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# 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:

- $\ell_1$ - 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.

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## 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:  $\ell_1$ -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:

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

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

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

(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.

**$\ell_1$ -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  $\ell_1$ -embeddable, i.e.  $d_{ij} = \|u_i - u_j\|_1$  for all  $i, j$ , for some vectors  $u_1, \dots, u_n \in \mathbb{R}^m$ . Hence, characterizing  $\ell_1$ -embeddable metrics by inequalities amounts to find the valid inequalities for the cut cone  $Cut_n$ . More detailed connections with  $\ell_1$ - and  $L_1$ -metrics are described in section 3.

For rational metrics,  $\ell_1$ -embeddability is equivalent to embeddability, up to multiplicative factor, in a hypercube. For the case of graphic metrics, both concepts of  $\ell_1$ - 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  $\mu(A_1 \cup \dots \cup A_n)$  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:

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

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  $A_1, \dots, A_n$  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  $\psi$ , which is a unit vector of a Hilbert space  $H(N)$ . For each wavefunction  $\psi$  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  $\Gamma$   $N$ -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  $\text{Conv}((x_i x_j)_{1 \leq i < j \leq n} : x \in \{0, 1\}^n, \sum_{1 \leq i < j \leq n} x_i = N)$ . 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 exceeded 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  $d \in \text{Met}_n$ . Hence, the metric cone  $\text{Met}_n$ , 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  $\text{Hyp}_n$  which is contained in the metric cone  $\text{Met}_n$  and contains the cut cone  $\text{Cut}_n$ . The hypermetrics  $d \in \text{Hyp}_n$  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  $2td(K_n) = (2t, \dots, 2t)$  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 disproof 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  $V_n = \{1, \dots, n\}$ ,  $E_n = \{(i, j) : 1 \leq i < j \leq n\}$ , 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  $1 \leq i < j \leq n$ .

- 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  $\mathcal{I}_{< m}$  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  $b_1, \dots, b_n$ , we consider the inequality:

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

When  $\sigma := \sum_{1 \leq i \leq n} b_i = 1$ , the inequality (3) is called a *hypermetric inequality* and denoted by  $Hyp_n(b_1, \dots, b_n)$ . 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  $b_1, \dots, b_n$  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:

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

referred 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  $b_1, \dots, b_n$ , 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:

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

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  $\sigma$  odd and when there exists a subset  $A$  such that  $\sum_{i \in A} b_i = \frac{\sigma-1}{2}$ ).

### 2.3 $\ell_1$ , Voronoi and covariance maps

We introduce three useful maps:

- the  $\ell_1$ -map  $\varphi_\ell : \mathbb{R}^n \rightarrow \mathbb{R}^{\binom{n}{2}}$  defined by  $\varphi_\ell(x) = (|x_i - x_j|)_{1 \leq i < j \leq n}$  for  $x \in \mathbb{R}^n$ .
- the Voronoi map  $\varphi_v : \mathbb{R}^n \rightarrow \mathbb{R}^{\binom{n+1}{2}}$  defined by  $\varphi_v(x) = (x_i x_j)_{1 \leq i < j \leq n}$  for  $x \in \mathbb{R}^n$ .
- the covariance map  $\varphi_{c_0} : \mathbb{R}^{\binom{n+1}{2}} \rightarrow \mathbb{R}^{\binom{n+1}{2}}$  defined by  $\varphi_{c_0}(x) = p$ , for  $x = (x_{ij})_{0 \leq i < j \leq n}$ ,  $p = (p_{ij})_{1 \leq i < j \leq n}$ , with

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

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

The cut and intersection vectors are linked via these maps. Namely, given a subset  $S \subseteq \{1, \dots, n\}$  and its incidence vector  $1_S \in \{0, 1\}^n$ , then  $\delta(S) = \varphi_{c_0}(1_S)$  and  $\pi(S) = \varphi_{c_0}(1_S)$ . Moreover, if  $S$  is a subset of  $\{0, 1, \dots, n\}$  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.

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

- 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.

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

- 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

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

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  $\varphi_{c_0}$ , since their generators are in one-to-one correspondance via  $\varphi_{c_0}$ . 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  $\{0, 1, \dots, n\}$ , then

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

It can be checked that

$$\varphi_{c_0}(Hyp_{n+1}) = \{p = (p_{ij})_{1 \leq i < j \leq n} : \sum_{1 \leq i, j \leq n} b_i b_j p_{ij} - \sum_{1 \leq i \leq n} b_i p_{ii} \geq 0 \text{ for all integers } b_1, \dots, b_n\} \quad (8)$$

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

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

We deduce the following inclusions.

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

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.  $\pi_G(S) = (\pi(S)_{ij})_{1 \leq i < j \leq n, (i,j) \in E \text{ if } i \neq j}$ . 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

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

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

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.  $d \in \text{Met}_n$ , 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*.

•  $d \in \text{Met}_n$  is said to be *metrically rigid* if  $d$  lies on a simplicial face of  $\text{Met}_n$ , 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  $\text{Met}_n$ .

•  $d$  is *hypermetric* if  $d$  satisfies the hypermetric inequalities (3), i.e.  $d \in \text{Hyp}_n$ , 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.  $d \in \text{Neg}_n$ , and  $d$  is  $2k$ -gonal if it satisfies all  $2k$ -gonal negative type inequalities.

- $d$  is  $\ell_p$ -embeddable if there exist  $n$  vectors  $x_1, \dots, x_n \in \mathbb{R}^m$  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  $x_1, \dots, x_n \in \{0, 1\}^m$ ,  $m \geq 1$ .
  - If  $d$  is rational valued, then  $d$  is  $\ell_1$ -embeddable if and only if  $\eta d$  is *h-embeddable* for some scalar  $\eta$  [10]. The smallest such  $\eta$  is called the *scale* of  $d$ . This fact is easy, but crucial, since it permits to link combinatorial and analytical aspects.
  - For  $d \in \text{Cut}_n$ , 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  $d \in \text{Cut}_n$  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  $d \in \text{Cut}_n$ , we have the following bounds on its minimum size  $s(d)$ :

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

- $d \in \text{Cut}_n$  is said to be  $\ell_1$ -rigid if it lies on a simplicial face of  $\text{Cut}_n$ , i.e.  $d$  has a unique  $\mathbb{R}_+$ -realization or, equivalently (in view of Theorem 3.3),  $d$  has a unique  $\ell_1$ -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  $\text{Cut}_{n+1}$  and the boolean quadric polytope  $BQP_n$  are in one-to-one correspondance via the covariance map  $\varphi_{e_0}$ . We now see in more detail how the covariance map acts on the valid inequalities. Consider the inequalities:

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

$$\sum_{1 \leq i \leq n} a_i p_{ii} + \sum_{1 \leq i < j \leq n} b_{ij} p_{ij} \leq d \quad (15)$$

where  $a, b, c$  are linked by

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

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  $\mathbb{R}^{\binom{n}{2}}$  by

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

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

Hence,  $r_{\delta(A)}$  is an affine map, called *switching map*, whose associated linear map is  $R_{\delta(A)}$ . Then, the inequality  $v^T x \leq v_0$  is valid (resp. facet defining) for  $CutP_n$  if and only if the inequality  $R_{\delta(A)}(v)^T x \leq v_0 - v^T \delta(A)$  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

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

into the inequality

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

where

$$\begin{aligned} d' &= d - \sum_{i \in A} a_i - \frac{1}{2} \sum_{1 \leq i < j \leq n, i, j \in A} b_{ij} \\ a'_i &= \begin{cases} a_i + \sum_{j \in A} b_{ij} & \text{if } i \notin A \\ -a_i - \sum_{j \in A - \{i\}} b_{ij} & \text{if } i \in A \end{cases} \\ b'_{ij} &= \begin{cases} -b_{ij} & \text{if } |A \cap \{i, j\}| = 1 \\ b_{ij} & \text{if } |A \cap \{i, j\}| \neq 1. \end{cases} \end{aligned}$$

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: $\ell_1$ - and $L_1$ -metrics

#### 3.1 The cut cone and $\ell_1$ -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  $d \in \text{Cut}_n$  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,  $\ell_1$ -embeddable or, equivalently,  $d \in \text{Cut}_n$  if and only if  $d_{ij} = \mu(A_i \Delta A_j)$ ,  $1 \leq i < j \leq n$ , for some non negative measure space  $(\Omega, \mathcal{A}, \mu)$  and some events  $A_1, \dots, A_n \in \mathcal{A}$ . The corresponding statement for the boolean quadric cone reads:  $p \in \text{BQ}_n$  if and only if  $p_{ij} = \mu(A_i \cap A_j)$ ,  $1 \leq i \leq j \leq n$ , for some non negative measure space  $(\Omega, \mathcal{A}, \mu)$  and some events  $A_1, \dots, A_n \in \mathcal{A}$ . 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  $\Omega$ , a  $\sigma$ -algebra  $\mathcal{A}$  of subsets of  $\Omega$ , and a measure  $\mu$  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  $\phi$  (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  $\| \cdot \|_1$  denotes the  $\ell_1$ -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)  $d \in \text{Cut}_n$  (resp.  $d \in \text{Cut}P_n$ ).
- (ii) *There exist a non negative measure space (resp. a probability space)  $(\Omega, \mathcal{A}, \mu)$  and  $A_1, \dots, A_n \in \mathcal{A}$  such that  $d_{ij} = \mu(A_i \Delta A_j)$  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  $A_1, \dots, A_n \in \mathcal{A}$  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,  $p = \sum_{S \subseteq \{1, \dots, n\}} \lambda_S \pi(S)$  for some  $\lambda_S \geq 0$ . We define a non negative measure space  $(\Omega, \mathcal{A}, \mu)$  as follows. Let  $\Omega$  denote the family of subsets of  $\{1, \dots, n\}$ , let  $\mathcal{A}$  denote the family of subsets of  $\Omega$  and let  $\mu$  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  $\{1, \dots, n\}$ ). 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  $1 \leq i \leq j \leq n$ . 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  $1 \leq i \leq j \leq n$ , where  $(\Omega, \mathcal{A}, \mu)$  is a nonnegative measure space and  $A_1, \dots, A_n \in \mathcal{A}$ . Set  $A^S = \bigcap_{i \in S} A_i \cap \bigcap_{i \notin S} (\Omega - A_i)$  for each  $S \subseteq \{1, \dots, n\}$ . 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,  $p = \sum_{S \subseteq \{1, \dots, n\}} \mu(A^S) \pi(S)$ , 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  $BQP_n$ .  $\blacksquare$

Another characterization of the cut cone is given in [6], [11] in terms of  $\ell_1$ -metrics.

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

- (i)  $d \in \text{Cut}_n$ .



(ii)  $(X, d)$  is  $\ell_1$ -embeddable, i.e. there exist  $n$  vectors  $u_1, \dots, u_n \in \mathbb{R}^m$  for some  $m$  such that  $d_{ij} = \|u_i - u_j\|_1$  for all  $1 \leq i < j \leq n$ .

PROOF. (i)  $\Rightarrow$  (ii). Let  $d \in \text{Cut}_n$ , then  $d = \sum_{1 \leq k \leq m} \lambda_k \delta(S_k)$  with  $\lambda_1, \dots, \lambda_m \geq 0$ . For  $1 \leq i \leq n$ , 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  $1 \leq k \leq m$ . Then  $d_{ij} = \|u_i - u_j\|_1$  holds, showing that  $(X, d)$  is  $\ell_1$ -embeddable.

(ii)  $\Rightarrow$  (i). Assume that  $(X, d)$  is  $\ell_1$ -embeddable, i.e. there exist  $n$  vectors  $u_1, \dots, u_n \in \mathbb{R}^m$  for some  $m \geq 1$  such that  $d_{ij} = \|u_i - u_j\|_1$ , for  $1 \leq i < j \leq n$ . We show that  $d \in \text{Cut}_n$ . It suffices to show the result for the case  $m = 1$  by additivity of the  $\ell_1$ -norm. Hence  $d_{ij} = |u_i - u_j|$  where  $u_1, \dots, u_n \in \mathbb{R}$ . Without loss of generality, we can suppose that  $0 = u_1 \leq u_2 \leq \dots \leq u_n$ . Then,  $d = \sum_{1 \leq k \leq n-1} (u_{k+1} - u_k) \delta(\{1, 2, \dots, k-1, k\})$  holds, showing that  $d \in \text{Cut}_n$ .  $\blacksquare$

There is an analogue characterization for  $h$ -embeddable metrics.

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

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

(ii)  $(X, d)$  is  $h$ -embeddable, i.e. there exist  $n$  vectors  $u_1, \dots, u_n \in \{0, 1\}^m$  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  $S_1, \dots, S_m$ . If  $u_1, \dots, u_n$  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  $u_1, \dots, u_n$ . Let  $S_1, \dots, S_m$  be the subsets of  $\{1, \dots, n\}$  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.  $\blacksquare$

### 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  $f : \Omega \rightarrow \mathbb{R}$ , 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  $\mathcal{A}_\mu = \{A \in \mathcal{A} : \mu(A) < \infty\}$  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  $\Omega$  is a set of cardinality  $m$ ,  $\mathcal{A} = 2^\Omega$  is the collection of subsets of  $\Omega$  and  $\mu$  is the cardinality measure, i.e.  $\mu(A) = |A|$  for  $A \subseteq \Omega$ , then  $L_1(\Omega, 2^\Omega, |\cdot|)$  is simply denoted as  $\ell_1(m)$ , or  $\ell_1$ . Hence, the  $m$ -dimensional hypercube  $(K_2)^m$  is the subspace of  $\ell_1$  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  $\phi$  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  $\lambda$  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  $f \mapsto E(f) \Delta E(0)$  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.  $\blacksquare$

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  $\delta_Y$  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  $\delta_Y$  is just the symmetrization of the usual cut metric  $\delta(Y)$ . Let  $\mathcal{D}(X)$  denote the set of all cut functions  $\delta_Y$  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  $\nu$  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  $x \mapsto A_x$  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  $\nu$  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,

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

(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.  $\blacksquare$

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  $\delta_Y$  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  $\mu_i$  to  $\Omega_1 \cup \Omega_2$ . If  $\phi_i$  denotes the embedding of  $(X_i, d_i)$  into  $L_1(\Omega_i, \mathcal{A}_i, \mu_i)$ , then we obtain an embedding  $\phi$  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  $x \mapsto (x, x)$ ) 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  $\delta$ . 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  $d$ .  $\blacksquare$

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

**THEOREM 3.8** *Let  $X = \{1, \dots, n\}$  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  $\ell_1$ -embeddable.
- (iii)  $d \in \text{Cut}_n$ .

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.  $\sum_{1 \leq i < j \leq n} b_i b_j d(x_i, x_j) \leq 0$  for all integers  $b_1, \dots, b_n$  with  $\sum_{1 \leq i \leq n} b_i = 1$ , for all  $x_1, \dots, x_n \in X$  and all  $n \geq 1$ . Let  $\text{Hyp}(X)$  denote the set of the hypermetrics  $d$  on  $X$ . Then,  $C(X) \subseteq \text{Hyp}(X)$  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 examples 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  $\ell_1$ -,  $\ell_2$ -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  $\sum_S \lambda_S \delta(S)$ ,  $\lambda_S$  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*:

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

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  $\ell_1$ -embeddable, we also say that the graph is an  $\ell_1$ -*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:

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

for all distinct  $i, j, k$ , i.e. each triangle is isocetes 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  $|\cdot|$  be a non-archimedean valuation on  $F$  (e.g. the  $p$ -adic valuation on the field of  $p$ -adic numbers), i.e.  $|\cdot|$  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*:

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

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  $\ell_2$ -embeddable (indeed, if  $d$  is ultrametric, then  $d^2$  too is ultrametric and, thus, of negative type, implying that  $d$  is  $\ell_2$ -embeddable - see Table 1 for the implications). In fact, it is easy to check that:

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

The inequality:  $\min\{m : d \text{ is } \ell_2\text{-embeddable into } \mathbb{R}^m\} \leq n - 1$ , holds for all  $\ell_2$ -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  $\ell_2$ -embeddable  $\iff d^2 \in Neg_n$ , 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  $\ell_1$ -rigid, but  $d$  is not metrically rigid. The path metric of  $K_4$  is  $\ell_1$ -embeddable, but not  $\ell_1$ -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  $\ell_1$ -rigid.

$d$ is $\ell_2$ - embeddable	$\iff$	$d^2 \in Neg_n$	$\iff$	$d$ is ultrametric
$\Downarrow$		$\Downarrow$		$\Updownarrow$
$d$ is $\ell_1$ - embeddable	$\iff$	$d \in Cut_n$		$d^a \in Met_n$ for all $a \in \mathbb{R}_+$
		$\Downarrow$		$\Downarrow$
$d \in Met_n$	$\iff$	$d \in Hyp_n$		$d$ is the path metric of a weighted tree
		$\Downarrow$		$\Uparrow$
$d$ has one positive eigenvalue	$\iff$	$d \in Neg_n$		$d$ is the path metric of a tree
				$\Downarrow$
$d$ is metrically rigid	$\iff$	$d$ is the path metric of a bipartite graph	$\iff$	$d$ is the path metric of an isometric subgraph of a hypercube
$\Downarrow$				$\Downarrow$
$d$ is $\ell_1$ - rigid (if $d \in Cut_n$ )		$d \in Cut_n \cap L_n$	$\iff$	$d$ is $h$ - embeddable
$\Downarrow$		$\Downarrow$		$\Downarrow$
$d$ is $h$ - rigid ( if $d$ is $h$ -embeddable)		$d \in Cut_n$ and $d$ is rational valued	$\iff$	$\eta d$ 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  $\{u \in \{0, 1\}^n : \sum_{1 \leq i \leq n} u_i \text{ is even}\}$  with two nodes adjacent if their Hamming distance is equal to 2. The *cocktail party* graph  $K_{n \times 2}$  has  $2n$  nodes:  $1, \dots, 2n$  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  $\ell_1$ -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  $2d \in \text{Cut}_{2n}$  (so  $K_{n \times 2}$  is an  $\ell_1$ -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 [14]:*

- $d_G$  is  $h$ -embeddable,
- $d_G$  is  $\ell_1$ -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  $\ell_1$ -rigid [62].

**THEOREM 4.3** [149]

- (i)  $G$  is an  $\ell_1$ -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  $\ell_1$ -graph on  $n$  nodes, then its scale  $\eta$  is equal to 1, or is even with  $\eta \leq n-1$ . Moreover, if  $G$  is  $\ell_1$ -rigid, then its scale  $\eta$  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  $\ell_1$ -graphs within the class of graphs having a universal node. Given a graph  $G$ ,  $\nabla G$  denotes the graph obtained by adding a node adjacent to all nodes of  $G$ . So the path metric of  $\nabla G$  takes only the values 1,2.

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

- $\nabla G$  is an  $\ell_1$ -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  $\nabla G$  is an  $\ell_1$ -graph if and only if its path metric is 5-gonal and of negative type; if  $n \geq 28$ , then  $\nabla G$  is an  $\ell_1$ -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,  $\ell_1$ -embeddability, and  $\ell_1$ -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  $\ell_1$ -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 neighbor of  $v^*$ ).*

Finally, we mention a characterization of trees within  $\ell_1$ -graphs, using the notion of minimum size.

**PROPOSITION 4.9** [52] *Let  $G$  be an  $\ell_1$ -graph and let  $s(d_G)$  denote the minimum size of its path metric. Then,  $2 - \frac{1}{\lfloor \frac{n}{2} \rfloor} \leq s(d_G) \leq n - 1$ . 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  $d \in \text{Cut}_n$ , 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  $\|\cdot\|$  on  $\mathbb{R}^d$  is of the form  $h(K, \cdot)$ , where  $K$  is the polar of the unit ball. Each norm  $\|\cdot\|$  on  $\mathbb{R}^d$  defines a metric  $d_{\|\cdot\|}$  on  $\mathbb{R}^d$ , called *norm* (or *Minkowski*) *metric*, by setting  $d_{\|\cdot\|}(x, y) = \|x - y\|$ . The following results give several equivalent characterizations for  $L_1$ -embeddable normed spaces.

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

- (i)  $d_{\|\cdot\|}$  is of negative type.
- (ii)  $d_{\|\cdot\|}$  is hypermetric.
- (iii)  $(\mathbb{R}^d, d_{\|\cdot\|})$  is  $L_1$ -embeddable.
- (iv) The polar of  $U$  is a zonoid, i.e.  $\|\cdot\| = h(U^*, \cdot)$  is the support function of a zonoid.
- (v) There exists a positive Borel measure  $\mu$  on the hyperplanesets of  $\mathbb{R}^d$  such that the norm  $\|\cdot\|$  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  $\| \cdot \|$  be a norm on  $\mathbb{R}^d$  for which the unit ball  $U$  is a polytope. The following assertions are equivalent:

(i)  $\| \cdot \|$  satisfies the Hlawka inequality:

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

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

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

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

(iv)  $(\mathbb{R}^d, d_{\|\cdot\|})$  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  $\mu$  on the hyperplanesets of  $\mathbb{R}^d$  satisfying

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

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  $v : L \rightarrow \mathbb{R}_+$  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  $x \mapsto S_x$  is the isomorphism from  $K$  to  $\mathcal{N}$ , then we have the embedding  $x \mapsto S_x$  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.  $\blacksquare$

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  $d_v(x, y) = \log\left(\frac{\text{l.c.m.}(x, y)}{\text{g.c.d.}(x, y)}\right)$  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  $v : S \mapsto \mathbb{R}$ , 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  $x \vee \dots \vee x = x$  for all  $x \in S$ , where the join  $x \vee \dots \vee x$  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  $\{x \in \mathbb{R}_+^E : x(C) \leq |C| - 1 \text{ for all odd cycles } C \text{ of } G\}$  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,

$$\begin{aligned} \max \quad & w^T x \\ \text{subject to} \quad & x \in \text{Cut}P(G). \end{aligned}$$

This is the polyhedral approach, classical in combinatorial optimization, which leads to the study of the facets of  $\text{Cut}P(G)$ . 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,  $\text{Cut}P(G) = \text{Met}(G)$ , 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  $\text{Cut}P(G)$ , 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

$$\begin{aligned} \max \quad & w^T x \\ \text{subject to} \quad & x \in \text{Cut}P_n \end{aligned}$$

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

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

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

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

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  $L_{ii} = \text{deg}_G(i)$  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

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

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

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

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

- (i)  $mc(G) \leq \varphi(G)$  [45]
- (ii)  $mc(G) \leq \psi(G)$  [146]

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

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

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

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*  $c : E \rightarrow \mathbb{R}_+$ , and the *demand graph*  $H = (T, U)$  together with a *demand function*  $r : U \rightarrow \mathbb{R}_+$ , 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  $f : \mathcal{P} \rightarrow \mathbb{R}_+$ . The instance  $(G, H, c, r)$  is said to be *feasible* if there exists a feasible multiflow, i.e. a multiflow  $f : \mathcal{P} \rightarrow \mathbb{R}_+$  satisfying the following capacity and demand requirements:

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

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

Using Farkas lemma, it can be checked that:

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

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

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*

$$(c - r)^T d \geq 0 \text{ for all } d \in \text{Met}_n. \quad (23)$$

Therefore, the metric cone  $\text{Met}_n$  is the dual cone to the cone of feasible multiflows.

An obvious way for testing feasibility of the pair  $(c, r)$  is to solve the linear program  $\min((c - r)^T d : d \in \text{Met}_n)$  which has  $\binom{n}{2}$  variables and  $3\binom{n}{3}$  constraints (the triangle inequalities (1)). An alternative way is to check the condition (23) for all extreme rays  $d$  of  $\text{Met}_n$ . This approach leads to the study of the extreme rays of the metric cone  $\text{Met}_n$  (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  $\text{Met}(G)$  (defined in relation (11)) arises naturally when studying multicommodity flows. It is shown in [148] that all extreme rays of  $\text{Met}(G)$  are 0, 1-valued (i.e.  $\text{Met}(G) = \text{Cut}(G)$ ) if and only if  $G$  is not contractible to  $K_5$ . The graphs for which all extreme rays of  $\text{Met}(G)$  are 0, 1, 2-valued are characterized in [147]. The graphs for which all the vertices of the metric polytope  $\text{Met}P(G)$  (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  $\text{Cut}_n$  is contained in the metric cone  $\text{Met}_n$ , a necessary condition for the existence of a feasible multiflow is the following *cut condition*:

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

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  $d \in \text{Met}_n$  having an extremal graph  $K = (V_0, W)$  such that  $W$  is a subset of the support of the demand function  $r$ .*

**THEOREM 5.6** [107] *If  $d \in \text{Met}_n$  has an extremal graph which is  $K_4$ ,  $C_5$ , or a union of two stars, then  $d \in \text{Cut}_n$ . Moreover, if  $d$  satisfies the parity condition (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  $A_1, \dots, A_n$  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  $\mu(A_1 \cup \dots \cup A_n)$  ?*

It is easy to see that the answer is:

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

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

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  $\mu(A_1 \cup \dots \cup A_n)$  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,

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

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

**Estimations for  $\mu(A_1 \cup \dots \cup A_n)$  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  $\{1, \dots, n\}$  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  $A_1, \dots, A_n \in \mathcal{A}$  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.

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

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

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  $p \in BQP_n^{\mathcal{I}}$ . 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**  $z_{min} \leq \mu(A_1 \cup \dots \cup A_n) \leq z_{max}$ .

**PROOF.** For  $S \subseteq \{1, \dots, n\}$ , set  $A^S = \bigcap_{i \in S} A_i \cap \bigcap_{i \notin S} (\Omega - A_i)$ . Then,  $\bigcap_{i \in I} A_i = \bigcup_{I \subseteq S \subseteq \{1, \dots, n\}} A^S$ ,  $\Omega = \bigcup_S A^S$  and  $A_1 \cup \dots \cup A_n = \bigcup_{S \neq \emptyset} A^S$ . We have  $p_I = \mu(\bigcap_{i \in I} A_i)$  for each  $I \in \mathcal{I}$ . Therefore,  $p = \sum_{S \neq \emptyset} \mu(A^S) \pi^{\mathcal{I}}(S)$  holds, with  $\mu(A^S) \geq 0$ . Hence  $(\mu(A^S) : \emptyset \neq S \subseteq \{1, \dots, n\})$  is a feasible solution to the program (25), or (26), with objective value  $\mu(A_1 \cup \dots \cup A_n)$ . This proves the result.  $\blacksquare$

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

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

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

By linear programming duality, we have:

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

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

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

(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  $\mu(A_1 \cup \dots \cup A_n)$  in terms of the joint probabilities  $p_I = \mu(\bigcap_{i \in I} A_i)$  for  $I \in \mathcal{I}$ . Examples of such lower bounds are exposed below (after Proposition 5.9).

The case when the collection  $\mathcal{I}$  of index sets is  $\mathcal{I}_{\leq m}$  is considered in [32]. The following estimations for  $\mu(A_1 \cup \dots \cup A_n)$  are given there:

$$y_{min} \leq \mu(A_1 \cup \dots \cup A_n) \leq y_{max} \quad (30)$$

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

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

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

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  $y_{min} \leq z_{min} \leq \mu(A_1 \cup \dots \cup A_n) \leq z_{max} \leq y_{max}$ .*

**PROOF.** Indeed, every feasible solution for (25) yields a feasible solution for (31) with the same objective value. Namely, let  $(\lambda_S, \emptyset \neq S \subseteq \{1, \dots, n\})$  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,

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

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

**Examples of bounds for  $\mu(A_1 \cup \dots \cup A_n)$ .** The best lower bound for  $\mu(A_1 \cup \dots \cup A_n)$  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  $\mathcal{I} = \mathcal{I}_{\leq 2}$ , 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  $\mu(A_1 \cup \dots \cup A_n)$ .

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

$$\begin{aligned} \frac{n \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{\lfloor \frac{n+1}{2} \rfloor \lceil \frac{n+1}{2} \rceil} &\leq \sum_{\emptyset \neq S \subseteq \{1, \dots, n\}} \lambda_S \\ \frac{n \sum_{1 \leq i \leq n} p_i - 2 \sum_{1 \leq i < j \leq n} p_{ij}}{n} &\geq \sum_{\emptyset \neq S \subseteq \{1, \dots, n\}} \lambda_S \end{aligned} \quad (33)$$

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

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

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:

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

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  $b_1 = \dots = b_n = 1$ , the inequality (35) corresponds (via the covariance map) to the inequality:

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

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

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



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  $b_1, \dots, b_n$  and  $k \geq 0$ , the inequality:

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

is valid for  $BQP_n$ . This yields the bound:

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

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 explicitly 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  $a_i = \left( \binom{i}{1}, \binom{i}{2}, \dots, \binom{i}{m} \right)$ , for  $1 \leq i \leq n$ . Set  $b = (S_1, \dots, S_m)$ . The matrix  $M$  is full rank, hence a basis  $B$  consists of a set of  $m$  linearly independent vectors among  $a_1, \dots, a_n$ . 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  $i \in \{1, \dots, n\} - B$ , 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  $1_m^T M_B^{-1} b \leq \mu(A_1 \cup \dots \cup A_n)$  holds. The dual feasible bases are explicitly described in [32] together with the corresponding bounds for  $\mu(A_1 \cup \dots \cup A_n)$ .

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

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

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  $\nu$  denotes the random variable counting the number of events that occur among  $A_1, \dots, A_n$ .

The inequality (38) can alternatively be written as

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

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  $b_1, \dots, b_n$  and  $k_1, \dots, k_m \geq 0$ , the inequality

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

is clearly valid for the polytope  $BQP_n^{\mathcal{I}_{\leq 2m}}$ . Thus arises the question of determining the parameters  $b_1, \dots, b_n, k_1, \dots, k_m$  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:

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

For  $d \in Hyp_n$ ,  $(V_n = \{1, \dots, n\}, d)$  is called a *hypermetric space*. It is convenient to work with the hypermetric cone  $Hyp_{n+1}$  defined on the  $n + 1$  points  $0, 1, 2, \dots, n$ .

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  $B = \{v_0, v_1, \dots, v_m\} \subseteq L$  is *generating* for  $L$  if, for each  $v \in L$ , there exist integers  $z_0, z_1, \dots, z_m$  such that  $\sum_{0 \leq i \leq m} z_i = 1$  and  $v = \sum_{0 \leq i \leq m} z_i v_i$ . If, moreover, there is unicity of the integers  $z_i$ , then  $B$  is an (affine) *basis* of  $L$ ; in this case,  $m = |B| - 1$  is called the *dimension* of  $L$ .

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

- $\|v - c\|_2 \geq r$  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  $\alpha_n$ , hypercube  $\gamma_n$ , cross polytope  $\beta_n := \text{Conv}(\pm e_i : 1 \leq i \leq n)$  (where  $e_1, \dots, e_n$  are the unit vectors in  $\mathbb{R}^n$ ). Both  $\beta_n$  and  $\gamma_n$  are centrally symmetric,  $\alpha_n$  is asymmetric. All types of *L-polytopes* in dimension  $k \leq 4$  have been classified in [80]:

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

The following polytope  $P_{p,q}^m$  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  $\text{Pyr}(P)$ . We define iteratively  $\text{Pyr}_m(P)$  as  $\text{Pyr}(\text{Pyr}_{m-1}(P))$ , setting  $\text{Pyr}_0(P) = P$ . Let  $S_p, S_q$  be two simplices of respective dimensions  $p, q$  and lying in affine spaces which intersect in one point. Then,  $P_{p,q}^m := \text{Pyr}_m(\text{Conv}(S_p \cup S_q))$  is called a *repartitioning polytope*; it has dimension  $m + p + q$  and  $m + p + q + 2$  vertices. In fact,  $P_{p,q}^m$  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  $d \in \text{Hyp}_{n+1}$ . 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  $f_d : \{0, 1, \dots, n\} \rightarrow V(P_d)$ ,  $f_d(i) = v_i$  for  $0 \leq i \leq n$ , such that

- $\{v_0, v_1, \dots, v_n\}$  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  $\varphi_{c_0}$ . Define  $p = \varphi_{c_0}(d)$ ,  $p = (p_{ij})_{1 \leq i \leq j \leq n}$ . By relation (8),  $d \in \text{Hyp}_{n+1}$  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  $b_1, \dots, b_n$ . Therefore, if  $d \in \text{Hyp}_{n+1}$ , 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  $v_1, \dots, v_n \in \mathbb{R}^k$ , 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,  $v_0 = 0, v_1, \dots, v_n$  lie on the sphere  $S(c, r := \|c\|_2)$ . Remains only

to show that  $\{v_1, \dots, v_n\}$  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 $P$
$d \in Cut_{n+1}$	[7] $\iff$	$V(P)$ is contained in the set of vertices of a parallelepiped
$d$ is a cut	$\iff$	$P = \alpha_1$
$F(d) = Hyp_{n+1}$	[7] $\iff$	$P = \alpha_n$
$F(d)$ is a facet	[17] $\iff$	$P$ is a repartitioning polytope
$F(d)$ is an extreme ray	[55] $\iff$	$P$ is extreme
$F(d) = F(d')$	[55] $\iff$	$P, P'$ 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  $b_{max}^n$  denote the largest value of  $\max_i |b_i|$  for which the inequality (41) defines a facet of  $Hyp_n$ . Then,  $b_{max}^n < \frac{2^{n-2}(n-1)!}{n+1}$  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  $\alpha_1$ .

**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,*

$$(i) \quad \binom{k+2}{2} \leq r(P) \leq \binom{k+2}{2} - |V(P)|,$$

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

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

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

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

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  $\beta_n$ , the simplex  $\alpha_n$ , 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  $\alpha_1$ , 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 know any other extreme  $L$ -polytope of dimension  $k \leq 7$  beside  $\alpha_1$ ,  $2_{21}$ ,  $3_{21}$ .

**Extreme  $L$ -polytopes in sections of the Leech lattice  $\Lambda_{24}$ .** The Leech lattice  $\Lambda_{24}$  is a lattice of dimension 24. By taking suitable sections of the sphere of minimal vectors of  $\Lambda_{24}$ , 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  $\Lambda_{16}$ .** The Barnes-Wall lattice  $\Lambda_{16}$  is a lattice of dimension 16. Several examples of extreme  $L$ -polytopes are constructed from  $\Lambda_{16}$  in [55]:

- $P$ , centrally symmetric (constructed from a deep hole of  $\Lambda_{16}$ ), 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  $Hy p_n$  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  $\nabla G$  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

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

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

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

$$\langle A \rangle_\psi := \langle \psi, A\psi \rangle = \int \psi^*(x)A\psi(x)dx.$$

Among the observables of the system, the simplest ones are those that the system may have (then the expected value of the observable is equal to one), or lack (then the expected value is zero). Such observables are represented by orthogonal projections on subspaces of  $H(N)$ .

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

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

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

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

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

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

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

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

$\Gamma_{\psi}^{(p)}(x_1 \dots x_p | x_1 \dots x_p)$  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,  $\binom{N}{2}^{-1} \Gamma_{\psi}^{(2)}(x_1 x_2 | x_1 x_2) dv_1 dv_2$  is the probability of finding a particle with spin  $s_1$  within the volume  $dv_1$  around the point  $r_1$ , and another particle with spin  $s_2$  within the volume  $dv_2$  around the point  $r_2$ , when all other particles have arbitrary spins and positions, etc...

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

Density matrices have been widely studied. In particular, they were the central topic of several conferences held at Queen's University, Kingston, Canada, yielding three volumes of proceedings ([39], [78], [81]).

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

$$A = A_0 + \sum_{1 \leq i \leq N} A_i + \frac{1}{2!} \sum_{1 \leq i \neq j \leq N} A_{ij} + \dots \quad (45)$$

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

$$\begin{aligned} \langle A \rangle_{\psi} &= A_0 + \int \{A_1 \Gamma_{\psi}^{(1)}(x'_1 | x_1)\}_{x'_1=x_1} dx_1 + \\ &+ \int \{A_{12} \Gamma_{\psi}^{(2)}(x'_1 x'_2 | x_1 x_2)\}_{x'_1=x_1, x'_2=x_2} dx_1 dx_2 + \dots \end{aligned} \quad (46)$$

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  $\Omega$  in relation (45) has only terms involving two particles at most, i.e.  $\Omega = \Omega_0 + \sum_{1 \leq i \leq N} \Omega_i + \frac{1}{2} \sum_{i \neq j} \Omega_{ij}$ . 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  $\Omega$  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  $\Phi_k, k \geq 1$ , be an orthonormal set (assumed to be discrete for the sake of simplicity) of functions of  $H(1)$  such that each function  $f \in H(1)$  can be expanded as

$$f = \sum_{k \geq 1} \langle \Phi_k, f \rangle \Phi_k. \quad (47)$$

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

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

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

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

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

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

where

$$\begin{aligned} C_K &= \langle \Phi_K, \psi \rangle \\ &= \sqrt{N!} \int \psi(x_1, \dots, x_N) \Phi_{k_1}^*(x_1) \dots \Phi_{k_N}^*(x_N) dx_1 \dots dx_N \end{aligned} \quad (51)$$

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

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

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

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

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

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

$$\gamma_\psi(ij|hk) = \sum C_I^* C_K \epsilon_{i,j,I-\{i,j\}}^I \epsilon_{h,k,K-\{h,k\}}^K \quad (54)$$

where the sum is over all subsets  $I, K \subseteq \{1, \dots, n\}$  of cardinality  $N$  such that  $i, j \in I$ ,  $h, k \in K$  and  $I - \{i, j\} = K - \{h, k\}$ , and we set  $\epsilon_{i_1 \dots i_p}^{j_1 \dots j_p} = \text{sign}(\sigma)$  if there is a permutation  $\sigma$  mapping  $i_1$  on  $j_1, \dots, i_p$  on  $j_p$  and  $\epsilon_{i_1 \dots i_p}^{j_1 \dots j_p} = 0$  otherwise. In particular, the diagonal terms are given by

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

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

and  $\sum w_\psi \langle \Omega \rangle_\psi$  have the same minimum (equal to the minimum eigenvalue of the Hamiltonian  $\Omega$  and attained at a corresponding eigenvector).

Let  $\mathcal{P}_N^{(2)}$  denote the convex set consisting of the convex combinations  $\sum_\psi w_\psi \Gamma_\psi^{(2)}$  ( $w_\psi \geq 0$ ,  $\sum_\psi w_\psi = 1$ ) of second order density matrices of normalized wavefunctions  $\psi \in H(N)$ . The question of finding a characterization of  $\mathcal{P}_N^{(2)}$  was formulated in [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 of the form  $\sum w_\psi \Gamma_\psi^{(1)}(x'_1|x_1)$  for  $w_\psi \geq 0$ ,  $\sum w_\psi = 1$ ,  $\langle \psi, \psi \rangle = 1$  and  $\psi \in H(N)$  if and only if  $\text{Tr}(\Gamma) = \int \Gamma(x_1|x_1) dx_1 = N$  and the eigenvalues of  $\Gamma$  satisfy  $0 \leq \lambda \leq 1$ . However, the ensemble  $N$ -representability problem is already difficult for density matrices of order  $p = 2$ . In fact, as stated in 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  $BQP_n^{I=2}(N)$  denote the polytope defined as the convex hull of the vectors  $\pi^{I=2}(K)$  for  $K \subseteq \{1, \dots, n\}$  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  $\gamma_{\Phi_K}$  coincide with the vector  $\pi^{I=2}(K)$ . For that reason, the polytope  $BQP_n^{I=2}(N)$  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  $BQP_n^{I=2}(N)$ .

**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  $\gamma$  belongs to  $BQP_n^{I=2}(N)$ .*

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),  $\gamma = \sum_{K \subseteq \{1, \dots, n\}, |K|=N} |C_K|^2 \pi^{\mathcal{I}=2}(K)$  with  $\sum |C_K|^2 = \langle \psi, \psi \rangle = 1$ . 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  $\langle \psi, \psi \rangle = 1$ . 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 additional extreme points besides the second order density matrices of the Slater determinants (even though those are the only extreme points when restricted to the diagonal terms). Other extreme points for  $\mathcal{P}_N^{(2)}$  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:

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

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  $K \subseteq \{1, \dots, n\}$ ,  $|K| = p$ .

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  $K = \{k_1, \dots, k_N\}$  with  $1 \leq k_1 < \dots < k_N$ ,

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

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

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

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

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  $\Phi_K$  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  $b := (b_0, b_i, 1 \leq i \leq n, b_{ij}, 1 \leq i < j \leq n)$  for which  $b(x) := b_0 + \sum_{1 \leq i \leq n} b_i x_i + \sum_{1 \leq i < j \leq n} b_{ij} x_i x_j \geq 0$  for each  $x \in \{0, 1\}^n$ . Therefore,  $Q^+(I^n)$  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  $BQ_{-n}$ .

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  $\varphi_{c_0}$ . Namely,

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

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  $A_1, \dots, A_n \in \mathcal{A}$  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  $\psi$  of a Hilbert space  $H$  ( $H = H(N)$  if the system has  $N$  particles). Let  $E_\psi$  denote the projection operator from  $H$  to the line spanned by  $\psi$ , i.e.  $E_\psi(\phi) = \langle \psi, \phi \rangle \psi$  for  $\phi \in H$ . Equivalently, a state of the system is given by such a projection operator  $E_\psi$ ; 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  $\langle \psi, \psi \rangle = 1$ ). Such states  $W$  are called *ensemble states*, or *mixtures*. Pure and ensemble states were already considered in section 7.2. Alternatively, a state of the system is a bounded linear operator  $W$  of  $H$  which is Hermitian, positive 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  $E_1, \dots, E_n$  (not necessarily distinct, nor commuting) such that

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

where  $E_i \wedge E_j$  denotes the projection from  $H$  to the subspace  $E_i(H) \cap E_j(H)$ . So  $p_{ij}$  represents the probability that the system has the properties associated with the projections  $E_i$  and  $E_j$  when it is in the state  $W$ . Let  $QCP_n$  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 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  $p = \sum_{K \subseteq \{1, \dots, n\}} \lambda_K \pi(K)$  where  $\lambda_K \geq 0$  and  $\sum_K \lambda_K = 1$ . Let  $H$  be a Hilbert space of dimension  $2^n$  and let  $(\psi_K, K \subseteq \{1, \dots, n\})$  be an orthonormal basis of  $H$  indexed by the subsets of  $\{1, \dots, n\}$ . Let  $W$  be the operator of  $H$  defined by  $W(\psi_K) = \lambda_K \psi_K$  for all  $K$ . Let  $E_i$  denote the projection from  $H$  to the subspace  $H_i$  spanned by the vectors  $\psi_K$  with  $i \in K$ ; then  $E_i \wedge E_j$  is the projection on the subspace spanned by  $\psi_K$  for  $i, j \in K$ . Note that the trace of the operator  $WE_i \wedge E_j$  is equal to  $\sum_{i, j \in K} \lambda_K = p_{ij}$ . This shows that  $p$  belongs to  $QCP_n$ .  $\blacksquare$

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 developed; 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,  $\text{trace}(WE_i) = (\cos \theta)^2 = p_{ii}$  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  $X : \Omega \rightarrow \mathbb{R}$  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.  $F_X(x) = \mu(\{\omega \in \Omega : X(\omega) \leq x\})$  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 ( $1 \leq p \leq \infty$ ) of the above metrics, especially of the first two, are also used in probability theory.

Several results are known, establishing links among the above metrics. One of the main such results is the Monge-Kantorovich mass-transportation theorem which shows that the second metric  $k(X, Y)$  can be viewed as a minimum of the first metric  $L_1(X, Y)$  over all joint distributions of  $X$  and  $Y$  with fixed marginal. A relationship between the  $L_1(X, Y)$  and the engineer metric  $EN(X, Y)$  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  $(H, \nu)$  and a map  $x \mapsto A_x \subseteq H$  with  $\nu(A_x) < \infty$  for  $x \in M$ , such that  $d(x, y) = \nu(A_x \Delta A_y)$  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  $(H, \nu)$  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 $\ell_1$ -metric in statistical data analysis

A *data structure* is a pair  $(I, d)$ , where  $I$  is a finite set, called *population*, and  $d : I \times I \rightarrow \mathbb{R}_+$  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  $\ell_2$ -embeddable are considered in factor analysis and multidimensional scaling. These two cases together with cluster analysis are the main three techniques for studying data structures. The case when  $d$  is  $\ell_1$ -embeddable is a natural extension of the ultrametric and  $\ell_2$  cases.

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

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

In fact, the  $\ell_1$  criterion has been increasingly used. Its importance has been pointed out, 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  $2td(K_n) = \sum_{1 \leq i < j \leq n} t\delta(\{i, j\})$ , 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 necessarily distinct) subsets of  $V_n = \{1, \dots, n\}$ , 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 necessarily distinct) subsets of  $V_n$ , the sets  $B \in \mathcal{B}$  are called *blocks*. Let  $r, k, \lambda$  be integers.

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

$\mathcal{B}$  is called a  $(n, k, \lambda)$ -*BIBD* (BIBD standing for balanced incomplete block design) if any two distinct points  $i, j \in V_n$  belong to  $\lambda$  common blocks and each block has cardinality  $k$ . This implies that each point  $i \in V_n$  belong to  $r = \frac{\lambda(n-1)}{k-1}$  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  $\pm 1$  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  $(n, k, \lambda)$ -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)

$$\begin{aligned}
 PG(2, t) \text{ exists} & \stackrel{[97] \text{ and } [142]}{\iff} z_{t^2+t+1}^t = t^2 + t + 1 \\
 & \stackrel{[48]}{\iff} 2td(K_{t^2+t+2}) \text{ is not } h\text{-rigid,} \\
 & \quad \text{i.e. } z_{t^2+t+2}^t < t(t^2 + t + 2) \\
 & \stackrel{[61]}{\iff} \begin{cases} z_{t^2+t+2}^t = t^2 + 2t \text{ if } t \geq 3 \\ t^2 + t + 1 \text{ if } t = 1, 2 \end{cases}
 \end{aligned}$$

(v) [142]

$$\begin{aligned}
 \text{There exists a Hadamard matrix of order } 4t & \iff z_{4t-1}^t = 4t - 1 \\
 & \iff z_{4t}^t = 4t - 1.
 \end{aligned}$$

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

Observe that  $a_{4t}^t = a_{4t-1}^t = 4t - 1$ , and  $a_{t^2+t+1}^t = a_{t^2+t+2}^t = 4t$  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  $z_n^t = a_n^t$ .

- If  $\lceil \frac{n}{2} \rceil$  divides  $2t$  and there exists a Hadamard matrix of order  $4t$ , then  $z_n^t = a_n^t$ .

#### 8.4 Miscellaneous

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

On the integers, beside the usual  $\ell_1$ -metric  $|a-b|$ , we have, for instance, the well known Hamming distance between the binary expansions of  $a, b$ , and  $\log\left(\frac{l.c.m.(a,b)}{g.c.d.(a,b)}\right)$  (mentioned after Theorem 4.13) which are both  $\ell_1$ -embeddable.

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

- The *Prevosti's genetic distance*:  $\frac{1}{2r} \sum_{1 \leq j < r} \sum_{1 \leq i < k_j} |p_{ij} - q_{ij}|$  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  $\ell_1$ -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  $\ell_1$ -distance  $\text{aire}(A \Delta B)$  is used in the treatment of images; see, for instance, [105].

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