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# Functional analysis on hypergraphs, density and Zeta functions: applications to molecular graphs and image processing.

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## Abstract

This paper introduces new descriptors and invariants for hypergraphs. We develop a new type of Zeta functions and density functions, that are proved to have useful invariance and monotony properties. Links with hypergraph entropies are established as well. New matrices linked with hypergraphs are also proposed, from which a new type of Laplacian associated with hypergraphs is derived.

*Keywords:* Hypergraphs - Entropy - Algebraic and graphical structures - Laplacian hypergraph - Molecular Topological indices- Image Processing.

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## 1. Introduction

The theory of networks and hyper-networks is explored in many fields of human activity. These structures are represented in most cases by graphs or hypergraphs. Their study often involves descriptors and invariant characteristics. As an example, many have been introduced, particularly in chemistry [32, 39, 23].

These indices are of various nature: arithmetic, topological geometric, algebraic, combinatorial, but also analytical [5, 6, 35, 29]. Over the past twenty years, many works have been carried out on these indices, which proved useful in other fields than those where they were introduced. This

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shows that finally this study has become an autonomous field of graph theory, as illustrated e.g. in [18, 44] .

The algebraic theory of graphs has demonstrated its relevance in several application fields. It is used in classification, deep learning, image analysis and many other sciences. The study of the spectrum of the adjacency matrix and the Laplacian matrix is key in these applications. The study of eigenvalues and eigenvectors gives excellent information on the combinatorics of graphs, thus making it possible to bring more precision on topological parameters of these structures. Most of the classical matrices associated with graphs can be seen as operators acting on a set of functions defined on vertices or edges. This led to the introduction of functional analysis in a discrete version. The tools derived from analysis, notably in physics such as Dirichlet's problem or Green's functions, were introduced in graph theories, and combinatorial versions of the great theorems of mathematical physics were developed, thus showing their usefulness for the different network applications [15, 16].

The theory of hypergraphs is more recent than that of graphs. For about fifteen years, given the development of algorithmics on hypergraphs, these are widely used in applied sciences [10]. Naturally several mathematicians and computer scientists have tried to adapt the tools of the graph theory to hypergraphs. Invariants, such as Randic index, Wiener index, Estrada index for example, have been generalized with more or less success. However, work on these generalizations is not as advanced as that on graphs. While the representation by adjacency matrix of a graph fully characterizes it, this is not the case for a hypergraph. This creates some problems, particularly in the definition of the Laplacian, for example. Consequently, there is a relatively large loss of information. Interesting attempts have been made to address these issues [13, 14, 2]. Starting from the diffusion processes of modern physics such as the heat equation or wave equations, some authors have given definitions of classical operators of functional analysis which have shown their validity in the study of hypergraphs [13, 14].

In this article we propose to extend the various analyzes that have been carried out in the work cited above. The philosophy of our work is to start from invariants inspired for example by Randic index and others, then to develop new basic parameters, associated with hypergraphs, and which allow us to introduce new matrices associated with hypergraphs. This, as we will see, is in our opinion more relevant than those which have been introduced so far because they take better into account the topology of the hypergraphs.

Thirdly, thanks to these matrices and therefore introduced invariants, we develop the classic tools of functional analysis.

The paper is organized as follows. Section 2 recalls the definitions related to hypergraphs which are used throughout the article. Section 3 introduces new hypergraph invariants. They are based on the combinatorial topology of these structures and are inspired by the notion of RIEMANN 's function. Elementary properties are developed in Section 4, which allows us on the one hand to connect different notions of entropies with our invariants, and on the other hand to identify the links between some hypergraph parameters and the Zeta function as well as the density function. A comparative study between the Zeta function and the density functions is carried out in Section 5. This shows that these functions could play an interesting role in additive-multiplicative number theory. This, to some extent, justifies the names given to these invariants. To illustrate the use of the invariants introduced in our work, some applications of the proposed Zeta-like functions are given in Section 6, in particular to characterize certain types of hypergraphs. Section 7 introduces new matrices associated with hypergraphs, which allow us to show that the proposed Zeta functions form bounds of the ESTRADA function, which is well known in mathematical chemistry for instance. Moreover a Laplacian operator is introduced, along with its properties.

in Section 8, we will introduce some applications in order to illustrate the relevance of the concepts introduced throughout this article. We approached two areas, chemistry and image analysis where the use of the tools forged in this work can be promising. Obviously, other sectors could be investigated, but this section is simply an introductory illustration.

In the last section we explore some avenues for future work, notably on dynamic hypergraphs which are increasingly important in (hyper)network theory.

## 2. Preliminaries

Let us first recall some useful notions on hypergraphs [10]. A hypergraph  $H$  denoted by  $H = (V, E)$  is defined as a pair of a finite set  $V$  of vertices and a finite family  $E = \{e_i, i = 1..m\}$  of hyperedges (only finite hypergraphs are considered in this paper). Hyperedges can be considered equivalently as subsets of vertices or as a relation between vertices of  $V$ . The first interpretation is considered here, and we will note  $x \in e_i$  the fact that a vertex

$x \in V$  belongs to the hyperedge  $e_i$ . In this paper, it is further assumed that  $E$  is non-empty, that each hyperedge is non-empty (i.e.  $\forall e_i \in E, e_i \neq \emptyset$ ), and that  $H$  is simple (i.e.  $\forall (e_i, e_j) \in E^2, e_i \subseteq e_j \Rightarrow i = j$ , which implies that  $H$  is without repeated hyperedges). The degree of a vertex  $x$  of  $V$  is defined as  $d(x) = \sum_{e \in E} 1_{x \in e}$ , where  $1_{x \in e} = 1$  if  $x$  is a vertex of  $e$  and 0 otherwise. For a simple hypergraph  $H$ , we have  $d(x) = |\{e \in E \mid x \in e\}| = |H(x)|$  where  $H$  is the star of  $x$  in  $H$  (see below).

In order to study the fine structure of an hypergraph, the following notions are important in this paper:

- A *partial hypergraph*  $H'$  of  $H$  generated by  $J \subseteq \{1 \dots m\}$  is a hypergraph  $(V', \{e_j, j \in J\})$ , where  $\cup_{j \in J} e_j \subseteq V' \subseteq V$ . This definition induces a partial ordering between hypergraphs, denoted by  $H' \leq H$ :  $H' \leq H$  if  $H'$  is a partial hypergraph of  $H$ .
- A hypergraph  $H = (V, E)$  is *isomorphic* to a hypergraph  $H' = (V', E')$  ( $H \simeq H'$ ), if there exist a bijection  $f : V \rightarrow V'$  and a bijection  $\pi : \{1 \dots m\} \rightarrow \{1 \dots m'\}$ , where  $m = |E|$  and  $m' = |E'|$ , which induce a bijection  $g : E \rightarrow E'$  (if  $H$  is simple,  $g(e) = \{f(x) \mid x \in e\}$ ) such that  $g(e_i) = e'_{\pi(i)}$  for all  $e_i \in E$  and  $e'_{\pi(i)} \in E'$ . The mapping  $f$  is then called *isomorphism* of hypergraphs. Obviously it implies  $m = m'$ .

Let  $H = (V, E)$  be a hypergraph with  $|V| = n$ ,  $|E| = m$ . The incidence matrix of  $H$  is defined by:  $I(H) = ((a_{i,j}))_{(i,j) \in \{1 \dots m\} \times \{1 \dots n\}}$  where  $a_{i,j} = 1$  if  $x_j \in e_i$ , and  $a_{i,j} = 0$  otherwise. Let  $H = (V, E)$  be a hypergraph with  $|V| = n$ ,  $|E| = m$ , the transposed of  $I(H)$ ,  $I(H)^t$ , gives rise to a new hypergraph called *dual hypergraph* denoted by  $H^* = (V^*, E^*)$ , with  $|V^*| = m$  and  $|E^*| = n$ , and the incidence matrix of  $H^*$  is  $I(H)^t$ .

A hypergraph  $H = (V, E)$  is said *connected* if  $\cup_{e \in E} e = V$  (i.e. there is not isolated vertex), and  $\forall (e, e') \in E^2, \exists k \in \mathbb{N}, \exists (e_1 \dots e_k) \in E^k, e_1 = e, e_k = e', \forall i < k, e_i \cap e_{i+1} \neq \emptyset$ .

A *star* centered at  $x$  in a hypergraph  $H = (V, E)$  is the collection of hyperedges which contain  $x$ :  $H(x) = \{e \in E \mid x \in e\}$  (which is a multiset if the hypergraph has repeated hyperedges), hence  $|H(x)| = d(x)$ . A hypergraph  $H = (V, E)$  is called a *star* if there exists a vertex  $x \in V$  such that  $H(x) = E$ .

A hypergraph  $H = (V, E)$  is *linear* if it is simple and  $\forall (e_i, e_j) \in E^2, i \neq j, |e_i \cap e_j| \leq 1$ .

Let  $H = (V, E)$  be a loopless hypergraph (i.e.  $\forall e \in E, |e| \geq 2$ ), a *hyper-path* in  $H$  is an ordered sequence  $(e_1, e_2, \dots, e_k)$  such that two consecutive

hyperedges intersect in exactly one vertex and non-consecutive hyperedges are disjoint. Moreover, if the sequence is cyclic, i.e.  $|e_k \cap e_1| = 1$ , then it is a *hypercycle*. By extension, a hypergraph  $H = (V, E)$  is called *hypercycle* if all the hyperedges can be numbered as  $e_1 \dots e_m$  such that the sequence  $(e_1 \dots e_m)$  is a hypercycle.

**Convention 1.** *In this paper, all considered hypergraphs are simple, without isolated vertex, without empty hyperedge, and finite, i.e. the cardinality of the sets of both vertices and hyperedges are finite.*

### 3. Hypergraph characteristics from Zeta function

#### 3.1. Combinatorial parameters

Let  $H = (V, E)$  be a hypergraph with  $|V| = n$ ,  $|E| = m$ .

**Definition 1.** *For any  $e \in E$  we define the multiplicative degree and the additive degree of  $e$  as*

$$d_e^\times = \prod_{x \in e} d(x) \text{ and } d_e^+ = \sum_{x \in e} (d(x) - 1).$$

Note that for a vertex  $x$  that belongs only to one hyperedge  $e$ , then  $d(x) = 1$  (and  $d(x) - 1 = 0$ ), which means that this vertex does not play any role in  $d_e^\times$  nor  $d_e^+$ . Moreover, isolated vertices are not involved at all in these characteristics.

**Definition 2.** *The hyperedge multiplicative degree and hyperedge additive degree of  $H$  are defined by:*

$$\delta^\times(H) = \sum_{e \in E} d_e^\times \text{ and } \delta^+(H) = \sum_{e \in E} d_e^+.$$

Note that these two characteristics of  $H$  only depend on hyperedges (hence their names), and are independent of potential isolated vertices in  $H$ . Since  $\forall e \in E, d_e^\times \geq 1$  (hyperedges are assumed to be non-empty),  $\delta^\times(H) \geq 1$ . By contrast, we can have  $\delta^+(H) = 0$  in the case where every vertex belongs at most to one hyperedge. Intuitively, these characteristics represent how much  $H$  is “connected”, i.e. they increase when vertices belong to more hyperedges.

From these parameters we define two discrete probability distributions on  $E$ , if  $\delta^+(H) \neq 0$  for the second one:

$$(p_e^\times)_{e \in E} = \left( \frac{d_e^\times}{\delta^\times(H)} \right)_{e \in E} \quad \text{and} \quad (p_e^+)_{e \in E} = \left( \frac{d_e^+}{\delta^+(H)} \right)_{e \in E}$$

Intuitively, these distributions illustrate how “homogeneous” is the topology of  $H$  among the hyperedges.

### 3.2. Zeta functions, density functions

In the sequel we use the notation  $\bullet$  to denote either  $\times$  or  $+$ . Recall that the Zeta function is defined for any  $s \in \mathbb{C}$ , as  $\zeta(s) = \sum_{n=1}^{+\infty} \frac{1}{n^s}$ . By analogy, we define Zeta functions on hypergraphs, as follows.

**Definition 3.** *The multiplicative-additive Zeta functions of a hypergraph  $H$ , or for short Zeta functions, as:*

$$\zeta_H^\bullet(s) = \sum_{e \in E} \left( \frac{1}{d_e^\bullet} \right)^s \quad (1)$$

where the sum is restricted to  $e$  such that  $(\frac{1}{d_e^\bullet})^s$  is well defined.

**Definition 4.** *Similarly, we define (multiplicative-additive) density functions of  $H$  as:*

$$\tau_H^\bullet(s) = \prod_{e \in E} \left( \frac{1}{d_e^\bullet} \right)^s \quad (2)$$

where the product restricted to  $e$  such that  $(\frac{1}{d_e^\bullet})^s$  is well defined.

Note that in these definitions, no restriction applies for  $d_e^\times$  since these values are always greater than or equal to 1. For  $d_e^+$ , the following result allows using a limit value when the real part of  $s$  is negative.

**Proposition 1.** *Let  $\sigma = \text{Re}(s)$ . We have  $\lim_{d_e^+ \rightarrow 0} (\frac{1}{d_e^+})^s = 0$  for  $\sigma < 0$ .*

Therefore, for  $d_e^+ = 0$ , we can set

$$\left( \frac{1}{d_e^+} \right)^s = \begin{cases} 0 & \text{if } \sigma < 0 \\ 1 & \text{if } s = 0 \\ \text{undefined} & \text{otherwise} \end{cases}$$

These two functions measure the complexity of the topology of  $H$ , as shown in the following examples.

**Example 1.** If  $H$  is such that there is no intersection between any two hyperedges (every hyperedge is “isolated” and there are as many connected components as hyperedges), then  $\forall e \in E, \forall x \in e, d(x) = 1$ , and  $d_e^\times = 1, d_e^+ = 0$ . Therefore  $\forall s \in \mathbb{C}, \zeta_H^\times(s) = |E| = m$ , and  $\Upsilon_H^\times(s) = 1$ . Using the convention in the previous proposition, we have  $\zeta_H^+(s) = \Upsilon_H^+(s) = 0$  if  $\text{Re}(s) < 0$ , and  $\zeta_H^+(0) = m, \Upsilon_H^+(0) = 1$ . Otherwise, these two quantities are undefined. A generalization of this example will be given in Section 4.

**Example 2.** If the hyperedges are “chained”, i.e.  $\forall i < m, e_i \cap e_{i+1} = \{x_i\}$  and  $x_i \neq x_j, \forall i \neq j$ , then  $d_{e_1}^+ = d_{e_m}^+ = 1, d_{e_i}^+ = 2, \forall i, i \neq 1, i \neq m$ , and  $d_{e_1}^\times = d_{e_m}^\times = 2, d_{e_i}^\times = 4, \forall i, i \neq 1, i \neq m$ . Therefore  $\forall s, \zeta_H^+(s) = 2 + (m - 2)2^{-s}, \Upsilon_H^+(s) = 2^{-s(m-2)}$ , while  $\zeta_H^\times(s) = 2 \cdot 2^{-s} + (m - 2)4^{-s}, \Upsilon_H^\times(s) = 2^{-2s(m-1)}$  (hence they depend on  $s$ ).

In the same way, we can define two functions for the dual  $H^*$  of  $H$ , as:

$$\zeta_{H^*}^\bullet(s) = \sum_{x \in V} \left( \frac{1}{d_x^\bullet} \right)^s \quad (3)$$

$$\Upsilon_{H^*}^\bullet(s) = \prod_{x \in V} \left( \frac{1}{d_x^\bullet} \right)^s \quad (4)$$

with similar restrictions on the  $x$  involved in the sums, where

$$d_x^\times = \prod_{e \ni x} |e| \text{ and } d_x^+ = \sum_{e \ni x} (|e| - 1),$$

and

$$\delta^\times(H^*) = \sum_{x \in V} d_x^\times \text{ and } \delta^+(H^*) = \sum_{x \in V} d_x^+.$$

**Remark 1.** In the following we will restrict the study to the analytic functions of  $H$ , while keeping in mind that other combinatorial parameters can be exploited by considering the dual.

**Remark 2.** While the definitions above are given in general for  $s \in \mathbb{C}$  (according to the definition of the Zeta function), some of the results in the sequel will be proved only for restricted cases, with  $s \in \mathbb{R}$  or  $s \in \mathbb{N}$ .



### 3.3. Hypergraph entropies

A usual way to measure complexity is via entropy. While several notions of graph or hypergraph entropy have been defined [7, 20, 17], here new definitions are proposed, using the probability distributions introduced in Section 3.1.

**Definition 5.** *Let  $H$  be a simple hypergraph such that  $\delta^+(H) \neq 0$ . We define three entropies:*

$$S^\bullet(H) = - \sum_{e \in E} p_e^\bullet \ln p_e^\bullet \quad \text{hypergraph Shannon entropy (5)}$$

$$R_s^\bullet(H) = \frac{1}{1-s} \ln \left( \sum_{e \in E} (p_e^\bullet)^s \right), \quad s \in \mathbb{R}^+ \setminus \{1\} \quad \text{hypergraph Renyi entropy (6)}$$

$$T_s^\bullet(H) = \frac{1 - \sum_{e \in E} (p_e^\bullet)^s}{s-1}, \quad s \in \mathbb{R} \setminus \{1\} \quad \text{hypergraph Tsallis entropy (7)}$$

For  $\delta^+(H) = 0$ , i.e.  $\forall x, d(x) \leq 1$  and  $\forall e, d_e^+ = 0$ , we set  $p_e^+ = \frac{1}{m}$ , expressing the “regularity” of  $H$ , where all hyperedges are disconnected from each other. Then  $S^+(H) = R_s^+(H) = \ln m$  and  $T_s^+(H) = \frac{1-m^{1-s}}{s-1}$ .

By duality we have similar formulas for  $H^*$ .

**Remark 3.** *For the sake of simplicity we use the natural logarithm in all these definitions.*

**Remark 4.** *The limit of the Tsallis entropy when  $s \rightarrow 1$  is the Shannon entropy, i.e.  $-\sum_{e \in E} p_e^\bullet \ln p_e^\bullet$  [42].*

## 4. Properties

In this section, we prove a number of properties of the defined functions, as well as some links between them.

### 4.1. Basic properties

The different analytic functions defined in Section 3 can be linked according to the following properties.

**Proposition 2.** *Let  $H = (V, E)$  be a hypergraph, we have the following properties:*

1. for all  $s \in \mathbb{R}^+$ ,  $\zeta_H^\bullet(-s) = (\delta^\bullet(H))^s e^{(1-s)R_s^\bullet(H)}$  (for  $s = 1$ , where the Renyi entropy is not defined, we take the limit, i.e.  $(1-s)R_s^\bullet(H) = \ln \sum_{e \in E} (p_e^\bullet)^s$ , which is defined for  $s = 1$ );
2. for all  $s \in \mathbb{R}$ ,  $\zeta_H^\bullet(-s) = \delta^\bullet(H)(1 - (s-1)T_s^\bullet(H))$ ;
3.  $\zeta_H^{\bullet\prime}(0) = -\ln(\mathcal{T}_H^\bullet(-1))$ , where  $\zeta'$  denotes the derivative of  $\zeta$  with respect to  $s$ ;
4.  $\zeta_H^{\bullet\prime}(-1) = \delta^\bullet(H) [-\ln \delta^\bullet(H) + S^\bullet(H)]$ .

*Proof:*

1.  $\ln \zeta_H^\bullet(-s) = \ln \sum_{e \in E} (d_e^\bullet)^s = \ln (\delta^\bullet(H))^s + \ln \sum_{e \in E} (p_e^\bullet)^s = \ln (\delta^\bullet(H))^s + (1-s)R_s^\bullet(H)$ ; consequently  $\zeta_H^\bullet(-s) = (\delta^\bullet(H))^s e^{(1-s)R_s^\bullet(H)}$ ;
2.  $\zeta_H^\bullet(-s) = \sum_{e \in E} (d_e^\bullet)^s = (\delta^\bullet(H))^s \sum_{e \in E} p_e^{\bullet s} = (\delta^\bullet(H))^s (1 - (s-1)T_s^\bullet(H))$  (and this also holds for  $s = 1$ );
3.  $\zeta_H^{\bullet\prime}(s) = -\sum_{e \in E} (d_e^\bullet)^{-s} \ln d_e^\bullet$ ; hence,  $\zeta_H^{\bullet\prime}(0) = -\sum_{e \in E} \ln d_e^\bullet = -\ln \prod_{e \in E} d_e^\bullet = -\ln(\mathcal{T}_H^\bullet(-1))$ ;
4.  $\zeta_H^{\bullet\prime}(-1) = -\sum_{e \in E} d_e^\bullet \ln d_e^\bullet = -\sum_{e \in E} \delta^\bullet(H) p_e^\bullet \ln (\delta^\bullet(H) p_e^\bullet) = -\delta^\bullet(H) \ln \delta^\bullet(H) + \delta^\bullet(H) S^\bullet(H)$ .

■

#### 4.2. Combinatorial parameters and analytic functions

**Proposition 3.** *Let  $H = (V, E)$  be a hypergraph with  $|V| = n$  and  $|E| = m$  ( $m > 0$ ). We have the two following properties:*

1.  $\zeta_H^\bullet(0) = m$ ;
2.  $\zeta_H^\bullet(-1) = \delta^\bullet(H)$ ;
3.  $\mathcal{T}_H^\bullet(0) = 1$ .

*Proof:* We have:  $\zeta_H^\bullet(s) = \sum_{e \in E} e^{-s \ln d_e^\bullet}$ . So

1.  $\zeta_H^\bullet(0) = |E| = m$ ;
2. and  $\zeta_H^\bullet(-1) = \sum_{e \in E} d_e^\bullet = \delta^\bullet(H)$ .
3. The proof of (3) is direct.

■

The following property is an important result, since it shows that the Zeta and density functions are invariant characteristics with respect to isomorphisms (which is not surprising since they only involve the topology of the hypergraph), and that they are monotonous with respect to the partial ordering  $\leq$ . These are important features to use these functions as hypergraph descriptors.

**Proposition 4.** *Let  $H = (V, E)$  and  $H' = (V', E')$  be two hypergraphs, then*

1. *If  $H \simeq H'$  then for all  $s \in \mathbb{C}$ ,  $\zeta_H^\bullet(s) = \zeta_{H'}^\bullet(s)$  and  $\tau_H^\bullet(s) = \tau_{H'}^\bullet(s)$ .*
2. *If  $H' \leq H$  then for all  $s \in \mathbb{R}$ ,  $s \leq 0$ ,  $\zeta_H^\bullet(s) \geq \zeta_{H'}^\bullet(s)$ ,  $\tau_H^\bullet(s) \geq \tau_{H'}^\bullet(s)$ .*

*Proof:*

1. Assume that  $H \simeq H'$ . Let  $f$  be an isomorphism between  $H$  and  $H'$ . Then the two hypergraphs have the same size, i.e.  $|V| = |V'|$  and  $|E| = |E'|$ , and the same topology. Hence, for all  $x \in V$ ,  $f(x) \in V'$  and  $d(x) = d(f(x))$ ; for all  $e \in E$ ,  $g(e) \in E'$  ( $g$  being the bijection induced by  $f$  between  $E$  and  $E'$ ) and  $d_e^\bullet = d_{g(e)}^\bullet$ . This implies that  $\zeta_H^\bullet(s) = \zeta_{H'}^\bullet(s)$  and  $\tau_H^\bullet(s) = \tau_{H'}^\bullet(s)$ .  
Note that the result also holds if  $H$  and  $H'$  are only isomorphic up to isolated vertices (although not considered in this paper), since only hyperedges are involved in the Zeta and density functions.
2. Assume now that  $H' \leq H$  (i.e.  $H'$  is a partial hypergraph of  $H$ ). Since by definition  $E' \subseteq E$ , the degree of a vertex in  $H$  is higher than in  $H'$ . Let  $g$  be the natural injection from  $E'$  into  $E$  (induced by the inclusion):  $\forall e \in E', g(e) = e$ . Then we have  $d_e^\bullet \leq d_{g(e)}^\bullet$  for all  $e \in E'$ , where  $d_e^\bullet$  is meant in  $H'$ , while  $d_{g(e)}^\bullet$  is in  $H$ , and for  $s \leq 0$ ,  $(\frac{1}{d_e^\bullet})^s \leq (\frac{1}{d_{g(e)}^\bullet})^s$ , and the reverse inequality for  $s > 0$ . Consequently, since  $\zeta_H^\bullet(s)$  contains terms for  $e$  also belonging to  $E'$  and additional terms for  $e \in E \setminus E'$  (which do not appear at all in  $\zeta_{H'}^\bullet(s)$ ), we can conclude for  $s \leq 0$  but not for  $s > 0$ . For  $\tau_H^\bullet(s)$ , the additional terms are greater than 1 for  $s \leq 0$  and involved in a product, so we can also conclude in this case. Finally we get: if  $s \leq 0$  then  $\zeta_H^\bullet(s) \geq \zeta_{H'}^\bullet(s)$ ,  $\tau_H^\bullet(s) \geq \tau_{H'}^\bullet(s)$ .

■

Recall that a hypergraph  $H = (V, E)$  is a *matching* if for all  $e, e' \in E$ ,  $e \neq e'$ , we have  $e \cap e' = \emptyset$  (i.e.  $E$  is a set of pairwise disjoint hyperedges).

**Proposition 5.** *Let  $H = (V, E)$  be a hypergraph, and  $s \in \mathbb{R}$ . We have the following properties:*

1.  *$H$  is a matching if and only if for all  $s > 0$ ,  $\zeta_H^+(-s) = 0$ .*
2.  *$H$  contains at least one isolated hyperedge if and only if for all  $s > 0$ ,  $\tau_H^+(-s) = 0$*

*Proof:*

1. Assume that  $\zeta_H^+(-s) = 0$  for  $s > 0$ .  
 We have  $\zeta_H^+(-s) = \sum_{e \in E} (d_e^+)^s$ . For all  $x \in e$ ,  $d(x) \geq 1$ , and therefore  $d_e^+ \geq 0$ , for all  $e$ . Hence  $\zeta_H^+(-s) = 0$  implies that for all  $e \in E$ ,  $d_e^+ = 0$  (since  $s > 0$ ), and therefore for all  $x \in V$ ,  $d(x) = 1$  if  $x$  belongs to a hyperedge (then exactly one), or  $d(x) = 0$  if  $x$  is isolated; so  $H$  is a matching.  
 Conversely suppose that  $H$  is a matching. In this case for any  $e \in E$ , we have  $\forall x \in e$ ,  $d(x) = 1$ ; consequently  $\sum_{e \in E} (\sum_{x \in e} (d(x) - 1))^s = 0$ , so  $\zeta_H^+(-s) = 0$ .
2. We have the following equivalences, for  $s > 0$ :  
 $\neg \zeta_H^+(-s) = 0 \Leftrightarrow \exists e \in E, d_e^+ = 0 \Leftrightarrow \exists e \in E, \forall x \in e, d(x) = 1 \Leftrightarrow \exists e \in E, e \text{ isolated.}$

■

**Remark 5.** *These results suggest a counter-example illustrating the fact that in the first item of Proposition 4 the converse is not true. For instance take two hypergraphs  $H, H'$  which are both matchings, and which have the same number  $m$  of hyperedges. Assume that in the first one there is an hyperedge whose cardinality is greater than the one of every hyperedge of the second one, then  $H \not\cong H'$ . Since  $H$  and  $H'$  are matchings, we have  $\zeta_H^+(-s) = \zeta_{H'}^+(-s)$  for all  $s > 0$ ,  $\zeta_H^+(0) = \zeta_{H'}^+(0) = m$ , and the two functions are undefined otherwise. This means that for all  $s$  for which the functions are defined, they are equal. But the two hypergraphs are not isomorphic.*

#### 4.3. Hypergraph entropy and regularity

A hypergraph  $H = (V, E)$  is *multiplicative degree regular* if there exists  $k \in \mathbb{N}$  such that  $d_e^\times = \prod_{x \in e} d(x) = k$  for all  $e \in E$ , and it is *additive degree regular* if there exists  $k' \in \mathbb{N}$  such that  $d_e^+ = \sum_{x \in e} (d(x) - 1) = k'$  for all  $e \in E$ .

**Proposition 6.** *Let  $H = (V, E)$  be a hypergraph with  $|E| = m$ . The two following properties are equivalent:*

1.  $H$  is multiplicative (respectively additive) degree regular;
2.  $S^\times(H) = \ln m$  (respectively  $S^+(H) = \ln m$ ).

*Proof:* Assume that  $H$  is multiplicative degree regular, and let  $k$  be the constant value of  $d_e^\times$ . We have:

$$\begin{aligned} \forall e \in E, d_e^\times = k &\implies \sum_{e \in E} d_e^\times = mk \\ &\implies \forall e \in E, p_e^\times = \frac{k}{mk} = \frac{1}{m} \\ &\implies S^\times(H) = - \sum_{e \in E} \frac{1}{m} \ln \frac{1}{m} = \ln m. \end{aligned}$$

Conversely, if  $S^\times(H) = \ln m$ , then the discrete distribution is uniform, and  $p_e^\times = \frac{1}{m}$  for all  $e$ . This implies that  $d_e^\times$  is constant for all  $e$ , i.e. there exists  $k \in \mathbb{N}$  such that  $d_e^\times = k$ .

The proof for  $S^+(H)$  is similar. ■

Note that a similar result holds for  $R_s^\bullet$  and  $T_s^\bullet$  for  $s \neq 0$ . Indeed the extremal values of  $R_s^\bullet$  (i.e.  $\ln m$ ) and of  $T_s^\bullet$  (i.e.  $\frac{1-m^{1-s}}{s-1}$ ) are achieved for uniform distributions (i.e.  $p_e^\bullet = \frac{1}{m}, \forall e$ ). The other direction ((1)  $\implies$  (2)) is direct. Note that for  $s = 0$ , these two entropies do not depend on  $p_e^\bullet$ , and (2) does not imply (1).

## 5. Comparison between the density function and the Zeta function

In this section we establish further relations between the Zeta function and the density function.

**Lemma 1.** *Let  $F = \{x_1, x_2, \dots, x_m\} \subset \mathbb{N}$  with  $x_i \geq 2$ , for all  $i \in \{1, 2, \dots, m\}$ . Let  $s \in \mathbb{R}$  and  $s \geq 1$ , then for all subfamily  $\{x_{i_1}, x_{i_2}, \dots, x_{i_k}\} \subseteq F$ ,  $1 \leq k \leq m$  we have:*

$$x_{i_1}^s + x_{i_2}^s + \dots + x_{i_k}^s \leq x_{i_1}^s x_{i_2}^s \dots x_{i_k}^s; \quad (8)$$

$$\frac{1}{x_{i_1}^s} \frac{1}{x_{i_2}^s} \dots \frac{1}{x_{i_k}^s} \leq \frac{1}{x_{i_1}^s} + \frac{1}{x_{i_2}^s} + \dots + \frac{1}{x_{i_k}^s}. \quad (9)$$

*Proof:* Let us prove the first inequality by induction on  $k$ .

- For  $k = 1$  the result is obvious.
- For  $k = 2$ , let us assume, without loss of generality, that  $x_{i_1} \leq x_{i_2}$ . Then  $x_{i_1}^s \leq x_{i_2}^s$  since  $s \geq 1$ . We also have  $2 \leq 2^s \leq x_{i_1}^s$ . Hence  $x_{i_1}^s + x_{i_2}^s \leq 2x_{i_2}^s \leq x_{i_1}^s x_{i_2}^s$ .

- Assume that Equation 8 is true for  $k$ , i.e.  $S_k \leq M_k$ , where  $S_k = \sum_{j=1}^k x_{i_j}^s$  and  $M_k = \prod_{j=1}^k x_{i_j}^s$ . Then  $S_k + s_{i_{k+1}}^s \leq M_k + s_{i_{k+1}}^s$ . Two cases may arise:
  - If  $x_{i_{k+1}}^s \leq M_k$ , then  $S_{k+1} \leq 2M_k \leq M_k x_{i_{k+1}}^s$  since  $x_{i_{k+1}} \geq 2$ , and therefore  $S_{k+1} \leq M_{k+1}$ , where  $S_{k+1}$  et  $M_{k+1}$  are defined similarly as  $S_k$  and  $M_k$ .
  - If  $x_{i_{k+1}}^s \geq M_k$ , then  $S_{k+1} \leq 2x_{i_{k+1}}^s \leq M_k x_{i_{k+1}}^s$ , and  $S_{k+1} \leq M_{k+1}$ .

Then, by the induction hypothesis, we can conclude that Equation 8 is true for all  $k \leq m$ .

Let us now prove the second inequality. From Equation 8 we have  $\prod_{j=1}^k \frac{1}{x_{i_j}^s} \leq \frac{1}{\sum_{j=1}^k x_{i_j}^s}$ . Let us assume without loss of generality that  $x_{i_1}^s \leq x_{i_j}^s$  for all  $j$ . We then have  $x_{i_1}^s \leq \sum_{j=1}^k x_{i_j}^s$  and  $\frac{1}{x_{i_1}^s} \geq \frac{1}{\sum_{j=1}^k x_{i_j}^s}$ . Finally

$$\prod_{j=1}^k \frac{1}{x_{i_j}^s} \leq \frac{1}{\sum_{j=1}^k x_{i_j}^s} \leq \frac{1}{x_{i_1}^s} \leq \sum_{j=1}^k \frac{1}{x_{i_j}^s}$$

■

**Theorem 1.** *Let  $H = (V, E)$  be a hypergraph, then*

1. *if for all  $x \in V$ ,  $d(x) \geq 2$ , then  $\Upsilon_H^\times(s) \leq \zeta_H^\times(s)$  if  $s \geq 1$ , and  $\Upsilon_H^\times(s) \geq \zeta_H^\times(s)$  if  $s \leq -1$ ;*
2. *if for all  $x \in V$ ,  $d(x) \geq 3$ , then  $\Upsilon_H^+(s) \leq \zeta_H^+(s)$  if  $s \geq 1$ , and  $\Upsilon_H^+(s) \geq \zeta_H^+(s)$  if  $s \leq -1$ ;*

*Note that while it is convenient to express general conditions on the degrees of the vertices, the result holds for weaker conditions. Indeed it is sufficient to have  $\forall e, d_e^\bullet \geq 2$  for the inequalities to be true. This means that for  $\bullet = \times$  it is sufficient to have  $\forall e, \exists x \in e, d(x) \geq 2$  (i.e. no isolated hyperedge), while for  $\bullet = +$  the condition would be  $\forall e, \exists x \in e, d(x) \geq 3$  or  $\exists x, x' \in e, x \neq x', d(x) \geq 2$  and  $d(x') \geq 2$  (which implicitly assumes that  $e$  contains at least two vertices).*

*Proof:* By applying Lemma 1. ■

Let us now show that, under some conditions, equality cannot occur.

**Lemma 2.** Let  $x_1, x_2, \dots, x_m \in \mathbb{N}$ , and  $m \geq 3$ . If  $x_i \geq 2$  for all  $i \in \{1, 2, \dots, m\}$ , then for all  $s \geq 1$ :

$$x_1^s + x_2^s + \dots + x_m^s \neq x_1^s x_2^s \dots x_m^s$$

In a similar way, for  $m \geq 3$  and  $s \geq 1$ ,  $\sum_{i=1}^m (\frac{1}{x_i})^s \neq \prod_{i=1}^m (\frac{1}{x_i})^s$ .

*Proof:* Let  $x_1, x_2, \dots, x_m \in \mathbb{N}$  with  $x_i \geq 2$  for all  $i \in \{1, 2, \dots, m\}$ , and  $m \geq 3$ . Let  $s \geq 1$ . Assume that  $x_1^s + x_2^s + \dots + x_m^s = x_1^s x_2^s \dots x_m^s$ . Suppose (without loss of generality) that  $x_1 \leq x_2 \leq \dots, x_{m-1} \leq x_m$ . Then  $x_1^s + x_2^s + \dots + x_m^s \leq m \cdot x_m^s$ . By hypothesis this is equivalent to  $x_1^s x_2^s \dots x_m^s \leq m \cdot x_m^s$ , and since  $x_m > 0$   $x_1^s x_2^s \dots x_{m-1}^s \leq m$ . Because  $x_i \geq 2$  for all  $i \in \{1, 2, \dots, m\}$  we have:

$$2^{s(m-1)} \leq x_1^s x_2^s \dots x_{m-1}^s \leq m$$

which is impossible since  $s \geq 1$  and  $m \geq 3$ . Hence the hypothesis is false and  $x_1^s + x_2^s + \dots + x_m^s \neq x_1^s x_2^s \dots x_m^s$ .

The proof for the product is similar. ■

**Theorem 2.** Let  $H = (V, E)$  be a hypergraph such that for all  $x \in V$ ,  $d(x) \geq 3$ . Then, for all  $s \geq 1$ :

$$\mathfrak{T}_H^\bullet(s) \neq \zeta_H^\bullet(s);$$

and

$$\mathfrak{T}_H^\bullet(-s) \neq \zeta_H^\bullet(-s).$$

As in Theorem 1, these results hold actually under the weaker condition that  $\forall e, d_e^\bullet \geq 2$ .

*Proof:* Directly by applying Lemma 1 and Lemma 2. ■

These results show that the two functions  $\mathfrak{T}_H^\bullet$  and  $\zeta_H^\bullet$  are actually different characteristics of hypergraphs.

**Remark 6.** If the conditions of Lemma 2 are not verified we can have the equality, for instance

$$x_1 = x_2 = 2 \text{ then } x_1 + x_2 = x_1 x_2;$$

$$x_1 = 3, x_2 = 2 \text{ and } x_3 = 1, \text{ then } x_1 + x_2 + x_3 = x_1 x_2 x_3$$

This theorem is very close to certain problems in number theory. This leads us to bring the following problem:

**Problem 1.** *Let  $x_1, x_2, \dots, x_m \in \mathbb{N}^*$ ,  $m \geq 2$ , and  $s \geq 2$ . What is the set of solutions of the following equation:*

$$x_1^s + x_2^s + \dots + x_m^s = x_1^s x_2^s \dots x_m^s?$$

*and is this set non-empty for any  $m \geq 2$  and  $s \geq 2$ ?*

These solutions exist, for instance: let  $s = 2$ ,  $m = 10$ , then  $(2, 2, 1, 1, 1, 1, 1, 1, 1, 1)$  is a solution of the above equation.

## 6. Hypergraphs characterization from $\Upsilon_H^\bullet$ and $\zeta_H^\bullet$ functions

We show in this section that some hypergraphs can be fully characterized by their  $\Upsilon_H^\bullet$  and  $\zeta_H^\bullet$  functions.

**Theorem 3.** *Let  $F = \{x_1, x_2, \dots, x_r\} \subset \mathbb{N}^*$  with  $r \geq 1$ , then the two following properties are equivalent:*

1.

$$\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = 1 - r; \quad (10)$$

2. *there is at most one element  $x_j \in F$  such that  $x_j > 1$ .*

*Proof:* Assume that (2) is true. Two cases have to be considered:

- $\forall i, x_i = 1$ , then  $\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = 1 - r$ .
- Let  $x_j \in F$  such that  $x_j > 1$  (and then  $\forall i \neq j, x_i = 1$ ); hence we have:

$$\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = x_j - (r - 1) \times 1 - x_j = 1 - r$$

This shows that in both cases (1) is true.

Now assume that (1) is true, i.e.  $\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = 1 - r$  (with  $r \geq 1$ ), and prove (2) by induction on  $r = |F|$ .

- If  $r = 1$ , it is obvious.



- If  $r = 2$ , then  $x_1x_2 - (x_1 + x_2) = -1$ ; hence,  $x_1x_2 < x_1 + x_2$ , and by Lemma 1 there is at least one  $i \in \{1, 2\}$ , such that  $x_i < 2$ . Since  $F \subset \mathbb{N}^*$ ,  $x_i = 1$  (and therefore at most one is strictly greater than 1).
- Assume now that our assertion is true for any  $r \geq 2$ , and prove it for  $F$  with  $|F| = r + 1 \geq 3$ . By hypothesis

$$\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = 1 - (r + 1) = -r$$

Since  $\prod_{x_i \in F} x_i < \sum_{x_i \in F} x_i$ , from Lemma 1 there is at least one  $l \in \{1, 2, \dots, r, r + 1\}$ , such that  $x_l = 1$ . Therefore

$$\prod_{x_i \in F} x_i - \sum_{x_i \in F} x_i = \prod_{x_i \in F \setminus \{x_l\}} x_i - \sum_{x_i \in F \setminus \{x_l\}} x_i - 1 = -r$$

Hence

$$\prod_{x_i \in F \setminus \{x_l\}} x_i - \sum_{x_i \in F \setminus \{x_l\}} x_i = 1 - r$$

By induction hypothesis, there is at most one element  $x_t \in F \setminus \{x_l\}$ , such that  $x_t > 1$ ; since  $x_l = 1$ , this concludes the proof.

■

**Proposition 7.** *Let  $H = (V, E)$  be a linear connected hypergraph with  $|E| = m$ ,  $m \geq 2$ , then the three following properties are equivalent, for  $s \neq 0$ :*

1.  $H$  is a star;
2.  $\zeta_H^+(s) = m \left(\frac{1}{m-1}\right)^s$ ,  $\zeta_H^\times(s) = m \left(\frac{1}{m}\right)^s$  and  $H$  is multiplicative and additive degree regular;
3.  $\mathfrak{T}_H^+(s) = \left(\frac{1}{m-1}\right)^{ms}$ ,  $\mathfrak{T}_H^\times(s) = \left(\frac{1}{m}\right)^{ms}$  and  $H$  is multiplicative and additive degree regular.

*Proof:*

- Let us first show (1)  $\Rightarrow$  (2). From the definition of a star (see Section 2), there exists a vertex  $x$  common to all hyperedges. Since  $H$  is linear, this  $x$  is unique, and we have  $d(x) = m$  and  $\forall x' \in V \setminus \{x\}, d(x') = 1$  if  $x'$  is not isolated (0 otherwise). Hence  $d_e^\times = m$  and  $d_e^+ = m - 1$  for each  $e \in E$ . This shows that  $H$  is multiplicative and additive regular. Moreover, we have  $\zeta_H^+(s) = \sum_{e \in E} \left(\frac{1}{d_e^+}\right)^s = m \left(\frac{1}{m-1}\right)^s$  and  $\zeta_H^\times(s) = \sum_{e \in E} \left(\frac{1}{d_e^\times}\right)^s = m \left(\frac{1}{m}\right)^s$ .

- Let us show (2)  $\Rightarrow$  (3). Since  $H$  is multiplicative regular, there is a constant  $k$  such that  $\forall e \in E, d_e^\times = k$ . From  $\zeta_H^\times(s) = m \left(\frac{1}{m}\right)^s = m \left(\frac{1}{k}\right)^s$  we derive  $k = m$  if  $s \neq 0$ . Therefore  $\mathfrak{T}_H^\times(s) = \prod_{e \in E} \left(\frac{1}{d_e^\times}\right)^s = \left(\frac{1}{k}\right)^{ms} = \left(\frac{1}{m}\right)^{ms}$  (which also holds for  $s = 0$ ). The proof for  $\mathfrak{T}_H^+(s)$  is similar, using the fact that  $H$  is additive regular and that  $m - 1 > 0$ .
- Let us now show (3)  $\Rightarrow$  (1). As above, it is easy to derive from the expression of  $\mathfrak{T}_H^\times(s)$  and from the fact that  $H$  is multiplicative regular that, for  $s \neq 0, \forall e \in E, d_e^\times = m$ . Similarly, from the expression of  $\mathfrak{T}_H^+(s)$  and from the fact that  $H$  is additive regular, we derive that  $\forall e \in E, d_e^+ = m - 1$ . Then  $d_e^\times - d_e^+ = 1$ , and we have:

$$\prod_{x_i \in e} d(x_i) - \sum_{x_i \in e} d(x_i) = 1 - |e|.$$

From Theorem 3, there is at most one  $x$  in  $e$  such that  $d(x) > 1$ . Two cases arise:

- There is none, then  $e$  is an isolated hyperedge, which is impossible since  $H$  is assumed to be connected with  $m \geq 2$ ;
- There is a unique  $x \in E$  such that  $d(x) = k, k > 1$ . Then there exists a family of  $k$  hyperedges which share the vertex  $x \in e$ , and since  $H$  is linear and connected this is the same  $x$  for each  $e \in E$ , and consequently  $H$  is a star.

Note that for  $s = 0$ , we have  $\mathfrak{T}_H^+(0) = \mathfrak{T}_H^\times(0) = 1$  whatever the values of  $d_e^+$  and  $d_e^\times$ , and we cannot conclude anything on  $H$ .

Finally we have (1)  $\Rightarrow$  (2)  $\Rightarrow$  (3)  $\Rightarrow$  (1) which shows the equivalence between all three propositions. ■

**Proposition 8.** *Let  $H = (V, E)$  be a loopless connected hypergraph with  $|E| = m, m \geq 2$ , then the three following properties are equivalent for  $s \neq 0$ :*

1.  $H$  is a hypercycle;
2.  $\zeta_H^+(s) = m \left(\frac{1}{2}\right)^s, \zeta_H^\times(s) = m \left(\frac{1}{4}\right)^s$  and  $H$  is multiplicative-additive degree regular;
3.  $\mathfrak{T}_H^+(s) = \left(\frac{1}{2}\right)^{ms}, \mathfrak{T}_H^\times(s) = \left(\frac{1}{4}\right)^{ms}$  and  $H$  is multiplicative-additive degree regular.

*Proof:*

- Let us show (1)  $\Rightarrow$  (2). From the definition of a hypercycle (see Section 2), it is easy to show that  $\forall e \in E, d_e^\times = 4$  and  $d_e^+ = 2$ . Then the proof of (2) is similar as the proof of Proposition 7.
- Proving that (2)  $\Rightarrow$  (3) is similar as for Proposition 7.
- Let us now show that (3)  $\Rightarrow$  (1) for  $s \neq 0$ . From (3) we have that  $d_e^\times = k, d_e^+ = k'$  where  $k, k'$  are constant, and:

$$\tau_H^+(s) = \prod_{e \in E} \left( \frac{1}{d_e^+} \right)^s = \left( \frac{1}{k'} \right)^{ms} = \left( \frac{1}{2} \right)^{ms}$$

hence  $k' = 2$ , and similarly

$$\tau_H^\times(s) = \prod_{e \in E} \left( \frac{1}{d_e^\times} \right)^s = \left( \frac{1}{k} \right)^{ms} = \left( \frac{1}{4} \right)^{ms}$$

hence  $k = 4$ . Therefore we have:  $d_e^+ = 2$  and  $d_e^\times = 4$ , for all  $e \in E$ .

Now, since  $d_e^\times = \prod_{x \in e} d(x) = 4$ , it follows that  $d(x)$  is a divisor of 4, i.e. equal to 1, 2 or 4. Assume that  $d(x) = 4$ , for  $x \in e$ . Then

$$d_e^+ = \sum_{x \in e} (d(x) - 1) \geq 3 > 2$$

which is impossible. Similarly it is impossible to have  $d(x) = 1$  for all  $x \in E$ . Therefore there exists at least one  $x \in E$  such that  $d(x) = 2$ . Then

$$d_e^+ = \sum_{x \in e} (d(x) - 1) = 2 = \sum_{y \in e \setminus \{x\}} (d(y) - 1) + d(x) - 1 \Rightarrow \sum_{y \in e \setminus \{x\}} (d(y) - 1) = 1$$

consequently, there is exactly another vertex  $z \in e$  such that  $d(z) = 2$ , and for all  $y \in e, y \neq x, y \neq z, d(y) = 1$ . This means that there exist two other hyperedges  $e', e'' \in E \setminus \{e\}, e' \neq e''$  such that  $x \in e', z \in e'', |e \cap e'| = 1, |e \cap e''| = 1$ . Therefore  $e', e, e''$  are consecutive. Since this holds for any  $e$  (by repeating the reasoning process to  $e''$  and so on), and  $E$  is finite, the set of all hyperedges can be organized in a cyclic hyperpath, and therefore  $H$  is a hypercycle.

Finally we have (1)  $\Rightarrow$  (2)  $\Rightarrow$  (3)  $\Rightarrow$  (1) which shows the equivalence between all three propositions. ■

## 7. Zeta-density matrices and Laplacian

In this section we introduce new matrices associated with hypergraphs and we define new types of Laplacians. The problem of the Laplacian associated with a hypergraph comes from the adjacency matrix, which does not convey the topological structure of the hypergraph (how the hyperedges intersect with each other). It is a vertex-vertex matrix, where if  $x, y$  are vertices then the coefficient of this matrix  $a_{x,y}$  is equal to the number of hyperedges which contain  $x$  and  $y$ . With this type of matrix we lose a lot of information. This loss is passed on to the associated Laplacian. For instance two different hypergraphs may have the same adjacency matrix. To overcome this problem, many authors have introduced a tensorial representation of hypergraphs [12, 27, 32, 34, 36, 45]. It is, in a way, a generalized matrix. Despite the interest of such a representation and the richness of the derived results, it raises other problems. For example the calculation of the eigenvalues is difficult.

Therefore, we propose new matrices which are relevant in the sense that they better represent the topology of the hypergraphs. In addition, they convey information on the hyperedges and on the vertices, such as the degrees. Furthermore, they are linked to the Zeta and density functions defined above.

### 7.1. Zeta-density matrices

Let  $H = (V, E)$  be a hypergraph, with  $E = \{e_1 \dots e_m\}$ . We assume that for all  $e \in E$ ,  $d_e^\bullet \geq 1$ . Note that this is always the case for  $d_e^\times$ . For  $d_e^+$  this imposes an additional constraint on the topology of the hypergraph, i.e. at least one vertex of each  $e$  is also belongs to another hyperedge. Let  $s \in \mathbb{N}$  (the results below can be easily generalized by taking  $s \in \mathbb{R}$ ).

*Zeta-density matrices* are defined as the matrices  $Z^+(s)$  and  $Z^\times(s)$  whose general terms are respectively:

$$Z^+(e_i, e_i)(s) = 0, \quad Z^\times(e_i, e_i)(s) = 0$$

and for  $i \neq j$

$$Z^+(e_i, e_j)(s) = \begin{cases} \left( \frac{1}{d_{e_i}^\bullet + d_{e_j}^\bullet} \right)^s & \text{if } e_i \cap e_j \neq \emptyset; \\ 0 & \text{if } e_i \cap e_j = \emptyset. \end{cases}$$

$$Z^\times(e_i, e_j)(s) = \begin{cases} \left( \frac{1}{d_{e_i}^\bullet d_{e_j}^\bullet} \right)^s & \text{if } e_i \cap e_j \neq \emptyset; \\ 0 & \text{if } e_i \cap e_j = \emptyset. \end{cases}$$

Note that in these definitions,  $d^\bullet$  can be either  $d^\times$  or  $d^+$  (i.e. we have four different matrices).

Note that these matrices are well defined thanks to the hypothesis that for any  $e \in E$ ,  $d_e^\bullet \geq 1$ .

## 7.2. Laplacian operator

Let  $\mathcal{F}$  denote the set of functions from  $E$  to  $\mathbb{R}$ :  $\mathcal{F} = \mathbb{R}^E$ . Let  $f \in \mathcal{F}$ . The *gradient*  $\nabla f$  of  $f$  on  $H = (V, E)$  is defined as follows:

$$\forall (e, e') \in E \times E, \nabla f(e, e') = (f(e) - f(e')) \mathbf{1}_{e, e'}$$

where

$$\mathbf{1}_{e, e'} = \begin{cases} 1 & \text{if } e \cap e' \neq \emptyset; \\ 0 & \text{otherwise.} \end{cases}$$

Let us again consider  $A_e = \{e' \in E \mid e' \neq e \text{ and } e \cap e' \neq \emptyset\}$ , and define, for  $s \in \mathbb{N}$ :

$$\zeta^+(e)(s) = \sum_{e' \in A_e} (d_e^\bullet + d_{e'}^\bullet)^s = \sum_{e' \in A_e} Z^+(e, e')(-s)$$

The *Laplacian operator*  $\Delta_s$  is defined by:

$$\begin{aligned} \Delta_s f(e) &= \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E} (f(e) - f(e')) Z^+(e, e')(-s) \\ &= f(e) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E} f(e') Z^+(e, e')(-s) \end{aligned} \tag{11}$$

and since  $Z^+(e, e')(-s) = 0$  when  $e = e'$  or  $e \cap e' = \emptyset$ , then

$$\Delta_s f(e) = f(e) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in A_e} f(e') Z^+(e, e')(-s) \tag{12}$$

By using the gradient operator we have:

$$\Delta_s f(e) = \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E} \nabla f(e, e') Z^+(e, e')(-s) \tag{13}$$

By duality, we can define an operator  $\Delta_s$  on the vertices by taking the dual  $H^*$ . In addition we can also take as basic operator  $Z^\times(s)$ .

### 7.3. Classical results

Let  $H = (V, E)$  be a hypergraph, such that for all  $e \in E$ ,  $d_e^+ \neq 0$ . Then for all  $f, f' \in \mathcal{F}$ , it is easy to show that

$$\langle f, f' \rangle_s = \sum_{e \in E} \zeta^+(e)(s) f(e) f'(e) \quad (14)$$

is an inner product.

**Proposition 9.** *Let  $H$  be a connected hypergraph, and  $s \geq 1$ . Then*

i) *the operator  $\Delta_s$  is positive semi-definite: for all  $f \in \mathcal{F}$ ,  $\langle \Delta_s f, f \rangle_s \geq 0$ ;*

ii) *the operator  $\Delta_s$  is symmetric:  $\Delta_s = \Delta_s^t$ .*

*Proof:*

$$\begin{aligned} \sum_{e \in E} \zeta^+(e)(s) \Delta_s f(e) f(e) &= \sum_{e \in E} \sum_{e' \in E} (f(e) - f(e')) f(e) Z^+(e, e')(-s) \\ &= \sum_{e' \in E} \sum_{e \in E} (f(e') - f(e)) f(e') Z^+(e, e')(-s) \end{aligned}$$

(by exchanging the roles of  $e$  and  $e'$ ). Now, by adding the two second members, we get:

$$\langle \Delta_s f, f \rangle_s = \frac{1}{2} \left( \sum_{e \in E} \sum_{e' \in E} (f(e) - f(e'))^2 Z^+(e, e')(-s) \right)$$

which is positive, hence

$$\langle \Delta_s f, f \rangle_s \geq 0.$$

Now take the difference:

$$\begin{aligned} \langle \Delta_s f, g \rangle_s - \langle f, \Delta_s g \rangle_s &= \sum_{e \in E} \sum_{e' \in E} (f(e) - f(e')) g(e) Z^+(e, e')(-s) - \sum_{e \in E} \sum_{e' \in E} f(e) (g(e) - g(e')) Z^+(e, e')(-s) \\ &= - \sum_{e \in E} \sum_{e' \in E} f(e') g(e) Z^+(e, e')(-s) + \sum_{e \in E} \sum_{e' \in E} f(e) g(e') Z^+(e, e')(-s) = 0 \end{aligned}$$

by exchanging  $e$  and  $e'$  and since  $e, e'$  run through the whole  $E$ .

Hence,  $\langle \Delta_s f, g \rangle_s = \langle f, \Delta_s g \rangle_s$ .

■

To the operator  $\Delta_s$  we can associate a matrix  $M_{\Delta_s}$  defined as:

$$M_{\Delta_s} = I_m - \left( \frac{1}{\zeta^+(\bullet)(s)} \right) \circ Z^+(-s) \quad (15)$$

where  $I_m$  is the identity matrix of size  $m$ , and  $\left( \frac{1}{\zeta^+(\bullet)(s)} \right)$  is a  $m \times m$ -matrix where lines are the repeated coefficient  $\frac{1}{\zeta^+(e_i)(s)}$   $m$  times for all  $i \in \{1, 2, \dots, m\}$ . By denoting  $e_i, i = 1 \dots m$ , the hyperedges of  $H$ , we have

$$M_{\Delta_s}(f(e_1), \dots, f(e_m))^t = \Delta_s(f(e_1), \dots, f(e_m))^t$$

From Proposition 9 this matrix is symmetric and positive semi-definite. Consequently its eigenvalues, denoted by  $\mu_i(s)$ , are real and positive with

$$0 \leq \mu_1(s) \leq \mu_2(s) \leq \dots \leq \mu_m(s)$$

They are associated to an orthogonal basis formed by the eigenfunctions  $\{\phi_i(s), i \in \{1, 2, \dots, m\}\}$ , that can be seen as functions of  $\mathcal{F}$ .

Let us define  $p_{e,e'} = \frac{Z^+(e,e')(-s)}{\zeta^+(e)(s)}$ . It is easy to verify that  $0 \leq p_{e,e'} \leq 1$  and  $\sum_{e' \in A_e} p_{e,e'} = 1$ . Let  $P = (p_{e,e'})_{e,e'}$ , which defines on  $\mathcal{F}$  the *Markov operator* by setting:

$$Pf(e) = \sum_{e' \in E} p_{e,e'} f(e') \quad (16)$$

Laplace operator and Markov operator are linked by:

$$M_{\Delta_s} = I_m - P = I_m - \left( \frac{1}{\zeta^+(\bullet)(s)} \right) \circ Z^+(-s) \quad (17)$$

**Lemma 3.** *Let  $H$  be a connected hypergraph, and  $s \geq 1$ . Then*

- i)  $\mu_1(s) = 0$ ;
- ii)  $\mu_2(s) \leq \frac{m}{m-1}$ ;
- ii)  $\text{Spect}(M_{\Delta_s}) \subseteq [0, 2]$ , where  $\text{Spect}(M_{\Delta_s})$  is the set of all eigenvalues of  $M_{\Delta_s}$ .

*Proof:* (i) Let  $f \in \mathcal{F}$ , such that for all  $e \in E$ ,  $f(e) = 1$  (i. e.  $f = \mathbf{1}$ ); then  $\Delta_s f(e) = \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E} (f(e) - f(e')) Z^+(e, e')(-s) = 0$ . Consequently,

thanks to the correspondence between  $\Delta_s$  and  $M_{\Delta_s}$ ,  $\mu_1(s) = 0$  is a eigenvalue associated to the eigenfunction  $f = \mathbf{1}$ .

(ii) We have  $\sum_{i=1}^m \mu_i(s) = \text{Tr}(M_{\Delta_s}) = m$ . Since  $\mu_1(s) = 0$  and  $\mu_2(s) \leq \mu_j(s)$  for all  $j \geq 2$ , it follows that  $(m-1)\mu_2(s) \leq m$ .

(iii) The *spectral radius* of a square matrix  $A$  denoted by  $\rho(A)$  is the largest of the absolute values of the eigenvalues, hence  $\rho(P) = \mu_m(s)$ , and by Gershgorin circle theorem [21] we have, for all  $i \in \{1, 2, \dots, m\}$ ,  $|\mu_i - p_{e_i, e_i}| \leq \sum_{e' \in E} p_{e, e'} = 1$ . Consequently  $\text{Spect}(P) \subseteq [-1, 1]$ , by Equation 17, then  $\text{Spect}(M_{\Delta_s}) \subseteq [0, 2]$ .

■

#### 7.4. Dirichlet problem

Dirichlet problem is fundamental in many areas of mathematics and physics [22]. It appears in electrostatics, in heat conduction, in elasticity, in theory of gravitation, among others. This problem has made it possible to significantly advance mathematical knowledge in many directions.

This classical problem fits very well on graphs. We will now show that we can also interpret it in the context of hypergraphs thanks to the matrices proposed in this paper.

Before giving the main result of this section, we need to introduce a few more definitions and a lemma.

Let  $H = (V, E)$  be a hypergraph and let  $f \in \mathcal{F}$ . The function  $f$  is said *s-harmonic or harmonic* on  $E' \subseteq E$ , if for  $s \in \mathbb{N}^*$  and for all  $e \in E'$

$$\Delta_s f(e) = 0.$$

This expresses an equivalent of the Laplace equation in the discrete setting provided by hypergraphs. If  $f$  satisfies this equation, then

$$f(e) = \frac{1}{\zeta^+(e)(s)} \sum_{e' \in A_e} f(e') Z^+(e, e')(-s)$$

We can interpret a harmonic function by saying that the average value of the function on the hyperedges which intersect a hyperedge  $e$  is equal to the value on the function on this hyperedge.

Let  $H = (V, E)$  be a hypergraph and let  $E' \subseteq E$ . The *adherence* of  $E'$  is defined as  $\overline{E'} = \{e \in E \mid \exists e' \in E' \text{ such that } e' \cap e \neq \emptyset\}$ , and the *boundary* of  $E'$  is defined as  $\text{Fr}(E') = \overline{E'} \setminus E'$ .



**Lemma 4.** *Let  $H = (V, E)$  be a connected hypergraph,  $H(E') = (V', E')$  its partial hypergraph induced by  $E' \subsetneq E$ ,  $E' \neq \emptyset$  and  $|E'| \geq 2$  ( $V'$  is the set of vertices of  $V$  that are covered by the hyperedges in  $E'$ ), and assume that  $H(E')$  is connected. Let  $f : E \rightarrow \mathbb{R}$ , and suppose that  $f$  verifies the two following properties:*

- a)  $f$  is  $s$ -harmonic on  $E'$ ,
- b)  $f$  reaches its maximum and minimum on  $E'$ .

Then  $f$  is constant on  $\overline{E'}$ .

*Proof:* Let  $M = \max_{e \in E} f(e)$  and denote by  $E'' = \{e \in E \mid f(e) = M\}$ . From b)  $E' \cap E'' \neq \emptyset$ , and since  $f$  is  $s$ -harmonic on  $E'$ , we have for all  $e \in E' \cap E''$ :  $\Delta_s f(e) = 0$ , i.e.

$$0 = \frac{1}{\zeta^+(e)(s)} \sum_{e' \in A'_e} (f(e) - f(e')) Z^+(e, e')(-s) = \frac{1}{\zeta^+(e)(s)} \sum_{e' \in A'_e} (M - f(e')) Z^+(e, e')(-s).$$

where  $A'_e = \{e' \in E' \mid e' \neq e \text{ and } e' \cap e \neq \emptyset\}$ . This set is not empty by definition. Since  $Z^+(e, e')(-s) > 0$  and  $(M - f(e')) \geq 0$  then  $f(e') = M$  for all  $e' \in A'_e$ . This means that every hyperedge that intersects an hyperedge of  $E' \cap E''$  has value  $M$  and hence belongs to  $E''$ . Since  $H(E')$  is connected, it follows recursively that  $E' \subseteq E''$ . And similarly we conclude that  $\overline{E'} \subseteq E''$  since  $\overline{E'}$  all hyperedges intersecting at least one hyperedge of  $E'$ .

The same reasoning applies for the minimum. ■

**Definition 6.** *Let  $H = (V, E)$  be a hypergraph,  $(E')$  its partial hypergraph, for  $E' \subsetneq E$ ,  $E' \neq \emptyset$  and such that  $H(E')$  is connected. Let  $h : E' \rightarrow \mathbb{R}$  and  $g : E \setminus E' \rightarrow \mathbb{R}$  be two fixed functions. The DIRICHLET problem on hypergraphs is expressed as follows: what are the functions  $f : E \rightarrow \mathbb{R}$  that satisfy the following differential system*

$$\begin{aligned} \Delta_s f(e) &= h(e) && \text{for all } e \in E', \\ f(e) &= g(e) && \text{for all } e \in E \setminus E'. \end{aligned}$$

Note that the boundary  $E \setminus E'$  can be “thick” in comparison to the classical Dirichlet problem.

**Theorem 4.** *The DIRICHLET problem for a connected hypergraph  $H = (V, E)$  and its connected partial hypergraph  $H(E')$  admits a unique solution  $f$ .*

Note that if the hypergraph is not connected, then the result applies on each connected component.

*Proof:* We must demonstrate the uniqueness of the solution as well as its existence.

**Uniqueness.** Assume that there are two solutions  $f_1$  and  $f_2$ ; hence  $f = f_1 - f_2$  is a solution of the following system:

$$\begin{aligned}\Delta_s f(e) &= 0 \quad \text{for all } e \in E', \\ f(e) &= 0 \quad \text{for all } e \in E \setminus E' .\end{aligned}$$

Assume that there is  $e \in E$  such that  $f(e) \neq 0$ .

1. If  $f(e) > 0$ , then  $f$  would reach its maximum  $M$  on  $E'$  (since  $f(e) = 0$  for all  $e \in E \setminus E'$ ), and from Lemma 4  $f$  would be constant ( $= M$ ) on  $\overline{E'} = E' \cup Fr(E')$ . Since  $E' \subsetneq E$ ,  $Fr(E') \neq \emptyset$ , and we would get a contradiction with  $f(e) = 0$  for all  $e \in E \setminus E'$ .
2. If  $f(e) < 0$ , then by applying Lemma 4 for minimum we have the result.

Finally  $f(e) = 0$  for all  $e \in E$ , and therefore  $f_1 = f_2$ .

**Existence.** We can write  $\Delta_s f(e) = h(e)$ , for all  $e \in E'$ , i.e.

$$f(e) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E'} f(e') Z^+(e, e')(-s) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E \setminus E'} f(e') Z^+(e, e')(-s) = h(e)$$

Since  $f(e') = g(e')$ , for all  $e' \in E \setminus E'$ , we obtain:

$$f(e) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E'} f(e') Z^+(e, e')(-s) = h(e) + \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E \setminus E'} g(e') Z^+(e, e')(-s)$$

Now for all  $e \in E'$  we denote by  $h_1(e) = h(e) + \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E \setminus E'} g(e') Z^+(e, e')(-s)$  and  $\Delta'_s f(e) = f(e) - \frac{1}{\zeta^+(e)(s)} \sum_{e' \in E'} f(e') Z^+(e, e')(-s)$ . Let  $\mathcal{F}' = \{f : E \rightarrow \mathbb{R} : f \text{ is a map with } f \equiv 0 \text{ on } E \setminus E'\}$ , which is a subspace of  $\mathbb{R}^E$ .

The operator  $\Delta'_s$  is equal to  $\Delta_s \upharpoonright_{\mathcal{F}'}$ . Let  $f'$  and  $h'_1$  be the functions of  $\mathcal{F}'$  that coincide with  $f$  and  $h_1$  on  $E'$ , respectively. The DIRICHLET problem of our theorem can be rewritten as

$$\begin{aligned}\Delta'_s f'(e) &= h'_1(e) \quad \text{for all } e \in E', \\ f'(e) &= g(e) \quad \text{for all } e \in E \setminus E' .\end{aligned}$$

Let  $f' \in \mathcal{F}'$  such that  $\Delta'_s f'(e) = 0$  on  $E'$ ,  $f'$  is harmonic on  $E'$ ; since by definition  $f' \equiv 0$  on  $E \setminus E'$ ; hence  $f' \equiv 0$  on  $Fr(E')$ ; moreover  $f'$  reach its maximum on  $E'$ ; by Lemma 4  $f'$  is constant on  $\overline{E'}$  so we can conclude that  $f' \equiv 0$  on  $E$ . Consequently  $\Delta'_s$  is an injective linear operator on  $\mathcal{F}'$  and since it is a  $\mathbb{R}$ -vectorial space with  $\dim(\mathcal{F}') = |E'|$ , it is bijective, we obtain a unique solution  $f$  of the DIRICHLET problem by asking:

$$\begin{aligned} f \upharpoonright_{E'} &= (\Delta'_s)^{-1} h'_1(e), \\ f \upharpoonright_{E \setminus E'} &= g. \end{aligned}$$

■

## 8. Some Applications

### 8.1. Mathematical Chemistry

In mathematical chemistry, a *molecular graph*, also *chemical graph* is a representation of a molecule or a chemical compound by a graph. The atoms of a molecule are represented by the vertices and the chemical bonds are represented by the edges. It is a good representation of a molecule when bonds are localized: localized bonding refers to the sharing of electron pairs (represented by an edge of the graph) between two atoms of a molecule.

There is another type of bonds. Delocalized bonds occur when electrons are not confined to the region between two particular atoms but are distributed across multiple atoms or regions within a molecule. This phenomenon arises from the concept of electron delocalization, in which electrons are given the freedom to move throughout a larger part of the molecule, this implies unique bonding properties and behaviors. In this case graph representation is not the more appropriate model.

A *molecular hypergraph*, also *chemical hypergraph* is a hypergraph  $H = (V, E)$  where  $V$  correspond to the individuals atoms of the molecule and hyperedges  $e \in E$  with degrees greater than two correspond to delocalized bonds and hyperedges  $e \in E$  such that  $|e| = 2$  correspond to simple covalent bonds (localized bonds) [31].

There are other definitions of molecular hypergraphs, for example see [30]. Properties of molecules are strongly linked to the geometric structures of the chemical compounds studied and which are modeled by graphs or hypergraphs. Consequently, the physical properties will depend on the topology of the (hyper)graphs. These are studied through *topological indices* which

are invariants of (hyper)graphs [11]. Most of these indices are based on combinatorial parameters of (hyper)graphs: lengths of chains or paths; degrees, connectivities, ... But also on the algebraic properties of (hyper)graphs: incidence matrix, adjacency matrix, Laplacian, eigenvalues and eigenvectors, ....

So it is easy to see that Zeta function and Density function are both invariants of (hyper)graphs and can be easily used in the context of molecular (hyper)graphs as topological indices. In order to show the relevance of these functions and matrices defined above it is necessary to be able to situate them in relation to classic topological indices which are intensely studied. Below, we introduce some classical topological indices and situate them in relation to the Zeta function and the density function.

**Remark 7.** *In the following, without losing generality, we will assume that the (hyper)graphs are connected because the molecular compounds are made in one piece.*

#### 8.1.1. Estrada index

The *closure* of  $Z^\bullet(s)$ , denoted by  $\overline{Z^\bullet(s)}$ , is defined by:

$$\overline{Z^\bullet(s)} = Z^\bullet(s) + I^\bullet(s)$$

where  $I^\bullet(s)$  is a diagonal matrix defined by:

$$I^+(s) = \text{Diag} \left( (2d_{e_1}^\bullet)^s ; (2d_{e_2}^\bullet)^s ; \dots , (2d_{e_m}^\bullet)^s \right)$$

$$I^\times(s) = \text{Diag} \left( (d_{e_1}^\bullet)^{2s} ; (d_{e_2}^\bullet)^{2s} ; \dots , (d_{e_m}^\bullet)^{2s} \right)$$

Let  $A$  and  $B$  be two  $m \times n$ -matrices, the HADAMARD product of the two matrices is defined by the element-wise product:

$$A \circ B = (a \circ b)_{i,j} = (a)_{i,j} (b)_{i,j}$$

We have:

**Proposition 10.** [37] *Let  $A, B \in \mathbb{R}^{n \times n}$  be two matrices such that  $A$  is positive semi-definite and  $B$  is positive definite. If all diagonal elements of  $A$  are positive then  $A \circ B$  is positive definite.*

The *Estrada index* [19] of a  $m \times m$ -matrix  $A$  is

$$EE(A) = \sum_{i=1}^m e^{\lambda_i}$$

where  $\lambda_i$  are the eigenvalues of  $A$ .

Let us introduce an additional notation, useful in the sequel to reason on intersecting hyperedges:  $A_e = \{e' \in E \mid e' \neq e \text{ and } e \cap e' \neq \emptyset\}$ .

**Theorem 5.** *Let  $H = (V, E)$  be a connected hypergraph <sup>1</sup> with  $|E| = m$  and  $m \geq 3$  let  $s \in \mathbb{R}$ ,  $s \geq 1$ . The matrices  $\overline{Z^\bullet}(s)$  are positive definite. Moreover, if  $\lambda_i^+(s), \lambda_i^\times(s), i = 1 \dots m$  denote the eigenvalues of  $\overline{Z^+}(s)$  and  $\overline{Z^\times}(s)$ , respectively, with  $0 < \lambda_1^+(s) \leq \lambda_2^+(s) \leq \lambda_3^+(s) \dots \leq \lambda_m^+(s)$  and  $0 < \lambda_1^\times(s) \leq \lambda_2^\times(s) \leq \lambda_3^\times(s) \dots \leq \lambda_m^\times(s)$ , then we have the following inequalities:*

$$2^s \zeta_H^\bullet(-s) < EE(\overline{Z^+}(s)) \leq e^{m+2^s \zeta_H^\bullet(-s)}, \quad (18)$$

and

$$\zeta_H^\bullet(-2s) < EE(\overline{Z^\times}(s)) \leq e^{m+\zeta_H^\bullet(-2s)}. \quad (19)$$

*Proof:*

Define

$$\mathbb{1}_{e_i, e_j} = \begin{cases} 1 & \text{if } e_i \cap e_j \neq \emptyset; \\ 0 & \text{otherwise.} \end{cases}$$

Define the matrix:

$$\mathcal{I} = (\mathbb{1}_{e_i, e_j})_{i,j} - \text{Diag}(1, 1, 1, \dots, 1)$$

Let

$$P = \text{Diag} \left( (2d_{e_1}^\bullet)^{2s}, (2d_{e_2}^\bullet)^{2s}, \dots, (2d_{e_m}^\bullet)^{2s} \right) + \mathcal{I}$$

and define

$$Q = \left( \left( \frac{1}{d_{e_i}^\bullet + d_{e_j}^\bullet} \right)^s \right)_{i,j}$$

For  $s = 1$ ,  $Q$  is a Cauchy matrix which is known as positive semi-definite [3].

---

<sup>1</sup>Note that this implies  $\forall e \in E, d_e^\bullet \geq 1$ .

For  $s > 1$ , let  $p_i$  be a row of  $P$ , we have on this row  $(2d_{e_i}^\bullet)^{2s}$  at position  $i$ , 1 for each position corresponding to the elements of  $A_{e_i}$ , and 0 elsewhere. Note that we have  $d_{e_i}^\bullet \geq |A_{e_i}|$ , since every time a hyperedge  $e'$  intersects  $e_i$  it counts at least for 1 in  $d_{e_i}^+$ , and for at least 2 in  $d_{e_i}^\times$ . Consequently, since  $s > 1$ ,  $(2d_{e_i}^\bullet)^{2s} > |A_{e_i}|$  which shows that  $P$  is positive definite. Note that for  $d^\times$  we even have  $(2d_{e_i}^\times)^{2s} > 2^{|A_i|}$ .

It is easy to see that  $\overline{Z^+(s)} = Q \circ P$  and from Proposition 10 this matrix is positive definite.

Define now

$$Q = \left( \left( \frac{1}{d_{e_i}^\bullet \cdot d_{e_j}^\bullet} \right)_{i,j}^s \right) \quad \text{and} \quad P = \text{Diag} \left( (d_{e_1}^\bullet)^{4s}; (d_{e_2}^\bullet)^{4s}; \dots, (d_{e_m}^\bullet)^{4s} \right) + \mathcal{I}$$

It is known [33] that if  $x_1, x_2, x_3, \dots, x_m$  is a family of real positive number then the matrix  $(x_i \cdot x_j)_{i,j}$  is positive semi-definite. Hence  $Q$  is positive semi-definite. As above we can show than  $P$  is positive definite. Consequently, since we have  $\overline{Z^\times(s)} = Q \circ P$ , we can conclude that  $\overline{Z^\times(s)}$  is positive definite.

Let  $\lambda_i, i = 1 \dots m$  be  $m$  real positive values, and let us show that  $\frac{\sum_{i=1}^m e^{\lambda_i}}{e^{\sum_{i=1}^m (1+\lambda_i)}} \leq 1$ . Indeed we have:

$$\frac{\sum_{i=1}^m e^{\lambda_i}}{e^{\sum_{i=1}^m (1+\lambda_i)}} = \frac{\sum_{i=1}^m e^{\lambda_i}}{e^m e^{\sum_{i=1}^m \lambda_i}} \quad (20)$$

$$= \frac{1}{e^m} \sum_{i=1}^m \left( \frac{e^{\lambda_i}}{\prod_{j=1}^m e^{\lambda_j}} \right) \quad (21)$$

$$= \frac{1}{e^m} \sum_{i=1}^m \frac{1}{e^{\sum_{i=1, i \neq j}^m \lambda_j}} \quad (22)$$

Let us assume that  $\lambda_1 \leq \lambda_j, \forall j$ . Then

$$\sum_{i=1, i \neq j}^m \lambda_j \geq (m-1)\lambda_1$$

and

$$\frac{1}{e^{\sum_{i=1, i \neq j}^m \lambda_j}} \leq \frac{1}{e^{(m-1)\lambda_1}}$$

So we get:

$$\frac{\sum_{i=1}^m e^{\lambda_i}}{e^{\sum_{i=1}^m (1+\lambda_i)}} \leq \frac{1}{e^m} \frac{m}{e^{(m-1)\lambda_1}} \leq 1.$$

From this, we have:

$$\sum_{i=1}^m e^{\lambda_i} \leq e^{\sum_{i=1}^m (1+\lambda_i)}$$

and

$$\log \sum_{i=1}^m e^{\lambda_i} \leq \log e^{\sum_{i=1}^m (1+\lambda_i)} = m + \sum_{i=1}^m \lambda_i$$

Let us now apply this result for  $\lambda_i = \lambda_i^\bullet(s)$ . We have

$$\sum_{i=1}^m \lambda_i^+(s) = Tr(\overline{Z^+(s)}) = 2^s \zeta_H^\bullet(-s)$$

and

$$\sum_{i=1}^m \lambda_i^\times(s) = Tr(\overline{Z^\times(s)}) = \zeta_H^\bullet(-2s)$$

Consequently

$$EE(\overline{Z^+(s)}) \leq e^{m+2^s \zeta_H^\bullet(-s)}.$$

Moreover, we have  $e^{\lambda_i} \geq \lambda_i$  for positive values of  $\lambda_i$ . Therefore

$$EE(\overline{Z^+(s)}) \geq Tr(\overline{Z^+(s)}) = 2^s \zeta_H^\bullet(-s).$$

In the same way we have:

$$\zeta_H^\bullet(-2s) \leq EE(\overline{Z^\times}) \leq e^{m+\zeta_H^\bullet(-2s)}.$$

■

These bounds allow us to compare the Estrada index, which is a classical index on graphs, in particular molecular graphs, with invariants proposed in this article. Therefore our indices could play an important role in mathematical chemistry.

### 8.1.2. Sombor index

Quite recently a new vertex-degree-based topological invariant for graphs was introduced [24], this one was named *Sombor index*. This can be easily generalized to hypergraphs:

*Sombor index* for the hypergraph  $H = (V, E)$ , [40] is given by

$$SO(H) = \sum_{e \in E} \left( \sum_{x \in e} (d(x))^2 \right)^{\frac{1}{2}}$$

**Proposition 11.** *Let  $H = (V, E)$  be a hypergraph such that for all  $x \in V$ ,  $d(x) \geq 2$ , then we have*

$$\zeta_H^+(-\frac{1}{2}) \leq SO(H) \leq \zeta_H^\times(-1) \quad (23)$$

*Proof:*

$$\begin{aligned} SO(H) &= \sum_{e \in E} \left( \sum_{x \in e} (d(x))^2 \right)^{\frac{1}{2}} \geq \sum_{e \in E} \left( \sum_{x \in e} (d(x) - 1) \right)^{\frac{1}{2}} = \sum_{e \in E} (d_e^+)^{\frac{1}{2}} = \zeta_H^+(-\frac{1}{2}) \\ SO(H) &= \sum_{e \in E} \left( \sum_{x \in e} (d(x))^2 \right)^{\frac{1}{2}} \leq \sum_{e \in E} \left( \prod_{x \in e} (d(x))^2 \right)^{\frac{1}{2}} = \sum_{e \in E} d_e^\times = \zeta_H^\times(-1) \end{aligned}$$

since, from Lemma 1:

$$\sum_{x \in e} (d(x))^2 \leq \prod_{x \in e} (d(x))^2.$$

■

Sombor index is a new invariant introduced around 2020, however a lot of work has been carried out on this invariant because it conveys a lot of information on molecular (hyper)graphs. Above proposition shows that it is in close relation with our Zeta function.

### 8.1.3. General Randić index

General Randić index is also a important topological index. It is defined for graphs as: let  $\Gamma = (V, E)$  be a graph

$$R(\Gamma)_\alpha = \sum_{\{x,y\} \in E} (d(x)d(y))^\alpha, \quad \alpha \in \mathbb{R}.$$

This definition has been generalized by [41] to k-uniform hypergraph as: let  $H = (V, E)$  be a k-uniform hypergraph

$$R(H)_\alpha = \sum_{e \in E} (d(x_1)d(x_2) \dots d(x_k))^\alpha, \quad e = \{x_1, x_2, x_3 \dots x_k\}$$

In fact, this is our Zeta function  $\zeta_H^\times(s)$ ,  $s \in \mathbb{R}$ , in the case where the hypergraph is uniform. Curiously, the authors of [41] did not extend the definition to non-uniform hypergraphs



#### 8.1.4. Topological Indices and Their Reciprocals

When we have a topological invariant, starting from it we can define a new index called *reciprocal index* [25]. Below we give some examples and show the relevance of our indicators in this context.

Let  $H = (V, E)$  be a molecular (hyper)graph, let

$$TI(H) = \sum_{\alpha} F(\alpha)$$

be a topological index of the graph  $H$ , the *reciprocal index* of  $TI$  is given by:

$$RTI(H) = \sum_{\alpha} \frac{1}{F(\alpha)}$$

For instance sum-connectivity index and nirmala index is

$$SC(H) = \sum_{e \in E} \left( \frac{1}{\sum_{x \in E} d(x)} \right)^{\frac{1}{2}}$$

and its reciprocal:

$$RSC(H) = \sum_{e \in E} \left( \sum_{x \in E} d(x) \right)^{\frac{1}{2}}$$

clearly

$$SC(H) = \zeta_H^+\left(\frac{1}{2}\right) \text{ and } RC(H) = \zeta_H^+\left(-\frac{1}{2}\right)$$

Randić index and reciprocal Randić index are

$$\zeta_H^{\times}(-s) \text{ and } \zeta_H^{\times}(s), \quad s \geq 1$$

Our functions allow us to encompass both concepts at the same time. There are many other topological indices, most of them are related to the zeta function or the density function. This allows us to say that our invariants are in some way a "generalization" of part of the topological invariants of molecular (hyper)graphs.

## 8.2. Hypergraph associated to an image

Functions and matrices introduced in this article can also be used in the context of image analysis. Indeed we know that we can associate a hypergraph with an image [5]. This construction is defined below.

A *grid*  $X \subseteq \mathbb{Z}^n, n \geq 2$  is a graph  $\Gamma = (V, E)$  defines by a distance  $d : X \times X \rightarrow \mathbb{N}$  such that  $\Gamma$  is connected, regular without both loop and multi edge; for instance if  $n = 2$  and the distance is given by

$$d_{\text{Chebyshev}}(\mathbf{x}, \mathbf{y}) = \max(|x_2 - x_1|, |y_2 - y_1|)$$

we obtain the 8-connected grid.

A digital image  $I$  on a grid is a  $n$ -dimensional function that has been digitalized both on a grid and in magnitude feature value; hence, it is given by:

$$I : X \subseteq \mathbb{Z}^n \rightarrow \mathcal{C} \subseteq \mathbb{Z}^m; n \geq 2 \text{ and } m \geq 1. \quad (24)$$

where  $\mathcal{C}$  is the feature intensity level and  $X$  identifies a set of points called *image points*. The couple  $(x, I(x))$  is called pixel.

Let  $\delta$  be a distance on  $\mathcal{C}$ ; we define the relation on a image by

$$\Gamma_{\alpha, \beta}(x) = \{y \in X, y \neq x : \delta(I(x), I(y)) \leq \alpha \wedge d((x, y)) \leq \beta\} \quad (25)$$

The neighborhood of  $x$  at level at most  $\beta$  will be denoted by  $\Gamma_{\beta}(x)$  From this we can define a hypergraph associated to a image (denoted by INH) by

$$\mathcal{H}_{\alpha, \beta} = (X, (\{x\} \cup \Gamma_{\alpha, \beta}(x))_{x \in X}) \quad (26)$$

The attribute  $\alpha$  can be compute in an adaptative way depending on local properties of the image. For instance, for all  $x \in X$ ,  $\alpha_x$  would be the standard deviation of  $I(y)$  for all elements  $y$  of  $\{x\} \cup \Gamma_{\beta}(x)$ ; in this case e will denote  $\alpha_x = \sigma_x$ .

### 8.2.1. Using INH to image analysis

An image being represented by its associated hypergraph, to process this image, it is now sufficient to use the properties of the hypergraphs in order to extract information.

Hypergraph classification, using algebraic tools, has been effectively developed in image analysis, for example [38]. This gives an image segmentation

algorithm which is of very good quality.

The idea of this algorithm is to construct the Laplacian associated with a hypergraph, to calculate the eigenvalues and starting from these, to develop the classification because certain eigenvalues play the role of threshold.

The Laplacian is constructed starting from the adjacency matrix of the hypergraph  $H$  which is the product of the incidence matrix by its transpose. The main problem with this matrix is that the information conveyed by it is not really relevant because it only takes into account the number of hyperedges containing a pair of vertices. If for example the hypergraph is linear (the cardinality of the intersection of the hyperedges is at most 1), then this matrix is the matrix of the line-graph of  $H$ , thus we fall back on a graph and we lose relevance hypergraphs.

The matrices defined in section 7 seem much more appropriate to us, because the information transmitted by them is much more important. Indeed it takes into account the topology and the geometry of the hypergraph and if it comes from an image, as for example defined above, then we take into account the geometry of the image but also, given the construction of INH the luminance and chrominance of this image. Naturally the Laplacian defined in this article can also be very useful for edge detection, for sharpness of the image and many other processes.

*Inpainting problem* is a restoration process in which damaged or missing parts of an image are reconstructed to obtain a complete image. This process is similar to image restoration, it is also used in removing parts of the image while maintaining a "harmonious" appearance. More precisely, let  $I$  be an image and a region  $R$  of it, the inpainting problem consists of modifying the values of the pixels image of  $R$  so that this region does not stand out in relation to its environment.

If the image is seen as a two-dimensional signal the inpainting problem can be seen as the extension of a function under certain conditions [1]. So it is quite natural to try to adapt the Dirichlet problem in such a process. This type of process has already been applied to hypergraphs [43] and gives interesting results, however it uses the classic Laplacian of hypergraphs and we run into the same problems as above. One way of research would consist of constructing a partial hypergraph of INH as above except on the region  $R$  and trying to extend it using the Dirichlet problem defined in subsection 7.4.

Naturally, hypergraph associated with an image defined as above can be used

for other types of processing, therefore the concepts introduced throughout this article can be used for these various treatments, for example the entropy presented Subsection 3.3. All this will be the subject of another work.

## 9. Conclusion

In this article we have introduced new invariants associated with hypergraphs. These are based on analytic functions on  $\mathbb{R}$  or  $\mathbb{C}$ . These functions come naturally from different parameters of the hypergraphs. This allowed us to link them to classical notions such as entropy. Moreover, this allowed us to redefine notions such as gradient and Laplacian on hypergraphs.

To illustrate the possible uses of these concepts defined in the preceding sections, Section 8 introduces applications to molecular (hyper)graphs by situating the Zeta functions and the density in relation to known molecular topological indices, but also by using the new matrices defined in this work. Another illustration of the relevance of these invariants and these matrices has also been introduced in image analysis. We introduce a hypergraph associated with an image (INH), which allows us to use all the tools developed in this article in image analysis.

Naturally other classical notions can be approached such as the notion of Ricci flow, functional analysis, differential calculus, Fourier transform...

Another perspective is to consider hypergraphs varying over time. For instance hypernetworks can be seen as discrete dynamic systems depending on a temporal parameter. We could then introduce time as a variable of our functions.

Instead of considering one value of  $s$ , we could consider a set of values, and extend our functions  $\zeta_H$  and  $\tau_H$  accordingly, as sets (or vectors) of values, in an approach similar as the one developed for entropy in [7].

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