H(N) \) and \( a_i^\dagger \), its adjoint, the creation operator (see [50]). Both are defined by their action on the Slater determinants. Namely, for \( K = \{k_1, \ldots, k_N\} \) with \( 1 \leq k_1 < \cdots < k_N \),

\[
a_i(\Phi_K) = \begin{cases} 0 & \text{if } i \notin K, \\
-(1)^{j-1} \Phi_{K-\{i\}} & \text{if } i = k_j \in K,
\end{cases}
\]

\[
a_i^\dagger(\Phi_K) = \begin{cases} 0 & \text{if } i \in K, \\
-(1)^{j-1} \Phi_{K\cup\{i\}} & \text{if } i \notin K \text{ and } k_{j-1} < i < k_j.
\end{cases}
\]

Hence, \( a_i^\dagger a_i(\Phi_K) = |K \cap \{i\}| \Phi_K \) for each \( K \subseteq \{1, \ldots, n\} \). Therefore, the Slater determinants \( \Phi_K \) are common eigenvectors for the operators \( a_i^\dagger a_i \), and thus for any two-body operator of the form

\[
B = b_0 + \sum_{1 \leq i \leq n} b_i a_i^\dagger a_i + \sum_{1 \leq i < j \leq n} b_{ij} a_i^\dagger a_j a_j.
\]

The cone \( \mathcal{Q}^+(I^*) \), consisting of the two-body operators \( B \) of the form (53) which are positive semidefinite, is considered in [40]. Since any such operator has the same eigenvectors \( \Phi_K \) associated with the eigenvalues \( b_0 + \sum_{i \in K} b_i + \sum_{i,j \in K} b_{ij} \), the cone \( \mathcal{Q}^+(I^*) \) can be equivalently defined as the cone of the vectors \( b := (b_0, b_i, 1 \leq i \leq n, b_{ij}, 1 \leq i < j \leq n) \) for which \( b(x) := b_0 + \sum_{1 \leq i \leq n} b_i x_i + \sum_{1 \leq i < j \leq n} b_{ij} x_i x_j \geq 0 \) for each \( x \in \{0,1\}^n \). Therefore, \( \mathcal{Q}^+(I^*) \) is the dual cone to \( \text{BQP}_n \), i.e., \( b \in \mathcal{Q}^+(I^*) \) if and only if the inequality \( b(x) \geq 0 \) is valid for \( \text{BQP}_n \).
The cone $Q^+(\mathbb{Z}^n) := \{ b : b(x) \geq 0 \text{ for all } x \in \mathbb{Z}^n \}$, which corresponds to the case of a system of bosons (when several particles may occupy the same spin-orbital) while $Q^+(\mathbb{I}^n)$ corresponds to a system of fermions (with at most one particle per spin-orbital), is also considered in [40].

Let us finally mention a connection between the hypermetric cone $\text{HYP}_{n+1}$ and the cone $Q^+(\mathbb{Z}^n)$. It can be established via the covariance map $\varphi_{c_0}$. Namely,

$$\varphi_{c_0}(\text{HYP}_{n+1}) = \left\{ a = (a_{ij})_{1 \leq i \leq j \leq n} : \sum_{1 \leq i < j \leq n} a_{ij}x_ix_j - \sum_{1 \leq i < n} a_{ii}x_i \geq 0 \text{ for } x \in \mathbb{Z}^n \right\}$$

and, therefore,

$$\varphi_{c_0}(\text{HYP}_{n+1}) = Q^+(\mathbb{Z}^n) \cap \{ b : b_0 = 0, b_i = -b_{ii} \text{ for } 1 \leq i \leq n \}$$

is a section of the cone $Q^+(\mathbb{I}^n)$.

### 7.3. The quantum correlation polytope

We address in this section a connection between the boolean quadric polytope $\text{BQP}_n$ and the quantum correlation polytope, considered in [77,78].

Recall that the boolean quadric polytope $\text{BQP}_n$ arises naturally in the theory of probability. Namely, from [31, Theorem 3.2], given $p = (p_{ij}, 1 \leq i \leq j \leq n) \in \mathbb{R}^{\left(\begin{smallmatrix} n+1 \\ 2 \end{smallmatrix}\right)}$, then $p \in \text{BQP}_n$ if and only if there exist a probability space $(\Omega, \mathcal{A}, \mu)$ and $n$ events $A_1, \ldots, A_n \in \mathcal{A}$ such that

$$p_{ij} = \mu(A_i \cap A_j) \text{ for all } 1 \leq i \leq j \leq n.$$ 

For that reason, the polytope $\text{BQP}_n$ is also called the correlation polytope in [77–79]. For $n = 3$, $\text{BQP}_n$ is also called the Bell–Wigner polytope.

As an extension, [77] introduces the quantum correlation polytope whose points represent the probability that a quantum mechanical system has the properties associated with two projection operators in a given state. We fix some notation.

As we saw before, the state of a quantum mechanical system is represented by a unit vector $\psi$ of a Hilbert space $H (H = H(N)$ if the system has $N$ particles). Let $E_\phi$ denote the projection operator from $H$ to the line spanned by $\psi$, i.e., $E_\phi(\phi) = \langle \psi, \phi \rangle \psi$ for $\phi \in H$. Equivalently, a state of the system is given by such a projection operator $E_\phi$; such a state is called a pure state. More generally, we consider also nonpure states, namely convex combinations of pure states: $W = \sum_\psi \lambda_\psi E_\phi (\lambda_\psi \geq 0, \sum_\psi \lambda_\psi = 1, \psi \in H$ with $\langle \psi, \psi \rangle = 1$). Such states $W$ are called ensemble states, or mixtures. Pure and ensemble states were already considered in Section 7.2. Alternatively, a state of the system is a bounded linear operator $W$ of $H$ which is Hermitian, positive semidefinite and has trace one.

Given $p = (p_{ij}, 1 \leq i \leq j \leq n) \in \mathbb{R}^{\left(\begin{smallmatrix} n+1 \\ 2 \end{smallmatrix}\right)}$, we say that $p$ has a quantum mechanical representation if there exists a Hilbert space $H$, a state $W$, $n$ projections $E_1, \ldots, E_n$ (not necessarily distinct, nor commuting) such that

$$p_{ij} = \text{trace}(WE_i \wedge E_j) \text{ for } 1 \leq i \leq j \leq n,$$

where $E_i \wedge E_j$ denotes the projection from $H$ to the subspace $E_i(H) \cap E_j(H)$. So $p_{ij}$ represents the probability that the system has the properties associated with the projections $E_i$ and $E_j$ when it is in the state $W$. Let $\text{QCP}_n$ denote the polytope in $\mathbb{R}^{\left(\begin{smallmatrix} n+1 \\ 2 \end{smallmatrix}\right)}$ consisting of those $p$ which admit a quantum mechanical representation; $\text{QCP}_n$ is called the quantum correlation polytope.
Finally let $T_n$ denote the set of the vectors $p \in \mathbb{R}^{n^2}$ satisfying

$$0 \leq p_{ij} \leq \min(p_{ii}, p_{jj}) \leq \max(p_{ii}, p_{jj}) \leq 1$$

for $1 \leq i \leq j \leq n$. It is easy to see that the extreme points of $T_n$ are exactly the vectors $p \in T_n$ with $0$–$1$ coordinates.

**Theorem 7.2.** (i) $\text{BQP}_n \subseteq \text{QCP}_n \subseteq T_n$.

(ii) $\text{QCP}_n$ is a convex set which contains the interior of $T_n$.

(iii) The subset of $\text{QCP}_n$ consisting of those $p$ admitting a quantum mechanical representation in which the state $W = E_\psi$ is pure is also convex and contains the interior of $T_n$.

For clarity, we give the proof of the statement (i) of Theorem 7.2.

**Proof.** The inclusion $\text{QCP}_n \subseteq T_n$ follows from the fact that each state $W$ is positive semidefinite with trace 1. We check the inclusion $\text{BQP}_n \subseteq \text{QCP}_n$. Let $p \in \text{BQP}_n$. Hence $p = \sum_{K \subseteq \{1, \ldots, n\}} \lambda_K \pi(K)$ where $\lambda_K \geq 0$ and $\sum_K \lambda_K = 1$. Let $H$ be a Hilbert space of dimension $2^n$ and let $\{\psi_K, K \subseteq \{1, \ldots, n\}\}$ be an orthonormal basis of $H$ indexed by the subsets of $\{1, \ldots, n\}$. Let $W$ be the operator of $H$ defined by $W(\psi_K) = \lambda_K \psi_K$ for all $K$. Let $E_i$ denote the projection from $H$ to the subspace $H_i$ spanned by the vectors $\psi_K$ with $i \in K$, then $E_i \wedge E_j$ is the projection on the subspace spanned by $\psi_K$ for $i, j \in K$. Note that the trace of the operator $WE_i \wedge E_j$ is equal to $\sum_{i, j \in K} \lambda_K = p_{ij}$. This shows that $p$ belongs to $\text{QCP}_n$. \qed

Note that, if $p \in \text{QCP}_n$ has a quantum mechanical representation in which the operators $E_i$ commute, then, in fact, $p \in \text{BQP}_n$.

Note also that every $p \in L_n$ with $0 < p_{ij} < 1$ for all $i, j$ belongs to $\text{QCP}_n$. Therefore, except for some boundary cases, every $p \in T_n$ has a quantum mechanical representation, i.e. the only requirements for joint probabilities in the quantum case are that probabilities be numbers between 0 and 1 and that the probability of the joint be less than or equal to the probability of each event. Hence the probabilities of quantum mechanical events do not obey the laws of classical probability theory. New theories of quantum probability and quantum logic have been developed; see, for instance, [77, 78].

The region $\text{QCP}_n - \text{BQP}_n$ is called the interference region. Several examples of physical experiments are described in [77, 78] that yield some pair distributions $p$ lying in the interference region. For example, the classical Einstein–Podolsky–Rosen experiment [36] yields $p \in \text{QCP}_3 - \text{BQP}_3$.

We conclude this section with a concrete example in the simplest case $n = 2$. Consider the vector $p = (p_{11} = p_{22} = (\cos \theta)^2, p_{12} = 0)$. Then, $p \notin \text{BQP}_2$ if $1 > (\cos \theta)^2 > \frac{1}{2}$, since it violates the inequality $p_{11} + p_{22} - p_{12} \leq 1$. On the other hand, $p \in \text{QCP}_2$. Indeed, let $H = \mathbb{R}^3$ be a Hilbert space with canonical basis $(e_1, e_2, e_3)$, $W$ be the projection on the line spanned by $e_3$ and let $E_i$ be the projection on the line spanned by $u_i$, for $i = 1, 2$, where $u_1 = (\sin \theta, 0, \cos \theta)$ and $u_2 = (-\sin \theta, 0, \cos \theta)$. Then, $\text{trace}(WE_i) = (\cos \theta)^2 = p_i$ for $i = 1, 2$ and $E_1 \wedge E_2 = 0$.

The vector $p$ has the following physical interpretation. Consider a source of photons all polarized in the $e_3$ direction in the space. Let $\psi = e_3$ be the quantum mechanical wavefunction associated with these photons, so $W = E_\psi$ is the state of the system. The projection $E_i$ corresponds to the property "the photon is polarized in the direction $u_i$"; this corresponds to the experiment where
a polarizer is located in front of the source, oriented in the direction \( u_i \) and \( p_{ii} \) counts the frequency of the photons which pass through the polarizer. The relation \( p_{12} = 0 \) should be understood as follows. There may be some photons having both properties \( E_1 \) and \( E_2 \), but no experiment exists which could detect the simultaneous existence of the properties \( E_1 \) and \( E_2 \).

Note that \( \text{BQP}_2 \) has the following extreme points: \((0,0,0), (1,0,0), (0,1,0), \) and \((1,1,1)\), while \( T_2 \) has one more extreme point \((1,1,0)\). In fact, \( \text{QCP}_2 = T_2 - \{(1,1,0)\} \).

8. Other applications

8.1. The \( L_1 \)-metric in probability theory

Let \((\Omega, \mathcal{A}, \mu)\) be a probability space and let \( X: \Omega \to \mathbb{R} \) be a random variable with finite expected value \( E(X) = \int_\Omega |X(\omega)| \mu(d\omega) < \infty \), i.e., \( X \in L_1(\Omega, \mathcal{A}, \mu) \). Let \( F_X \) denote the distribution function of \( X \), i.e., \( F_X(x) = \mu(\{\omega \in \Omega: X(\omega) = x\}) \) for \( x \in \mathbb{R} \); when it exists, its derivative \( F_X' \) is called the density of \( X \). A great variety of metrics on random variables are studied in the monograph [84]; among them, the following are based on the \( L_1 \)-metric:

- the usual \( L_1 \)-metric between the random variables,
  \[
  L_1(X, Y) = E(|X - Y|) = \int_\Omega |X(\omega) - Y(\omega)| \mu(d\omega);
  \]

- the Monge-Kantorovich Wasserstein metric (i.e., the \( L_1 \)-metric between the distribution functions), \( k(X, Y) = \int_{\mathbb{R}} |F_X(x) - F_Y(x)| \, dx \);

- the total valuation metric (i.e., the \( L_1 \)-metric between the densities when they exist), \( \sigma(X, Y) = \frac{1}{2} \int_{\mathbb{R}} |F_X'(x) - F_Y'(x)| \, dx \);

- the engineer metric (i.e., the \( L_1 \)-metric between the expected values), \( E_\text{N}(X, Y) = |E(X) - E(Y)| \);

- the indicator metric,
  \[
  i(X, Y) = E(1_{X \neq Y}) = \mu(\{\omega \in \Omega: X(\omega) \neq Y(\omega)\}).
  \]

In fact, the \( L_p \)-analogues \((1 \leq p \leq \infty)\) of the above metrics, especially of the first two, are also used in probability theory.

Several results are known, establishing links among the above metrics. One of the main such results is the Monge–Kantorovich mass-transportation theorem which shows that the second metric \( k(X, Y) \) can be viewed as a minimum of the first metric \( L_1(X, Y) \) over all joint distributions of \( X \) and \( Y \) with fixed marginal. A relationship between the \( L_1(X, Y) \) and the engineer metric \( E_\text{N}(X, Y) \) is given by [84] as solution of a moment problem. Similarly, a connection between the total valuation metric \( \sigma(X, Y) \) and the indicator metric \( i(X, Y) \) is given in Dobrushin's theorem on the existence and uniqueness of Gibbs fields in statistical physics. See [84] for a detailed account of the above topics.

We mention another example of use of the \( L_1 \)-metric in probability theory, namely for Gaussian random fields. We refer to [73, 74] for a detailed account. Let \( B = (B(x); x \in M) \) be a centered
Gaussian system with parameter space $M$, $0 \in M$. The variance of the increment is denoted by:

$$d(x, y) := E((B(x) - B(y))^2) \quad \text{for } x, y \in M.$$ 

When $(M, d)$ is a metric space which is $L_1$-embeddable, the Gaussian system is called a Lévy’s Brownian motion with parameter space $(M, d)$. The case $M = \mathbb{R}^n$ and $d(x, y) = \|x - y\|_2$ gives the usual Brownian motion with $n$-dimensional parameter. By [31, Lemma 3.51], $(M, d)$ is $L_1$-embeddable if and only if there exist a nonnegative measure space $(H, \nu)$ and a map $x \mapsto A_x \subseteq H$ with $\nu(A_x) < \infty$ for $x \in M$, such that $d(x, y) = \nu(A_x \triangle A_y)$ for $x, y \in M$. Hence, a Gaussian system admits a representation called of Chentsov type

$$B(x) = \int_{A_x} W(dh) \quad \text{for } x \in M$$

in terms of a Gaussian random measure based on the measure space $(H, \nu)$ with $d(x, y) = \nu(A_x \triangle A_y)$ if and only if $d$ is $L_1$-embeddable.

This Chentsov-type representation can be compared with the Crofton formula for projective metrics from [31, Theorem 4.12]. Actually both come naturally together in [1] (see parts A.8 and A.9 of Appendix A there).

8.2. The $\ell_1$-metric in statistical data analysis

A data structure is a pair $(I, d)$, where $I$ is a finite set, called population, and $d : I \times I \to \mathbb{R}_+$ is a symmetric map with $d_{ii} = 0$ for $i \in I$, called dissimilarity index. The typical problem in statistical data analysis is to choose a “good representation” of a data structure; usually, “good” means a representation allowing to represent the data structure visually by a graphic display. Each sort of visual display corresponds, in fact, to a special choice of the dissimilarity index as a distance and the problem turns out to be the classical isometric embedding problem in special classes of metrics.

For instance, in hierarchical classification, the case when $d$ is ultrametric corresponds to the possibility of a so-called indexed hierarchy (see [57]). A natural extension is the case when $d$ is the path metric of a weighted tree, i.e., $d$ satisfies the four-point condition (see [31, Section 4.11]); then the data structure is called an additive tree. Also, data structures $(I, d)$ for which $d$ is $\ell_2$-embeddable are considered in factor analysis and multidimensional scaling. These two cases together with cluster analysis are the main three techniques for studying data structures. The case when $d$ is $\ell_1$-embeddable is a natural extension of the ultrametric and $\ell_2$ cases.

An $\ell_p$-approximation consists of minimizing the estimator $\|e\|_p$, where $e$ is a vector or a random variable (representing an error, deviation, etc.). The following criteria are used in statistical data analysis:

- the $\ell_2$-norm, in the least-square method or its square;
- the $\ell_\infty$-norm, in the minimax or Chebychev method;
- the $\ell_1$-norm, in the least absolute values (LAV) method.

In fact, the $\ell_1$ criterion has been increasingly used. Its importance can be seen, for instance, from the volume [34] of proceedings of a conference entitled “Statistical data analysis based on the $L_1$-norm and related methods”; we refer, in particular, to [15, 33, 44, 91].
8.3. Hypercube embeddings and designs

In this section, we describe how some questions about the existence of special classes of designs are connected with questions about $\mathbb{Z}_+\,$-realizations of the equidistant metric $2td(K_n)$ and, in particular, about its minimum $h$-size.

We recall some definitions.

Given integers $n, t \geq 1$, $d(K_n)$ denotes the path metric of the complete graph $K_n$ and $2td(K_n)$ is the equidistant metric with components all equal to $2t$. The metric $2td(K_n)$ is clearly $h$-embeddable, since $2td(K_n) = \sum_{1 \leq i \leq n} t\delta(\{i\})$, called its starcut realization. Any decomposition of $2td(K_n)$ as $\sum_{S \in \mathcal{B}} \delta(S)$, where $\mathcal{B}$ is a collection of (nonnecessarily distinct) subsets of $V_n = \{1, \ldots, n\}$, is called a $\mathbb{Z}_+\,$-realization of $2td(K_n)$ and $|\mathcal{B}|$ (counting the multiplicities) is its size. The $\mathbb{Z}_+\,$-realization is called $k$-uniform if $|S| = k$ holds for all $S \in \mathcal{B}$. Let $z^t_n$ denote the minimum size of a $\mathbb{Z}_+\,$-realization of $2td(K_n)$. The metric $2td(K_n)$ is $h$-rigid if the starcut realization is its only $\mathbb{Z}_+\,$-realization, i.e., $z^t_n = n$. If, in fact, the set families $\mathcal{B}$ giving $\mathbb{Z}_+\,$-realizations of $2td(K_n)$, i.e., for which $2td(K_n) = \sum_{S \in \mathcal{B}} \delta(S)$, correspond to some designs. Let us first recall some notions about designs; for details about designs, see, e.g., [30].

Let $\mathcal{B}$ be a collection of (nonnecessarily distinct) subsets of $V_n$, the sets $B \in \mathcal{B}$ are called blocks. Let $r, k, \lambda$ be integers.

Then, $\mathcal{B}$ is called a $(r, \lambda; n)$-design if each point $i \in V_n$ belongs to $r$ blocks and any two distinct points $i, j \in V_n$ belong to $\lambda$ common blocks.

$\mathcal{B}$ is called an $(n, k, \lambda)$-BIBD (BIBD standing for balanced incomplete block design) if any two distinct points $i, j \in V_n$ belong to $\lambda$ common blocks and each block has cardinality $k$. This implies that each point $i \in V_n$ belong to $r = \frac{n(n - 1)}{(k - 1)}$ blocks and the total number of blocks is $b := |\mathcal{B}| = r n / k$. It is well known that $b \geq n$ holds. The BIBD is called symmetric if $b = n$ or, equivalently, $r = k$ holds. Two important cases of symmetric BIBD are

- the projective plane $\mathrm{PG}(2, t)$, i.e. $(t^2 + t + 1, t + 1, 1)$-BIBD,
- the Hadamard design of order $4t - 1$, i.e. $(4t - 1, 2t, t)$-BIBD.

It is well known that a Hadamard design of order $4t - 1$ corresponds to a Hadamard matrix of order $4t$ (i.e., a matrix with ±1 entries whose rows are pairwise orthogonal).

We have the following links between the $\mathbb{Z}_+\,$-realizations of $2td(K_n)$ and designs [30]:

(i) There is a one-to-one correspondence between the $\mathbb{Z}_+\,$-realizations of $2td(K_n)$ and the $(2t, t, n - 1)$-designs.

(ii) There is a one-to-one correspondence between the $k$-uniform $\mathbb{Z}_+\,$-realizations of $2td(K_n)$ and the $(n, k, \lambda)$ BIBD, where the parameters satisfy:

$$r = \frac{t(n - 1)}{n - k}, \quad \lambda = r - t = \frac{t(k - 1)}{n - k}.$$ 

(iii) If there exists a symmetric $(n, \lambda + t, t)$-BIBD with $n \neq 4t$, $n = 2t + \lambda + t(t - 1)/\lambda$, then $z^t_n = n$ [35]. In the cases $\lambda = 1$, $t$, the implication of (iii) is, in fact, an equivalence. Namely, we have:

(iv) $\mathrm{PG}(2, t)$ exists $\iff z^t_{2t + t + 1} = t^2 + t + 1$
2td(K, + 1 + 2) is not h-rigid,
\[ i.e., \ z^t_1 + 1 + 2 < t(t^2 + t + 2) \]
\[ \iff \]
\[ z^t_1 + 1 + 2 = t^2 + 2t \text{ if } t \geq 3 \]
\[ = t^2 + t + 1 \text{ if } t = 1, 2. \]

(v) There exists a Hadamard matrix of order 4t \iff \ z^t_4t - 1 = 4t - 1 \iff \ z^t_4t = 4t - 1 \ [85].

The following bounds hold for \( z^t_n \):

(vi) by [31, (13)], \( z^t_n \leq nt \), with equality if and only if 2td(K,\( n \)) is h-rigid,

(vii) \( z^t_n \geq n - 1 \), with equality if and only if \( n = 4t \) and there exists a Hadamard matrix of order 4t \ [85];

(viii) \( z^t_n \geq n \) if we are not in the case of equality of (vii);

(ix) by [31, (13)],
\[
\frac{n(n - 1)t}{\left[ \frac{1}{2}n \right]^2} = 4t - \frac{2t}{\left[ \frac{1}{2}n \right]}. 
\]

Observe that \( a^t_n = a^t_{n+1} = 4t - 1 \), and \( a^t_{n+1} = a^t_{n+2} = 4t \) if \( t \geq 3 \).

From (iv), there exists a projective plane PG(2, t) if and only if equality holds in the bound (viii) for \( n = t^2 + t + 1 \) or, equivalently, there is a strict inequality in the bound (vii) for \( n = t^2 + t + 2 \).

From (v), there exists a Hadamard matrix of order 4t if and only if equality holds in the bounds (vii) and (ix) for \( n = 4t \) or, equivalently, equality holds in the bounds (viii) and (ix) for \( n = 4t - 1 \).

Therefore, the \( Z_+ \)-realizations of minimum size of 2td(K,\( n \)) provide a common generalization of the two most interesting cases of symmetric BIBD, namely finite projective planes and Hadamard designs.

Finally, we mention a conjecture which generalizes the implication (iii) in the case \( \lambda = t \); it is stated and partially proved in [30].

**Conjecture 8.1.** (a) For \( n \leq 4t \), if there exists a Hadamard matrix of order 4t, then \( z^t_n = a^t_n \).

(b) If \( \left\lfloor \frac{1}{2}n \right\rfloor \) divides 2t and there exists a Hadamard matrix of order 4t, then \( z^t_n = a^t_n \).

8.4. Miscellaneous

The variety of uses of the \( \ell_1 \)-metric is very vast as we already saw in Sections 8.1 and 8.2. We group here several other examples where \( \ell_1 \)-embeddable metrics are useful.

On the integers, besides the usual \( \ell_1 \)-metric \( |a - b| \), we have, for instance, the well-known Hamming distance between the binary expansions of \( a, b \), and \( \log(l.c.m.(a, b)/g.c.d.(a, b)) \) (mentioned after [31, Theorem 4.13]) which are both \( \ell_1 \)-embeddable.

Two examples of \( \ell_1 \)-embeddable metrics are used in biology:

- The *Prevosti's genetic distance:* \( (1/2r) \sum_{1 \leq j \leq r} \sum_{1 \leq i \leq k_j} |p_{ij} - q_{ij}| \) between two populations \( P \) and \( Q \), where \( r \) is the number of loci or chromosomes, \( p_{ij} \) (resp. \( q_{ij} \)) is the frequency of the chromosomal ordering \( i \) in the locus or chromosome \( j \) within the population \( P \) (resp. \( Q \)); the literature on this distance started in [83].
The biotope distance: $|A \triangle B|/|A \cup B|$ between biotopes $A, B$ (sets of species in, say, forests); it was introduced in [71] and it is shown in [2] to be $\ell_1$-embeddable.

The so-called chemical distance between two graphs $G_1, G_2$ on $n$ nodes: $\min \| A_i - P^T A_j P \|$ , where the minimum is taken over all $n \times n$ permutation matrices $P$, and $A_i$ denotes the adjacency matrix of $G_i$, for $i = 1, 2$ [65].

The Hamming distance $\{(a, b) \in G^2: a \cdot b \neq a \ast b\}$ between the multiplication tables of two groups $A = (G, \cdot)$ and $B = (G, \ast)$ on the same underlying set $G$ is used in [35].

Given compact subsets $A, B$ of the plane $\mathbb{R}^2$, the $\ell_1$-distance $\text{aire}(A \triangle B)$ is used in the treatment of images; see, for instance, [58].

References


