Applications of Cut Polyhedra

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Abstract

We group in this paper, within a unified framework, many applications of the following polyhedra: cut, boolean quadric, hypermetric and metric polyhedra. We treat, in particular, the following applications:

- ℓ_1- and L_1-metrics in functional analysis,
- the max-cut problem, the Boole problem and multicommodity flow problems in combinatorial optimization,
- lattice holes in geometry of numbers,
- density matrices of many-fermions systems in quantum mechanics.

We present some other applications, in probability theory, statistical data analysis and design theory.

Contents

1 Introduction

In this paper, we show that cut polyhedra are exceptional, among other polyhedra, by the great diversity of their applications and connections. The main fields of applications include: ℓ_1-metrics in functional analysis, combinatorial optimization, geometry of numbers, quantum mechanics. We give some other connections, in particular, with probability theory, statistical data analysis, multicommodity flows, designs. Another purpose of this paper is to present an extended bibliography on cut polyhedra and related areas.

We present more extensively the applications which were not well documented outside of their specific context. For example, we treat at length the connection with quantum mechanics and with the Boole problem.

Examples of important applications, but already well presented elsewhere, include applications of the maximum cut problem to VLSI circuit designs and spin glass problems.

The more peripheric applications are presented briefly, but references are always supplied in case of absence of definitions.

On the other hand, we do not cover at all generalizations of cut polyhedra and their applications, as multicut polytopes (with applications to clustering and qualitative data analysis) (see e.g. [56]) and cycle polytopes of binary matroids (see e.g. [22]). Many complexity results are known on cut and embeddings problems, but we do not survey them here.

Our central objects are the cut cone Cut_n, the cut polytope $CutP_n$ and the boolean quadric polytope BQP_n, respectively defined by:

$$Cut_n = \text{Cone}((|x_i - x_j|)_{1 \leq i < j \leq n} : x \in \{0,1\}^n),$$

$$CutP_n = \text{Conv}(|x_i - x_j|)_{1 \leq i < j \leq n} : x \in \{0,1\}^n),$$

$$BQP_n = \text{Conv}((x_i x_j)_{1 \leq i \leq j \leq n} : x \in \{0,1\}^n),$$

(where "Cone" denotes the operation of taking the conic hull and "Conv" that of taking the convex hull). In fact, the cut polytope $CutP_{n+1}$ and the boolean quadric polytope BQP_n are in one-to-one correspondence (via the covariance linear bijective map, see section 2.4). Also, all the facets of the cut polytope $CutP_n$ can be deduced from those of the cut cone Cut_n (via the switching map, see section 2.6).

Cut polyhedra have been extensively studied, in particular, from the following points of view: facets (see the survey [60] and references there), simplicial faces (see the survey [58]), geometrical questions ([25], [54], [68]); see section 2.4 for a detailed bibliography. We refer to section 1 for a catalogue of definitions and basic facts about the objects considered in the paper.

Cut polyhedra arise naturally in various contexts. We now list some of the main fields or questions in which cut polyhedra are directly involved. This will also give a flavor of the contents of the paper and of the type of questions which have been considered about cut polyhedra.

ℓ_1-metrics. The points of the cut cone Cut_n have the following interpretation: a semi-metric d on n points belongs to Cut_n if and only if it is isometrically ℓ_1-embeddable, i.e. $d_{ij} = \| u_i - u_j \|_1$ for all i, j, for some vectors $u_1, \ldots, u_n \in \mathbb{R}^m$. Hence, characterizing ℓ_1-embeddable metrics by inequalities amounts to find the valid inequalities for the cut cone Cut_n. More detailed connections with ℓ_1- and L_1-metrics are described in section 3.

For rational metrics, ℓ_1-embeddability is equivalent to embeddability, up to multiplicative factor, in a hypercube. For the case of graphic metrics, both concepts of ℓ_1- and hypercube embeddability (binary addressing) have important applications, in particular, for the design of communication networks and hypercube multiprocessors. For a graph, hypercube embeddability of its path metric means that the graph is an isometric subgraph of a hypercube. See section 4.2 for details.

Combinatorial optimization. The cut polytope and the boolean quadric polytope are used in combinatorial optimization. Indeed, the max-cut problem can be formulated as a linear program on the cut polytope and, thus, the polyhedral approach to the max-cut problem leads to the study of the facet defining inequalities for the cut polytope. Similarly, the polyhedral approach to unconstrained boolean quadratic programming leads to the study of the facets of the boolean quadric polytope. See section 5.1 for details.

The Boole problem. Given n events in a probability space $(\Omega, \mathcal{A}, \mu)$, the Boole problem consists of finding the best estimation of $\mu(A_1 \cup \ldots \cup A_n)$ in terms of the joint probabilities $p_{ij} = \mu(A_i \cap A_j)$ for $1 \leq i \leq j \leq n$. In fact, the answer relies directly on the knowledge of the facets of the boolean quadric polytope; namely, we have:

$$\mu(A_1 \cup \ldots \cup A_n) \geq \max(w^T p : w^T x \leq 1 \text{ is facet defining for } BQP_n)$$

where $p = (p_{ij})_{1 \leq i \leq j \leq n}$. See section 5.3 for details. The above fact relies on the following probabilistic interpretation of BQP_n: a point p belongs to BQP_n if and only if $p_{ij} = \mu(A_i \cap A_j)$ for $1 \leq i \leq j \leq n$, for some events $A_1, \ldots, A_n$ in some probability space $(\Omega, \mathcal{A}, \mu)$ (see section 3.1).

Quantum mechanics. The physical state of a quantum mechanical system of N particles is represented by a wavefunction ψ, which is a unit vector of a Hilbert space $H(N)$. For each wavefunction ψ is defined its density matrix $\Gamma_{\psi}^{(2)}(x|x')$ of second order. An important problem in quantum mechanics is the N-representability problem: given a function $\Gamma(x|x')$, when is Γ N-representable, i.e. $\Gamma(x|x') = \Gamma_{\psi}^{(2)}(x|x')$ for some wavefunction $\psi \in H(N)$? In fact, when restricted to the diagonal terms, i.e. asking only that $\Gamma(x|x) = \Gamma_{\psi}^{(2)}(x|x)$, this problem is equivalent to the membership problem in the polytope $\mathrm{Conv}((x_i x_j)_{1 \leq i \leq j \leq n} : x \in \{0,1\}^n, \sum_{1 \leq i \leq n} x_i = N)$. For a variable number N of particles, the N-representability problem in its diagonal form leads to the membership problem in the boolean quadric polytope. See section 7 for details. Moreover, the dual of BQP_n can be interpreted as the cone of positive semi definite two-body operators (see relation (56) in section 7.2).

Multicommodity flows. Let (G, H, c, r) be an instance of the multicommodity flow problem, where G is the supply graph with capacities c_e on its edges, and H is the demand graph with demands r_e on its edges. The instance is said to be feasible if there exists a multiflow such that the capacities are not exceded and the demands are fulfilled. The well known so-called Japanese theorem asserts that the problem is feasible if and only if $(c-r)^T d \geq 0$ holds for all $d \in Met_n$. Hence, the metric cone Met_n, consisting of all semi-metrics on n points, is the dual cone to the cone of feasible multiflows. When restricting the condition $(c-r)^T d \geq 0$ to the cut metrics d, we obtain the well known cut condition, which is always necessary, and sometimes sufficient for some classes of graphs. See section 5.2 for details.

Hypermetrics and L-polytopes. The hypermetric inequalities are a natural strengthening of the metric condition, which are still satisfied by the cuts. They define the hypermetric cone Hyp_n which is contained in the metric cone Met_n and contains the cut cone Cut_n. The hypermetrics $d \in Hyp_n$ are in one-to-one correspondence with L-polytopes of holes in lattices. Therefore, the study of the extreme rays of the hypermetric cone translates into the study of "rigid" L-polytopes (see Theorem 6.5). See section 6 for details.

Designs. Each hypercube embedding of the equidistant metric $2td(K_n) = (2t, \ldots, 2t)$ corresponds to some design. The embeddings of minimum size, i.e. in a hypercube of minimum dimension, correspond to special classes of designs (Hadamard designs and projective planes), depending on the parameters. These connections are described in section 8.3.

Several additional applications are described, in particular, in section 8.

One more interesting application of cuts is for the disproval of the following conjecture by Borsuk: Every set of diameter one in the space $\mathbb{R}^d$ can be partitioned into $d+1$ subsets of diameter smaller than one. For $n = 4k$ with k prime power, consider the set X of the incidence vectors of the equicuts, i.e. corresponding to a partition into two sets of size $\frac{n}{2}$, of the complete graph K_n. Then X cannot be partitioned into fewer than 1.1^n parts so that each part has diameter smaller than the diameter of X. This is a counterexample to Borsuk's conjecture; it is given in [106].

Finally, a curiosity about cuts is the link existing between the cut cone and Fibonacci numbers. Namely, the number of cuts on one of its facets is expressed directly in terms of the Fibonacci numbers [67].

2 Objects

2.1 Cut and intersection vectors

Set $V_n = \{1, \ldots, n\}$, $E_n = \{(i,j) : 1 \leq i < j \leq n\}$, then $K_n = (V_n, E_n)$ denotes the complete graph on n nodes.

• For $S \subseteq V_n$, $\delta(S) \subseteq E_n$ denotes the *cut* defined by S, with $(i,j) \in \delta(S)$ if and only if $|S \cap \{i,j\}| = 1$. The incidence vector of the cut $\delta(S)$ is called a *cut vector* and, by abuse of language, is also denoted as $\delta(S)$. Hence, $\delta(S) \in \{0,1\}^{\binom{n}{2}}$ with $\delta(S)_{ij} = 1$ if and only if $|S \cap \{i,j\}| = 1$ for $1 \leq i < j \leq n$. Therefore, $\delta(S) = \delta(V_n - S)$ holds, i.e. a cut can be defined by any of its two *shores* S or $V_n - S$.

• For $S \subseteq V_n$, $\pi(S) \in \{0,1\}^{\binom{n+1}{2}}$ is the *intersection vector* defined by S with $\pi(S)_{ij} = 1$ if and only if $i, j \in S$ for $1 \leq i \leq j \leq n$.

• Let $\mathcal{I}$ be a collection of subsets of V_n. For $S \subseteq V_n$, we define its $\mathcal{I}$-*intersection vector* $\pi^{\mathcal{I}}(S) \in \{0,1\}^{\mathcal{I}}$ by $\pi^{\mathcal{I}}(S)_I = 1$ if and only if $I \subseteq S$, for

$I \in \mathcal{I}$. We shall consider, in particular, the following set families $\mathcal{I}$: $\mathcal{I}_{=m}$ consisting of all $I \subseteq V_n$ with $|I| = m$, and $\mathcal{I}_{\leq m}$ consisting of all $I \subseteq V_n$ with $1 \leq |I| \leq m$, for $1 \leq m \leq n$. For instance, for $\mathcal{I} = \mathcal{I}_{=1}$, $\pi^{\mathcal{I}}(S)$ is simply the incidence vector of S and, for $\mathcal{I} = \mathcal{I}_{\leq 2}$, $\pi^{\mathcal{I}}(S)$ coincides with the usual intersection vector $\pi(S)$.

2.2 Inequalities

• For distinct $i, j, k \in V_n$, the inequalities:

$$x_{ij} - x_{ik} - x_{jk} \leq 0 \tag{1}$$

and

$$x_{ij} + x_{ik} + x_{jk} \leq 2 \tag{2}$$

are called *triangle inequalities*; (1) is homogeneous while (2) is not.
• Given n integers $b_1, \ldots, b_n$, we consider the inequality:

$$\sum_{1 \leq i < j \leq n} b_i b_j x_{ij} \leq 0. \tag{3}$$

When $\sigma := \sum_{1 \leq i \leq n} b_i = 1$, the inequality (3) is called a *hypermetric inequality* and denoted by $Hyp_n(b_1, \ldots, b_n)$. The triangle inequality (1) is the special case $b_i = b_j = 1$, $b_k = -1$, $b_h = 0$ for $h \in V_n - \{i, j, k\}$, of the hypermetric inequality (3). When $\sum_{1 \leq i \leq n} |b_i| = 2k + 1$, the inequality (3) is called $2k+1$-*gonal*. The 5-*gonal* inequality is $Hyp_5(1, 1, 1, -1, -1)$.

When $\sigma = 0$, the inequality (3) is called a *negative type inequality* and when $\sum_{1 \leq i \leq n} |b_i| = 2k$, it is called $2k$-*gonal*.
• More generally, let $b_1, \ldots, b_n$ be integers such that $\sigma = \sum_{1 \leq i \leq n} b_i$ is odd and such that there exists a subset $A \subseteq V_n$ with $\sum_{i \in A} b_i = \frac{\sigma - 1}{2}$. Then, we consider the inequality:

$$\sum_{1 \leq i < j \leq n} b_i b_j x_{ij} \leq \frac{\sigma^2 - 1}{4} \tag{4}$$

refered to as the *non homogeneous hypermetric inequality*. The triangle inequality (2) is the special case $b_i = b_j = b_k = 1$, $b_h = 0$ for $h \in V_n - \{i, j, k\}$ of the inequality (4).

• Given integers $b_1, \ldots, b_n$, set $\sigma = \sum_{1 \leq i \leq n} b_i$ and $\gamma = \min(|\sigma - 2\sum_{i \in S} b_i| : S \subseteq V_n)$, called the *gap* of the b_i's. The inequality:

$$\sum_{1 \leq i < j \leq n} b_i b_j x_{ij} \leq \frac{\sigma^2 - \gamma^2}{4} \tag{5}$$

is valid for the cut polytope $CutP_{n+1}$; it is called a *gap inequality* [117]. The class of gap inequalities includes the negative type inequalities (for $\sigma = 0$), the hypermetric inequalities (for $\sigma = 1$) and the non homogeneous hypermetric inequalities (4) (for σ odd and when there exists a subset A such that $\sum_{i \in A} b_i = \frac{\sigma - 1}{2}$).

2.3 ℓ_1, Voronoi and covariance maps

We introduce three useful maps:
• the ℓ_1-*map* $\varphi_\ell : \mathbb{R}^n \longrightarrow \mathbb{R}^{\binom{n}{2}}$ defined by $\varphi_\ell(x) = (|x_i - x_j|)_{1 \leq i < j \leq n}$ for $x \in \mathbb{R}^n$.
• the *Voronoi map* $\varphi_v : \Re^n \longrightarrow \Re^{\binom{n+1}{2}}$ defined by $\varphi_v(x) = (x_i x_j)_{1 \leq i \leq j \leq n}$ for $x \in \mathbb{R}^n$.
• the *covariance map* $\varphi_{c_0} : \mathbb{R}^{\binom{n+1}{2}} \longrightarrow \mathbb{R}^{\binom{n+1}{2}}$ defined by $\varphi_{c_0}(x) = p$, for $x = (x_{ij})_{0 \leq i < j \leq n}$, $p = (p_{ij})_{1 \leq i \leq j \leq n}$, with

$$\begin{cases} p_{ii} &= x_{0i} \quad \text{for } 1 \leq i \leq n \\ p_{ij} &= \frac{x_{0i} + x_{0j} - x_{ij}}{2} \quad \text{for } 1 \leq i < j \leq n \end{cases} \tag{6}$$

The subscript "0" in φ_{c_0} refers to the fact that the index "0" has been specialized in relation (6), but any other index $i \in \{0, 1, \ldots, n\}$ can be specialized as well yielding the map φ_{c_i}.

The cut and intersection vectors are linked via these maps. Namely, given a subset $S \subseteq \{1, \ldots, n\}$ and its incidence vector $1_S \in \{0,1\}^n$, then $\delta(S) = \varphi_\ell(1_S)$ and $\pi(S) = \varphi_v(1_S)$. Moreover, if S is a subset of $\{0, 1, \ldots, n\}$ with $0 \notin S$ and if $\delta(S)$ denotes the cut vector defined by S in K_{n+1}, then $\pi(S) = \varphi_{c_0}(\delta(S))$.

2.4 Polyhedra

We define now a list of polytopes and cones to be considered in the paper. For a general account of the theory of polyhedra, we refer e.g. to [145].

• The *cut cone* Cut_n is the cone generated by all cut vectors $\delta(S)$ for $S \subseteq V_n$.
• The *cut polytope* $CutP_n$ is the convex hull of all cut vectors $\delta(S)$ for $S \subseteq V_n$. Both Cut_n and $CutP_n$ are full dimensional polyhedra in $\mathbb{R}^{\binom{n}{2}}$.
• The *boolean quadric cone* BQ_n is the cone generated by all intersection vectors $\pi(S)$ for $S \subseteq V_n$.
• The *boolean quadric polytope* BQP_n is the convex hull of all intersection vectors $\pi(S)$ for $S \subseteq V_n$. Both BQ_n and BQP_n are full dimensional polyhedra in $\mathbb{R}^{\binom{n+1}{2}}$.
• More generally, given a family $\mathcal{I}$ of subsets of V_n, the cone $BQ_n^{\mathcal{I}}$ (resp. the polytope $BQP_n^{\mathcal{I}}$) is defined as the conic hull (resp. convex hull) of the $\mathcal{I}$-intersection vectors $\pi^{\mathcal{I}}(S)$ for $S \subseteq V_n$. Hence, for $\mathcal{I} = \mathcal{I}_{=1}$, $BQP_n^{\mathcal{I}}$ is the n-dimensional cube and, for $\mathcal{I} = \mathcal{I}_{\leq 2}$, $BQP_n^{\mathcal{I}}$ coincides with BQP_n.
• The *hypermetric cone* Hyp_n is the cone defined by the hypermetric inequalities (3), i.e.

$$Hyp_n = \{x \in \mathbb{R}^{\binom{n}{2}} : \quad \textstyle\sum_{1\leq i<j\leq n} b_ib_jx_{ij} \leq 0 \quad \text{for all integers } b_1, \ldots, b_n \text{ with } \sum_{1\leq i\leq n} b_i = 1\}.$$

• The *hypermetric polytope* $HypP_n$ is the polytope defined by the inequalities (4).
• The *negative type cone* Neg_n is the cone defined by the negative type inequalities (3), i.e.

$$Neg_n = \{x \in \mathbb{R}^{\binom{n}{2}} : \quad \textstyle\sum_{1\leq i<j\leq n} b_ib_jx_{ij} \leq 0 \quad \text{for all integers } b_1, \ldots, b_n \text{ with } \sum_{1\leq i\leq n} b_i = 0\}.$$

• The *metric cone* Met_n is the cone defined by the triangle inequalities (1) and the *metric polytope* $MetP_n$ is the polytope defined by the triangle inequalities (1) and (2).
• The cone Q_n of the positive semi-definite quadratic forms can be defined as

$$Q_n = \{x \in \mathbb{R}^{\binom{n+1}{2}} : \sum_{1\leq i,j\leq n} b_ib_jx_{ij} \geq 0 \text{ for all } b_1, \ldots, b_n \in \mathbb{R}\}.$$

There are several connections between the above polyhedra. An easy, but fundamental, fact is that Cut_{n+1} and BQ_n (resp. $CutP_{n+1}$ and BQP_n) are in linear one-to-one correspondance via the covariance map φ_{c_0}, since their generators are in one-to-one correspondance via φ_{c_0}. It was rediscovered, independently, by several authors, e.g. [98], [47], [150].

Namely, let Cut_{n+1} and $CutP_{n+1}$ be defined on the $n+1$ points of $\{0,1,\ldots,n\}$, then

$$BQ_n = \varphi_{c_0}(Cut_{n+1}), BQP_n = \varphi_{c_0}(CutP_{n+1}). \tag{7}$$

It can be checked that

$$\begin{aligned}\varphi_{c_0}(Hyp_{n+1}) = \quad & \{p = (p_{ij})_{1\leq i\leq j\leq n} : \textstyle\sum_{1\leq i,j\leq n} b_ib_jp_{ij} - \sum_{1\leq i\leq n} b_ip_{ii} \geq 0 \\ & \text{for all integers } b_1,\ldots,b_n\}\end{aligned} \tag{8}$$

$$\varphi_{c_0}(Neg_{n+1}) = Q_n \tag{9}$$

since $p \in \varphi_{c_0}(Neg_{n+1})$ if and only if $\sum_{1\leq i,j\leq n} b_ib_jp_{ij} \geq 0$ for all integers $b_1,\ldots,b_n$.

We deduce the following inclusions.

$$\left\{\begin{array}{lll} Cut_n \subseteq Hyp_n \subseteq Met_n, & & CutP_n \subseteq HypP_n \subseteq MetP_n \\ Cut_n \subseteq Hyp_n \subseteq Neg_n, & \text{i.e.} & BQ_n \subseteq \varphi_{c_0}(Hyp_{n+1}) \subseteq Q_n. \end{array}\right. \tag{10}$$

Some of the above cones and polytopes can be defined, more generally, for an arbitrary graph $G=(V_n,E)$, where the edge set E is a subset of E_n.

Given a subset $S \subseteq V_n$, let $\delta_G(S) \in \mathbb{R}^E$ denote the cut vector defined by S in G, i.e. $\delta_G(S)$ is the projection of $\delta(S)$ on the edge set E of G. Similarly, let $\pi_G(S)$ denote the projection of the intersection vector $\pi(S)$ on $\mathbb{R}^E$, i.e. $\pi_G(S) = (\pi(S)_{ij})_{1\leq i\leq j\leq n, (i,j)\in E \text{ if } i\neq j}$. The corresponding cut cone, cut polytope, boolean quadric cone, boolean quadric polytope, are denoted, respectively, by $Cut(G)$, $CutP(G)$, $BQ(G)$, $BQP(G)$. For the complete graph $G=K_n$, they coincide, respectively, with Cut_n, $CutP_n$, BQ_n, BQP_n. The projection of the metric cone Met_n and of the metric polytope $MetP_n$ on the edge set E of G are the cone $Met(G)$ and the polytope $MetP(G)$ defined, respectively, by

$$\begin{aligned}Met(G) = \{x \in \mathbb{R}^E : \quad & x_e - x(C-e) \leq 0 \quad && \text{for } C \text{ cycle of } G \text{ and } e \in C \\ & 0 \leq x_e \leq 1 && \text{for } e \in E\}\end{aligned} \tag{11}$$

$$MetP(G) = \{x \in \mathbb{R}^E : \begin{array}{ll} x(F) - x(C-F) \leq |F| - 1 & \text{for } C \text{ cycle of } G \\ & \text{and } F \subseteq C, |F| \text{ odd} \\ 0 \leq x_e \leq 1 & \text{for } e \in E\}. \end{array} \quad (12)$$

We list now briefly the main papers where the above cones and polytopes have been considered. The papers are listed by alphabetic order.

The metric cone was considered in [12], [13], [92], [123], [124] (and references there), [101], [122], [147] and the metric polytope in [68], [116], [118], [119].

The hypermetric cone was considered in [7], [8], [17], [50], [51], [53], [55], [112] and the negative type cone in [99].

The boolean quadric cone was considered in [47] and the boolean quadric polytope in [31], [79], [127], [131], [135], [150].

The cut cone and polytope are considered in [2], [16], [19], [21], [23], [25], [46], [47], [54], [58], [64], [65], [66], [68], [91], [152]. A detailed survey on the valid inequalities and facets for the cut cone can be found in [60].

The uniform cut cone (generated by cuts with the same shore size) is considered in [63], the uniform boolean quadric polytope $BQP_n(N)$ in [79] (and references there), [127], [161], the equicut polytope in [40], [41], [49], [153], and even cut polyhedra (generated by the cuts whose shores have both an even cardinality) in [57].

2.5 Metric notions

Let $d = (d_{ij})_{1 \leq i < j \leq n} \in \mathbb{R}^{\binom{n}{2}}$. It may be convenient to view d as a symmetric $n \times n$-matrix by setting $d_{ij} = d_{ji}$ and $d_{ii} = 0$ for $i, j \in V_n$.

• d is a *semi-metric* if d satisfies the triangle inequalities (1), i.e. $d \in Met_n$, and d is a *metric* if, moreover, $d_{ij} \neq 0$ for distinct $i, j \in V_n$. However, we often use the term "metric" even if $d_{ij} = 0$ for some distinct i, j. We also say that (V_n, d) is a *metric space*.

• $d \in Met_n$ is said to be *metrically rigid* if d lies on a simplicial face of Met_n, i.e. on a face whose generators (the extreme rays lying on it) are linearly independent; d is an *extreme metric* if d lies on an extreme ray of Met_n.

• d is *hypermetric* if d satisfies the hypermetric inequalities (3), i.e. $d \in Hyp_n$, and d is $2k+1$-gonal if it satisfies all $2k+1$-gonal hypermetric inequalities; d is of *negative type* if it satisfies the negative type inequalities, i.e. $d \in Neg_n$, and d is $2k$-gonal if it satisfies all $2k$-gonal negative type inequalities.

• d is *ℓ_p-embeddable* if there exist n vectors $x_1, \ldots, x_n \in \mathbb{R}^m$ for some $m \geq 1$ such that $d_{ij} = \| x_i - x_j \|_p$ for $1 \leq i < j \leq n$, where $\| x \|_p = (\sum_{1 \leq h \leq m} |x_h|^p)^{\frac{1}{p}}$ for $x \in \mathbb{R}^m$. We consider here especially the cases $p = 1, 2$.

• d is *hypercube embeddable* (*h-embeddable*, for short) if $d_{ij} = \| x_i - x_j \|_1$ for $1 \leq i < j \leq n$, for some binary vectors $x_1, \ldots, x_n \in \{0,1\}^m$, $m \geq 1$.

• If d is rational valued, then d is ℓ_1-embeddable if and only if ηd is h-embeddable for some scalar η [10]. The smallest such η is called the *scale* of d. This fact is easy, but crucial, since it permits to link combinatorial and analytical aspects.

• For $d \in Cut_n$, any decomposition of d as $d = \sum_S \lambda_S \delta(S)$ with $\lambda_S \geq 0$ (resp. $\lambda_S \geq 0$, integer) is called a *$\mathbb{R}_+$-realization* (resp. *$\mathbb{Z}_+$-realization*) of d; $\sum_S \lambda_S$ is its *size*. The minimum size of a $\mathbb{R}_+$-realization of $d \in Cut_n$ is denoted as $s(d)$ and the minimum size of a $\mathbb{Z}_+$-realization (if exists) of d is called its *h-size* and denoted by $s_h(d)$.

If $d = \sum_S \lambda_S \delta(S)$ with $\lambda_S \geq 0$, then $\sum_{1 \leq i < j \leq n} d_{ij} = \sum_S \lambda_S |S|(n - |S|)$, with $n - 1 \leq |S|(n - |S|) \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ for $1 \leq |S| \leq n - 1$. Therefore, for $d \in Cut_n$, we have the following bounds on its minimum size $s(d)$:

$$\frac{\sum_{1 \leq i < j \leq n} d_{ij}}{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil} \leq s(d) \leq \frac{\sum_{1 \leq i < j \leq n} d_{ij}}{n-1}. \tag{13}$$

• $d \in Cut_n$ is said to be *ℓ_1-rigid* if it lies on a simplicial face of Cut_n, i.e. d has a unique $\mathbb{R}_+$-realization or, equivalently (in view of Theorem 3.3), d has a unique ℓ_1-embedding. Similarly, if d is h-embeddable, d is said to be *h-rigid* if d has a unique h-embedding or, equivalently, a unique $\mathbb{Z}_+$-realization.

2.6 Operations on faces

We saw above that the cut polytope Cut_{n+1} and the boolean quadric polytope BQP_n are in one-to-one correspondance via the covariance map φ_{c_0}. We now see in more detail how the covariance map acts on the valid inequalities. Consider the inequalities:

$$\sum_{0 \leq i < j \leq n} c_{ij} x_{ij} \leq d \tag{14}$$

$$\sum_{1\le i\le n} a_i p_{ii} + \sum_{1\le i<j\le n} b_{ij}p_{ij} \le d \tag{15}$$

where a, b, c are linked by

$$\begin{cases} c_{0i} &= a_i + \frac{1}{2}\sum_{1\le j\le n, j\neq i} b_{ij} \quad \text{for } 1\le i\le n \\ c_{ij} &= -\frac{1}{2}b_{ij} \quad \text{for } 1\le i<j\le n. \end{cases} \tag{16}$$

Then, the inequality (14) is valid (resp. facet defining) for $CutP_{n+1}$ if and only if the inequality (15) is valid (resp. facet defining) for BQP_n.

The cut polytope enjoys a lot of symmetries, namely the symmetries induced by the permutations of V_n and the switching maps that we now describe. The full symmetry group of the cut polytope $CutP_n$ is described in [54].

Given a cut $\delta(A)$ of K_n and $v\in\mathbb{R}^{\binom{n}{2}}$, we define the maps $R_{\delta(A)}$ and $r_{\delta(A)}$ from $\mathbb{R}^{\binom{n}{2}}$ to $\Re^{\binom{n}{2}}$ by

$$R_{\delta(A)}(v)_{ij} = \begin{cases} -v_{ij} & \text{if } (i,j)\in\delta(A) \\ v_{ij} & \text{otherwise} \end{cases} \tag{17}$$

$$r_{\delta(A)}(v)_{ij} = \begin{cases} 1-v_{ij} & \text{if } (i,j)\in\delta(A) \\ v_{ij} & \text{otherwise.} \end{cases} \tag{18}$$

Hence, $r_{\delta(A)}$ is an affine map, called *switching map*, whose associated linear map is $R_{\delta(A)}$. Then, the inequality $v^Tx\le v_0$ is valid (resp. facet defining) for $CutP_n$ if and only if the inequality $R_{\delta(A)}(v)^Tx\le v_0 - v^T\delta(A)$ is valid (resp. facet defining) for $CutP_n$. An important consequence is that all the facets of the cut polytope can be deduced from those of the cut cone, via the switching map [25].

For instance, the non homogeneous triangle inequality (2) is a switching of the homogeneous triangle inequality (1) and the inequalities (4) are all possible switchings of the hypermetric inequalities (3).

The switching operation was introduced in [47] for the cut cone Cut_n and in [25] for the cut polytope $CutP(G)$ of an arbitrary graph.

Via the covariance map, we have also an analogue of switching for the boolean quadric polytope, namely, the map $\varphi_{c_0} r_{\delta(A)} \varphi_{c_0}^{-1}$ which acts on the boolean quadric polytope BQP_n as follows. It transforms the inequality

$$\sum_{1 \le i \le n} a_i p_{ii} + \sum_{1 \le i < j \le n} b_{ij} p_{ij} \le d$$

into the inequality

$$\sum_{1 \le i \le n} a'_i p_{ii} + \sum_{1 \le i < j \le n} b'_{ij} p_{ij} \le d'$$

where

$$d' = d - \sum_{i \in A} a_i - \tfrac{1}{2} \sum_{1 \le i < j \le n, i,j \in A} b_{ij}$$

$$a'_i = \begin{cases} a_i + \sum_{j \in A} b_{ij} & \text{if } i \notin A \\ -a_i - \sum_{j \in A - \{i\}} b_{ij} & \text{if } i \in A \end{cases}$$

$$b'_{ij} = \begin{cases} -b_{ij} & \text{if } |A \cap \{i,j\}| = 1 \\ b_{ij} & \text{if } |A \cap \{i,j\}| \neq 1. \end{cases}$$

Several other operations on the faces of the cut polytope were considered, see e.g. [25], [63],[64], [151], [152].

3 Applications in functional analysis: ℓ_1- and L_1-metrics

3.1 The cut cone and ℓ_1-metrics

In this section, we mention how the members of the cut cone and polytope, or of the boolean quadric cone and polytope, can be interpreted in terms of metrics and measure spaces. We essentially follow [6] and [11].

Clearly, every member $d \in Cut_n$ defines a semi-metric on n points. Hence arises the question of characterizing the class of semi-metrics defined by the cut cone. As stated in Theorems 3.1, 3.3 and 3.8, the semi-metrics belonging to the cut cone are those that are L_1-embeddable or, equivalently, ℓ_1-embeddable or, equivalently, $d \in Cut_n$ if and only if $d_{ij} = \mu(A_i \Delta A_j)$, $1 \le i < j \le n$, for some non negative measure space $(\Omega, \mathcal{A}, \mu)$ and some events $A_1, \ldots, A_n \in \mathcal{A}$. The corresponding statement for the boolean quadric cone reads: $p \in BQ_n$ if and only if $p_{ij} = \mu(A_i \cap A_j)$, $1 \le i \le j \le n$, for some non negative measure space $(\Omega, \mathcal{A}, \mu)$ and some events $A_1, \ldots, A_n \in \mathcal{A}$. The polytope case corresponds to the case when $(\Omega, \mathcal{A}, \mu)$ is a probability space, i.e. $\mu(\Omega) = 1$.

Before stating the results, we recall some definitions.

A *measure space* $(\Omega, \mathcal{A}, \mu)$ consists of a set Ω, a σ-algebra $\mathcal{A}$ of subsets of Ω, and a measure μ defined on $\mathcal{A}$ which is additive, i.e. $\mu(\bigcup_{n\geq 1} A_n) = \sum_{n\geq 1} \mu(A_n)$ for all pairwise disjoint sets $A_n \in \mathcal{A}$, and satisfies $\mu(\emptyset) = 0$. The measure space is *non negative* if $\mu(A) \geq 0$ for all $A \in \mathcal{A}$. A *probability space* is a non negative measure space with total measure $\mu(\Omega) = 1$.

If (X, d) and (X', d') are two semi-metric spaces, (X, d) is said to be *isometrically embeddable* into (X', d') if there exists a map ϕ (the *embedding*) from X to X' such that $d(x, y) = d'(\phi(x), \phi(y))$ for all $x, y \in X$. One also says that (X, d) *is a subspace of* (X', d').

Recall that $\| \ \|_1$ denotes the ℓ_1-norm, defined by $\| u \|_1 = \sum_{1\leq j\leq m} |u_j|$ for $u \in \mathbb{R}^m$.

THEOREM 3.1 *Let $d = (d_{ij})_{1\leq i<j\leq n} \in \mathbb{R}^{\binom{n}{2}}$. The following assertions are equivalent.*

(i) $d \in Cut_n$ (resp. $d \in CutP_n$).

(ii) There exist a non negative measure space (resp. a probability space) $(\Omega, \mathcal{A}, \mu)$ and $A_1, \ldots, A_n \in \mathcal{A}$ such that $d_{ij} = \mu(A_i \Delta A_i)$ for all $1 \leq i < j \leq n$.

THEOREM 3.2 *Let $p = (p_{ij})_{1\leq i\leq j\leq n} \in \mathbb{R}^{\binom{n+1}{2}}$. The following assertions are equivalent.*

(i) $p \in BQ_n$ (resp. $p \in BQP_n$).

(ii) There exist a non negative measure space (resp. a probability space) $(\Omega, \mathcal{A}, \mu)$ and $A_1, \ldots, A_n \in \mathcal{A}$ such that $p_{ij} = \mu(A_i \cap A_j)$ for all $1 \leq i \leq j \leq n$.

Theorem 3.1 was given in [6] and Theorem 3.2 was given in [133], [135]. This interpretation of BQP_n is already used in [127] for describing the pair distributions of particles in lattice sites. In fact, both Theorems 3.1 and 3.2 are easily seen to be equivalent using the covariance map. We give the proof of Theorem 3.2, following [133].

PROOF. Assume $p \in BQ_n$. Then, $p = \sum_{S\subseteq\{1,\ldots,n\}} \lambda_S \pi(S)$ for some $\lambda_S \geq 0$. We define a non negative measure space $(\Omega, \mathcal{A}, \mu)$ as follows. Let Ω denote the family of subsets of $\{1, \ldots, n\}$, let $\mathcal{A}$ denote the family of subsets of Ω and let μ denote the measure on $\mathcal{A}$ defined by $\mu(A) = \sum_{S\in A} \lambda_S$ for each $A \in \mathcal{A}$

(i.e. A is a collection of subsets of $\{1,\ldots,n\}$). Define $A_i = \{S \in \Omega : i \in S\}$. Then, $\mu(A_i \cap A_j) = \mu(\{S \in \Omega : i,j \in S\}) = \sum_{S\in\Omega: i,j\in S} \lambda_S = p_{ij}$ holds, for all $1 \le i \le j \le n$. Moreover, if $p \in BQP_n$, then we have $\sum_S \lambda_S = 1$, i.e. $\mu(\Omega) = 1$, that is $(\Omega, \mathcal{A}, \mu)$ is a probability space.

Conversely, assume $p_{ij} = \mu(A_i \cap A_j)$ for $1 \le i \le j \le n$, where $(\Omega, \mathcal{A}, \mu)$ is a nonnegative measure space and $A_1, \ldots, A_n \in \mathcal{A}$. Set $A^S = \bigcap_{i\in S} A_i \cap \bigcap_{i\notin S}(\Omega - A_i)$ for each $S \subseteq \{1,\ldots,n\}$. Then, $A_i = \bigcup_{S: i\in S} A^S$, $A_i \cap A_j = \bigcup_{S: i,j\in S} A_S$ and $\Omega = \bigcup_S A^S$. Therefore, $p = \sum_{S\subseteq\{1,\ldots,n\}} \mu(A^S)\pi(S)$, showing that p belongs to the boolean quadric cone BQ_n. Moreover, if $(\Omega, \mathcal{A}, \mu)$ is a probability space, i.e. $\mu(\Omega) = 1$, then $\sum_S \mu(A^S) = 1$, implying that p belongs to the boolean quadric polytope BQP_n. ∎

Another characterization of the cut cone is given in [6], [11] in terms of ℓ_1-metrics.

THEOREM 3.3 *Let (X,d) be a semi-metric space with $X = \{1,\ldots,n\}$. The following assertions are equivalent.*

(i) $d \in Cut_n$.

(ii) (X,d) is ℓ_1-embeddable, i.e. there exist n vectors $u_1,\ldots,u_n \in \mathbb{R}^m$ for some m such that $d_{ij} = \| u_i - u_j \|_1$ for all $1 \le i < j \le n$.

PROOF. $(i) \Rightarrow (ii)$. Let $d \in Cut_n$, then $d = \sum_{1\le k\le m} \lambda_k \delta(S_k)$ with $\lambda_1,\ldots,\lambda_m \ge 0$. For $1 \le i \le n$, define the vector $u_i \in \mathbb{R}^m$ with components $(u_i)_k = \lambda_k$ if $i \in S_k$ and $(u_i)_k = 0$ otherwise, for $1 \le k \le m$. Then $d_{ij} = \| u_i - u_j \|_1$ holds, showing that (X,d) is ℓ_1-embeddable.

$(ii) \Rightarrow (i)$. Assume that (X,d) is ℓ_1-embeddable, i.e. there exist n vectors $u_1,\ldots,u_n \in \mathbb{R}^m$ for some $m \ge 1$ such that $d_{ij} = \| u_i - u_j \|_1$, for $1 \le i < j \le n$. We show that $d \in Cut_n$. It suffices to show the result for the case $m = 1$ by additivity of the ℓ_1-norm. Hence $d_{ij} = |u_i - u_j|$ where $u_1,\ldots,u_n \in \mathbb{R}$. Without loss of generality, we can suppose that $0 = u_1 \le u_2 \le \ldots \le u_n$. Then, $d = \sum_{1\le k\le n-1}(u_{k+1} - u_k)\delta(\{1,2,\ldots,k-1,k\})$ holds, showing that $d \in Cut_n$. ∎

There is an analogue characterization for h-embeddable metrics.

THEOREM 3.4 *Let (X,d) be a semi-metric space with $X = \{1,\ldots,n\}$. The following assertions are equivalent.*

(i) $d = \sum_S \lambda_S \delta(S)$ *for some non negative integer scalars* λ_S.

(ii) (X, d) *is h-embeddable, i.e. there exist n vectors* $u_1, \ldots, u_n \in \{0,1\}^m$ *for some m such that* $d_{ij} = \| u_i - u_j \|_1$ *for all* $1 \leq i < j \leq n$.

Proof. The proof is analogous to that of Theorem 3.3. Namely, for $(i) \Rightarrow (ii)$, assume $d = \sum_{1 \leq k \leq m} \delta(S_k)$ (allowing repetitions). Consider the binary $n \times m$ matrix M whose columns are the incidence vectors of the sets $S_1, \ldots, S_m$. If $u_1, \ldots, u_n$ denote the rows of M, then $d_{ij} = \| u_i - u_j \|_1$ holds, providing an embedding of (X, d) in the hypercube of dimension m. Conversely, for $(ii) \Rightarrow (i)$, consider the matrix M whose rows are the n given vectors $u_1, \ldots, u_n$. Let $S_1, \ldots, S_m$ be the subsets of $\{1, \ldots, n\}$ whose incidence vectors are the columns of M. Then, $d = \sum_{1 \leq k \leq m} \delta(S_k)$ holds, giving a decomposition of d as a non negative integer combination of cuts. ∎

3.2 The cut cone and L_1-metrics (infinite case)

In fact, there is a deeper connection between the cut cone and functional analysis, namely with L_1-spaces. It was established in [6] (see also [11]). For this, we need some more definitions. In what follows, we shall consider a semi-metric space (X, d) where the set X may be finite or infinite, since some results remain valid in the infinite case.

Given a measure space $(\Omega, \mathcal{A}, \mu)$ and given a function $f : \Omega \longrightarrow \mathbb{R}$, its L_1-norm is defined by:

$$\| f \|_1 = \int_\Omega |f(\omega)| \mu(d\omega).$$

Then $L_1(\Omega, \mathcal{A}, \mu)$ denotes the set of measurable functions f, i.e. with $\| f \|_1 < \infty$. Hence the L_1-norm defines a metric structure on $L_1(\Omega, \mathcal{A}, \mu)$.

Given a non negative measure space $(\Omega, \mathcal{A}, \mu)$, another metric space $(\mathcal{A}_\mu, d_\mu)$ can be defined, where $\mathcal{A}_\mu = \{\mathcal{A} \in \mathcal{A} : \mu(\mathcal{A}) < \infty\}$ and $d_\mu(A, B) = \mu(A \Delta B)$ for $A, B \in \mathcal{A}_\mu$. In fact, $(\mathcal{A}_\mu, d_\mu)$ is the subspace of $L_1(\Omega, \mathcal{A}, \mu)$ consisting of its 0-1 valued functions.

When Ω is a set of cardinality m, $\mathcal{A} = 2^\Omega$ is the collection of subsets of Ω and μ is the cardinality measure, i.e. $\mu(A) = |A|$ for $A \subseteq \Omega$, then $L_1(\Omega, 2^\Omega, |.|)$ is simply denoted as $\ell_1(m)$, or ℓ_1. Hence, the m-dimensional hypercube $(K_2)^m$ is the subspace of ℓ_1 consisting only of the binary sequences.

A semi-metric space (X, d) is L_1-*embeddable* if it is a subspace of some $L_1(\Omega, \mathcal{A}, \mu)$ for some non negative measure space, i.e. there is a map ϕ from X to $L_1(\Omega, \mathcal{A}, \mu)$ such that $d(x, y) = \| \phi(x) - \phi(y) \|_1$ for $x, y \in X$.

LEMMA 3.5 *For a semi-metric space (X, d), the following assertions are equivalent.*

(i) (X, d) is L_1-embeddable.

(ii) (X, d) is a subspace of $(\mathcal{A}_\mu, d_\mu)$ for some non negative measure space $(\Omega, \mathcal{A}, \mu)$.

PROOF. The implication $(ii) \Rightarrow (i)$ is clear, since $(\mathcal{A}_\mu, d_\mu)$ is a subspace of $L_1(\Omega, \mathcal{A}, \mu)$. We check $(i) \Rightarrow (ii)$. It suffices to show that each space $L_1(\Omega, \mathcal{A}, \mu)$ is a subspace of $(\mathcal{B}_\nu, d_\nu)$ for some non negative measure space $(T, \mathcal{B}, \nu)$. Set $T = \Omega \times \mathbb{R}$, $\mathcal{B} = \mathcal{A} \times \mathcal{R}$ where $\mathcal{R}$ is the family of Borel subsets of $\mathbb{R}$, and $\nu = \mu \otimes \lambda$ where λ is the Lebesgue measure on $\mathbb{R}$. For $f \in L_1(\Omega, \mathcal{A}, \mu)$, let $E(f) = \{(\omega, s) \in \Omega \times \mathbb{R} : s > f(\omega)\}$ denote its epigraph. Then, the map $f \longmapsto E(f)\Delta E(0)$ provides an isometric embedding from $L_1(\Omega, \mathcal{A}, \mu)$ to $(\mathcal{B}_\nu, d_\nu)$, since $\| f - g \|_1 = \nu(E(f)\Delta E(g))$ holds. ∎

The next theorem is an analogue of Theorem 3.3 for the general case when the set X may be infinite.

For each subset Y of X, let δ_Y denote the cut function induced by Y defined by $\delta_Y(x, y) = 1$ if $|Y \cap \{x, y\}| = 1$, $\delta_Y(x, y) = 0$ otherwise, for $x, y \in X$; so δ_Y is just the symmetrization of the usual cut metric $\delta(Y)$. Let $\mathcal{D}(X)$ denote the set of all cut functions δ_Y for $Y \subseteq X$.

THEOREM 3.6 *Given a semi-metric space (X, d), the following assertions are equivalent.*

(i) (X, d) is L_1-embeddable.

(ii) There exists a non negative measure ν on $\mathcal{D}(X)$ such that $d(x, y) = \int_{\mathcal{D}(X)} \delta(x, y)\nu(d\delta)$ for $x, y \in X$.

PROOF. $(i) \Rightarrow (ii)$. Assume (X, d) is L_1-embeddable. Then, by Lemma 3.5, there exist a non negative measure space $(\Omega, \mathcal{A}, \mu)$ and a map $x \longmapsto A_x$

from X to $\mathcal{A}_\mu$ such that $d(x,y)=\mu(A_x \Delta A_y)$ for $x,y \in X$. For $\omega \in \Omega$, set $A^\omega = \{x \in X : \omega \in A_x\}$. We define a measure ν on $\mathcal{D}(X)$ additively by setting: $\nu(\{\delta_Y\}) = \mu(\{\omega \in \Omega : A^\omega = Y\})$ for each $Y \subseteq X$.
Note that $\omega \in A_x$ if and only if $x \in A^\omega$ and $\omega \in A_x \Delta A_y$ if and only if $|A^\omega \cap \{x,y\}| = 1$. Therefore,

$$\begin{aligned} d(x,y) &= \mu(A_x \Delta A_y) = \mu(\{\omega \in \Omega : |A^\omega \cap \{x,y\}| = 1\}) \\ &= \mu(\{\omega \in \Omega : \delta_{A^\omega}(x,y) = 1\}) \\ &= \mu(\textstyle\bigcup_{Y \subseteq X : \delta_Y(x,y)=1} \{\omega \in \Omega : A^\omega = Y\}) \\ &= \textstyle\int_{\mathcal{D}(X)} \delta(x,y)\nu(d\delta). \end{aligned}$$

$(ii) \Rightarrow (i)$. Conversely, assume that $d = \int_{\mathcal{D}(X)} \delta\nu(d\delta)$ for some non negative measure on $\mathcal{D}(X)$. Fix $s \in X$ and set $A_x = \{\delta \in \mathcal{D}(X) : \delta(s,x) = 1\}$ for each $x \in X$. Then, $d(x,y) = \nu(A_x \Delta A_y)$ holds, since $\delta(x,y) = 0$ if $\delta \notin A_x \Delta A_y$ and $\delta(x,y) = 1$ if $\delta \in A_x \Delta A_y$. This shows, using Lemma 3.5, that (X,d) is L_1-embeddable. ∎

Let $C(X)$ denote the set of all semi-metrics d on X for which (X,d) is L_1-embeddable.

Theorem 3.7 *(i) $C(X)$ is a convex cone.*

(ii) The extremal rays of $C(X)$ are the rays generated by the non zero cut functions δ_Y for $Y \subseteq X$, $\emptyset \neq Y \neq X$.

Proof. The proof of (i) is based on the fact that the direct sum of two L_1-subspaces is again an L_1-subspace. Namely, assume that (X_i,d_i) is a subspace of $L_1(\Omega_i,\mathcal{A}_i,\mu_i)$ for $i=1,2$. Consider their direct sum $(X = X_1 \times X_2, d = d_1 \oplus d_2)$, where $d((x_1,x_2),(y_1,y_2)) = d_1(x_1,y_1) + d_2(x_2,y_2)$ for $x_1,y_1 \in X_1$ and $x_2,y_2 \in X_2$. Let $(\Omega = \Omega_1 \cup \Omega_2, \mathcal{A}, \mu)$ denote the measure space obtained by extending $\mathcal{A}_i$ and μ_i to $\Omega_1 \cup \Omega_2$. If ϕ_i denotes the embedding of (X_i,d_i) into $L_1(\Omega_i,\mathcal{A}_i,\mu_i)$, then we obtain an embedding ϕ of $(X_1 \times X_2, d_1 \oplus d_2)$ into $L_1(\Omega,\mathcal{A},\mu)$ by setting $\phi(x_1,x_2)(\omega) = \phi_i(x_i)(\omega)$ if $\omega \in \Omega_i$, for $i=1,2$. Indeed,

$$\begin{aligned} d_1 \oplus d_2((x_1,x_2),(y_1,y_2)) &= d_1(x_1,y_1) + d_2(x_2,y_2) \\ &= \| \phi_1(x_1) - \phi_1(y_1) \| + \| \phi_2(x_2) - \phi_2(y_2) \| \\ &= \| \phi(x_1,x_2) - \phi(y_1,y_2) \| . \end{aligned}$$

We check that $d_1 + d_2 \in C(X)$ if $d_1, d_2 \in C(X)$. Indeed, if (X,d_1) and (X,d_2) are L_1-embeddable, then $(X, d_1 + d_2)$ is L_1-embeddable, since it is a subspace of $(X \times X, d_1 \oplus d_2)$ (via the embedding $x \longmapsto (x,x)$) which is L_1-embeddable by the previous argument.

We now check (ii). It is easy to see that each cut function lies on an extreme ray of $C(X)$ (it lies, in fact, on an extreme ray of the metric cone). Consider now $d \in C(X)$ which is not a cut function. We can suppose that $d(x_1,x_2) = 1$, $d(x_1,x_3) = \alpha > 0$ and $d(x_2,x_3) = \beta > 0$ for some $x_1,x_2,x_3 \in X$ with $\alpha \geq \beta$. Set $d_1 = \int_{\mathcal{D}(X)} \delta(x_1,x_2)\delta(x_1,x_3)\delta\nu(d\delta)$ and $d_2 = d - d_1$. Then, $d_1, d_2 \in C(X)$ by Theorem 3.6. But $d_1(x_1,x_2) = \frac{1+\alpha-\beta}{2} > 0$, since $2\delta(x_1,x_2)\delta(x_1,x_3) = \delta(x_1,x_2) + \delta(x_1,x_3) - \delta(x_2,x_3)$ for each cut function δ. Also, $d_1(x_2,x_3) = 0$ and $d_2(x_2,x_3) = \beta$. Therefore d does not lie on an extreme ray of $C(X)$ since $d = d_1 + d_2$ where d_1 and d_2 are not proportional to d. ∎

In the case X finite, the following result is an immediate consequence of Theorems 3.3 and 3.6.

THEOREM 3.8 *Let $X = \{1,\ldots,n\}$ be a finite set and let d be a semi-metric on X. The following assertions are equivalent.*

(i) (X,d) is L_1-embeddable.

(ii) (X,d) is ℓ_1-embeddable.

(iii) $d \in Cut_n$.

In fact, even for X infinite, the study of the L_1-embeddable semi-metrics on X can be reduced in some sense to the finite case and thus to the study of the cut cone. Indeed, based on the fact that $C(X)$ is closed for the topology of the pointwise convergence, it was shown in [33] that (X,d) is L_1-embeddable if and only if $(Y,d_{|Y})$ is L_1-embeddable for each finite subset Y of X, where $d_{|Y}$ denotes the restriction of d to the set Y.

Let d be defined on a set X; d is said to be *hypermetric* if its restriction to any finite subset Y of X is hypermetric, i.e. $\sum_{1\leq i<j\leq n} b_ib_jd(x_i,x_j) \leq 0$ for all integers $b_1,\ldots,b_n$ with $\sum_{1\leq i\leq n} b_i = 1$, for all $x_1,\ldots,x_n \in X$ and all $n \geq 1$. Let $Hyp(X)$ denote the set of the hypermetrics d on X. Then, $C(X) \subseteq Hyp(X)$ holds clearly. However, the inclusion is, in general, strict. It is strict, for instance, if $7 \leq |X| < \infty$ or if X is the set of non negative integers.

However, there are many examples of classes of semi-metric spaces (X,d) for which the properties of being hypermetric and L_1-embeddable are equivalent. Such examples are given in section 4; see sections 4.3 and 4.4 for examples with X infinite.

4 Metric properties

In this section, we give a hierarchy of metric properties, together with exemples showing the irreversibility of the one-way implications. Then, we consider three classes of metrics: graphic metrics, metrics from normed spaces, metrics from lattices, for which the hierarchy partially collapses.

4.1 A hierarchy of metric properties

In this section, we consider several metric properties, in particular, hypermetricity, hypercube and ℓ_1-, ℓ_2-embeddability, ultrametricity, the negative type, four point and rigidity conditions. We indicate which implications exist among them.

We first recall some facts about the cut lattice, graphic metrics, ultrametrics and the four point condition.

Let L_n denote the *cut lattice*, consisting of the integer combinations $\sum_S \lambda_S \delta(S)$, λ_S integer, of the cut vectors of K_n. It is easy to check that, for d integral, $d \in L_n$ if and only if d satisfies the following *parity condition*:

$$d_{ij} + d_{ik} + d_{jk} \equiv 0 \pmod 2 \text{ for } i, j, k \in V_n. \tag{19}$$

Therefore, every h-embeddable metric satisfies the above parity condition.

Given a graph $G = (V, E)$, its *path metric* d_G is defined by letting $d_G(i, j)$ denote the length of a shortest path from i to j in G, for $i, j \in V$. If non negative weights w_e are assigned to the edges e of G, the path metric of the weighted graph (G, w) is defined similarly by defining the length of a path as the sum of the weights of its edges. When its path metric is ℓ_1-embeddable, we also say that the graph is an *ℓ_1-graph.* A metric is called *graphic* if it is the path metric of some graph. Specific results on graphic metrics are grouped in section 4.2.

A metric d is called *ultrametric* if it satisfies the condition:

$$d_{ij} \leq \max(d_{ik}, d_{jk}) \tag{20}$$

for all distinct i, j, k, i.e. each triangle is isoceles with the third side shorter or equal to the two others; this implies that any two distinct balls with the same radius are disjoint. See [4] and references there for a description of applications of ultrametric spaces. An important class of ultrametric spaces arises from valuated fields (see e.g. [35]). Let F be a field and let $|.|$ be a non-archimedean valuation on F (e.g. the p-adic valuation on the field of p-adic numbers), i.e. $|.|$ is a map from F to $\mathbb{R}_+$ satisfying:

- $|a| = 0$ if and only if $a = 0$, for $a \in F$,
- $|ab| = |a||b|$ for $a, b \in F$,
- $|a+1| \leq 1$ for all $a \in F$ such that $|a| \leq 1$, or equivalently, $|a+b| \leq \max(|a|, |b|)$ for $a, b \in F$.

Then, $d(a,b) = |a-b|$ defines an ultrametric on F.

Ultrametrics can be represented by weighted trees in the following way (see [4]).

Let $T = (V, E)$ be a rooted tree with root $r \in V$ and let X denote its set of leaves (nodes of degree 1) other than the root. Let $w_e, e \in E$, be non negative weights assigned to the edges of T and let $d_{T,w}$ denote the path metric of the weighted tree (T, w). We suppose that $d_{T,w}(r, x) = h$ for all leaves $x \in X$, for some constant h, called the height of the tree; then, the weighted tree is called a *dendogram* (or *indexed hierarchy*). The *height* $h(v)$ of a node v of T is defined as the length of a shortest path connecting v to a leaf of T. A metric space (X, d_X) is defined on the set X of leaves by defining $d_X(x,y)$ as the height of the first predecessor of the leaves x, y. Then, d_X is ultrametric and, moreover, every ultrametric is of the form d_X for some dendogram.

This tree representation for ultrametrics is used in classification theory, especially in taxonomy (see [88] and references there for details).

We give another connection with weighted trees. The following condition is called the *four point condition*:

$$d_{ij} + d_{kl} \leq \max(d_{ik} + d_{jl}, d_{il} + d_{jk}) \tag{21}$$

for $i, j, k, l \in V_n$. It implies the triangle inequality (1) (for $k = l$).

The metrics satisfying the four point condition (21) are exactly the path metrics of weighted trees (with non negative weights); for this reason, they also called *tree metrics*.

It is easy to see that the condition (20) implies the condition (21), i.e. every ultrametric satisfies the four point condition. Actually, every tree metric can be characterized in terms of an associated ultrametric (see [20]). Given $r \in V_n$ and a constant $c \geq \max(d_{ij} : i, j \in V_n)$, define $d^{(r)}$ by:

$$d_{ij}^{(r)} = c + \frac{1}{2}(d_{ij} - d_{ir} - d_{jr}) \text{ for } i, j \in V_n.$$

Then, d is a tree metric, i.e. satisfies the four point condition (21), if and only if $d^{(r)}$ is ultrametric.

Observe that each ultrametric d is ℓ_2-embeddable (indeed, if d is ultrametric, then d^2 too is ultrametric and, thus, of negative type, implying that d is ℓ_2-embeddable - see Table 1 for the implications). In fact, it is easy to check that:

$$\begin{array}{lcl} d \text{ is ultrametric} & \Longleftrightarrow & d^a \text{ is ultrametric for all } a \in \mathbb{R}_+ \\ & \Longleftrightarrow & d^a \text{ is } \ell_2\text{-embeddable for all } a \in \mathbb{R}_+ \\ & \Longleftrightarrow & d^a \text{ is a metric for all } a \in \mathbb{R}_+. \end{array}$$

The inequality: $\min(m : d \text{ is } \ell_2\text{-embeddable into } \mathbb{R}^m) \leq n - 1$, holds for all ℓ_2-metrics with equality for ultrametrics [100].

We summarize in Table 1 below the implications existing between the various metric properties considered here.

First, we add some examples showing that the one-way implications shown in Table 1 are irreversible, and some additional remarks. P_n denotes the path on n nodes and C_n the cycle on n nodes.

- If d is $2k+1$-gonal, then d is $2k+2$-gonal; if d is $n+3$-gonal, then d is $n+1$-gonal ([46]). Counterexamples to the reverse implications are given in [11].
- The equivalence: d is ℓ_2-embeddable $\Longleftrightarrow d^2 \in Neg_n$, was proved in [144].
- Let d be the path metric of $K_4 - P_3$, then $d \in Cut_n$, but $d^2 \notin Neg_n$; also, d is metrically rigid, but not h-embeddable.
- Let d be the path metric of $K_7 - P_3$, or $K_7 - P_4$, or $K_7 - C_5$, then $d \in Hyp_n$, but $d \notin Cut_n$.
- Let d be the path metric of $K_5 - K_3$, or $K_9 - P_3$, then $d \in Neg_n$, but $d \notin Hyp_n$.
- Let d be the path metric of $K_7 - K_5$, or $K_{11} - P_3$, then d (considered as the symmetric matrix $(d_{ij})_{1 \leq i,j \leq n}$, with $d_{ij} = d_{ji}$ and $d_{ii} = 0$) has exactly one positive eigenvalue, but $d \notin Neg_n$. Note that the path metric of $K_{n+1} - K_{n-1}$, $n \geq 6$, has eigenvalues $2n-1, -1, -2$ with respective multiplicities

1,1,$n-1$ [159]. Also, the path metric of $K_{n+2}-P_3$ has one positive eigenvalue if $n \leq 9$ and two otherwise [18].

• Let d be the path metric of P_3, then $d^2 \in Neg_n$ and d satisfies the four point condition, but d is not ultrametric.

• Let d be the path metric of $K_5 - P_3$, or $K_6 - P_3$, then d is ℓ_1-rigid, but d is not metrically rigid. The path metric of K_4 is ℓ_1-embeddable, but not ℓ_1-rigid.

• Let d be the path metric of $K_6 - P_2$, then $2d \in Cut_n \cap L_n$, but $2d$ is not h-embeddable. The path metric of $K_{2,3}$ is not hypermetric, since it is not 5-gonal.

• For $n = 7, 8$, the path metric of $K_n - P_3$ lies on a simplicial face (in fact, on an extreme ray) of Hyp_n, but it does not lie on a simplicial face of Met_n, i.e. it is not metrically rigid; moreover, it does not belong to Cut_n.

• Let d be the path metric of K_5, then $2d$ is h-embeddable and h-rigid, but not ℓ_1-rigid.

d is ℓ_2 − embeddable	$\Longleftrightarrow$	$d^2 \in Neg_n$	$\Longleftarrow$	d is ultrametric
$\Downarrow$		$\Downarrow$		$\Updownarrow$
d is ℓ_1 − embeddable	$\Longleftrightarrow$	$d \in Cut_n$		$d^a \in Met_n$ for all $a \in \mathbb{R}_+$
		$\Downarrow$		$\Downarrow$
$d \in Met_n$	$\Longleftarrow$	$d \in Hyp_n$		d is the path metric of a weighted tree
		$\Downarrow$		$\Uparrow$
d has one positive eigenvalue	$\Longleftarrow$	$d \in Neg_n$		d is the path metric of a tree
				$\Downarrow$
d is metrically rigid	$\Longleftarrow$	d is the path metric of a bipartite graph	$\Longleftarrow$	d is the path metric of an isometric subgraph of a hypercube
$\Downarrow$				$\Downarrow$
d is ℓ_1 − rigid (if $d \in Cut_n$)		$d \in Cut_n \cap L_n$	$\Longleftarrow$	d is h − embeddable
$\Downarrow$		$\Downarrow$		$\Downarrow$
d is h − rigid (if d is h-embeddable)		$d \in Cut_n$ and d is rational valued	$\Longleftrightarrow$	ηd is h − embeddable for some integer $\eta \geq 1$

Table 1

4.2 Metric properties of graphs

We group here several results on the metric properties of graphs.

A graph $G = (V, E)$ is said to be an *isometric subgraph* of a graph $H = (W, F)$ if there is a map (embedding) f from V to W such that $d_G(i, j) = d_H(f(i), f(j))$ for all nodes i, j of G.

A typical question in the metric theory of graphs is whether G is an isometric subgraph of another graph H, where H has a simpler structure, e.g. H is a hypercube, a half-cube, or a product of complete graphs (see [90], [160]). One of the motivations comes from the applications to the problem of designing addressing schemes for computer communication networks (see [28], [89]).

Recall that the n-dimensional *hypercube* is the graph $(K_2)^n$ (also denoted by $H(n, 2)$) whose node set is $\{0, 1\}^n$ with two nodes $u, v \in \{0, 1\}^n$ adjacent if their Hamming distance is equal to 1. The *half-cube* $\frac{1}{2}H(n, 2)$ has node set $\{u \in \{0, 1\}^n : \sum_{1 \leq i \leq n} u_i$ is even $\}$ with two nodes adjacent if their Hamming distance is equal to 2. The *cocktail party* graph $K_{n \times 2}$ has $2n$ nodes: $1, \ldots, 2n$ and its edges are all pairs except the n pairs $(i, i + n)$ for $1 \leq i \leq n$.

It is clear from the definition that, for a graph G, its path metric d_G is h-embeddable if and only if G is an isometric subgraph of some hypercube. Also, d_G is ℓ_1-embeddable with scale 2, i.e. $2d_G$ is h-embeddable, if and only if G is an isometric subgraph of some half-cube. Note that, if d is the path metric of the cocktail party graph $K_{n \times 2}$ and $n \geq 5$, then $2d \in Cut_{2n}$ (so $K_{n \times 2}$ is an ℓ_1-graph), $2d \in L_{2n}$, but $2d$ is not h-embeddable.

The question of isometric embedding is directly linked to the problematic of cuts; namely, by Theorem 3.4, G is an isometric subgraph of a hypercube if and only if its path metric d_G can be written as a non negative integer combination of cut vectors.

The following results are known for graphic metrics.

THEOREM 4.1 *The graph G is an isometric subgraph of a hypercube if and only if G is bipartite and, for all nodes a, b of G, the set $G(a, b) := \{u \in V : d_G(u, a) < d_G(u, b)\}$ is closed under taking shortest paths ([70]), or equivalently, if and only if G is bipartite and d_G is 5-gonal ([14]).*

THEOREM 4.2 *Let G be a bipartite graph. The following properties are equivalent [141]:*

- *d_G is h-embeddable,*

- *d_G is ℓ_1-embeddable,*
- *d_G is hypermetric,*
- *d_G is 5-gonal,*
- *d_G is of negative type,*
- *d_G (as symmetric matrix with zero on its diagonal) has exactly one positive eigenvalue.*

Moreover, every bipartite graph is metrically rigid [122], implying that every isometric subgraph of the hypercube is ℓ_1-rigid [62].

Theorem 4.3 *[149]*

(i) G is an ℓ_1-graph if and only if G is an isometric subgraph of a cartesian product of half-cubes and cocktail party graphs.

(ii) If G is an ℓ_1-graph on n nodes, then its scale η is equal to 1, or is even with $\eta \leq n-1$. Moreover, if G is ℓ_1-rigid, then its scale η is equal to 1, or 2.

Theorem 4.4 *[154] Let G be a graph. Then its path metric d_G is hypermetric if and only if G is an isometric subgraph of a cartesian product of half-cubes, cocktail party graphs and copies of the Gosset graph G_{56}. (The Gosset graph G_{56} is a graph on 56 nodes arising as the 1-skeleton of the Gosset polytope 3_{21} [34].)*

The following result gives a characterization of ℓ_1-graphs within the class of graphs having a universal node. Given a graph G, ∇G denotes the graph obtained by adding a node adjacent to all nodes of G. So the path metric of ∇G takes only the values 1,2.

Theorem 4.5 *[9] Let G be a connected graph on n nodes. The following assertions are equivalent:*

- *∇G is an ℓ_1-graph.*
- *G is an induced subgraph of a cocktail party graph, or G is a line graph (i.e. G does not contain any of nine given graphs [26]).*

Moreover, if $n \geq 37$, then ∇G is an ℓ_1-graph if and only if its path metric is 5-gonal and of negative type; if $n \geq 28$, then ∇G is an ℓ_1-graph if and only if its path metric is hypermetric.

THEOREM 4.6 *[50] Let G be a regular graph of diameter 2. The following assertions are equivalent:*

(i) d_G is of negative type,

(ii) d_G is hypermetric,

(iii) $d_{\nabla G}$ is of negative type,

(iv) the minimum eigenvalue of the adjacency matrix of G is greater or equal to -2.

Moreover, the path metric d_G of a regular graph G of diameter 2 is hypermetric if and only if $G = K_{n\times 2}$ for some integer n, or G is an isometric subgraph of a half-cube, or d_G lies on an extreme ray of the hypermetric cone.

The classification of hypermetricity, ℓ_1-embeddability, and ℓ_1-rigidity was done for many classes of regular graphs (see, in particular, [50], [62], [113]).

The following result is an analogue of Theorems 4.5 and 4.6 for the class of (non necessarily graphic) metrics with values $1, 2, 3$.

THEOREM 4.7 *(i) [10] Let d be a metric with values in $\{1,2\}$. Then, d is h-embeddable if and only if d is 5-gonal and satisfies (19), or equivalently, if and only if d is the path metric of $K_{1,n-1}$, $K_{2,2}$, or $\frac{d}{2}$ is the path metric of K_n.*

(ii) [15] Let d be a metric on $n \geq 9$ points with values in $\{1,2,3\}$ and satisfying (19). The following assertions are equivalent:

- *d is h-embeddable,*
- *d is ℓ_1-embeddable,*
- *d is hypermetric,*
- *d is 11-gonal.*

In [59], a characterization of h-embeddability is given for a larger class of metrics including those whose values are all odd, or equal to 2.

We mention another application of isometric subgraphs of the cube in terms of oriented matroids.

Theorem 4.8 *[85] A graph G is isomorphic to the tope graph of an oriented matroid of rank at most three if and only if G is planar, isometrically embeddable in some hypercube, and antipodal (i.e. for each vertex v, there is a unique vertex v^* which is not closer to v than any neighboor of v^*).*

Finally, we mention a characterization of trees within ℓ_1-graphs, using the notion of minimum size.

Proposition 4.9 *[52] Let G be an ℓ_1-graph and let $s(d_G)$ denote the minimum size of its path metric. Then, $2 - \frac{1}{\lceil \frac{n}{2} \rceil} \leq s(d_G) \leq n-1$. Equality holds in the lower bound if and only if $G = K_n$ and in the upper bound if and only if G is a tree.*

Note also that, for $d \in Cut_n$, equality holds in the upper bound of (13), i.e. $s(d) = \frac{\sum_{1 \leq i < j \leq n} d_{ij}}{n-1}$, if and only if d is the path metric of a weighted star $K_{1,n-1}$.

4.3 L_1-metrics from normed spaces

A convex polytope is called a *zonotope* if it is the vector sum of some line segments. A convex body which can be approximated by zonotopes with respect to the Hausdorff metric is called a *zonoid*. Zonotopes and zonoids are central objects in convex geometry and they are also relevant to many other fields (see e.g. [143] for a survey). They are, in particular, relevant to the topic of L_1-metrics as we now explain.

We first recall some definitions.

Let K be a convex body (i.e. a convex compact set) in $\mathbb{R}^d$, K is centered if it has a center of symmetry. Its *support function* is defined by:

$$h(K,x) = \max(x^T y : y \in K)$$

for $x \in \mathbb{R}^d$. It is easy to see that, if K is a centered convex body, then $\| x \| := h(K,x)$ defines a norm on $\mathbb{R}^d$ with K^* as unit ball. Conversely, every norm $\| . \|$ on $\mathbb{R}^d$ is of the form $h(K,.)$, where K is the polar of the unit ball. Each norm $\| . \|$ on $\mathbb{R}^d$ defines a metric $d_{\|.\|}$ on $\mathbb{R}^d$, called *norm* (or *Minkowski*) *metric*, by setting $d_{\|.\|}(x,y) = \| x - y \|$. The following results give several equivalent characterizations for L_1-embeddable normed spaces.

THEOREM 4.10 *(see [1], [6], [143]). Let* $\| \, . \, \|$ *be a norm on* $\mathbb{R}^d$ *and let* U *be its unit ball. The following assertions are equivalent:*

(i) $d_{\|.\|}$ *is of negative type.*

(ii) $d_{\|.\|}$ *is hypermetric.*

(iii) $(\mathbb{R}^d, d_{\|.\|})$ *is* L_1*-embeddable.*

(iv) The polar of U *is a zonoid, i.e.* $\| \, . \, \| = h(U^*, .)$ *is the support function of a zonoid.*

(v) There exists a positive Borel measure μ *on the hyperplanesets of* $\mathbb{R}^d$ *such that the norm* $\| \, . \, \|$ *is defined by the following formula (called* Crofton formula*):*

$$\| x - y \| = \mu([[x, y]])$$

where $[[x, y]]$ *denotes the set of hyperplanes meeting the segment* $[x, y]$*.*

THEOREM 4.11 *(see [6], [143]). Let* $\| \, . \, \|$ *be a norm on* $\mathbb{R}^d$ *for which the unit ball* U *is a polytope. The following assertions are equivalent:*

(i) $\| \, . \, \|$ *satisfies the Hlawkla inequality:*

$$\| x \| + \| y \| + \| z \| + \| x + y + z \| \geq \| x + y \| + \| x + z \| + \| y + z \|$$

for all $x, y, z \in \mathbb{R}^d$*.*

(ii) $d_{\|.\|}$ *is 7-gonal.*

(iii) The polar of U *is a zonotope.*

(iv) $(\mathbb{R}^d, d_{\|.\|})$ *is* L_1*-embeddable.*

These results can be partially extended to the more general concept of projective metrics. A continuous metric d on $\mathbb{R}^d$ is called a *projective metric* if it satisfies $d(x, z) = d(x, y) + d(y, z)$ for any collinear points x, y, z lying in that order on a common line. Clearly, every norm metric is projective. The cone of projective metrics is the object considered by the unsolved fourth Hilbert problem in $\mathbb{R}^n$ (see [1], [3]).

We have the following characterization of L_1-embeddability for projective metrics.

THEOREM 4.12 *[1] Let d be a projective metric on $\mathbb{R}^d$. The following assertions are equivalent:*

(i) d is hypermetric.

(ii) There exists a positive Borel measure μ on the hyperplanesets of $\mathbb{R}^d$ satisfying

$$\begin{array}{rl} \mu([[x]]) = 0 & \textit{for all } x \in \mathbb{R}^d \\ 0 < \mu([[x,y]]) < \infty & \textit{for all } x \neq y \in \mathbb{R}^d \end{array}$$

such that $d(x,y) = \mu([[x,y]])$ for $x, y \in \mathbb{R}^d$. (As in Theorem 4.10, $[[x,y]]$ is the set of hyperplanes that meet the segment $[x,y]$).

(iii) $(\mathbb{R}^d, d)$ is L_1-embeddable (namely, $d(x,y) = \mu([[x,y]]) = \mu([[0,x]]\Delta[[0,y]])$).

Remark that, for $d = 2$, Theorem 4.12 (ii) always holds, i.e. every projective metric on $\mathbb{R}^2$ is L_1-embeddable. On the other hand, the projective metric arising from the norm $\| x \| = \max(|x_1|, |x_2|, |x_3|)$ in $\mathbb{R}^3$ is not even hypermetric (it is not 5-gonal).

4.4 L_1-metrics from lattices

We give in this section results on the metrics arising from lattices. A good reference on lattices is [27].

Let $(L, \preceq)$ be a lattice (possibly infinite), i.e. a partially ordered set in which any two elements $x, y \in L$ have a join $x \vee y$ and a meet $x \wedge y$. A *valuation* on L is a function $v : L \longrightarrow \mathbb{R}_+$ satisfying

$$v(x \vee y) + v(x \wedge y) = v(x) + v(y)$$

for all $x, y \in L$. The valuation v is *isotone* if $v(x) \leq v(y)$ whenever $x \preceq y$ and it is *positive* if $v(x) < v(y)$ whenever $x \preceq y, x \neq y$. Set

$$d_v(x,y) = v(x \vee y) - v(x \wedge y)$$

for $x, y \in L$. Then, (L, d_v) is a semi-metric space if v is an isotone valuation on L and (L, d_v) is a metric space if v is a positive valuation on L; in the latter case, L is called a *metric lattice* (see [27]). Clearly, every metric lattice is *modular*, i.e. satisfies: $x \wedge (y \vee z) = (x \wedge y) \vee z$ for all x, y, z with $z \preceq x$. A lattice is called *distributive* if $x \wedge (y \vee z) = (x \wedge y) \vee (x \wedge z)$ for all x, y, z. The metric lattices which are distributive are characterized in [111]:

THEOREM 4.13 *Let L be a metric lattice with positive valuation v. The following assertions are equivalent:*

(i) L is a distributive lattice.

(ii) (L, d_v) is 5-gonal.

(iii) (L, d_v) is hypermetric.

(iv) (L, d_v) is L_1-embeddable.

PROOF. It suffices to show the implications $(ii) \Rightarrow (i)$ and $(i) \Rightarrow (iv)$.

$(ii) \Rightarrow (i)$. Using the definition of the valuation v and applying the 5-gonal inequality to the points $t_1 = x \vee y$, $t_2 = x \wedge y$, $t_3 = z$, $s_1 = x$, $s_2 = y$, we obtain the inequality: $2(v(x \vee y \vee z) - v(x \wedge y \wedge z)) \leq v(x \vee y) + v(x \vee z) + v(y \vee z) - v(x \wedge y) - v(x \wedge z) - v(y \wedge z)$. By applying again the 5-gonal inequality to the points $t_1 = x$, $t_2 = y$, $t_3 = z$, $s_1 = x \vee y$, $s_2 = x \wedge y$, we obtain the reverse inequality. Therefore, the equality holds in the above inequality. In fact, this condition of equality is equivalent to L being distributive (see [27]).

$(i) \Rightarrow (iv)$. Take a finite subset L_0 of L. We show that (L_0, d_v) is L_1-embeddable. Let K be the sublattice of L generated by L_0. Suppose K has length n. Then, K is isomorphic to a ring $\mathcal{N}$ of subsets of a set X, $|X| = n$ ("ring" means closed under $\cup$ and $\cap$). Via this isomorphism, we have a valuation, again denoted by v, defined on $\mathcal{N}$. We can assume without loss of generality that $v(\emptyset) = 0$. Then, v can be extended to a valuation v^* on 2^X satisfying: $v^*(S) = \sum_{x \in S} v^*(\{x\})$ for $S \subseteq X$. Now, if $x \longmapsto S_x$ is the isomorphism from K to $\mathcal{N}$, then we have the embedding $x \longmapsto S_x$ from (L_0, d_v) to $(2^X, v^*)$ which is isometric. Indeed, $d_v(x, y) = v(x \vee y) - v(x \wedge y) = v(S_x \cup S_y) - v(S_x \cap S_y) = v^*(S_x \cup S_y) - v^*(S_x \cap S_y) = v^*(S_x \Delta S_y)$. This shows that every finite subset of (L, d_v) is L_1-embeddable, and thus (L, d_v) is L_1-embeddable. ∎

The following example was given in [5]. Let L be the set of positive integers with order relation $x \preceq y$ if x divides y. Then, $x \wedge y$ is the g.c.d. of x and y, $x \vee y$ is their l.c.m. and $(L, \preceq)$ is a distributive lattice. Hence, (L, d_v) is L_1-embeddable for every positive valuation v on L. For instance, $v(x) = \log x$ is a positive valuation on L, hence $d_v(x, y) = \log(\frac{l.c.m.(x,y)}{g.c.d.(x,y)})$ is L_1-embeddable.

The following result was proved in [5], [6]; it implies Theorem 4.13.

Theorem 4.14 *Let $(S, \vee)$ be a commutative semi-group. Given $v : S \longmapsto \mathbb{R}$, set $d_v(x,y) = 2v(x \vee y) - v(x \vee x) - v(y \vee y)$ for $x, y \in S$. Suppose that, either S is a group, or $x \vee \ldots \vee x = x$ for all $x \in S$, where the join $x \vee \ldots \vee x$ is repeated $2n$ times, for some integer $n \geq 1$. Then, the following assertions are equivalent:*

(i) (S, d_v) is L_1-embeddable.

(ii) (S, d_v) is of negative type.

This result applies, in particular, to the case when S is a subset of a lattice L which is stable under the join operation $\vee$ of L and contains the least element of L. Therefore, when applied to $S = L$, it gives that, for a metric lattice L, (L, d_v) is of negative type if and only if (L, d_v) is L_1-embeddable.

5 Applications in combinatorial optimization

5.1 The maximum cut problem

Given a graph $G = (V_n, E)$ and non negative 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 [87]. If we replace "as large" by "as small", then we obtain the min-cut problem which can be solved using network flow techniques [84]. 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 [96], for graphs not contractible to K_5 [21], 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 C of $G\}$ has all its vertices integral [95]. In fact, the class of weakly bipartite graphs includes the graphs not contractible to K_5 ([83], or [136]).

For definitions of the terms used in this section, see e.g. [94], [145].

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

$$\begin{array}{ll} \max & w^T x \\ \text{subject to} & x \in CutP(G). \end{array}$$

This is the polyhedral approach, classical in combinatorial optimization, which leads to the study of the facets of $CutP(G)$. This approach has been used in practice for solving large instances of the max-cut problem (see e.g. [23], [24]). 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, $CutP(G) = Met(G)$, i.e. the inequalities

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

are sufficient for describing $CutP(G)$, if and only if G is not contractible to K_5 [25]. 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 [25].

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

$$\begin{array}{ll} \max & w^T x \\ \text{subject to} & x \in CutP_n \end{array}$$

after setting $w_e = 0$ if e is not an edge of G. This permits to fully exploit 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 [23] for a detailed description of these two applications, together with a computational treatment. In fact, the spin glass problem was already mentioned in [127] as an optimization problem over the boolean quadric polytope.

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

$$\begin{array}{ll} \max & \sum_{1 \leq i \leq j \leq n} c_{ij} x_i x_j \\ \text{subject to} & x \in \{0, 1\}^n \end{array}$$

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

$$\begin{array}{ll} \max & c^T p \\ \text{subject to} & p \in BQP_n. \end{array}$$

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 section

2.4), the max-cut problem and the unconstrained quadratic programming problem are equivalent.

Other approaches, beside the polyhedral approach, have been proposed for attacking the max-cut problem. In particular, an approach based on eigenvalue methods is investigated in [45], [138]. 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 $L_{ii} = deg_G(i)$ for $i \in V_n$ and $L_{ij} = -a_{ij}$ for $i \neq j \in V_n$, where $A = (a_{ij})_{1 \leq i,j \leq n}$ is the adjacency matrix of G. Set

$$\varphi(G) = \frac{n}{4} \min(\lambda_{max}(L + diag(u)) : u \in \mathbb{R}^n, \sum_{1 \leq i \leq n} u_i = 0)$$

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

$$\psi(G) = \max(\frac{1}{2} Trace(AY) : \frac{1}{2} J - Y \, is \text{ positive semi definite and } Y_{ii} = 0 \text{ for } 1 \leq i \leq n)$$

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) $mc(G) \leq \varphi(G)$ [45]

(ii) $mc(G) \leq \psi(G)$ [146]

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

$$\psi(G) = \max(\sum_{1 \leq i < j \leq n} a_{ij} x_{ij} : x \text{ satisfies the inequalities (22) for all integers } b_1, \ldots, b_n),$$

$$\sum_{1 \leq i < j \leq n} b_i b_j x_{ij} \leq \frac{(\sum_{1 \leq i \leq n} b_i)^2}{4} \tag{22}$$

The inequalities (22) are clearly valid for the cut polytope $CutP_n$, but they are never facet defining since they are dominated by the gap inequalities (5) (defined in section 2.2).

In fact, using general duality theory, it is shown that $\varphi(G) = \psi(G)$ holds by [137].

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

$$\sum_{P\in\mathcal{P},e\in P} f_P \le c_e \text{ for } e \in E,$$

$$\sum_{P\in\mathcal{P}_{st}} f_P \ge r_{st} \text{ for } (s,t) \in U.$$

Using Farkas lemma, it can be checked that:

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

$$C(G,H) = \{(y,z) \in \mathbb{R}_+^E \times \mathbb{R}_+^U : \sum_{e\in P} y_e - z_{st} \ge 0 \textit{ for } P \in \mathcal{P}_{st} \textit{ and } (s,t) \in U\}.$$

The cone $C(G, H)$ is studied in detail in [109] 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 [103], [130], restated in [123], [124]).

THEOREM 5.2 *The pair (c, r) is feasible if and only if*

$$(c - r)^T d \ge 0 \textit{ for all } d \in Met_n. \tag{23}$$

Therefore, the metric cone 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 $\min((c - r)^T d : d \in Met_n)$ which has $\binom{n}{2}$ variables and $3\binom{n}{3}$

constraints (the triangle inequalities (1)). An alternative way is to check the condition (23) for all extreme rays d of Met_n. This approach leads to the study of the extreme rays of the metric cone Met_n (see references on it in section 2.4).

There are other variants of the Japanese theorem, in particular, in the more general setting of binary matroids (see [148]). In particular, the metric cone $Met(G)$ (defined in relation (11)) arises naturally when studying multicommodity flows. It is shown in [148] that all extreme rays of $Met(G)$ are $0,1$-valued (i.e. $Met(G) = Cut(G)$) if and only if G is not contractible to K_5. The graphs for which all extreme rays of $Met(G)$ are $0,1,2$-valued are characterized in [147]. The graphs for which all the vertices of the metric polytope $MetP(G)$ (defined in relation (12)) are $\frac{1}{3}$-integral are studied in [119] (x is said to be $\frac{1}{3}$-integral if $3x$ is integral).

Since the cut cone Cut_n is contained in the metric cone Met_n, a necessary condition for the existence of a feasible multiflow is the following *cut condition*:

$$\sum_{e \in \delta(S)} (c_e - r_e) \geq 0 \text{ for all } S \subseteq V_n. \tag{24}$$

The well known Ford-Fulkerson theorem [84] 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 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 (24) holds [132]. Moreover, if c, r are integral, $(c - r)^T \delta(S)$ is even for all cuts and (24) holds, then there exists an integral multiflow (see [124] and references there).*

Theorem 5.4 *[108], [110]. 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 multiflow if and only if (23) holds or, equivalently, if and only if (24) 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 [16]. Given a semi metric d on V_n, an *extremal graph* ([123], [124]) 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 $d_{sx} + d_{xy} + d_{yt} = d_{st}$, 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 multiflows.

Proposition 5.5 *([123], [124]). The pair (c, r) is feasible if and only if $(c-r)^T d \geq 0$ holds for all $d \in Met_n$ 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 *[107] If $d \in Met_n$ has an extremal graph which is K_4, C_5, or a union of two stars, then $d \in Cut_n$. Moreover, if d satisfies the parity condition (19), 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 multiflow problem* consists of finding a multiflow 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 [109]; in particular, the demand graphs H for which all vertices of $P(G,H)$ are $\frac{1}{4}$-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 [30], 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 $\mu(A_1 \cup \ldots A_n)$?

It is easy to see that the answer is:

$$\max(p_1,\ldots,p_n) \leq \mu(A_1 \cup \ldots A_n) \leq \min(1, \sum_{1\leq i\leq n} p_i).$$

More generally, let $\mathcal{I}$ be a collection of subsets of $\{1,\ldots,n\}$.

Suppose we are given the values of the joint probabilities $p_I = \mu(\cap_{i\in I} A_i)$, for all $I \in \mathcal{I}$. What is the best estimation of $\mu(A_1 \cup \ldots \cup A_n)$ in terms of the p_I's ?

In fact, the answer to this problem is given by the facet defining inequalities for the polytope $BQP_n^{\mathcal{I}}$ (defined in section 2.4). Namely,

$$\mu(A_1 \cup \ldots \cup A_n) \geq \max(w^T p : w^T z \leq 1 \text{ is facet defining for } BQP_n^{\mathcal{I}})$$

(see Proposition 5.8 and relation (29)). In particular, when $\mathcal{I}$ consists of all pairs and singletons, then the lower bound for $\mu(A_1 \cup \ldots \cup A_n)$ is in terms of the facets of the boolean quadric polytope BQP_n.

Estimations for $\mu(A_1 \cup \ldots \cup A_n)$ via linear programming.

First, we observe that Theorem 3.2 remains valid for the polytope $BQP_n^{\mathcal{I}}$, for an arbitrary non empty set family $\mathcal{I}$.

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

(i) $p \in BQ_n^{\mathcal{I}}$ (resp. $p \in BQP_n^{\mathcal{I}}$).

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

PROOF. It is identical to that of Theorem 3.2. ∎

Given $p \in BQ_n^{\mathcal{I}}$, consider the following two linear programming problems.

$$\begin{array}{lll} \text{minimize} & \sum_{\emptyset\neq S\subseteq\{1,\ldots,n\}} \lambda_S & \\ \text{subject to} & \sum_{\emptyset\neq S\subseteq\{1,\ldots,n\}} \lambda_S \pi^{\mathcal{I}}(S) = p & \\ & \lambda_S \geq 0 & \text{for } \emptyset \neq S \subseteq \{1,\ldots,n\} \end{array} \qquad (25)$$

$$\begin{array}{lll} \text{maximize} & \sum_{\emptyset\neq S\subseteq\{1,\ldots,n\}} \lambda_S & \\ \text{subject to} & \sum_{\emptyset\neq S\subseteq\{1,\ldots,n\}} \lambda_S \pi^{\mathcal{I}}(S) = p & \\ & \lambda_S \geq 0 & \text{for } \emptyset\neq S\subseteq\{1,\ldots,n\} \end{array} \tag{26}$$

Let z_{min} (resp. z_{max}) denote the optimum value of the program (25) (resp. (26)).

So, the program (25) (resp. (26)) is evaluating the minimum value (resp. the maximum value) of $\sum_S \lambda_S$ for a decomposition $p = \sum_S \lambda_S \pi^{\mathcal{I}}(S)$, $\lambda_S \geq 0$, of $p \in BQ_n^{\mathcal{I}}$. In particular, in the case $\mathcal{I} = \mathcal{I}_{\leq 2}$, if we set $d = \varphi_{c_0}^{-1}(p)$, then $d \in Cut_{n+1}$ and z_{min} coincides with the minimum size $s(d)$ (defined in section 2.5). This approach, in the case of $\mathcal{I}_{\leq 2}$, is considered in [114], [135].

PROPOSITION 5.8 $z_{min} \leq \mu(A_1 \cup \ldots \cup A_n) \leq z_{max}$.

PROOF. For $S \subseteq \{1,\ldots,n\}$, set $A^S = \bigcap_{i\in S} A_i \cap \bigcap_{i\notin S}(\Omega - A_i)$. Then, $\cap_{i\in I} A_i = \cup_{I\subseteq S\subseteq\{1,\ldots,n\}} A^S$, $\Omega = \cup_S A^S$ and $A_1 \cup \ldots A_n = \cup_{S\neq\emptyset} A^S$. We have $p_I = \mu(\cap_{i\in I} A_i)$ for each $I \in \mathcal{I}$. Therefore, $p = \sum_{S\neq\emptyset} \mu(A^S)\pi^{\mathcal{I}}(S)$ 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 (25), or (26), with objective value $\mu(A_1 \cup \ldots \cup A_n)$. This proves the result. ∎

The dual programs to (25) and (26) are the following programs (27) and (28), respectively.

$$\begin{array}{lll} \text{maximize} & w^T p & \\ \text{subject to} & w^T \pi^{\mathcal{I}}(S) \leq 1 & \text{for } \emptyset\neq S\subseteq\{1,\ldots,n\} \end{array} \tag{27}$$

$$\begin{array}{lll} \text{minimize} & w^T p & \\ \text{subject to} & w^T \pi^{\mathcal{I}}(S) \geq 1 & \text{for } \emptyset\neq S\subseteq\{1,\ldots,n\} \end{array} \tag{28}$$

By linear programming duality, we have:

$$z_{min} = \max(w^T p : w^T z \leq 1 \text{ is a valid inequality for } BQP_n^{\mathcal{I}}) \tag{29}$$

and it is easily verified that, in relation (29), it is sufficient to consider facet defining inequalities. Similarly,

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

(The latter polytope is distinct from $BQP_n^{\mathcal{I}}$ since it does not contain the origin).

Therefore, by (29), every valid inequality for $BQP_n^{\mathcal{I}}$ yields a lower bound for $\mu(A_1 \cup \ldots \cup A_n)$ in terms of the joint probabilities $p_I = \mu(\cap_{i \in I} A_i)$ 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 [32]. The following estimations for $\mu(A_1 \cup \ldots \cup A_n)$ are given there:

$$y_{min} \leq \mu(A_1 \cup \ldots \cup A_n) \leq y_{max} \tag{30}$$

where y_{min} is the optimum value of the linear program (31) below and y_{max} is the optimum value of (32) below, setting $S_k = \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq n} \mu(A_{i_1} \cap A_{i_2} \cap \ldots \cap A_{i_k})$ for $1 \leq k \leq n$.

$$\begin{array}{lll} \text{minimize} & \sum_{1 \leq i \leq n} v_i & \\ \text{subject to} & \sum_{1 \leq i \leq n} \binom{i}{k} v_i = S_k & \text{for } 1 \leq k \leq m \\ & v_i \geq 0 & \text{for } 1 \leq i \leq n \end{array} \tag{31}$$

$$\begin{array}{lll} \text{maximize} & \sum_{1 \leq i \leq n} v_i & \\ \text{subject to} & \sum_{1 \leq i \leq n} \binom{i}{k} v_i = S_k & \text{for } 1 \leq k \leq m \\ & v_i \geq 0 & \text{for } 1 \leq i \leq n \end{array} \tag{32}$$

In fact, the programs (25), (26) give sharper bounds than the programs (31), (32), respectively. Namely, we have:

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

Proof. Indeed, every feasible solution for (25) yields a feasible solution for (31) with the same objective value. Namely, let $(\lambda_S, \emptyset \neq S \subseteq \{1, \ldots, n\})$ be a feasible solution for (25), i.e. $\lambda_S \geq 0$ and $p = \sum_S \lambda_S \pi^{\mathcal{I}_{\leq m}}(S)$. Set $v_i = \sum_{S:|S|=i} \lambda_S$ for $1 \leq i \leq n$. Then,

$$\begin{aligned}
\sum_{1\le i\le n} \binom{i}{k} v_i &= \sum_{1\le i\le n} \binom{i}{k} \sum_{S:|S|=i} \lambda_S \\
&= \sum_{1\le i_1<\ldots<i_k\le n} \sum_{S:i_1,\ldots,i_k\in S} \lambda_S \\
&= \sum_{1\le i_1<\ldots<i_k\le n} p_{\{i_1,\ldots,i_k\}} \\
&= \sum_{1\le i_1<\ldots<i_k\le n} \mu(A_{i_1}\cap\ldots\cap A_{i_k}) \\
&= S_k.
\end{aligned}$$

Therefore, $(v_1,\ldots,v_n)$ is a feasible solution for (31) with $\sum_{1\le i\le n} v_i = \sum_S \lambda_S$. This shows that $y_{min} \le z_{min}$. The inequality $z_{max} \le y_{max}$ follows from the same argument. ∎

Examples of bounds for $\mu(A_1\cup\ldots\cup A_n)$. The best lower bound for $\mu(A_1\cup\ldots\cup A_n)$ is given by z_{min}, defined by relation (29), whose evaluation relies on the knowledge of the facets of the polytope $BQP_n^{\mathcal{I}}$. In the case $\mathcal{I} = \mathcal{I}_{\le 2}$, the facet structure of the boolean quadric polytope 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 BQP_n, together with the lower bounds they yield for $\mu(A_1\cup\ldots\cup A_n)$.

First, note that, if $p = \sum_S \lambda_S \pi(S)$ with $\lambda_S \ge 0$, then $n\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij} = \sum_S \lambda_S |S|(n+1-|S|)$, where $n \le |S|(n+1-|S|) \le \lfloor\frac{n+1}{2}\rfloor\lceil\frac{n+1}{2}\rceil$ if $S\ne\emptyset$. Hence, we have:

$$\begin{aligned}
\frac{n\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij}}{\lfloor\frac{n+1}{2}\rfloor\lceil\frac{n+1}{2}\rceil} &\le \sum_{\emptyset\ne S\subseteq\{1,\ldots,n\}} \lambda_S \\
\frac{n\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij}}{n} &\ge \sum_{\emptyset\ne S\subseteq\{1,\ldots,n\}} \lambda_S
\end{aligned} \tag{33}$$

and, therefore, from the definition of z_{min}, z_{max} and from Proposition 5.8,

$$\frac{n\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij}}{\lfloor\frac{n+1}{2}\rfloor\lceil\frac{n+1}{2}\rceil} \le \mu(A_1\cup\ldots\cup A_n) \le \frac{n\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij}}{n}. \tag{34}$$

Note that the inequalities equivalent to (33) in the context of the cut cone are the bounds on the minimum size of $d \in Cut_{n+1}$ given in (13).

The inequality:

$$2k\sum_{1\le i\le n} p_i - 2\sum_{1\le i<j\le n} p_{ij} \le k(k+1) \tag{35}$$

is valid for the boolean quadric polytope 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 $b_1 = \ldots = b_n = 1$, the inequality (35) corresponds (via the covariance map) to the inequality:

$$\sum_{0 \leq i < j \leq n} b_i b_j x_{ij} \leq k(k+1) \tag{36}$$

which is valid for the cut polytope $CutP_{n+1}$; (36) is a switching of the hypermetric inequality $Hyp_{n+1}(2k+1-n, 1, \ldots, 1, -1, \ldots, -1)$ (with $n-k$ coefficients +1 and k coefficients -1). (See e.g. [60].) Therefore, we have the following lower bound for $\mu(A_1 \cup \ldots \cup A_n)$:

$$\frac{2}{k+1} \sum_{1 \leq i \leq n} p_i - \frac{2}{k(k+1)} \sum_{1 \leq i < j \leq n} p_{ij} \leq \mu(A_1 \cup \ldots \cup A_n) \tag{37}$$

for each k, $1 \leq k \leq n-1$; it was found independently by several authors, including [36], [44], [86]. Note that (37) coincides with the lower bound of (34) in the case $n = 2k$.

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

$$\sum_{1 \leq i \leq n} b_i(2k+1-b_i)p_i - 2 \sum_{1 \leq i < j \leq n} b_i b_j p_{ij} \leq k(k+1) \tag{38}$$

is valid for BQP_n. This yields the bound:

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

The programs (31), (32) provide weaker bounds than the programs (25), (26), but they present the advantage of being easier to handle, especially for small values of m. Exploiting their special structure, the bounds y_{min} and y_{max} were explicitely described in [32] in terms of the S_k's (defined in relation (30)).

Let M denote the matrix corresponding to the program (25) or (26). its columns are the n vectors a_i, where $a_i = (\binom{i}{1}, \binom{i}{2}, \ldots, \binom{i}{m})$, for $1 \leq i \leq n$.

Set $b = (S_1, \ldots, S_m)$. 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 $y = 1_m^T M_B^{-1}$ is feasible for the dual program of (31), 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 $1_B^T M_B^{-1} b \leq \mu(A_1 \cup \ldots \cup A_n)$ holds. The dual feasible bases are explicitely described in [32] together with the corresponding bounds for $\mu(A_1 \cup \ldots \cup A_n)$.

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

$$\mu(A_1 \cup \ldots \cup A_n) \geq S_1 - S_2 + S_3 - S_4 \ldots + (-1)^{m-1} S_m$$

which was first given in [29]. For $m = 2$, this is the special case $k = 1$ of the bound (37); another choice of basis yields the general bound (37).

In fact, the method from [32] also works for finding estimates of the probabilities $\mu(\{\nu \geq r\})$ and $\mu(\{\nu = r\})$, where ν denotes the random variable counting the number of events that occur among $A_1, \ldots, A_n$.

The inequality (38) can alternatively be written as

$$(\sum_{1 \leq i \leq n} b_i p_i - k)(\sum_{1 \leq i \leq n} b_i p_i - k - 1) \geq 0 \qquad (39)$$

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 under this form by many authors (e.g. [79], [114], [127], [135], [161]). This suggests naturally the following generalization of the inequality (39) in the case $\mathcal{I}_{\leq m}$, when m is an even integer. Given integers $b_1, \ldots, b_n$ and $k_1, \ldots, k_m \geq 0$, the inequality

$$\prod_{1 \leq l \leq m} (\sum_{1 \leq i \leq n} b_i p_i - k_l)(\sum_{1 \leq i \leq n} b_i p_i - k_l - 1) \geq 0 \qquad (40)$$

is clearly valid for the polytope $BQP_n^{\mathcal{I}_{\leq 2m}}$. Thus arises the question of determining the parameters $b_1, \ldots, b_n, k_1, \ldots, k_m$ for which (40) defines a facet of $BQP_n^{\mathcal{I}_{\leq 2m}}$. 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 [42], [55].

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

$$\sum_{1 \le i < j \le n} b_i b_j x_{ij} \le 0 \text{ for } b_1, \ldots, b_n \text{ integers with } \sum_{1 \le i \le n} b_i = 1. \qquad (41)$$

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 section 4.4. 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 $\sum_{0 \le i \le m} z_i = 1$ and $v = \sum_{0 \le i \le m} z_i v_i$. 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:

- $\| v - c \|_2 \ge r$ holds for all $v \in L$,
- $S \cap L$ 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 α_n, hypercube γ_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 β_n and γ_n are centrally symmetric, α_n is asymmetric. All types of L-polytopes in dimension $k \leq 4$ have been classified in [80]:

- for $k = 1$, there is only $\alpha_1 = \beta_1 = \gamma_1$,
- for $k = 2$, they are: α_2 and $\beta_2 = \gamma_2$,
- for $k = 3$, they are: α_3, β_3, γ_3, the prism (with triangular base) and the pyramid (with square base),
- for $k = 4$, there are 19 types.

The following polytope $P^m_{p,q}$ was studied and named *repartitioning polytope* by Voronoi (see also [17]). 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 $Pyr(P)$. We define iteratively $Pyr_m(P)$ as $Pyr(Pyr_{m-1}(P))$, setting $Pyr_0(P) = P$. Let S_p, S_q be two simplices of respective dimensions p, q and lying in affine spaces which intersect in one point. Then, $P^m_{p,q} := Pyr_m(\text{Conv}(S_p \cup S_q))$ is called a *repartitioning polytope*; it has dimension $m+p+q$ and $m+p+q+2$ vertices. In fact, $P^m_{p,q}$ 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 [51]. 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_c is a set of equiangular lines. (See section 6.4 below.)

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 $\{x \in \mathbb{R}^k : \| x - v_0 \|_2 \leq \| x - v \|_2 \text{ for all } v \in L\}$. 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 *[7]*

(i) Let P be an L-polytope with set of vertices $V(P)$. Then, $(V(P), d_0)$ is a hypermetric space.

(ii) Let $d \in Hyp_{n+1}$. Then, there exist a lattice $L_d \subseteq \mathbb{R}^k$ of dimension $k \leq n$, an L-polytope P_d in L_d and a map $f_d : \{0, 1, \ldots, n\} \longrightarrow V(P_d)$, $f_d(i) = v_i$ for $0 \leq i \leq n$, such that

- *$\{v_0, v_1, \ldots, v_n\}$ generates L_d,*
- *$d_{ij} = d_0(v_i, v_j) = (\| v_i - v_j \|_2)^2$ for $0 \leq i \leq j \leq n$.*

Moreover, the triple (L_d, P_d, f_d) is unique, up to translation and orthogonal transformation.

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

PROOF. (i) Let $S(c, r)$ denote the empty sphere circumscribed to P. Let b_v, $v \in V(P)$, be integers with $\sum_{v \in V(P)} b_v = 1$. Then,

$$\begin{aligned} \sum_{u,v \in V(P)} b_u b_v d_0(u, v) &= \sum_{u,v \in V(P)} b_u b_v (\| (u - c) + (c - v) \|_2)^2 \\ &= \sum_{u,v \in V(P)} b_u b_v (2r^2 + 2(u - c)^T (c - v)) \\ &= 2r^2 - 2(\| \sum_{u \in V(P)} b_u u - c \|_2)^2 \leq 0, \end{aligned}$$

because $\sum_{u \in V(P)} b_u u \in L$.

We now give a sketch of the proof of (ii). One of the basic tools used in the proof is the covariance map φ_{c_0}. Define $p = \varphi_{c_0}(d)$, $p = (p_{ij})_{1 \leq i \leq j \leq n}$. By relation (8), $d \in Hyp_{n+1}$ if and only if $\sum_{1 \leq i,j \leq n} b_i b_j p_{ij} - \sum_{1 \leq i \leq n} b_i p_{ii} \geq 0$ for all integers $b_1, \ldots, b_n$. Therefore, if $d \in Hyp_{n+1}$, then the symmetric matrix $(p_{ij})_{1 \leq i,j \leq n}$ is positive semi definite and, thus, $p_{ij} = v_i^T v_j$, $1 \leq i \leq j \leq n$, for some vectors $v_1, \ldots, v_n \in \mathbb{R}^k$, where k is the rank of the matrix $(p_{ij})_{1 \leq i,j \leq n}$, $k \leq n$.

Moreover, one can show the existence of $c \in \mathbb{R}^k$ such that $2c^T v_i = (\| v_i \|_2)^2$ for $1 \leq i \leq n$. Therefore, $v_0 = 0, v_1, \ldots, v_n$ lie on the sphere $S(c, r := \| c \|_2)$. Remains only to show that $\{v_1, \ldots, v_n\}$ generates a lattice L and that the sphere S is empty in L. ∎

PROPOSITION 6.2 *[55] 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, d_0). Then, $V(P') \subseteq V(P)$ 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 below the correspondences between some special hypermetrics and their associated L-polytopes. Given $d \in Hyp_{n+1}$, $F(d)$ denotes the smallest face of Hyp_{n+1} containing d.

hypermetric d		associated L-polytope P
$d \in Cut_{n+1}$	$\overset{[7]}{\Longleftrightarrow}$	$V(P)$ is contained in the set of vertices of a parallepiped
d is a cut	$\Longleftrightarrow$	$P = \alpha_1$
$F(d) = Hyp_{n+1}$	$\overset{[7]}{\Longleftrightarrow}$	$P = \alpha_n$
$F(d)$ is a facet	$\overset{[17]}{\Longleftrightarrow}$	P is a repartitioning polytope
$F(d)$ is an extreme ray	$\overset{[55]}{\Longleftrightarrow}$	P is extreme
$F(d) = F(d')$	$\overset{[55]}{\Longleftrightarrow}$	P, P' are affinely equivalent

Table 2

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 (41) only a finite number is non redundant. The answer is yes, as stated in the following result.

THEOREM 6.3 *[53] The hypermetric cone Hyp_n is polyhedral.*

The proof given in [53] is based on the following two facts:

- the correspondence between the hypermetrics of 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 [157], [158] (a direct proof is given in [53]).

Let b^n_{max} denote the largest value of $\max_i |b_i|$ for which the inequality (41) defines a facet of Hyp_n. Then, $b^n_{max} < \frac{2^{n-2}(n-1)!}{n+1}$ is shown in [17].

6.3 Rank of an L-polytope

Let $d \in Hyp_{n+1}$ and let $F(d)$ denote the smallest face of Hyp_{n+1} containing d. The dimension of $F(d)$ is called the *rank* of d and denoted as $r(d)$, or $r(V_{n+1}, d)$. Hence, $r(d) = 1$ if d lies on an extreme ray of Hyp_{n+1}, $r(d) = \binom{n+1}{2}$ if d lies in the interior of Hyp_{n+1} and $r(d) = \binom{n+1}{2} - 1$ if $F(d)$ is a facet of 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 *[55] 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 *[55] 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 $n \leq 5$, $Hyp_{n+1} = Cut_{n+1}$, i.e. the only extreme rays are the cut vectors. Therefore, the only extreme L-polytope of dimension $k \leq 5$ is α_1.

PROPOSITION 6.6 *[55] 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 *[55] Let P be a basic L-polytope of dimension k. Then,* *(i)* $\binom{k+2}{2} \leq r(P) \leq \binom{k+2}{2} - |V(P)|$,

(ii) for P centrally symmetric, $r(P) \geq \binom{k+1}{2} - \frac{|V(P)|}{2} + 1$.

For instance, for α_k, $r(\alpha_k) = k+1$ yielding equality in both inequalities of (i); for β_k, $r(\beta_k) = \binom{k+1}{2} - k + 1$ 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:

$$|V(P)| \geq \frac{k(k+3)}{2} \tag{42}$$

$$|V(P)| \geq k(k+1) \text{ if } P \text{ is centrally symmetric.} \tag{43}$$

There is a striking analogy between the bounds (42) and (43) and some known upper bounds (see [121]) for the number N_p of points in a spherical two-distance set of dimension k and the number N_l of lines in a set of equiangular lines of dimension k, namely,

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

Moreover, if $N_l = \frac{k(k+1)}{2}$, then $k+2 = 4, 5$, or $k+2 = q^2$ for some odd integer $q \geq 3$ (see [121]). The first case of equality is for $q = 3$, $k = 7$, $N_l = 28$; 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 set of equiangular lines exists.

However, there are examples of extreme L-polytopes realizing equality in the bounds (42) or (43), 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, P^{16} constructed from the Barnes-Wall lattice (see below). There are also examples of extreme L-polytopes not realizing equality in the bounds (42), or (43).

We have given in [55] several examples of extreme L-polytopes achieving or not equality in the bounds (42) or (43). We refer to [55] for a detailed account and to [42] 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 [154], or [75]. They are the half-cube $h\gamma_n$, the cross polytope β_n, the simplex α_n, the Gosset polytope 3_{21} and the Schläfli polytope 2_{21} (whose 1-skeletons are, respectively, the half-cube graph $\frac{1}{2}H(n,2)$, the cocktail party graph $K_{n\times 2}$, the complete graph K_{n+1}, the Gosset graph G_{56} and the Schläfli graph G_{27}). Among them, the extreme polytopes are: the segment α_1, the Schläfli 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 (42). The polytope 3_{21} is centrally symmetric with 56 vertices, realizing equality in the bound (43). Both are basic. We do not known any other extreme L-polytope of dimension $k \leq 7$ beside α_1, 2_{21}, 3_{21}.

Extreme L-polytopes in sections of the Leech lattice Λ_{24}. The Leech lattice Λ_{24} is a lattice of dimension 24. By taking suitable sections of the sphere of minimal vectors of Λ_{24}, two extreme L-polytopes are constructed in [55]:

- P_{23}, centrally symmetric, with 552 vertices, dimension 23, realizing equality in the bound (43),
- P_{22}, asymmetric, with 275 vertices, dimension 22, realizing equality in the bound (42).

Extreme L-polytopes in sections of the Barnes-Wall lattice Λ_{16}. The Barnes-Wall lattice Λ_{16} is a lattice of dimension 16. Several examples of extreme L-polytopes are constructed from Λ_{16} in [55]:

- P, centrally symmetric (constructed from a deep hole of Λ_{16}), with 512 vertices, dimension 16 (equality does not hold in (43)),
- Q, centrally symmetric, with 272 vertices, dimension 16, realizing equality in the bound (43),
- P^8, P^{16}, asymmetric, with 135 vertices, dimension 15, realizing equality in the bound (42),

- Q', asymmetric, with 1080 vertices, dimension 15 (equality does not hold in (42)).

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 [50] that, if G is an extreme hypermetric graph, i.e. 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 ∇G is extreme of type I.

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

7 Applications in quantum mechanics

7.1 Preliminaries on quantum mechanics

The object of (non relativistic) 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. J. von Neumann [156] 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 [81], [93], [125], [127], [161].

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

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

for $\psi_1, \psi_2 \in H(N)$. The physical state of the system is represented by a unit vector $\psi \in H(N)$, 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 functions of $H(N)$ 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 functions $\psi \in H(N)$ with $< \psi, \psi >= 1$. 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 ψ is given by

$$< A >_\psi := < \psi, A\psi >= \int \psi^*(x)A\psi(x)dx.$$

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 $A = \sum_{i \geq 1} \lambda_i E_i$, where the λ_i's are the eigenvalues of A and E_i denotes the projection on the eigenspace associated with the eigenvalue λ_i. So, the projection E_i corresponds to the property "The observable A has value λ_i". If the system is in the state ψ, then it has the property associated with E_i if $< E_i >_\psi = 1$, i.e. if $A\psi = \lambda_i \psi$, that is ψ is an eigenvector of A corresponding to the eigenvalue λ_i.

The *standard deviation* of the observable A in the state ψ is given by

$$\Delta_\psi(A) = | < A^2 >_\psi -(< A >_\psi)^2|^{\frac{1}{2}}.$$

Heisenberg's uncertainty principle states that, if A, B are two observables of the system in the state ψ, then $\Delta_\psi(A)\Delta_\psi(B) \geq \frac{1}{2}| < \psi, (AB - BA)\psi > |$, 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 Ω. The average energy of the system in the state ψ is given by $< \Omega >_\psi$. A fundamental problem in quantum mechanics is to derive bounds on the average energy of the system without knowing explicitely the state ψ 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:

$$\Gamma_\psi^{(p)}(x'_1 \ldots x'_p | x_1 \ldots x_p) = \binom{N}{p} \int_{y \in X^{N-p}} \psi^*(x'_1, \ldots, x'_p, y) \psi(x_1, \ldots, x_p, y) dy \quad (44)$$

Density matrices were introduced in [102] (see also [125]); Dirac [69] 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, $\binom{N}{2}^{-1}\Gamma_\psi^{(2)}(x_1x_2|x_1x_2)dv_1dv_2$ 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 ψ, $\Gamma_\psi^{(p)}(x_1 \ldots x_p | x_1 \ldots x_p) = 0$ 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 particuler, they were the central topic of several conferences held at Queen's University, Kingston, Canada, yielding three volumes of proceedings ([39], [78], [81]).

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

$$A = A_0 + \sum_{1 \le i \le N} A_i + \frac{1}{2!} \sum_{1 \le i \ne j \le N} A_{ij} + \ldots \quad (45)$$

where the n-th term is an $(n-1)$-particle operator. Therefore, the expected value of A in the state ψ can be expressed, in terms of the density matrices, as follows:

$$\begin{aligned} < A >_\psi &= A_0 + \int\{A_1\Gamma_\psi^{(1)}(x_1'|x_1)\}_{x_1'=x_1} dx_1 + \\ &+ \int\{A_{12}\Gamma_\psi^{(2)}(x_1'x_2'|x_1x_2)\}_{x_1'=x_1, x_2'=x_2} dx_1 dx_2 + \ldots \end{aligned} \quad (46)$$

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

By the Hartree-Fock approximation (see [93]), one can assume that the expansion of the Hamiltonian Ω in relation (45) has only terms involving two particles at most, i.e. $\Omega = \Omega_0 + \sum_{1\le i\le N}\Omega_i + \frac{1}{2}\sum_{i\neq j}\Omega_{ij}$. 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 Ω can then be expressed as $\Omega = \frac{1}{2}\sum_{i\neq j} G_{ij}$, where $G_{ij} = \Omega_{ij} + \frac{1}{N-1}(\Omega_i + \Omega_j) + \frac{2}{N(N-1)}\Omega_0$. Therefore, from relation (46), 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 $\Phi_k, k \ge 1$, 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

$$f = \sum_{k\ge 1} < \Phi_k, f > \Phi_k. \quad (47)$$

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

$$\Phi_K(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} det(\Phi_{k_1}(x), \ldots, \Phi_{k_N}(x)) \quad (48)$$

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

$$\Phi_K(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in Sym(n)} sign(\sigma) \Phi_{k_{\sigma(1)}}(x_1) \ldots \Phi_{k_{\sigma(N)}}(x_N). \quad (49)$$

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

$$\psi(x_1, \ldots, x_N) = \sum_{K=\{k_1,\ldots,k_N\}, 1 \leq k_1 < \ldots < k_N} C_K \Phi_K \quad (50)$$

where

$$\begin{aligned} C_K &= < \Phi_K, \psi > \\ &= \sqrt{N!} \int \psi(x_1, \ldots, x_N) \Phi^*_{k_1}(x_1) \ldots \Phi^*_{k_N}(x_N) dx_1 \ldots dx_N \end{aligned} \quad (51)$$

with $\sum_K |C_K|^2 =< \psi, \psi >= 1$.

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

$$\sum_{K \subseteq \{1,\ldots,n\}, |K|=N} C_K \Phi_K \quad (52)$$

constitutes a good approximation of the wavefunction ψ. From now on, we assume that ψ is, in fact, equal to the finite sum in (52). It can be shown ([125]) that the 2nd-order density matrix $\Gamma^{(2)}_\psi$ can also be expanded in terms of the Slater determinants. Namely, if ψ is given by (52) where the coefficients C_K are given by (51), then

$$\Gamma^{(2)}_\psi(x'_1 x'_2 | x_1 x_2) = \sum_{1 \leq i < j \leq n, 1 \leq h < k \leq n} \gamma_\psi(ij|hk) \Phi^*_{\{i,j\}}(x'_1, x'_2) \Phi_{\{h,k\}}(x_1, x_2) \quad (53)$$

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

$$\gamma_\psi(ij|hk) = \sum C^*_I C_K \epsilon^I_{i,j,I-\{i,j\}} \epsilon^K_{h,k,K-\{h,k\}} \quad (54)$$

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 $\epsilon_{i_1 \ldots i_p}^{j_1 \ldots j_p} = sign(\sigma)$ if there is a permutation σ mapping i_1 on j_1, ..., i_p on j_p and $\epsilon_{i_1 \ldots i_p}^{j_1 \ldots j_p} = 0$ otherwise. In particular, the diagonal terms are given by

$$\gamma_\psi(ij|ij) = \sum_{i,j \in K \subseteq \{1,\ldots,n\}, |K|=N} |C_K|^2 \tag{55}$$

They have the following physical meaning: $\binom{N}{2}^{-1} \gamma_\psi(ij|ij)$ 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 Γ defined on $X^2 \times X^2$, Γ is said to be *N-representable* if there exists a wavefunction $\psi \in H(N)$ such that $\Gamma = \Gamma_\psi^{(2)}$. The *pure state representability problem* consists of finding the conditions that Γ must satisfy in order to be N-representable. This problem can be relaxed to the *ensemble representability problem* as follows. Instead of asking whether Γ is the second order density matrix of a single wavefunction ψ, 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 $\Gamma = \sum w_\psi \Gamma_\psi^{(2)}$ 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 $< \Omega >_\psi$ and $\sum w_\psi < \Omega >_\psi$ have the same minimum (equal to the minimum eigenvalue of the Hamiltonian Ω 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 [37] as the ensemble N-representability problem. The convex structure of $\mathcal{P}_N^{(2)}$ was studied e.g. in [38], [43], [76].

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 [37] (see also [115]). Namely, a matrix $\Gamma(x_1'|x_1)$ is is of the form $\sum w_\psi \Gamma_\psi^{(1)}(x_1'|x_1)$ for $w_\psi \geq 0$, $\sum w_\psi = 1$,

$<\psi,\psi>=1$ and $\psi\in H(N)$ if and only if $Tr(\Gamma)=\int\Gamma(x_1|x_1)dx_1=N$ and the eigenvalues of Γ 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 the next 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 $BQP_n^{\mathcal{I}=2}(N)$ denote the polytope defined as the convex hull of the vectors $\pi^{\mathcal{I}=2}(K)$ for $K\subseteq\{1,\ldots,n\}$ of cardinality N. From relation (55), 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 γ_{Φ_K} coincide with the vector $\pi^{\mathcal{I}=2}(K)$. For that reason, the polytope $BQP_n^{\mathcal{I}=2}(N)$ is sometimes called the *N-Slater hull* (e.g. in [77],[79]).

From (53), 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 $BQP_n^{\mathcal{I}=2}(N)$.

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 $\sum w_\psi\psi$ ($w_\psi\geq 0$, $\sum w_\psi=1$) of normalized wavefunctions $\psi\in H(N)$ such that $\gamma(ij)=\sum w_\psi\gamma_\psi(ij|ij)$ for $1\leq i<j\leq n$.

(iii) The vector γ belongs to $BQP_n^{\mathcal{I}=2}(N)$.

PROOF. $(i)\Rightarrow(ii)$ is clear.
$(ii)\Rightarrow(iii)$: Suppose first that $\gamma(ij)=\gamma_\psi(ij|ij)$ for some normalized $\psi\in H(N)$ given by (52). Then, from (55), $\gamma=\sum_{K\subseteq\{1,\ldots,n\},|K|=N}|C_K|^2\pi^{\mathcal{I}=2}(K)$ with $\sum|C_K|^2=<\psi,\psi>=1$. Hence $\gamma\in BQP_n^{\mathcal{I}=2}(N)$. Suppose now that $\gamma(ij)=\sum w_\psi\gamma_\psi(ij|ij)$ with $w_\psi\geq 0, \sum w_\psi=1$, $\psi\in H(N)$ and $<\psi,\psi>=1$.

Then, $\gamma = \sum_K t_K \pi^{\mathcal{I}_{=2}}(K)$, where $t_K = \sum_\psi w_\psi |C_K^\psi|^2 \geq 0$ and $\sum_K t_K = 1$. Therefore, $\gamma \in BQP_n^{\mathcal{I}_{=2}}(N)$.
$(iii) \Rightarrow (i)$: Assume $\gamma = \sum_K t_K \pi^{\mathcal{I}_{=2}}(K)$ 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. ∎

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 additionnal 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 $\mathcal{P}_N^{(2)}$ are given in [38], [76].

We conclude with some additional remarks.

• The N-representability problem for variable N leads to the study of the boolean quadric polytope BQP_n.

• The polytopes $BQP_n^{\mathcal{I}_{=2}}(N)$ and $BQP_n(N) = BQP_n^{\mathcal{I}_{\leq 2}}(N)$, lying respectively in $\mathbb{R}^{\binom{n}{2}}$ and $\mathbb{R}^{\binom{n+1}{2}}$, are in one-to-one correspondance. Indeed, each point $x \in BQP_n(N)$ satisfies the equations:

$$\begin{array}{ll} \sum_{1 \leq i < j \leq n} x_{ij} & = \binom{N}{2}, \\ \sum_{1 \leq j \leq n, j \neq i} x_{ij} & = (N-1) x_{ii} \text{ for } 1 \leq i \leq n. \end{array}$$

Hence both polytopes have the dimension $\binom{n}{2} - 1$.
• The combinatorial interpretation of the N-representability problem from Theorem 7.1 was given in [162]. 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 problematic of cuts. For arbitrary $p \geq 2$, the analogue of Theorem 7.1 leads to the study of the polytope $BQP_n^{\mathcal{I}_{=p}}(N)$ in $\mathbb{R}^{\binom{n}{p}}$, defined as the convex hull of the $\mathcal{I}_{=p}$-intersection vectors $\pi^{\mathcal{I}_{=p}}(K)$, for $K \subseteq \{1, \ldots, n\}$, $|K| = N$.

The facial structure of the polytope $BQP_n^{\mathcal{I}_{=p}}(N)$ is studied in [161]; 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.

• An additional alternative interpretation of the boolean quadric polytope BQP_n is given in [79], in terms of positive semi-definite two-body operators.

Let a_i denote the *annihilation operator* of the Fock space $\cup_{N\geq 1}H(N)$ and $a_i^\dagger$, its adjoint, the *creation operator* (see [93]). Both are defined by their action on the Slater determinants. Namely, for $K = \{k_1, \ldots, k_N\}$ with $1 \leq k_1 < \ldots < k_N$,

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

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

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

$$B = b_0 + \sum_{1\leq i\leq n} b_i a_i^\dagger a_i + \sum_{1\leq i\leq j\leq n} b_{ij} a_i^\dagger a_i a_j^\dagger a_j. \tag{56}$$

The cone $Q^+(I^n)$, consisting of the two-body operators B of the form (56) which are positive semi-definite, is considered in [79]. Since any such operator has the same eigenvectors Φ_K associated with the eigenvalues $b_0 + \sum_{i\in K} b_i + \sum_{i,j\in K} b_{ij}$, the cone $Q^+(I^n)$ can be equivalently defined as the cone of the vectors $b := (b_0, b_i\ 1 \leq i \leq n, b_{ij}\ 1 \leq i \leq j \leq n)$ for which $b(x) := b_0 + \sum_{1\leq i\leq n} b_i x_i + \sum_{1\leq i\leq j\leq n} b_{ij} x_i x_j \geq 0$ for each $x \in \{0,1\}^n$. Therefore, $Q^+(I^n)$ is the dual cone to BQP_n, i.e. $b \in Q^+(I^n)$ if and only if the inequality $b(x) \geq 0$ is valid for 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 $Q^+(I^n)$ corresponds to a system of fermions (with at most one particle per spin-orbital), is also considered in [79].

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

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

and, therefore,

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

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

7.3 The quantum correlation polytope

We address in this section a connection between the boolean quadric polytope BQP_n and the quantum correlation polytope, considered in [133], [134].

Recall that the boolean quadric polytope BQP_n arises naturally in the theory of probability. Namely, from Theorem 3.2, given $p = (p_{ij}, 1 \leq i \leq j \leq n) \in \mathbb{R}^{\binom{n+1}{2}}$, then $p \in BQP_n$ 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 BQP_n is also called the *correlation polytope* in [133], [134], [135]. For $n = 3$, BQP_n is also called the Bell-Wigner polytope.

As an extension, [133] 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 ψ of a Hilbert space H ($H = H(N)$ if the system has N particles). Let E_ψ denote the projection operator from H to the line spanned by ψ, i.e. $E_\psi(\phi) = <\psi, \phi> \psi$ for $\phi \in H$. Equivalently, a state of the system is given by such a projection operator E_ψ; such a state is called a *pure state*. More generally, we consider also non pure states, namely convex combinations of pure states: $W = \sum_\psi \lambda_\psi E_\psi$ ($\lambda_\psi \geq 0$, $\sum_\psi \lambda_\psi = 1$, $\psi \in H$ with $<\psi, \psi> = 1$). 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 semi-definite and has trace one.

Given $p = (p_{ij}, 1 \leq i \leq j \leq n) \in \mathbb{R}^{\binom{n+1}{2}}$, 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 necessarly distinct, nor commuting) such that

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

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 QCP_n denote the polytope in $\mathbb{R}^{\binom{n+1}{2}}$ consisting of those p which admit a quantum mechanical representation; QCP_n is called the *quantum correlation polytope*.

Finally let T_n denote the set of the vectors $p \in \mathbb{R}^{\binom{n+1}{2}}$ 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) $BQP_n \subseteq QCP_n \subseteq T_n$.*

(ii) QCP_n is is a convex set which contains the interior of T_n.

(iii) The subset of 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 $QCP_n \subseteq T_n$ follows from the fact that each state W is positive semi-definite with trace 1. We check the inclusion $BQP_n \subseteq QCP_n$. Let $p \in BQP_n$. 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 ψ_K with $i \in K$; then $E_i \wedge E_j$ is the projection on the subspace spanned by ψ_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 QCP_n. ∎

Note that, if $p \in QCP_n$ has a quantum mechanical representation in which the operators E_i commute then, in fact, $p \in BQP_n$.

Note also that every $p \in L_n$ with $0 < p_{ij} < 1$ for all i, j belongs to 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 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 developped; see, for instance, [133], [134].

The region $QCP_n - BQP_n$ is called the *interference region*. Several examples of physical experiments are described in ([133], [134]) that yield some pair distributions p lying in the interference region. For example, the classical Einstein-Podolsky-Rosen experiment ([74]) yields $p \in QCP_3 - BQP_3$.

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, $p \notin BQP_2$ 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, $p \in QCP_2$. 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, $trace(WE_i) = (\cos\theta)^2 = p_{ii}$ 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 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, $QCP_2 = T_2 - \{(1,1,0)\}$.

8 Other applications

8.1 The L_1-metric in probability theory

Let $(\Omega, \mathcal{A}, \mu)$ be a probability space and let $X : \Omega \longrightarrow \mathbb{R}$ 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 monography [140]; 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): $EN(X,Y) = |E(X) - E(Y)|$,
- 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 ($1 \le p \le \infty$) 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 $EN(X,Y)$ is given by [140] 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 [140] 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 [128], [129] 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:

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

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 Lemma 3.5, (M,d) is L_1-embeddable if and only if there exist a non negative measure space (H,ν) and a map $x \mapsto A_x \subseteq H$ with $\nu(A_x) < \infty$ for $x \in M$, such that $d(x,y) = \nu(A_x \Delta A_y)$ for $x, y \in M$. Hence, a Gaussian system admits a representation called of Chentsov type

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

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

This Chentsov type representation can be compared with the Crofton formula for projective metrics from Theorem 4.12. Actually both come naturally together in [3] (see parts A.8-A.9 of Appendix A there).

8.2 The ℓ_1-metric in statistical data analysis

A *data structure* is a pair (I, d), where I is a finite set, called *population*, and $d : I \times I \longrightarrow \mathbb{R}_+$ 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 [104]). 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 section 4.1); then the data structure is called an *additive tree*. Also, data structures (I, d) for which d is ℓ_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 ℓ_1-embeddable is a natural extension of the ultrametric and ℓ_2 cases.

An ℓ_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 ℓ_2-norm, in the least square method; or its square,
- the ℓ_∞-norm, in the minimax or Chebychev method,
- the ℓ_1-norm, in the least absolute values (LAV) method.

In fact, the ℓ_1 criterion has been increasingly used. Its importance can be seen, for instance, from the volume [72] of proceedings of a conference entitled "Statistical data analysis based on the L_1 norm and related methods"; we refer, in particular, to [71], [82], [120], [155].

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 (non necessarly 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_n^t 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. $z_n^t = nt$.

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. [142].

Let $\mathcal{B}$ be a collection of (non necessarly distinct) subsets of V_n, the sets $B \in \mathcal{B}$ are called *blocks.* Let r, k, λ 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 λ common blocks.

$\mathcal{B}$ is called a (n, k, λ)-*BIBD* (BIBD standing for balanced incomplete block design) if any two distinct points $i, j \in V_n$ belong to λ common blocks and each block has cardinality k. This implies that each point $i \in V_n$ belong to $r = \frac{\lambda(n-1)}{k-1}$ blocks and the total number of blocks is $b := |\mathcal{B}| = \frac{rn}{k}$. 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 $PG(2, t)$, 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 [61]:

(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, λ)-BIBD, where the parameters satisfy: $r = \frac{t(n-1)}{n-k}$, $\lambda = r - t = \frac{t(k-1)}{n-k}$.

(iii)[142] If there exists a symmetric $(n, \lambda + t, t)$-BIBD with $n \neq 4t$, $n = 2t + \lambda + \frac{t(t-1)}{\lambda}$, then $z_n^t = n$.

In the cases $\lambda = 1$, t, the implication of (iii) is, in fact, an equivalence. Namely, we have:

(iv)

$$PG(2,t) \text{ exists} \overset{[97] \text{ and } [142]}{\iff} z^t_{t^2+t+1} = t^2+t+1$$

$$\overset{[48]}{\iff} 2td(K_{t^2+t+2}) \text{ is not } h-\text{rigid, i.e. } z^t_{t^2+t+2} < t(t^2+t+2)$$

$$\overset{[61]}{\iff} z^t_{t^2+t+2} = \begin{cases} t^2+2t & \text{if } t \geq 3 \\ t^2+t+1 & \text{if } t = 1,2 \end{cases}$$

(v) [142]

$$\text{There exists a Hadamard matrix of order } 4t \iff z^t_{4t-1} = 4t-1$$

$$\iff z^t_{4t} = 4t-1.$$

The following bounds hold for z_n^t:

(vi) by (13), $z_n^t \leq nt$, with equality if and only if $2td(K_n)$ is h-rigid,

(vii) [142] $z_n^t \geq n-1$, with equality if and only if $n = 4t$ and there exists a Hadamard matrix of order $4t$,

(viii) $z_n^t \geq n$, if we are not in the case of equality of (vii),

(ix) by (13), $z_n^t \geq a_n^t := \lceil \frac{n(n-1)t}{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil} \rceil = 4t - \lfloor \frac{2t}{\lceil \frac{n}{2} \rceil} \rfloor$.

Observe that $a^t_{4t} = a^t_{4t-1} = 4t-1$, and $a^t_{t^2+t+1} = a^t_{t^2+t+2} = 4t$ 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 $\mathbb{Z}_+$-realizations of minimum size of $2td(K_n)$ provide a common generalization of the two most interesting cases of symmetric BIBD, namely 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 [61].

Conjecture 8.1
- *For $n \leq 4t$, if there exists a Hadamard matrix of order $4t$, then $z^t_n = a^t_n$.*
- *If $\lceil \frac{n}{2} \rceil$ divides $2t$ and there exists a Hadamard matrix of order $4t$, then $z^t_n = a^t_n$.*

8.4 Miscelleneous

The variety of uses of the ℓ_1-metric is very vast as we already saw in sections 8.1 and 8.2. We group here several other examples where ℓ_1-embeddable metrics are useful.

On the integers, beside the usual ℓ_1-metric $|a-b|$, we have, for instance, the well known Hamming distance between the binary expansions of a, b, and $\log(\frac{l.c.m.(a,b)}{g.c.d.(a,b)})$ (mentioned after Theorem 4.13) which are both ℓ_1-embeddable.

Two examples of ℓ_1-embeddable metrics are used in biology:

- The *Prevosti's genetic distance*: $\frac{1}{2r}\sum_{1\leq j\leq r}\sum_{1\leq i\leq k_j}|p_{ij}-q_{ij}|$ 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 litterature on this distance started in [139].
- The *biotope distance*: $\frac{|A\Delta B|}{|A\cup B|}$ between biotopes A, B (sets of species in, say, forests); it was introduced in [126] and it is shown in [5] to be ℓ_1-embeddable.

The Hamming distance $|\{(a,b) \in G^2 : a \cdot b \neq a * b\}|$ between the multiplication tables of two groups $A = (G, \cdot)$ and $B = (G, *)$ on the same underlying set G is used in [73].

Given compact subsets A, B of the plane $\mathbb{R}^2$, the ℓ_1-distance aire$(A \Delta B)$ is used in the treatment of images; see, for instance, [105].

References

[1] R. Alexander. Zonoid theory. *Geometriae Dedicata*, 28:199–211, 1988.

[2] N. Alon. The CW-inequalities for vectors in ℓ_1. *European Journal of Combinatorics*, 11:1–6, 1990.

[3] R.V. Ambarzumian. *Combinatorial integral geometry.* John Wiley and Sons, 1982.

[4] M. Aschbacher, P. Baldi, E.B. Baum, and R.M. Wilson. Embeddings of ultrametric spaces in finite dimensional structures. *SIAM Journal on Algebraic and Discrete Methods*, 8(4):564–577, 1987.

[5] P. Assouad. Produit tensoriel, distances extrémales et réalisation de covariances. *Comptes Rendus de l'Académie des Sciences de Paris*, 288(A):649–652 and 675–677, 1979.

[6] P. Assouad. Plongements isométriques dans L^1: aspect analytique. volume 14 of *Séminaire Choquet (Initiation à l'Analyse).* Paris VI, 1979-1980.

[7] P. Assouad. Sous espaces de L^1 et inégalités hypermétriques. *Comptes Rendus de l'Académie des Sciences de Paris*, 294(A):439–442, 1982.

[8] P. Assouad. Sur les inégalités valides dans L^1. *European Journal of Combinatorics*, 5:99–112, 1984.

[9] P. Assouad and C. Delorme. Graphes plongeables dans L^1. *Comptes Rendus de l'Académie des Sciences de Paris*, 291(A):369–372, 1980.

[10] P. Assouad and M Deza. Espaces métriques plongeables dans un hypercube: aspects combinatoires. In M. Deza and I.G. Rosenberg, editors, *Combinatorics 79 Part I*, volume 8 of *Annals of Discrete Mathematics*, pages 197–210, 1980.

[11] P. Assouad and M. Deza. Metric subspaces of L^1. *Publications mathématiques d'Orsay*, 3, 1982.

[12] D. Avis. Extremal metrics induced by graphs. *Annals of Discrete Mathematics*, 8:217–220, 1980.

[13] D. Avis. On the extreme rays of the metric cone. *Canadian Journal of Mathematics XXXII*, 1:126–144, 1980.

[14] D. Avis. Hypermetric spaces and the Hamming cone. *Canadian Journal of Mathematics*, 33(4):795–802, 1981.

[15] D. Avis. On the complexity of isometric embedding in the hypercube . In *Lecture Notes in Computer Science*, volume Algorithms 450, pages 348–357. Springer Verlag, 1990.

[16] D. Avis and M. Deza. The cut cone, L^1-embeddability, complexity and multicommodity flows. *Networks*, 21:595–617, 1991.

[17] D. Avis and V.P. Grishukhin. A bound on the k-gonality of the hypermetric cone and related complexity problems. Technical Report SOCS-92.4, School of Computer Science, Mc Gill University, Montreal, Canada, 1992.

[18] D. Avis and H. Maehara. Metric extensions and L_1-hierarchy. Technical report SOCS-90.4, School of Computer Science, McGill University, Montreal, Canada, 1990.

[19] D. Avis and Mutt. All facets of the six point Hamming cone. *European Journal of Combinatorics*, 10:309–312, 1989.

[20] H-J. Bandelt. Recognition of tree metrics. *SIAM Journal on Algebraic Discrete Methods*, 3(1):1–6, 1990.

[21] F. Barahona. The max-cut problem on graphs not contractible to K_5. *Operations Research Letters*, 2:107–111, 1983.

[22] F. Barahona and M. Grötschel. On the cycle polytope of a binary matroid. *Journal of Combinatorial Theory B*, 40:40–62, 1986.

[23] F. Barahona, M. Grötschel, M. Jünger, and G. Reinelt. An application of combinatorial optimization to statistical physics and circuit layout design. *Operations Research*, 36(3):493–513, 1988.

[24] F. Barahona, M. Jünger, and G. Reinelt. Experiments in quadratic 0-1 programming. *Mathematical Programming*, 44:127–137, 1989.

[25] F. Barahona and A.R. Mahjoub. On the cut polytope. *Mathematical Programming*, 36:157–173, 1986.

[26] L.W. Beineke. Characterization of derived graphs. *Journal of Combinatorial Theory*, 9:129–135, 1970.

[27] G. Birkoff. *Lattice theory*. American Mathematical Society, Providence, Rhode Island, 1967.

[28] I.F. Blake and J.H. Gilchrist. Addresses for graphs. *IEEE Transactions on Information Theory*, (5):683–688, 1973.

[29] C.E. Bonferroni. Il calcolo delle assicurazioni su grouppi di teste. *Studi in Onore del Professor S.O. Carboni (Roma)*, 1936.

[30] G. Boole. *An investigation of the laws of thought on which are founded the mathematical thories of logic and probabilities*. Dover Publications, Inc., original edition 1854.

[31] E. Boros and P.L. Hammer. Cut polytopes, boolean quadratic polytopes and nonnegative quadratic pseudo-boolean functions. Research report rrr 24-90, Rutgers University, USA, 1990.

[32] E. Boros and A. Prékopa. Closed form two-sided bounds for probabilities that at least r and exactly r out of n events occur. *Mathematics of Operations Research*, 14(2):317–342, 1989.

[33] J. Bretagnolle, D. Dacuna Castelle, and J-L Krivine. Lois stables et espaces L^p. *Annales de l'Institut Henri Poincaré*, 2(3):231–259, 1966.

[34] A.E. Brouwer, A.M. Cohen, and A. Neumaier. *Distance regular graphs*. Springer Verlag, 1989.

[35] J.H.H. Chalk. Algebraic lattices. In P. Gruber and J. Wills, editors, *Convexity and its applications*, pages 97–110. Birkhäuser Verlag Basel, 1983.

[36] K.L. Chung. On the probability of the occurrence of at least m events among n arbitrary events. *Annals of Mathematical Statistics*, 12:328–338, 1941.

[37] A.J. Coleman. The structure of Fermion density matrices I. *Review Mod. Physics*, 35:668–, 1963.

[38] A.J. Coleman. Necessary conditions for N-representability of reduced density matrices. *Journal of Mathematical Physics*, 13(2):214–222, 1972.

[39] A.J. Coleman and R.M. Erdahl, editors. *Reduced density operators with applications to physical and chemical systems I* , Queen's papers on pure and applied mathematics No. 11, Queen's University, Kingston, Ontario, Canada, 1968.

[40] M. Conforti, M.R. Rao, and A. Sassano. The equipartition polytope: part I. *Mathematical Programming*, 49:49–70, 1990.

[41] M. Conforti, M.R. Rao, and A. Sassano. The equipartition polytope: part II. *Mathematical Programming*, 49:71–91, 1990.

[42] J.V. Conway and N.J.A. Sloane. *Sphere Packings, lattices and groups*, volume 290 of *Grundlehren der mathematischen Wissenschaften.* Springer Verlag, Berlin, 1987.

[43] E. Davidson. Linear inequalities for density matrices. *Journal of Mathematical Physics*, 10(4):725–734, 1969.

[44] D.A. Dawson and D. Sankoff. An inequality for probabilities. *Proceedings of the American Mathematical Society*, 18:504–507, 1967.

[45] C. Delorme and S. Poljak. Laplacian eigenvalues and the maximum cut problem. *Mathematical Programming*, submitted.

[46] M. Deza. On the Hamming geometry of unitary cubes. *Doklady Akademii Nauk SSR (in Russian) (resp. Soviet Physics Doklady (English translation))*, 134 (resp. 5):1037–1040 (resp. 940–943), 1960 (resp. 1961).

[47] M. Deza. Matrices de formes quadratiques non négatives pour des arguments binaires. *Comptes rendus de l'Académie des Sciences de Paris*, 277(A):873–875, 1973.

[48] M. Deza. Une propriété extrémale des plans projectifs finis dans une classe de codes equidistants. *Discrete Mathematics*, 6:343–352, 1973.

[49] M. Deza, K. Fukuda, and M. Laurent. The inequicut cone. *Discrete Mathematics*, To appear.

[50] M. Deza and V.P. Grishukhin. Hypermetric graphs. Rapport LIENS-92-9, Ecole Normale Supérieure (Paris), 1992.

[51] M. Deza and V.P. Grishukhin. L-polytopes and equiangular lines. Technical report, 1992.

[52] M. Deza and V.P. Grishukhin. Hypermetric and ℓ_1-addressable graphs II. 1993.

[53] M. Deza, V.P. Grishukhin, and M. Laurent. The hypermetric cone is polyhedral. *Combinatorica*, To appear.

[54] M. Deza, V.P. Grishukhin, and M. Laurent. The symmetries of the cut polytope and of some relatives. In P. Gritzman and B. Sturmfels, editors, *Applied Geometry and Discrete Mathematics - The Victor Klee Festschrift*, volume 4 of *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, pages 205–220, 1991.

[55] M. Deza, V.P. Grishukhin, and M. Laurent. Extreme hypermetrics and L-polytopes. In *Sets, Graphs and Numbers, Budapest (Hungary), 1991*, volume 60 of *Colloquia Mathematica Societatis János Bolyai*, 1992.

[56] M. Deza, M. Grötschel, and M. Laurent. Clique-web facets for multicut polytopes. *Mathematics of Operations Research*, 17(3), 1992.

[57] M. Deza and M. Laurent. The even and odd cut polytopes. Research report B-231, Tokyo Institute of Technology (Tokyo), 1989.

[58] M. Deza and M. Laurent. The cut cone: simplicial faces and linear dependencies. Research report 90671-OR, Institut für Diskrete Mathematik, Universität Bonn, 1990.

[59] M. Deza and M. Laurent. Isometric hypercube embedding of generalized bipartite metrics. Research report 91706-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[60] M. Deza and M. Laurent. A survey of the known facets of the cut cone. Research report 91722-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[61] M. Deza and M. Laurent. Variety of hypercube embeddings of the equidistant metric and designs. Research report 91720-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[62] M. Deza and M. Laurent. ℓ_1-rigid graphs. Research report 92743-OR, Institut für Diskrete Mathematik, Universität Bonn, 1992.

[63] M. Deza and M. Laurent. Extension operations for cuts. *Discrete Mathematics*, 106-107:163–179, 1992.

[64] M. Deza and M. Laurent. Facets for the cut cone I. *Mathematical Programming*, 56(2):121–160, 1992.

[65] M. Deza and M. Laurent. Facets for the cut cone II: clique-web facets. *Mathematical Programming*, 56(2):161–188, 1992.

[66] M. Deza and M. Laurent. New results on facets of the cut cone. *Journal of Combinatorics, Information and System Sciences (R.C.Bose memorial issue)*, 17(1-2):19–38, 1992.

[67] M. Deza and M. Laurent. The Fibonacci and parachute inequalities for ℓ_1-metrics. *Fibonacci Quaterly*, 30(1):54–65, 1992.

[68] M. Deza, M. Laurent, and S. Poljak. The cut cone III: on the role of triangle facets. *Graphs and Combinatorics*, 8:125–142, 1992.

[69] P.A.M. Dirac. Note on exchange phenomena in the Thomas atom. *Proceedings of the Cambridge Philosophical Society*, 26:376–385, 1930.

[70] D.Z. Djokovic. Distance preserving subgraphs of hypercubes. *Journal of Combinatorial Theory B*, 14:263–267, 1973.

[71] Y. Dodge. An introduction to statistical data analysis L_1-norm based. In Y. Dodge, editor, *Statistical data analysis based on the L_1-norm and related methods*, pages 1–22. Elsevier Science Publishers B.V. (North Holland), 1987.

[72] Y. Dodge, editor. *Statistical data analysis based on the L_1-norm and related methods*. Elsevier Science Publishers B.V. (North Holland), 1987.

[73] A. Drápal. How far apart can the group multiplication tables be ? *European Journal of Combinatorics*, 13(5):335–344, 1992.

[74] A. Einstein, B. Podolsky, and W. Rosen. Can quantum mechanical description of physical reality be considered complete? *Physical Review*, 47 777(reprinted in Wheeler and Zurek (1983)), 1935.

[75] R.M. Erdahl. A cone of inhomogeneous second order polynomials. *Discrete and Computational Geometry*, To appear.

[76] R.M. Erdahl. The convex structure of the set of N-representable reduced 2-matrices. *Journal of Mathematical Physics*, 13(10):1608–1621, 1972.

[77] R.M. Erdahl. A convex set of second order inhomogeneous polynomials with applications to reduced density matrices. In R.M. Erdahl, editor, *Reduced density operators with applications to physical and chimical systems II*, volume 40 of *Queen's papers on pure and applied mathematics*, pages 28–35, 1974.

[78] R.M. Erdahl, editor. *Reduced density operators with applications to physical and chemical systems II*, Queen's papers on pure and applied mathematics No. 40, Queen's University, Kingston, Ontario, Canada, 1974.

[79] R.M. Erdahl. Representability conditions. In R.M. Erdahl and V.H. Smith, editors, *Density matrices and density functionals*, pages 51–75. D. Reidel, 1987.

[80] R.M. Erdahl and S.S. Ryshkov. The empty sphere. *Canadian Journal of Mathematics*, 39(4):794–824, 1987.

[81] R.M. Erdahl and V.H. Smith, editors. *Density matrices and density functionals*, Proceedings of the A.John Coleman Symposium. D.Reidel, Dordrecht, 1987.

[82] B. Fichet. The role played by L_1 in data analysis. In Y. Dodge, editor, *Statistical data analysis based on the L_1-norm and related methods*, pages 185–193. Elsevier Science Publishers B.V. (North Holland), 1987.

[83] J. Fonlupt, A.R. Mahjoub, and J.P. Uhry. compositions in the bipartite subgraph polytope. *Discrete Mathematics*, 105:73–91, 1992.

[84] L.R. Ford and D.R. Fulkerson. *Flows in networks.* Princeton University, Princeton, 1962.

[85] K. Fukuda and K. Handa. Antipodal graphs and oriented matroids. *Discrete Mathematics, to appear.*

[86] J. Galambos. Bonferroni inequalities. *Annals of Probabilities*, 5:577–581, 1977.

[87] M.R. Garey and D.S. Johnson. *Computers and intractability: A guide to the theory of NP-completeness.* Freeman, San Francisco, 1979.

[88] A.D. Gordon. A review of hierarchical classification. *Journal of the Royal Statistical Society A*, 150(2):119–137, 1987.

[89] R.L. Graham and H.O. Pollack. On the addressing problem for loop switching. *Bell System Tech. Journal*, 50:2495–2519, 1971.

[90] R.L. Graham and P.M. Winkler. On isometric embeddings of graphs. *Transactions of the American mathematical Society*, 288(2):527–536, 1985.

[91] V.P. Grishukhin. All facets of the cut cone $\mathcal{C}_n$ for $n = 7$ are known. *European Journal of Combinatorics*, 11:115–117, 1990.

[92] V.P. Grishukhin. Computing extreme rays of the metric cone for seven points. *European Journal of Combinatorics*, 13:153–165, 1992.

[93] E.K.U. Gross, E. Runge, and O. Heinonen. *Many-particle theory.* IOP Publishing, 1991.

[94] M. Grötschel, L. Lovász, and A. Schrijver. *Geometric algorithms and combinatorial optimization.* Springer Verlag, 1988.

[95] M. Grötschel and W.R. Pulleyblank. Weakly bipartite graphs and the max-cut problem. *Operations Research Letters*, 1:23–27, 1981.

[96] F.O. Hadlock. Finding a maximum cut of planar graphs in polynomial time. *SIAM Journal on Computing*, 4:221–225, 1975.

[97] J.I. Hall. Bounds for equidistant codes and projective planes. *Discrete Mathematics*, 17(1):85–94, 1977.

[98] P.L. Hammer. Some network flow problems solved with pseudo-boolean programming. *Operations Research*, 13:388–399, 1965.

[99] T.L. Hayden, J. Wells, Wei-Min Liu, and P. Tarazaga. The cone of distance matrices. *Linear Algebra and its applications*, 144:153–169, 1991.

[100] E.W. Holman. The relation between hierarchical and classical models for psychological distances . *Journal of the Royal Statistical Society A*, 37(4):417–423, 1972.

[101] E. Howe, C.R. Johnson, and J. Lawrence. The structure of distances in networks. *Networks*, 16:87–106, 1986.

[102] K. Husimi. *Proceedings of the physico-mathematical society of Japan*, 22:264–, 1940.

[103] M. Iri. On an extension of the maximum-flow minimum-cut theorem to multicommodity flows. *Journal of the Operational Society of Japan*, 13:129–135, 1970-71.

[104] S.C. Johnson. Hierarchical clustering schemes. *Psychometrika*, 32(3):241–254, 1967.

[105] M. Jourlin. Métriques de formes et applications. *Proceedings of the conference* Distancia *(Rennes 1992)*, pages 279–282, 1992.

[106] J. Kahn and G. Kalai. A counterexample to Borsuk's conjecture. 1992.

[107] A.V. Karzanov. Metrics and undirected cuts. *Mathematical Programming*, 32:183–198, 1985.

[108] A.V. Karzanov. Half-integral five-terminus flows. *Discrete Applied Mathematics*, 18:263–278, 1987.

[109] A.V. Karzanov. Polyhedra related to undirected multicommodity flows. *Linear Algebra and its Applications*, 114-115:293–328, 1989.

[110] A.V. Karzanov. Sums of cuts and bipartite metrics. *European Journal of Combinatorics*, 11:473–484, 1990.

[111] J.B. Kelly. Metric inequalities and symmetric differences. In O.Shisha, editor, *Inequalities II*, pages 193–212. Academic Press, New York, 1970.

[112] J.B. Kelly. Hypermetric spaces. In *Lecture Notes in Mathematics*, volume 490, pages 17–31. Springer Verlag, 1975.

[113] J. Koolen. On metric properties of regular graphs. Master's thesis, Eindhoven University of Technology, 1990.

[114] S. Kounias and J. Marin. Best linear Bonferroni bounds. *SIAM Journal of Applied Mathematics*, 30(2):307–323, 1976.

[115] H.W. Kuhn. Linear inequalities and the Pauli principle. In *Proceedings of the Symposium on Applied Mathematics*, volume 10, pages 141–147, 1960.

[116] M. Laurent. Graphic vertices of the metric polytope. Research report No. 91737-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[117] M. Laurent and S. Poljak. In preparation.

[118] M. Laurent and S. Poljak. The metric polytope. In E. Balas, G. Cornuejols, and R. Kannan, editors, *Integer Programming and Combinatorial Optimization*, pages 274–286. Carnegie Mellon University, GSIA, Pittsburgh, USA, 1992.

[119] M. Laurent and S. Poljak. One-third-integrality in the metric polytope. Report BS-R9209, Centrum voor Wiskunde en Informatica, 1992.

[120] G. LeCalve. L_1-embeddings of a data structure (I, D). In Y. Dodge, editor, *Statistical data analysis based on the L_1-norm and related methods*, pages 195–202. Elsevier Science Publishers B.V. (North Holland), 1987.

[121] P.W.H. Lemmens and J.J. Seidel. Equiangular lines. *Journal of Algebra*, 24:494–512, 1973.

[122] M. Lomonossov and A. Sebö. On the geodesics of graphs. 1992.

[123] M.V. Lomonossov. On a system of flows in a network (in Russian). *Probl. Peredatchi Infor.*, 14:60–73, 1978.

[124] M.V. Lomonossov. Combinatorial approaches to multiflow problems. *Discrete Applied Mathematics*, 11:1–93, 1985.

[125] P.O. Löwdin. Quantum theory of many particles systems I. Physical interpretation by means of density matrices, natural spin-orbitals, and

convergence problems in the method of configurational interaction. *Physical Review*, 97(6):1474–1489, 1955.

[126] F. Marczewski and H. Steinhaus. On a certain distance of sets and the corresponding distance of functions. *Colloquium Mathematicum*, 6:319–327, 1958.

[127] W.B. McRae and E.R. Davidson. Linear inequalities for density matrices II . *Journal of Mathematical Physics*, 13(10):1527–1538, 1972.

[128] A. Noda. Generalized Radon transform and Lévy's Brownian motion I and II. *Nagoya Mathematical Journal*, 105:71–87 and 89–107, 1987.

[129] A. Noda. White noise representation of some Gaussian random fields. *The bulletin of Aichi University of Education*, 38:35–45, 1989.

[130] K. Onaga and O. Kakusho. On feasibility conditions of multicommodity flows in networks. *IEEE Transactions on Circuit Theory*, 18:425–429, 1971.

[131] M. Padberg. The boolean quadric polytope: some characteristics, facets and relatives. *Mathematical Programming*, 45:139–172, 1989.

[132] B.A. Papernov. On existence of multicommodity flows. *Studies in Discrete Optimization (in Russian), Nauka, Moscow*, pages 230–261, 1976.

[133] I. Pitowsky. The range of quantum probability. *Journal of Mathematical Physics*, 27(6):1556–1565, 1986.

[134] I. Pitowsky. *Quantum probability - Quantum logic*, volume 321 of *Lecture Notes in Physics*. Springer Verlag, 1989.

[135] I. Pitowsky. Correlation polytopes: their geometry and complexity. *Mathematical Programming*, 50:395–414, 1991.

[136] S. Poljak. Polyhedral and eigenvalue approximations of the max-cut problem. In *Sets, graphs and Numbers, Budapest (Hungary), 1991*, volume 60 of *Colloquia Mathematica Societatis János Bolyai*, 1992.

[137] S. Poljak and F. Rendl. Semiinfinite relaxation of the graph bisection problem. In preparation.

[138] S. Poljak and F. Rendl. Solving the max-cut problem using eigenvalues. Research report No. 91735-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[139] A. Prevosti, J. Ocana, and G. Alonso. Distances between populations of drosophila subobscura based on chromosome arrangement frequencies. *Theoretical and Applied Genetics*, 45:231–241, 1975.

[140] S.T. Rachev. *Probability metrics and the stability of stochastic models.* John Wiley and Sons, 1991.

[141] R.L. Roth and P.M. Winkler. Collapse of the metric hierarchy for bipartite graphs. *European Journal of Combinatorics*, 7:371–375, 1986.

[142] H.J. Ryser. *Combinatorial mathematics*, volume 14 of *The Carus Mathematical Monographs.* The Mathematical Association of America, 1963.

[143] R. Schneider and W. Weil. Zonoids and related topics. In P. Gruber and J. Wills, editors, *Convexity and its applications*, pages 296–317. Birkhäuser Verlag Basel, 1983.

[144] I.J. Schoenberg. Metric spaces and positive definite functions. *Transactions of the American Mathematical Society*, 44:522–536, 1938.

[145] A. Schrijver. *Theory of linear and integer programming.* Wiley, 1986.

[146] A. Schrijver. Private communication. 1992.

[147] W. Schwärzler and A. Sebö. A generalized cut condition for multiflows in matroids. Research report 869-M, Artemis, IMAG, Université Joseph Fourier (Grenoble), 1992.

[148] P.D. Seymour. Matroids and multicommodity flows. *European Journal of Combinatorics*, 2:257–290, 1981.

[149] S.V. Shpectorov. On scale embeddings of graphs into hypercubes. *European Journal of Combinatorics*, 1993.

[150] C. De Simone. The cut polytope and the boolean quadric polytope. *Discrete Mathematics*, 79:71–75, 1989/90.

[151] C. De Simone. Lifting facets of the cut polytope. *Operations Research Letters*, 9:341–344, 1990.

[152] C. De Simone, M. Deza, and M. Laurent. Collapsing and lifting for the cut cone. Report n. 265, IASI-CNR, Roma, 1989.

[153] C.C. De Souza and M. Laurent. Some new classes of facets for the equicut polytope. Report 91738-OR, Institut für Diskrete Mathematik, Universität Bonn, 1991.

[154] P. Terwiliger and M. Deza. Classification of finite connected hypermetric spaces. *Graphs and Combinatorics*, 3:293–298, 1987.

[155] I. Vajda. L_1-distances in statistical inference: comparison of topological functional and statistical properties. In Y. Dodge, editor, *Statistical data analysis based on the L_1-norm and related methods*, pages 177–184. Elsevier Science Publishers B.V. (North Holland), 1987.

[156] J. von Neumann. *Mathematical foundations of quantum mechanics.* Princeton University Press, Princeton, original German edition in 1933 edition, 1955.

[157] G.F. Voronoi. Nouvelles applications des paramètres continus à le théorie des formes quadratiques, Deuxième mémoire. *Journal Reine Angewandte Mathematik*, 134:198–287, 1908.

[158] G.F. Voronoi. Nouvelles applications des paramètres continus à l e théorie des formes quadratiques, Deuxième mémoire. *Journal Reine Angewandte Mathematik*, 136:67–178, 1909.

[159] P.M. Winkler. On graphs which are metric spaces of negative type. In J. Alavi et al., editor, *Graph Theory with applications to Algorithms and Computer Science*, pages 801–810. Wiley, 1985.

[160] P.M. Winkler. The metric structure of graphs: theory and applications. In C. Whitehead, editor, *Surveys in Combinatorics 1987*, London Mathematical Society, Lecture Note Series 123, pages 197–221. Cambridge University Press, Cambridge, 1987.

[161] M.L. Yoseloff. *A combinatorial approach to the diagonal N-representability problem.* PhD thesis, Princeton University, 1970.

[162] M.L. Yoseloff and H.W. Kuhn. Combinatorial approach to the N-representability of p-density matrices. *Journal of Mathematical Physics*, 10(4):703–706, 1969.