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Topological scale framework for hypergraphs

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ABSTRACT

In this paper, a new computational topological framework for hypergraph analysis and recognition is developed. "Topology provides scale" is the principle at the core of this set of algebraic topological tools, whose fundamental notion is that of a scale-space topological model (s^2-model). The scale of this parameterized sequence of algebraic hypergraphs, all having the same Euler-Poincaré characteristic than the original hypergraph G, is provided by its relational topology in terms of evolution of incidence or adjacency connectivity maps. Its algebraic homological counterpart is again an s^2-model, allowing the computation of new topological characteristics of G, which far exceeds current homological analytical techniques. Both scale-space algebraic dynamical systems are hypergraph isomorphic invariants. The hypergraph isomorphism problem is attacked here to demonstrate the power of the proposed framework, by proving the ability of s^2-models to differentiate challenging cases that are difficult or even infeasible for state-of-the-art practical polynomial solvers. The processing, analysis, classification and learning power of the s^2-model, at both combinatorial and algebraic levels, augurs positive prospects with respect to its application to physical, biological and social network analysis.

1. Introduction

Detection and understanding of topological features and invariants of relational objects (such as graphs and hypergraphs) have recently gained increasing attention in the analysis of a wide variety of processes that are modeled by networks. In a different but related subject, it is well-known that one way to endow an image with a topology is to embed it into a one-parameter family of images, known as a scale-space representation [1]. The main goal of this paper is to develop a powerful topological analysis and representation learning framework for hypergraphs, which allows to progress in hard problems like those of hypergraph isomorphism, classification, matching and learning. The idea here is to redefine the notion of hypergraph in such a way that they can be managed as true cellular structures and to appropriately mimic the aforementioned classical scale-space modus operandi for such generalized hypergraph structures. The resulting systems, called topological scale-space models or simply s^2-models, are non-negative integer sequences of algebraic hypergraphs such that all of them have the same Euler-Poincaré characteristic and consecutive scale levels are connected by algebraic transition functions. The topological scale is provided by the incidence or adjacency connectivity degree of the hypergraph we want to analyze.

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Working with s^2-models having the same number of vertices and edges in each hypergraph, the incidence s^2-models compile much more uncorrelated information than adjacency ones. New combinatorial and algebro-topological invariants based on this type of construction are discovered. The high number and low correlation of these topological characteristics lay the foundations for a deep and complete topological analysis of hypergraphs. We demonstrate that the topological scale-space models presented here are isomorphism-invariant and that they constitute a powerful strategy for attacking, in particular, the Graph (GI) and Hypergraph Isomorphism (HI) problems, clearly outperforming current isomorphism solvers.

The paper is organized as follows. An overview of the state of the art is given in Section 2. In Section 3, basic combinatorial and algebraic topological notions, algorithms and techniques are introduced. Section 4 is devoted to theoretically develop the scale-space models of the proposed framework. Section 5 is dedicated to the homological information transfer. Experiments showing the applicability of the proposed framework are presented in Section 6. Conclusions are discussed in Section 7.

2. Related works

In the last century, the interest of the mathematical community to progress in the generation of solutions of topological nature to data science problems has enormously increased [2]. The adaptation of topological techniques of reconstruction and analysis to the study of data from real systems is commonly known as Topological Data Analysis (TDA). The ubiquitous preprocessing used in TDA consists of transforming any kind of data into a sequence of topological approximation spaces ruled by different kinds of scale. The subsequent process is to analyze this topological data by calculating some topological invariant or characteristic on it. Currently, the most used type of scale is a geometrical one provided by the notion of filtration and persistent homology (PH). The homology of successive stages of a filtration in a topological space is the most used topological feature implemented in the analysis [3]. The relational structures of graphs and hypergraphs have been studied using these PH tools [4], [5]. With respect to the graph and hypergraph isomorphism problem, several approaches have been developed. In [6] for instance, dynamical systems are used to tackle this problem. However, most competitive graph isomorphism/automorphism solvers like Nauty/Traces, Bliss, Saucy, Conauto, and Dejavu fall within the individualization-refinement framework [7]. These tools alternate color-refinement techniques (such as the Weisfeiler-Leman test [8]) with backtracking steps. In [9] the authors prove the suitability of TDA to differentiate isomorphic graphs, demonstrating that PH is at least as expressive as a corresponding Weisfeiler–Leman test for graph isomorphism. In [10] a new TDA framework is proposed, in which the scale is purely based on the intrinsic connectivity information of the hypergraph and therefore no filtration or clique identification is needed. Its applications on connectome analysis have been published in [11]. An extension of this framework as well as its usability in testing GI and HI is proposed here.

3. Preliminaries

This section is divided in three parts: firstly, the relational setting of the proposed framework will be introduced, followed by its cellular and algebraic topological settings. Let us first introduce some basic concepts that will be used throughout the paper. Sets are denoted here using curly braces { }. A multiset is an ordered pair (A, m_A) where A is the underlying set of the multiset, formed by its distinct elements, and $m_A : A \to \mathbb{N}$ is the function giving the multiplicity, that is, the number of occurrences of the element a in the multiset as the number $m_A(a)$. From now on, we use the additive notation $\sum_{i=1}^{r} m_A(a_i)\cdot a_i$ to represent the multiset $(\{a_1,\dots,a_r\}, m_A)$. Given a finite set A, the set 2^A (resp. $\overline{2}^A$) is the power set (resp. power multiset) of A. Given a finite set $A = \{a_1,\dots,a_r\}$, the number r of elements of A is denoted by $|A|$. $\mathbb{F}[A]$ denotes the vector space of finite linear combinations of elements of A with coefficients in some ring $\mathbb{F}$. Given a function $h : A \to B$ between two A and B, the $\mathbb{F}$-linearization of h, $\mathbb{F}[h] : \mathbb{F}[A] \to \mathbb{F}[B]$, is the linear map canonically associated to h.

3.1. Relational setting

Classically, hypergraphs are defined as data capturing multiway (adjacency) relationships (edges) within a group of entities (vertices) [12]. We handle here a topological incidence version of the hypergraph combinatorial notion, in which edges are as well considered as primary entities (which are not necessarily identified with subsets of vertices) and potential multiple degrees of "contact" between entities are contemplated [13]. Note that the definition we plan to use throughout this paper generalizes the most commonly used one [14].

Definition 1. A (cellular) hypergraph is a tuple $G = ((V, \ell^V), (E, \ell^E), \mathcal{I}_G)$, where:

- The set of vertices V and edges E of a hypergraph are considered to be ordered by enumeration maps $\ell^V : V \to \mathbb{N}$ and $\ell^E : E \to \mathbb{N}$ respectively;
- $\mathcal{I}_G : V \times E \to \overline{\mathbb{N}}$ is the vertex-edge incidence map of G.

The *degree* of a vertex $v_0 \in V$ is defined by $|v_0| := |\{e \in E / \mathcal{I}(v_0, e) \neq 0\}|$. The *degree of contact* of a vertex $v_0 \in V$ is defined by $|v_0|_c := \sum_{e\in E} \mathcal{I}(v_0, e)$. Analogously, the respective notions of degree and degree of contact for an edge can be defined. The following identities are straightforwardly proven: (a) $\sum_{v\in V} |v| = \sum_{e\in E} |e|$ and (b) $\sum_{v\in V} |v|_c = \sum_{e\in E} |e|_c$. An empty hypergraph $G = (V, E, \mathcal{I}_G)$ satisfies that $\mathcal{I}_G(v, e) = 0$, $\forall (v, e) \in V \times E$. A classical graph structure is here understood as an hypergraph, such that the degree and contact degree of each edge are both 2.

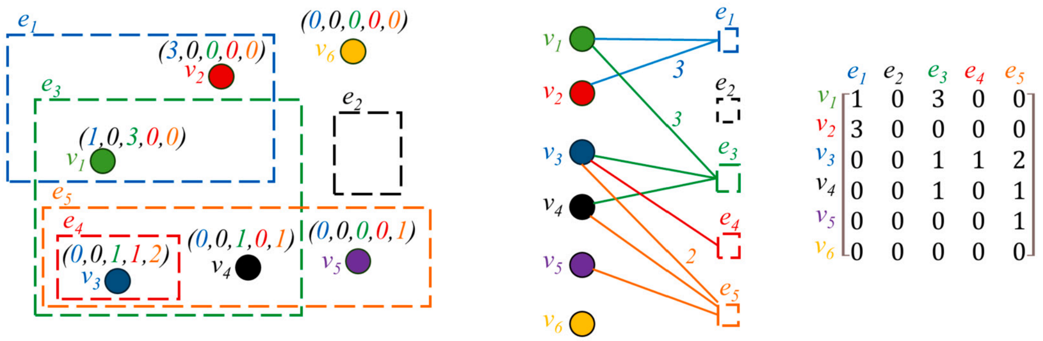


Fig. 1. A simple cellular hypergraph G, having $|V| = 6$ and $|E| = 5$, represented under three different formats. From left to right: relational description, connectivity representation and vertex-edge incidence matrix.

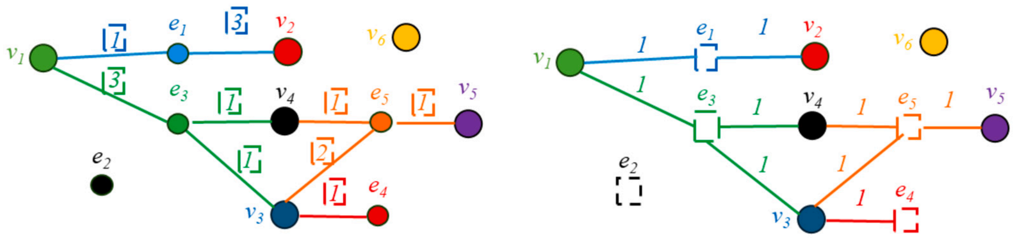


Fig. 2. The connectivity graph $gC(G)$ and hypergraph of minimum connectivity $mC(G)$ of the hypergraph G in Fig. 1. $|V| = 11$, $|E| = 9$ in $gC(G)$ and $|V| = 6$, $|E| = 5$ in $mC(G)$ (as in the original hypergraph G).

Associated to any non-empty hypergraph $G = (V, E, \mathcal{I}_G)$, there are two key combinatorial structures: (a) its *hypergraph of minimum connectivity* $mC(G) = (V, E, \mathcal{I}_{mC(G)})$, with all non-null degrees of contact of $mC(G)$ equal to one. Formally, if $\mathcal{I}_G(v, e) = n_0$, with $n_0 \in \mathbb{N}$, for a pair $(v, e) \in V \times E$, then $\mathcal{I}_{mC(G)}(v, e) = 1$; (b) its *(edge-weighted) connectivity graph* $gC(G) = (V \bigcup E, V \times E, \mathcal{I}_{gC(G)})$, whose incidence map satisfies that $\mathcal{I}_{gC(G)}(a, (v, e)) = 1$ if and only if $\mathcal{I}_G(v, e) \neq 0$ and $a = v$ or $a = e$, $\forall a, v, e \in V \bigcup E$. The weight on the edge (v, e) is precisely $\mathcal{I}_G(v, e)$.

A non-empty hypergraph $G = ((V, \ell^V), (E, \ell^E), \mathcal{I}_G)$ can also be identified: (a) by using a *boundary combinatorial map* $\partial_G : E \to \overline{2}^V$ defined by $\partial_G(e) := \sum n_v \cdot v$, s.t. $\mathcal{I}_G(v, e) = n_v \neq 0$; or (b) by using *a vertex-edge incidence matrix* $M_{ve}(G)$ of dimensions $|V| \times |E|$ with $M_{ve}(G)(i, j) = \mathcal{I}_G(v, e) \in \overline{\mathbb{N}}$ if $\ell^V(i) = v$; $\ell^E(j) = e$, with $1 \leq i \leq |V|$, $1 \leq j \leq |E|$. The different columns of $M_{ve}(G)$ determine the multiset action of ∂ over the edges of G. Reciprocally, given a matrix $M \in \overline{\mathbb{N}}^{|V|\times|E|}$, there is a hypergraph with $|V|$ vertices and $|E|$ edges having M as its vertex-edge incidence matrix.

Fig. 1 shows three possible descriptions of a simple cellular hypergraph G: relational description, connectivity representation and vertex-edge incidence matrix. Its connectivity graph $gC(G)$ and hypergraph of minimum connectivity $mC(G)$ are depicted in Fig. 2.

From now on, we intentionally omit the enumeration functions and the function's dependency on G, unless it is strictly necessary. The dual concepts of edge-vertex incidence relation $\mathcal{I}^{dual}$, coboundary map $\delta : V \to \overline{2}^E$ and edge-vertex incidence matrix M_{ev} can be straightforwardly constructed. Note that M_{ev} coincides with the transpose matrix M_{ve}^T of the vertex-edge incidence matrix. The notion of hypergraph map using the aforementioned notation is now defined.

Definition 2. Let $f = (f_0, f_1) : G = (V, E, \mathcal{I}) \to G' = (V', E', \mathcal{I}')$ be a pair of maps $f_0 : V \to V'$ and $f_1 : E \to E'$. f is a hypergraph map if the following condition holds: $0 \leq \mathcal{I}(v, e) \leq \mathcal{I}'(f_0(v), f_1(e))$ $\forall (v, e) \in V \times E$.

Given a sub-hypergraph $G' = (V', E', \mathcal{I}')$ of G (that means that $V' \subset V$, $E' \subset E$ and $\mathcal{I}(v', e') \geq \mathcal{I}'(v', e')$ $\forall v', e' \in V' \times E'$) the inclusion map $inc : G' \to G$ is a hypergraph map.

Definition 3. A hypergraph isomorphism $G \simeq G'$ between $G = (V, E, \mathcal{I})$ and $G' = (V', E', \mathcal{I}')$ is a bijective hypergraph map $f = (f_0, f_1) : G \to G'$ and $\mathcal{I}(v, e) = \mathcal{I}'(f_0(v), f_1(e))$, $\forall v \in V$ and $\forall e \in E$.

As usual in graph theory, given a hypergraph $G = (V, E, M_{ve})$ defined by its vertex-edge incidence matrix, permutations of rows or columns in M_{ve} generate hypergraphs that are isomorphic to G. The following result can be now deduced:

Proposition 1. *Given a hypergraph G, its associated hypergraph of minimum connectivity $mC(G)$ and its connectivity graph $gC(G)$ are isomorphism invariants.*

At this point, considering the relational setting, the set of non-negative integers $\overline{\mathbb{N}}$ is employed without any algebraic operation, and the composition of hypergraph maps is missing. Subsection 3.3 provides an algebraic framework to properly work with hypergraphs and s^2-models.

3.2. Celullar setting

Let us now recall the simplest topological characteristics of a hypergraph $G=(V,E,\mathcal{I})$, that is the Euler-Poincaré characteristic $\chi(G)=|V|-|E|$. Due to Proposition 1, the Euler-Poincaré characteristic of the connectivity graph $\chi(g\mathcal{C}(G))=|V|+|E|-|\{(v,e)\in V\times E \quad \mathcal{I}(v,e)\neq 0\}|$ is as well a hypergraph index of G that is invariant up to isomorphism. For instance, for the hypergraph G in Fig. 1, $\chi(G)=\chi(m\mathcal{C}(G))=6-5=1$ and $\chi(g\mathcal{C}(G))=11-9=2$ (see Fig. 2).

As we are planning here to construct a topological analytical framework, relational hypergraphs need to be considered as true topological spaces and must be embedded within abstract cell complex structures (ACCs) [15]. Let us recall that an ACC is a classical structure consisting of a dimension-graded set of cells endowed with a transitive bounding relation connecting two cells of different dimensions. The most natural and simple method for a non-empty hypergraph $G=(V,E,\mathcal{I})$ to become an ACC (called *1D-cellulation*) is to be used here. This ACC description (slightly different from the classical one) is simply given by $ACC(G)=(V\bigcup E, dim, \mathcal{I})$, with dimension function $dim: V\bigcup E\to\{0,1\}$ defined by $dim(v)=0$, $\forall v\in V$ and $dim(e)=1$, $\forall e\in E$. Informally speaking, we only need to incorporate a dimension function to the hypergraph representation. From now on, any hypergraph G is topologically analyzed by exclusively using its associated $1D$-cellulation and we confuse G and $ACC(G)$. This choice is mainly motivated by the fact that a hypergraph can be identified with this cellular version in the sense that both use the same structural space (set of vertices and edges) and the notions between hypergraphs can be automatically transferred to their homologous notions in the context of 1D cell complexes. A wide variety of cellulation schemes based on the stronger notion of simplicial complex have been extensively treated in the literature: flag complex, neighborhood complexes, clique-based complexes, Whitney complex, etc. [16]. Let us limit to say that the framework developed here runs correctly for any kind of hypergraph's cellulation.

3.3. Algebraic setting

We opt here for the hypergraph description $G=(V,E,\partial)$ in terms of the boundary function. Given hypergraph $G=(V,E,\partial)$, it is possible to construct an algebraic version of its 1D-cellulation in terms of the classical notion of chain complex [17].

First of all, let us embed the set of non-negative integer numbers $\overline{\mathbb{N}}$ into a ring algebraic structure $(\mathbb{F},+_{\mathbb{F}},\cdot_{\mathbb{F}},0_{\mathbb{F}},1_{\mathbb{F}})$. More formally, we deal here with a commutative Euclidean ring $\mathbb{F}$ equipped with a map $\lambda_{\mathbb{F}}:\mathbb{F}\to\overline{\mathbb{N}}$, called *euclidean or norm function*, assigning a non-negative integer to each element of the ring, such that for each $a,b\in\mathbb{F}$, $b\neq 0_{\mathbb{F}}$, there exist $q,r\in\mathbb{F}$ such that $a=q\cdot_{\mathbb{F}} b+_{\mathbb{F}} r$, with $\lambda_{\mathbb{F}}(r)<\lambda_{\mathbb{F}}(b)$. Besides, it is well-known that there is a unique semiring map $\vartheta_{\mathbb{F}}:\overline{\mathbb{N}}\to\mathbb{F}$ determined by $\vartheta_{\mathbb{F}}(1)=1_{\mathbb{F}}$. From now on, $\mathbb{F}$ is chosen to be either a field or the ring of integer numbers.

A *chain complex* $C_*(G,\mathbb{F})$ associated to a hypergraph $G=(V,E,\partial)$ is a graded vector space over the ring $\mathbb{F}$ (also called graded module in homological algebra) endowed with an algebraic boundary map. Formally, it is a family $\{C_q(G,\mathbb{F}),\mathbb{F}_q[\partial]\}_{q=0,1}$ where: (a) the sub-index q represents dimension and $C_0(G,\mathbb{F})=\mathbb{F}[V]$, $C_1(G,\mathbb{F})=\mathbb{F}[E]$; (b) the linear map $\mathbb{F}[\partial]=(\mathbb{F}_0[\partial],\mathbb{F}_1[\partial]):C_*(G,\mathbb{F})\to C_{*-1}(G,\mathbb{F})$, called *differential* of G is defined by: $\mathbb{F}_0[\partial](v):=0_F$ $\forall v\in V$ (note that $C_{-1}(G,\mathbb{F})$ is defined by the trivial or zero group) and $\mathbb{F}_1[\partial](e)=\mathbb{F}[\partial(e)]=\mathbb{F}[\sum_i n_{v_i}\cdot v_i]:=\sum_i\vartheta_{\mathbb{F}}(n_{v_i})\cdot v_i$, $\forall e\in E$.

The elements of $C_q(G,\mathbb{F})$ are called *q-chains*, $q=0,1$. A q-chain a is called a q-cycle if $\mathbb{F}_q[\partial](a)=0$. If $a=\mathbb{F}_{q+1}[\partial](b)$, for some $b\in C_{q+1}(G,\mathbb{F})$, then a is called a q-boundary. Denote the q-cycles and q-boundaries vector spaces by Z_q and B_q, respectively. We say that two q-cycles are *homologous* if $a-b$ is a q-boundary. Define the q^{th} homology vector space $\mathcal{H}_q(G,\mathbb{F})$ to be the quotient Z_q/B_q. For all $q=0,1$, there exists a finite number of elements of $C_q(G,\mathbb{F})$ from which we can deduce all the elements of $\mathcal{H}_q(G,\mathbb{F})$. Those elements are called *homology generators* of dimension q. We say that *a representative q–cycle a of a homology generator* α of $\mathcal{H}_q(G,\mathbb{F})$ if $\alpha=a+B_q$. In this case, α is also denoted by $[a]_{\mathcal{H}}$. Analogously, it is possible to define the *codifferential* $\{\mathbb{F}_q[\delta]\}_{q=0,1}$ from $C_*(G,\mathbb{F})$ to $C_{*+1}(G,\mathbb{F})$ and the cochain complex associated to G.

A *chain map* $f=(f_0,f_1):C_*(G,\mathbb{F})\to C_*(G',\mathbb{F})$ between two chain complexes $C_*(G,\mathbb{F})$ and $C_*(G',\mathbb{F})$ associated to their respective hypergraphs $G=(V,E,\partial)$ and $G'=(V',E',\partial')$ is a linear map such that $f_0\ \mathbb{F}_1[\partial]=\mathbb{F}_1[\partial']\ f_1$. It induces a well-defined map on homology $[f]_{\mathcal{H}}:\mathcal{H}_*(G,\mathbb{F})\to\mathcal{H}_*(G,\mathbb{F})$ where $[f]_{\mathcal{H}}([a]_{\mathcal{H}})=[f_q(a)]_{\mathcal{H}}$, $\forall a\in C_q(G,\mathbb{F})$, $q=0,1$.

It is straightforward to show that the $\mathbb{F}$-linearization of an isomorphism of hypergraphs $f=(f_0,f_1):(V,E,\partial)\simeq(V',E',\partial')$ is a chain isomorphism and a cochain isomorphism.

As an example of the different settings that are considered here, matrix and connectivity representations of the relational, cellular and algebraic settings for the hypergraph in Fig. 1 are shown in Fig. 3. Note that for instance, $\partial(v_5)=2\cdot v_3+v_4+v_5$ in the relational setting, and $\partial(v_5)=v_4+v_5$ in the algebraic one considering coefficients in the integers modulo 2, that is $\mathbb{F}=\mathbb{Z}_2$.

The following well known result can now be deduced:

Proposition 2. *Given a hypergraph $G=(V,E,\partial)$, its chain complex $C_*(G,\mathbb{F})$ with coefficients in $\mathbb{F}$ as well as its homology are hypergraph isomorphism invariants.*

The chain complex $C_*(G)$ of a hypergraph $G=(V,E,\partial)$ can be seen as an algebraic hypergraph of the kind $(\tilde{V},\tilde{E},\mathbb{F}[\partial])$, where $\tilde{V}$ and $\tilde{E}$ are basis of the vector spaces $\mathbb{F}[V]$ and $\mathbb{F}[E]$, respectively. A particular relevant choice for $\tilde{V}$ and $\tilde{E}$ are the combinatorial basis V and E. In what follows, chain complexes will be described in these terms.

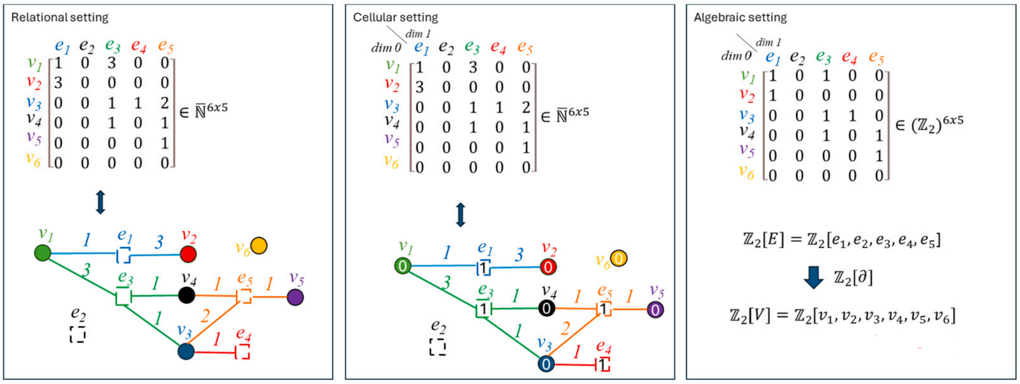


Fig. 3. Matrix and connectivity representations of the relational (left), cellular (center) and algebraic (right) settings for the hypergraph in Fig. 1, $G = (V, E, \mathcal{I}) = (V, E, \partial) = (V, E, M_{ve})$. The ground field $\mathbb{F}$ chosen in this example for the algebraic setting is the finite field $\mathbb{Z}_2$.

$$G(1) = (V, E, \partial) \underset{\rho^-(2)}{\overset{\rho^+(1)}{\rightleftarrows}} G(2) = (V(2), E(2), \partial(2)) \underset{\rho^-(3)}{\overset{\rho^+(2)}{\rightleftarrows}} \cdots$$

Fig. 4. Diagram showing the relations among the first two algebraic hypergraph components within a s^2-model $S^2(\{V(s), E(s), \partial(s), \rho^{\pm}(s)\}_{s\geq 1})$ of a hypergraph $G = (V, E, \partial)$.

4. Scale-space models of a hypergraph

In [10] an algebraic topological model of a geometric n-dimensional cell complex based on topological scale is presented. In this section, we design an improved and much more general scale-space model adapted to 1D-cellulations of hypergraphs, allowing a rich structural and dynamical topological analysis. In what follows, we omit the dependency with regards to $\mathbb{F}$ when describing (co)differentials, chain complexes and scale-space representations. In particular, the linear maps $\mathbb{F}[\partial]$ and $\mathbb{F}[\delta]$) are simply expressed by ∂ and δ, respectively. Let us now define the main representational tool of this new TDA framework.

Definition 4. Let $G = (V, E, \partial)$ be a non-empty hypergraph. A *scale-space model* (s^2-model) $S^2(\{V(s), E(s), \partial(s), \rho^{\pm}(s)\}_{s\geq 1})$ of G is a one-parameter family of chain complexes $G(s) = (V(s), E(s), \partial(s))$ endowed with transition functions $\rho^+(s) : G(s) \to G(s+1)$ and $\rho^-(s) : G(s) \to G(s-1)$, $\forall s \in \mathbb{N}$. More specifically, the following conditions must be satisfied for each scale s of the model:

S^2.1. [Original hypergraph as initial state]: $G(1) = C_*(G)$ and $\rho^-(1)$ from $C_*(G)$ to the trivial vector space with one element is the unique admissible linear map between them;

S^2.2. [Preservation of the Euler-Poincaré characteristic]: $|V(s)| \setminus |E(s)| = \chi(G)$, being $|V(s)|$ and $|E(s)|$ their respective basis dimensions.

S^2.3. [Algebraic Hypergraph Components]: The map $\partial(s) : G(s) \to G(s)$ is a differential for $G(s)$. The differential $\partial(1)$ agrees with ∂;

S^2.4. [Chain compatibility of the transition maps]: The transition maps $\rho^{\pm}(s) : G(s) \to G(s \pm 1)$ are chain maps.

S^2.5: [Invariance of transition map compositions]: $\forall m, n \geq 1$, the composition map (if doable) $\rho^-(s+n-m+1) \ldots \rho^-(s+n)\rho^+(s+n-1) \ldots \rho^+(s) : G(s) \to G(s+n-m)$ coincides with any other possible composition map from $G(s)$ to $G(s+n-m)$ of n maps $\rho^+(s)$ and m maps $\rho^-(s)$.

Summing up, a s^2-model associated to a hypergraph G is then a sequence of algebraic hypergraphs having the same Euler-Poincaré characteristic than G and connected by appropriate transition maps. In homological algebra terms, an algebraic topological s^2-model is simply a particular direct-inverse system over the positive integers of 1-dimensional chain complexes [18]. From a calculus viewpoint, it can be seen as a special type of discrete algebraic dynamical system of hypergraphs.

A *truncated* s^2*-model* containing the first $\mathbf{k} \geq 1$ algebraic hypergraphs $G(s)$ and their corresponding transition maps is denoted by $S^2_k(\{V(s), E(s), \partial(s), \rho^{\pm}(s)\})$. Fig. 4 shows a diagram representing the first two levels of the s^2-model for a hypergraph $G = (V, E, \partial)$.

Applicable choices for the linear transition functions in order that the [S^2.4] condition holds can be: (a) $(\rho^+(s), \rho^-(s+1)) = (f(s), f^{-1}(s))$, where $f(s) : G(s) \to G(s+1)$ is a chain isomorphism, $\forall s \geq 1$; (b) if $G(s) = G(1)$ $\forall s \geq 1$, $(\rho^+(s), \rho^-(s+1)) = (f, f)$, $\forall s \geq 1$, being $f : G(1) \to G(1)$ a chain map.

Let us emphasize that it is also possible to see an s^2-model in combinatorial terms, thanks to the euclidean function $\lambda_{\mathbb{F}} : \mathbb{F} \to \overline{\mathbb{N}}$ and the semiring map $\vartheta_{\mathbb{F}} : \overline{\mathbb{N}} \to \mathbb{F}$. For instance, if $\mathbb{F}$ is a field, the resulting combinatorial scale-space system of an s^2-model

$S^2(\{V(s), E(s), \partial(s), \rho^+(s)\}_{s\geq 1})$ is the sequence of the minimum connectivity hypergraphs of the components, having as transition maps the compositions $\lambda\rho^+(s)\vartheta$.

Definition 5. Let $G=(V,E,\partial)$ and $G'=(V',E',\partial')$ be two non-empty hypergraphs. Let $S^2(\{V(s), E(s), \partial(s), \rho^{\pm}(s)\}_{s\geq 1})$ and $S^2(\{V'(s), E'(s), \partial'(s), \rho'^{\pm}(s)\}_{s\geq 1})$ be two s^2-models respectively associated to them. A *scale-space map* (s^2-map) $\{f(s)\}_{s\geq 1} = \{(f_0(s), f_1(s))\}_{s\geq 1} : S^2(\{V(s), E(s), \partial(s), \rho^{\pm}(s)\}_{s\geq 1}) \to S^2(\{V'(s), E'(s), \partial'(s), \rho'^{\pm}(s)\}_{s\geq 1})$ is the one that satisfies:

(a) [Compatibility with boundary functions] Each pair $(f_0(s), f_1(s)) : G(s) \to G'(s)$ is a chain map;
(b) [Compatibility with transition functions] $f(s\pm 1)\rho^{\pm}(s) = \rho'^{\pm}(s\pm 1)f(s)$, $\forall s \geq 1$.

Note that due to the fact that the map $f(0)$ does not exist, we consider that the condition $f(0)\rho^-(1) = \rho^{-1}f(1)$ trivially holds. If each $f(s)$ component map is bijective and its inverse is as well a chain map, then both models are s^2-*isomorphic* via $\{f(s)\}_{s\geq 1}$.

Definition 6. Being $S^2(V, E, \{\partial(s), \rho^{\pm}(s)\}_s)$ and $S^2(V', E', \{\partial', \rho'^{\pm}(s)\}_s)$ two s^2-models associated to $G=(V,E,\partial)$ and $G' = (V',E',\partial')$ such that $V(s)=V$, $E(s)=E$ and respectively $V'(s)=V'$, $E'(s)=E$, $\forall s\geq 1$. Associated to a hypergraph map $f=(f_0,f_1) : G=(V,E,\partial) \to G'=(V',E',\partial')$, the *canonical map* $f^c := \{f^c(s)\}_{s\geq 1} = \{f_0^c(s), f_1^c(s))\}_{s\geq 1} : S^2(V, E, \{\partial(s), \rho^{\pm}(s)\}_s) \to S^2(V', E', \{\partial', \rho'^{\pm}(s)\}_s)$ is the map satisfying that $(f_0^c(s), f_1^c(s)) : G(s) \to G'(s)$ agrees with the $\mathbb{F}$-linearization of the original map $(f_0, f_1) = (f_0(1), f_1(1)) : G(1) \to G'(1)$.

Note that the canonical map associated to a chain map is not, in general a s^2-map. This is due to a lack of support regarding differential or transition functions. For the sake of a better understanding of the new concepts, from now on, s^2-models, having the same set of vertices and edges than G will be considered. The next two subsections are devoted to distinguish two main types of s^2-models that can be defined depending on the type of relations within the model that is "prioritize": adjacency vs incidence relation.

4.1. Adjacency s^2-models

These s^2-models are the simplest one and they follow the pattern $S^2(V, E, \{\partial(s), \rho^+(s), \rho^-(s)\}_{s\geq 1})$, such that $\partial(s)=\partial$, $\forall s\geq 1$. A trivial example of an adjacency s^2-model of $G=(V,E,\partial)$ with coefficients in $\mathbb{F}$ is the structure $S^2(V, E, \partial, (1_{\mathbb{F}[V]}, 1_{\mathbb{F}[E]}), (1_{\mathbb{F}[V]}, 1_{\mathbb{F}[E]}))$. A more interesting system is inspired by the classical Weisfeiler-Lehman (WL) and color refinement algorithms. WL was firstly developed in [8] for the graph class, and in [19] a hypergraph version was proposed. Its application to machine learning as foundational pillar of graph neural networks is developed in [20,21]. An adaptation of this process to the s^2-model setting is provided by the so-called *color refinement (or simply CR) s^2-model*, defined by $S^2(V, E, \partial, (\partial\delta, \delta\partial), (\partial\delta, \delta\partial))$ in which the differential and transition maps are not dependent on s. Note that $\delta\partial$ (resp. $\partial\delta$) is the classical signless edge (resp. vertex) Laplacian matrix of G [22]. As previously stated, an adjacency s^2-model can be automatically generated if a unique chain map $f : C_*(G) \to C_*(G)$ determines all the transition maps $\rho^+(s)$ and $\rho^-(s)$. The chain map $(\sum_{i=0}^{k}(-1_{\mathbb{F}})^i(\partial\delta)^i, \sum_{i=0}^{k}(-1_{\mathbb{F}})^i(\delta\partial)^i)$, for any $k\geq 0$, provides an important generalization of the CR s^2-model involving iterated Laplacian operators. Note that $(\partial\delta)^0 = (\delta\partial)^0 = 1_{C_*(G)}$.

4.2. Incidence s^2-models: the boundary-scale case

Incidence s^2-models for a hypergraph $G=(V,E,\partial)=(V,E,M)$ (being M the vertex-edge incidence matrix of G) are systems $S^2(V, E, \{\partial(s), \rho^{\pm}(s)\}_s)$ in which $\partial(s)\neq\partial$ for some $s>1$.

A first example of incidence s^2-model given in matrix terms is provided by respective changes of basis for vertices and edges. Given two square invertible matrices $P\in\mathbb{F}^{|V|\times|V|}$ and $Q\in\mathbb{F}^{|E|\times|E|}$, we can construct the s^2-model $S^2(V, E, \{P^{s-1} * M * Q^{s-1}, (P, Q^{-1}), (P^{-1}, Q)\}_{s\geq 1})$ where $*$ is the matrix multiplication operation with coefficients in the euclidean domain $\mathbb{F}$.

In order to investigate the applicability of s^2-models in profoundly studying hypergraph's connectivity, we focus here in a specific instance of this type of incidence models, that are named *boundary-scale model*. The main characteristic of this kind of representation, is that both, boundary and coboundary maps are deeply involved in every scale. With the aim of producing non-redundant and non-correlated topological information, we work with k-truncated boundary-scale models, with k no greater than half the diameter of the hypergraph.

Definition 7. Given a non-empty hypergraph $G=(V,E,\partial)$, the *boundary-scale model of G* is the s^2-model of the form: $S^2(V, E, \{\partial(\delta\partial)^s, (\partial\delta, 1_{\mathbb{F}[E]}), (1_{\mathbb{F}[V]}, \delta\partial)\}_{s\geq 1})$.

Given a hypergraph $G=(V,E,M)$ (where M is its vertex-edge incidence matrix), it is possible to redefine the boundary-scale model in matrix terms as follows: $S^2(V, E, \{M * (M^T * M)^{s-1}, (M * M^T, \mathbb{I}_{|E|\times|E|}), (\mathbb{I}_{|V|\times|V|}, M^T * M)\}_{s\geq 1})$, where $\mathbb{I}_{n\times m}$ represents the identity matrix of dimensions $n\times m$. An example of the second and third level of this model for the hypergraph G in Fig. 1 (being $\mathbb{F}$ the integers modulo 2 and graphically expressing its component chain complexes as (algebraic) hypergraphs) is shown in Fig. 5. Note that, for instance, the 1^{st} and 2^{nd} Betti numbers are $\beta_0(G(1))=2$ and $\beta_1(G(1))=1$ on the initial hypergraph, while moving to the second and third levels of the model they become $\beta_0(G(2))=3$, $\beta_1(G(2))=2$, $\beta_0(G(3))=4$ and $\beta_1(G(3))=3$.

$$\partial(1) = \mathbb{Z}_2[\partial] = \begin{array}{c|ccccc} & e_1 & e_2 & e_3 & e_4 & e_5 \\ \hline v_1 & 1 & 0 & 1 & 0 & 0 \\ v_2 & 1 & 0 & 0 & 0 & 0 \\ v_3 & 0 & 0 & 1 & 1 & 0 \\ v_4 & 0 & 0 & 1 & 0 & 1 \\ v_5 & 0 & 0 & 0 & 0 & 1 \\ v_6 & 0 & 0 & 0 & 0 & 0 \end{array}$$

$$\rho^{+}(2) = \left(\mathbb{Z}_2\,[\partial\delta] = \begin{array}{c|cccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \\ \hline v_1 & 0 & 1 & 1 & 1 & 0 & 0 \\ v_2 & 1 & 1 & 0 & 0 & 0 & 0 \\ v_3 & 1 & 0 & 0 & 1 & 0 & 0 \\ v_4 & 1 & 0 & 1 & 0 & 1 & 0 \\ v_5 & 0 & 0 & 0 & 1 & 1 & 0 \\ v_6 & 0 & 0 & 0 & 0 & 0 & 0 \end{array},\ 1_{\mathbb{Z}_2[\mathbb{E}]} \right)$$

$$\partial(2) = \mathbb{Z}_2[\partial(\delta\partial)] = \begin{array}{c|ccccc} & e_1 & e_2 & e_3 & e_4 & e_5 \\ \hline v_1 & 1 & 0 & 0 & 1 & 1 \\ v_2 & 0 & 0 & 1 & 0 & 0 \\ v_3 & 1 & 0 & 0 & 0 & 1 \\ v_4 & 1 & 0 & 0 & 1 & 1 \\ v_5 & 0 & 0 & 1 & 0 & 0 \\ v_6 & 0 & 0 & 0 & 0 & 0 \end{array} \qquad \partial(3) = \mathbb{Z}_2[\partial(\delta\partial)^2] = \begin{array}{c|ccccc} & e_1 & e_2 & e_3 & e_4 & e_5 \\ \hline v_1 & 0 & 0 & 1 & 1 & 0 \\ v_2 & 1 & 0 & 1 & 1 & 1 \\ v_3 & 0 & 0 & 0 & 0 & 0 \\ v_4 & 0 & 0 & 1 & 1 & 0 \\ v_5 & 1 & 0 & 1 & 1 & 1 \\ v_6 & 0 & 0 & 0 & 0 & 0 \end{array}$$

$$\rho^{-}(3) = \left(1_{\mathbb{Z}_2[\mathbb{V}]}\ ,\mathbb{Z}_2\,[\delta\partial] = \begin{array}{c|ccccc} & e_1 & e_2 & e_3 & e_4 & e_5 \\ \hline e_1 & 0 & 0 & 1 & 0 & 0 \\ e_2 & 0 & 0 & 0 & 0 & 0 \\ e_3 & 1 & 0 & 1 & 1 & 1 \\ e_4 & 0 & 0 & 1 & 1 & 0 \\ e_5 & 0 & 0 & 1 & 0 & 0 \end{array} \right)$$

Fig. 5. Algebraic setting of the hypergraph in Fig. 1 (top). Hypergraph components and its respective boundary and transition maps, of levels $s = 2$ and $s = 3$ for the boundary-scale s^2-model of the hypergraph in Fig. 1 (bottom).

5. Homology of s^2-models

The passing to homology of an s^2-model is analyzed here and leads to the main result of this paper. Note that the homology of the algebraic hypergraphs of the model can be taken with coefficients in a different ground ring than that employed for the construction of the s^2-model. For the purpose of simplifying, we will consider here both rings to be the same.

The content of Appendix *A* about homology computation using the classical Smith Normal Form factorization allows to determine the homology transfer within the context of scale-space models. The results obtained in this Section are valid for both, the free and torsion homology of a given s^2-model. Let us start with the definition of the homology of a s^2-model. To describe the resulting scale-space homological structure $\mathcal{H}(S^2(V, E, \{\partial(s), \rho^{\pm}(s)\}_s))$ we make use of the following tools:

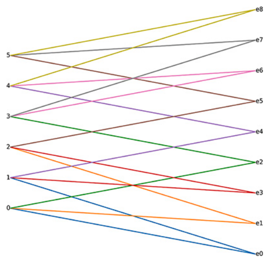
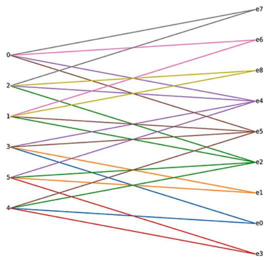
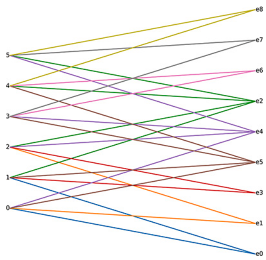
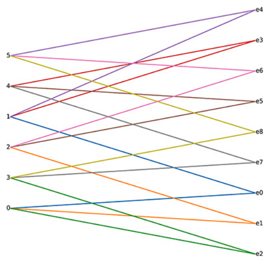
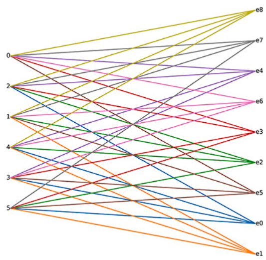
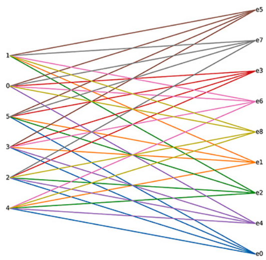
- The homology of a chain complex $G(s) = (V, E, M(s))$ (being $M(s)$ its vertex-edge incidence matrix with coefficients in $\mathbb{F}$) is represented by the algebraic hypergraph $\mathcal{H}_*(G(s)) = (\mathcal{B}^{\mathcal{H}}_{\mathbf{0}}(M(s)), \mathcal{B}^{\mathcal{H}}_{\mathbf{1}}(M(s)), D^{\mathcal{H}}_{SNF}(M(s)))$.
- Since $\rho^{\pm}(s) : G(s) \to G(s \pm 1)$ is a chain map for each scale index s, then each $[\rho^{\pm}(s)]_{\mathcal{H}} : \mathcal{H}_*(G(s)) \to \mathcal{H}_*(G(s \pm 1))$ is well defined and can be computed using the classical linear algebra tools explained in Appendix A.

Definition 8. Let $G = (V, E, \partial)$ be a non-empty hypergraph and $\mathbf{S}^2(G) = S^2(V, E, \{\partial(s), \rho^{\pm}(s)\}_{s\geq 1})$ be an s^2-model associated to it. The *homology of the s^2-model* $\mathcal{H}(\mathbf{S}^2(G))$ is the new s^2-model:

$$\mathcal{H}(\mathbf{S}^2(G)) = S^2(\{\mathcal{B}^{\mathcal{H}}_{\mathbf{0}}(M(s)),\ \mathcal{B}^{\mathcal{H}}_{\mathbf{1}}(M(s)), D^{\mathcal{H}}_{SNF}(M(s)), [\rho^{\pm}(s)]_{\mathcal{H}}\}_{s\geq 1})$$

Due to the fact that the transition maps are chain maps, the homology of an admissible composition of such maps coincides with the composition of its corresponding homology maps. That means, in particular, that condition $[S^2.4]$ of s^2-models holds. Note that the homology of an incidence s^2-model is again incidence s^2-models in which the sets of vertices and edges of the algebraic hypergraphs components are possibly different. Due to the fact that Smith Normal Form factorization of the vertex-edge incidence matrix of a hypergraph is a node and edge permutation invariant (see Appendix A), the fundamental result of this paper can be derived.

Table 1
Connectivity representation of the hypergraph components of the boundary-scale s^2-model in levels $s = 1, 2, 3$, that are generated for the two graphs in cubic06. Vertices and edges are nodes on the left and right, respectively.

	$s = 1$	$s = 2$	$s = 3$
$cubic06-0$			
$cubic06-1$			

Theorem 3. *Let* $\mathbf{S}^2(G) = S^2(V, E, \{\partial(s), \rho^{\pm}(s)\})_{s\geq 1}$ *be a* s^2*-model associated to a hypergraph* $G = (V, E, \partial)$*. Then,* $\mathbf{S}^2(G)$ *and* $\mathcal{H}(\mathbf{S}^2(G))$ *are hypergraph isomorphic invariants (up to* s^2*-isomorphism).*

Proof. Let us consider the matrix version $S^2(V, E, \{M(s), T_*^+(s), T_*^-(s)\}_{s\geq 1})$ of the s^2-model $\mathbf{S}^2(G)$, being $T_*^{\pm} = (T_0^{\pm}, T_1^{\pm})$ the corresponding matrix form of the transition maps. Let us construct its associated s^2-SNF-model $SNF(\mathbf{S}^2(G))$ having at scale s, $C_*^{snf}(G(s)) = (B_{\mathbf{0}}^{snf}(M(s)), B_{\mathbf{1}}^{snf}(M(s)), D_{snf}(M(s)))$ as chain complex components and $snf(\rho^+(s))$ and $snf(\rho^-(s))$ as transition maps. The resulting scale-space system, called the s^2-SNF-model, is a true s^2-model s^2-isomorphic to the original system, due to the fact that the SNF factorization of the matrices determining the boundary and transition maps of the model simply boils down to basis changes for the vertices and edges of a hypergraph G. The s^2-model $\mathcal{H}_*(\mathbf{S}^2(G))$ is automatically extracted from this intermediary system. If G and G' are isomorphic hypergraphs, the s^2-SNF-models of the corresponding s^2-models $\mathbf{S}^2(G)$ and $\mathbf{S}^2(G')$ are s^2-isomorphic. This is due to the fact that the Smith Normal Form is a hypergraph invariant. Moreover, the algebraic boundary map of each chain complex component of both systems must be the same. In consequence, the appropriate composition of s^2-isomorphisms linking the original s^2-models to their SNF versions provides us the desired s^2-isomorphism between $\mathbf{S}^2(G)$ and $\mathbf{S}^2(G')$. Now, we directly extract the homology of $\mathbf{S^2}(G)$ from its s^2-SNF-model. In fact, $\mathcal{H}(\mathbf{S}^2(G))$ is defined here using submatrices of the model connecting representative cycles of the corresponding homology vector spaces $\mathcal{H}(G(s))$ (see Appendix A). Then, by removing appropriate "vertices" and "edges" of the algebraic hypergraphs components of the isomorphic s^2-SNF-models of G and G', it is a simple exercise to show that $\mathcal{H}(\mathbf{S}^2(G))$ and $\mathcal{H}(\mathbf{S}^2(G'))$ are s^2-isomorphic. □

This theory can be analogously developed for free and torsion homology s^2-models. The chain compatibility condition for transition maps in the s^2-model definition can be relaxed (for instance, maps preserving cycles or boundaries) in such a way that some homological information of the s^2-model is preserved up to hypergraph isomorphism. This important issue as well as the use of non-linear transition functions will be discussed in a future paper.

6. Isomorphism test algorithms for hypergraphs based on s^2-model

GI and HI are computable problems strictly related to the time efficiency of the algorithms to detect (and if positive, construct one) isomorphism between two combinatorial structures. It is well known that the GI problem is polynomial-time reducible to that of HI and vice versa [23]. A generic HI Test takes a hypergraph and returns a string certificate that is identical for isomorphic hypergraphs. In other words, the chosen certificate musts be a hypergraph invariant (also called *topological index*). If a certificate always outputs a different answer for non-isomorphic hypergraphs, it is called *complete*. It is well known that there is a complete certificate that can be computed in exponential time (obtained via the canonical labeling algorithm [24]), but there is no known complete certificate that can be obtained in polynomial time for a general hypergraph. The tree class is an exception to this fact [25]. We distinguish here three different types of HI Test algorithms based on an s^2-model:

- *Intra-analysis* s^2*-HI*. The certificate associated to the test exclusively depends on local or global hypergraph indices [26] applied to the corresponding hypergraph components of truncated s^2-models of two given hypergraphs, as well as to their homology. If this certificate is different for some scale of the model, then the hypergraphs are non-isomorphic. Examples of these indices are the sequence of vertex and/or edge degrees, the Euler-Poincaré characteristic of their connectivity graph $\chi(g\mathcal{C}(G))$ at each scale, the WL algorithm applied to each scale, etc.

- *Inter-analysis s^2-HI.* Involves relationships determined by transition maps between vertices, edges and homology generators of the same dimension of different levels of the s^2-model. These algorithms can be implemented using both adjacency and incidence s^2-models. For instance, considering the CR s^2-model $S^2(V, E, \partial, (\partial\delta, \delta\partial), (\partial\delta, \delta\partial))$, a certificate based on vertex inter-degree is defined for each vertex $v \in V$, as the formal sum $\sum_{1\leq i\leq k} |(\partial\delta)^{i-1}(v)|$. Note that here the degree function $|\;|$ goes from $\mathbb{F}[V]$ to $\mathbb{F}[\mathbb{N}\bigcup\{0\}]$.
- *Hybrid Scale-Space HI.* This kind of certificates combines both, inter and intra analysis. An example of this type of algorithms is given by the following algorithm inspired in the WL-strategy. Given a truncated boundary-scale model with k hypergraph components $S^2_k(V, E, \{\partial(\delta\partial)^s, (\partial\delta, 1_E), (1_V, \delta\partial)\}_s)$, the certificate for each vertex $v \in V$ is given by the formal sum $\sum_{0\leq i\leq k}(\delta(\partial\delta)^i + (\partial\delta)^i)(v)$ in $\mathbb{F}[V\bigcup E]$ and for each edge $e \in E$ is $\sum_{0\leq i\leq k}(\partial(\delta\partial)^i + (\delta\partial)^i)(e)$ in $\mathbb{F}[V\bigcup E]$. A homology-based certificate of this kind can be automatically derived.

Finally, HI inspection at any level (intra-analysis, inter-analysis or hybrid) based on invariant features of the matrix description of the s^2-model need to be considered separately. We distinguish two main groups: *Spectral and SNF based*. Given any truncated s^2-model $S^2_k(V, E, \{\partial(s), \rho^{\pm}(s)\}_s)$, all the boundary $\partial(s)$ and transition $\rho^{\pm}(s)$ functions can be expressed in $\mathbb{F}$-matrix form. Spectral-based (respectively SNF-based) s^2-HI test algorithms are those related to the eigenvalues and eigenvectors (resp. elementary divisors) on the euclidean domain $\mathbb{F}$ of those matrices. To find efficient certificates resting on s^2-model approaches is out of the scope of this paper and will be studied in a near future.

6.1. Experiments testing graph isomorphism

In this subsection, we limit ourselves to provide a competitive GI testing algorithm demonstrating the discrimination power of the proposed framework. We use truncated boundary-scale s^2-models with $\mathbb{Z}_2$ coefficients to pursue this goal. Note that SNF is applied in the following using the integers $\mathbb{Z}$ as ground ring (see Appendix A). More concretely, three main intra-analysis measures are to be tested for comparison among isomorphic and non-isomorphic graphs:

a) ω_d: The increasing ordered sequence of vertex's degrees for each hypergraph generated at every scale of the s^2-model.
b) ω_β: The $\mathbb{Z}_2$ Betti number sequences computed for each hypergraph generated at every scale of the s^2-model. In this way, the free homology of each hypergraph is studied.
c) ω_i: The increasing ordered sequence of elementary divisors, that are not equal to $1_\mathbb{Z}$, of the incidence matrices (with coefficients in $\mathbb{Z}$) for each hypergraph generated at every scale of the s^2-model. In this way, the torsion homology (at dimension zero) of each hypergraph is studied.

As inter-analysis metric, we consider:

a) ω_{ρ^+}: The ordered sequence of the SNF multisets of all matrices (with integer coefficients) corresponding to the composition of the ρ^+ transition maps generated throughout the model. These compositions are constructed as: $\rho^+(1)$ for the first level of the model, $\rho^+(2)\circ\rho^+(1)$ for the second, $\rho^+(3)\circ\rho^+(2)\circ\rho^+(1)$ for the third, and so on. Note that in boundary-scale models, $\rho^+(s) = \rho^+(1), \forall s \geq 1$.
b) ω_{ρ^-}: Similarly, the ordered sequence of the SNF multisets of all matrices (with integer coefficients) corresponding to the composition of the ρ^- transition maps generated throughout the model. These compositions are constructed as: $\rho^-(2)$, $\rho^-(2)\circ\rho^-(3)$, and so on. Note that in boundary-scale models, $\rho^-(s) = \rho^-(1), \forall s \geq 1$.

Here, we analyze to what extent the proposed model is capable of distinguishing between different non-isomorphic graphs. To do so, we use different data sets that are known to be challenging for graph isomorphism tests. Connected cubic graphs and minimal Cayley graphs [27,28], for example, cannot be distinguished by 1-WL. The strongly regular graphs database [29] contains instances that cannot be distinguished by 3-WL. Recent attempts based on Persistent Homology [9] and Graph Neural Networks [30] demonstrate the limitations of these approaches when dealing with such datasets. Three levels of the boundary-scale s^2-model (from $s = 1$ to $s = 3$) have been generated for every database in our experiments. Table 2 shows the percentage of graphs that are univocally distinguished by using the metrics mentioned above for each level of the model. Note that level $s = 3$ of the model is sufficient to distinguish every graph within these three datasets.

Table 3 shows the results obtained for the connected cubic graph database with three levels of the model. Each cubic set (cubic06, cubic08, cubic10, cubic12 and cubic14) contains non-isomorphic graphs (2, 5, 19, 85 and 509 graphs, respectively) that have the same number of vertices and edges. Most of them show different ordered sequences of degrees for the vertices of the generated hypergraphs throughout the model, ω_d (100%, 100%, 89.5%, 96.5% and 97.6% respectively). Graphs that were not distinguished by using this metric, have either unique ω_β, ω_i, ω_{ρ^-} or ω_{ρ^+}. In conclusion, every graph within the cubic database can be uniquely distinguished (see column 6 in Table 3). Table 1 shows the hypergraph components of the boundary-scale s^2-model in levels $s = 1, 2, 3$, which are generated for the two graphs in cubic06, showing how incidence relations change throughout the model. Considering these two cases, level $s = 1$ of the model is sufficient to differentiate them (see Table 2), since the increasing ordered sequence of elementary divisors of the incidence matrices (ω_i) differs. Hypergraph representations were produced using PNNL's open source HyperNetX [31].

Table 2
Percentage of graphs that can be unequivocally distinguished by using boundary scale s^2-models with $s = 1$, $s = 2$ and $s = 3$ levels. Metrics considered here are ω_d, ω_β, ω_i, ω_{ρ^+} and ω_{ρ^-}.

	$s = 1$	$s = 2$	$s = 3$		$s = 1$	$s = 2$	$s = 3$
cayley12-24	25	100.0	100.0	cayley60-150	0	92.0	100.0
cayley16-24	0	33.3	100.0	cayley60-180	0	100.0	100.0
cayley16-32	0	100.0	100.0	cayley63-126	0	100.0	100.0
cayley20-30	100	100.0	100.0	cayley63-189	0	100.0	100.0
cayley20-40	0	100.0	100.0	sr261034	0	10.0	100.0
cayley24-36	0	100.0	100.0	sr281264	0	25.0	100.0
cayley24-48	0	100.0	100.0	sr291467	0	0.0	100.0
cayley24-60	25	100.0	100.0	sr351899	0	0.4	100.0
cayley24-72	0	100.0	100.0	sr361446	0	0.6	100.0
cayley32-48	0	28.6	100.0	sr401224	0	21.4	100.0
cayley32-64	0	89.5	100.0	cubic06	100	100.0	100.0
cayley32-80	0	85.7	100.0	cubic08	20	100.0	100.0
cayley32-96	0	100.0	100.0	cubic10	0	68.4	100.0
cayley60-90	0	90.0	100.0	cubic12	0	80.0	100.0
cayley60-120	0	100.0	100.0	cubic14	0	40.1	100.0

Table 3
Results obtained for the connected cubic graph database. The last column shows the percentage of graphs that can be uniquely distinguished throughout the s^2-model.

	#	ω_β	ω_d	ω_i	ω_ρ^-	ω_ρ^+	Disting.
cubic06	2	0	100	100	0	0	100
cubic08	5	60	100	60	100	100	100
cubic10	19	5.3	89.5	84.2	68.4	42.1	100
cubic12	85	1.2	96.5	38.8	80	52.9	100
cubic14	509	0.2	97.6	22.6	47.3	37.1	100

Table 4
Results obtained for the strongly regular database. The last column shows the percentage of graphs that can be uniquely distinguished throughout the s^2-model.

	#	ω_β	ω_d	ω_i	ω_ρ^-	ω_ρ^+	Disting.
sr16622	2	0	0	100	100	0	100
sr251256	15	0	0	0	100	0	100
sr261034	10	0	0	0	100	0	100
sr2812642	4	25	0	25	100	25	100
sr291467	41	0	0	0	100	0	100
sr351899	227	0	0	0.4	100	0.4	100
sr361446	180	0.6	0	0.6	100	0.6	100
sr4012243	28	3.6	0	21.4	100	3.6	100

Similar results for the strongly regular database are shown in Table 4. Datasets sr16622, sr251256, sr261034, sr281264, sr291467, sr351899, sr361446 and sr401224 contain 2, 15, 10, 4, 41, 227, 180 and 28 graphs, respectively. Each graph within each of these sets produces a unique ordered sequence of the SNF multisets of the transition map composition matrices generated throughout the model (ω_{ρ^-}) and it is, therefore, distinguishable from the others. Note, for instance, that the sr16622 dataset comprises 2 strongly regular graphs on 16 nodes, namely the Shrikhande and the 4×4 Rook's graph, which are 3-WL equivalent [32]. Likewise, for the Cayley dataset, the vast majority of graphs are distinguishable using this metric (see Table 5). Only one pair of graphs within cayley24-48 and one pair in cayley60-90 produce the same ω_{ρ^-}. These two pairs are, however, distinguishable as they produce a different sequence of Betti numbers ω_β.

The explanation of why some metrics allow to distinguish within certain group of graphs and other metrics do not, requires a hard and exhaustive analysis (not only topological but also statistical) that is not intended to be treated in our experiments. We limit ourselves to give an intuitive interpretation in the case of the strongly regular graphs database. For this group with strong properties of local topological regularity involving adjacent and non-adjacent connected vertices, the ordered sequence of the SNF multisets of the transition map composition matrices generated throughout the model ω_ρ^- is, by far, the most discriminative metric (see Table 4). This fact could be explained considering that ω_ρ^- is a global measure that primarily deals with adjacent and non-adjacent edges, whereas the other metrics considered in our experiment mainly deal with vertex information.

Table 5
Results obtained for the Cayley dataset. The last column shows the percentage of graphs that can be uniquely distinguished throughout the s^2-model.

	#	ω_β	ω_d	ω_i	ω_ρ^-	ω_ρ^+	Disting.
cayley12-18	2	100	100	100	100	100	100
cayley12-24	4	50	100	100	100	50	100
cayley16-24	3	33.3	100	100	100	100	100
cayley16-32	3	100	33.3	100	100	100	100
cayley20-30	2	100	100	100	100	100	100
cayley20-40	5	40	100	100	100	60	100
cayley24-36	8	50	25	100	100	100	100
cayley24-48	20	45	30	100	90	65	100
cayley24-60	4	50	100	100	100	100	100
cayley24-72	4	50	50	100	100	50	100
cayley32-48	7	0	14.3	100	100	100	100
cayley32-64	19	10.5	5.3	89.5	100	89.5	100
cayley32-80	14	0	14.3	74.1	100	74.1	100
cayley32-96	12	8.3	0	100	100	100	100
cayley60-90	20	25	10	100	90	100	100
cayley60-12	68	14.7	16.2	63.2	100	58.8	100
cayley60-15	25	20	36	92	100	92	100
cayley60-18	31	9.7	48.4	100	100	74.2	100
cayley63-12	11	45.5	36.4	81.8	100	63.6	100
cayley63-18	4	100	100	100	100	100	100

7. Conclusions

A new framework of algebraic topological analysis of hypergraphs based on the notion of s^2-model is developed here. An s^2-model is a kind of dynamical system satisfying some topological constraints, whose components are algebraic hypergraphs. We prove that the s^2-model representation and its homology are hypergraph invariants (up to s^2-model isomorphism). A boundary-scale model with only three levels is employed here to demonstrate the applicability of this framework to topologically discriminate graphs. Note that hypergraph topological discrimination could similarly be tested. More concretely, the graph isomorphism problem is tackled here using databases that are difficult or out of reach for most isomorphism solvers. Furthermore, the proposed framework is susceptible to be extended in multiple mathematical directions, depending of the different types of notions involved in s^2-models: dimension and cellulation (simplicial complex, clique, ...), topological identity (homology, homotopy, homeomorphism), topological scale parameters, ground ring chosen, relaxed conditions on s^2-models, extension to attributed hypergraphs, etc. Advances in any of these aspects might impact the power of analysis, classification, matching and learning of the framework. Going further, the proposed framework appears as a universal strategy for processing the topology of complex networks, aiming to improve the efficiency and learning capacity of topological analysis, classification and recognition of relational patterns.

Data availability

Data will be made available on request.

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Appendix A. Classical Homology Computation: Smith Normal Form

The following theoretical development about homology computation via Smith normal form has been extracted from [17] and adapted to the notation and nomenclature of the present paper. Let $G(V, E, \partial)$ be a non-empty hypergraph, being $\partial : E \to \overline{2}^V$ its boundary map. The linear map $\mathbb{F}[\partial]$ can be simply described by a matrix M of dimensions $|V| \times |E| = n \times m$, with coefficients in $\mathbb{F}$. In fact, M is obtained from the vertex-edge incidence matrix of G, applying the semiring function $\vartheta : \overline{\mathbb{N}} \to \mathbb{F}$ to each matrix coefficient. Let $\mathcal{B}_{\mathbf{0}}^{cmb}(M) = \{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ and $\mathcal{B}_{\mathbf{1}}^{cmb}(M) = \{\mathbf{e}_1, \dots, \mathbf{e}_m\}$ be the combinatorial bases of vertices and edges of G, respectively. Bold notation is used for vertices and edges to emphasize their treatment as elements of a vector space. In fact, the chain complex associated to G can be seen as an algebraic hypergraph of the form: $C_*(G) = (\mathcal{B}_{\mathbf{0}}^{cmb}(M), \mathcal{B}_{\mathbf{1}}^{cmb}(M), M)$. Homology has been classically computed via the *Smith Normal Form*, $M = U_{SNF}(M) * D_{SNF}(M) * V_{SNF}(M)$, where $*$ is the matrix multiplication with coefficients in $\mathbb{F}$, $U_{SNF}(M)$ and $V_{SNF}(M)$ are invertible (over $\mathbb{F}$) square matrices and $D_{SNF}(M)$ is a diagonal matrix in which each non-null diagonal entry d_{ii} divides the next $d_{i+1,i+1}$, $1 \le i \le r(G) - 1$, for some $r(G) = r \le \min(n, m)$ [17,33]. The multiset $SNF(G) = \{d_{11}, d_{22}, \dots, d_{rr}\}$ is called *the multiset of elementary divisors of G*. They are unique up to multiplication by units of $\mathbb{F}$. For $\mathbb{F} = \mathbb{Z}$, there may be a first index $t(G) = t$ $(1 \leq t \leq r \leq \min\{m, n\})$ such that $d_{tt} \neq 1_{\mathbb{Z}}$. All the elementary divisors are normalized to $1_{\mathbb{F}}$ if the ground ring is a field, and in this case, $t(G) = r(G)$.

It is also common knowledge that $SNF(M) = SNF(M^T) = SNF(P * M * Q)$, being $P \in \mathbb{F}^{|V|\times|V|}$ and $Q \in \mathbb{F}^{|E|\times|E|}$ two permutation matrices (that is, their coefficients are $0_{\mathbb{F}}$ or $1_{\mathbb{F}}$ and their inverses coincide with their transposes). Moreover a strong relation exists between the elementary divisors of the product of matrices with coefficients in $\mathbb{F}$ and the product of elementary divisors of the factor matrices [34].

In particular, $SNF(G) = SNF(G')$ for two isomorphic hypergraphs G and G'. SNF matrix factorization can also be described as a chain isomorphism $snf(G) = (U^{-1}_{snf}(M), V_{snf}(M)))$ from $C_*(G)$ to the chain complex $C^{snf}_*(G)$. In fact, the matrices $U_{snf}(M) \in \mathbb{F}^{|V|\times|V|}$ and $V_{snf}(M) \in \mathbb{F}^{|E|\times|E|}$ can be interpreted as respective changes of basis in $\mathbb{F}[V]$ and $\mathbb{F}[E]$. Let $\mathcal{B}^{snf}_{\mathbf{0}}(M) = \{\mathbf{w}_1, \ldots, \mathbf{w}_n\}$ and $\mathcal{B}^{snf}_1(M) = \{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_m\}$ be the bases of $\mathbb{F}[V]$ and $\mathbb{F}[E]$, respectively, with respect to which the matrix $D_{snf}(M)$ is defined. Then, the chain complex $C^{snf}_*(G)$ is defined as an algebraic hypergraph of the kind $(\mathcal{B}^{snf}_{\mathbf{0}}(M), \mathcal{B}^{snf}_{\mathbf{1}}(M), D_{snf}(M))$, where:

- The sets $\mathcal{B}^{f\mathcal{H}}_{\mathbf{0}}(M) = \{\mathbf{w}_{r+1}, \ldots, \mathbf{w}_n\}$ and $\mathcal{B}^{f\mathcal{H}}_{\mathbf{1}}(M) = \{\mathbf{c}_{r+1}, \ldots, \mathbf{c}_m\}$ are, respectively, basis of the free part of the 0^{th} and 1^{st} homology vector spaces of G. Note that homology of dimension one is always free. Hence, the *free part of homology* (or, simply, the *free homology*) of G can be rewritten as an algebraic hypergraph of the kind $f\mathcal{H}_*(G) = (\mathcal{B}^{f\mathcal{H}}_{\mathbf{0}}(M), \mathcal{B}^{f\mathcal{H}}_{\mathbf{1}}(M), D^{f\mathcal{H}}_{SNF}(M))$, where $D^{f\mathcal{H}}_{SNF}(M)$ is the submatrix of $D_{SNF}(M)$ obtained after removing its first r rows and columns. In fact, the matrix $D^{f\mathcal{H}}_{SNF}(M)$ is the zero matrix (all its element are $0_{\mathbb{F}}$) of dimensions $(n-r) \times (m-r)$. Precisely, the q^{th} Betti number $\beta_q(G)$ represents the rank (number of linearly independent generators) of the free part of the q^{th} homology vector space. Therefore, $\beta_0(G, \mathbb{F}) = |V| - r$ and $\beta_1(G, \mathbb{F}) = |E| - r$. In consequence, the Euler-Poincaré characteristic $\chi(G)$ of the hypergraph G can be computed using the formula $\chi(G) := \beta_0(G, \mathbb{F}) \setminus \beta_1(G, \mathbb{F}) = n - m$.
- The sets $\mathcal{B}^{\mathcal{H}}_{\mathbf{0}}(M) = \{\mathbf{w}_t, \ldots, \mathbf{w}_n\}$ and $\mathcal{B}^{\mathcal{H}}_{\mathbf{1}}(M) = \{\mathbf{c}_t, \ldots, \mathbf{c}_m\}$ are, respectively, bases of representative cycles of the 0^{th} and 1^{st} homology vector spaces of G. The homology of G can be rewritten as an algebraic hypergraph of the kind $\mathcal{H}_*(G) = (\mathcal{B}^{\mathcal{H}}_{\mathbf{0}}(M), \mathcal{B}^{\mathcal{H}}_{\mathbf{1}}(M), D^{\mathcal{H}}_{SNF}(M))$, where $D^{\mathcal{H}}_{SNF}(M)$ is the submatrix of $D_{SNF}(M)$ obtained after removing its first $t-1$ rows and columns.
- Assuming that $t(G)$ exists, the *torsion part of the homology (or, simply, torsion homology) of a hypergraph G* can be determined in the following way. The sets of vectors $\mathcal{B}^{t\mathcal{H}}_{\mathbf{0}}(M) = \{\mathbf{w}_t, \ldots, \mathbf{w}_r\}$ and $\mathcal{B}^{t\mathcal{H}}_{\mathbf{1}}(M) = \{\mathbf{c}_t, \ldots, \mathbf{c}_r\}$ are necessary. The torsion homology of G can be rewritten as an algebraic hypergraph $t\mathcal{H}_*(G) = (\mathcal{B}^{t\mathcal{H}}_{\mathbf{0}}(M), \mathcal{B}^{t\mathcal{H}}_{\mathbf{1}}(M), D^{t\mathcal{H}}_{SNF}(M))$, where $D^{t\mathcal{H}}_{SNF}(M)$ is the submatrix of $D_{SNF}(M)$) obtained after removing its first $t-1$ rows and columns, and the last $r+1$ rows and columns. In the case in which $\mathbb{F}$ is a field, $t = r+1$ and homology of G at both dimension 0 and 1 is free. For $\mathbb{F} = \mathbb{Z}$, the representative cycle of a torsion homology class defined by the elementary divisor $d_{ii} \neq 1_{\mathbb{Z}}$ (with $t \leq i \leq r$) is specified by the couple $(\mathbf{w}_i, \mathbf{c}_i)$.

Let $G = (V, E, M(G))$ and $G' = (V', E', M(G')$ be two non-empty hypergraphs, being $M(G) \in \mathbb{F}^{|V|\times|E|}$ and $M(G') \in \mathbb{F}^{|V'|\times|E'|}$ their respective vertex-edge incidence matrices with coefficients in $\mathbb{F}$. Let $q = (q_0, q_1) : C^*(G) \to C^*(G')$ be a chain map defined by an associated pair (Q_0, Q_1) of matrices ($Q_0 \in \mathbb{F}^{|V|\times|V'|}$ and $Q_1 \in \mathbb{F}^{|E|\times|E'|}$). The SNF factorizations $(Q_i = U_{SNF}(Q_i) * D_{SNF}(Q_i) * V_{SNF}(Q_i),\ i = 0, 1)$ of the square matrices Q_0 and Q_1, and the multisets $SNF(Q_i)$ (with $i = 0, 1$) are both invariants up to permutation of vertices and edges in G and G'. On the other hand, it is possible to determine the image of homology generators via the chain map q. Let $G = (V, E, M(G))$ and $G' = (V', E', M(G')$ be two non-empty hypergraphs, being $M(G) \in \mathbb{F}^{|V|\times|E|}$ and $M(G') \in \mathbb{F}^{|V'|\times|E'|}$ their respective vertex-edge incidence matrices with coefficients in $\mathbb{F}$. There are two chain isomorphisms $snf(G) = (U^{-1}_{snf}(M(G)), V_{snf}(M(G))) : C_*(G) \to C^{snf}_*(G)$ and $snf(G') = (U^{-1}_{snf}(M(G')), V_{snf}(M(G))) : C_*(G') \to C^{snf}_*(G')$.

The chain map $(snf(q_0), snf(q_1))$ from $(\mathcal{B}^{snf}_{\mathbf{0}}(M(G)),\ \mathcal{B}^{snf}_{\mathbf{1}}(M(G)), D_{snf}\ (M(G)))$ to $(\mathcal{B}^{snf}_{\mathbf{0}}(M(G')), \mathcal{B}^{snf}_{\mathbf{1}}(M(G')), D_{snf}(M(G')))$ is defined in matrix terms by:

- $snf(q_0) = U_{snf}(M(G')) * Q_0 * U^{-1}_{snf}(M(G))$ and
- $snf(q_1) = V^{-1}_{snf}(M(G')) * Q_1 * V_{snf}(M(G))$.

Restricting $snf(q_i)$ $(i = 0, 1)$ to the corresponding bases of representative cycles of homology vector spaces of G and G', unequivocally determines the associated homology map $[q]_{\mathcal{H}}$ between their algebraic homology hypergraphs $\mathcal{H}_*(G)$ and $\mathcal{H}_*(G')$. That amounts to removing from the matrix defining $snf(q_i)$ $(i = 0, 1)$ its first $t(G') - 1$ rows and $t(G) - 1$ columns. In this way, the following classical result can be constructively proven:

Theorem 4. *Given two non-empty isomorphic hypergraphs, their (co)homological graded vector spaces with coefficient in $\mathbb{F}$ are chain isomorphic.*

Proof. If $q = (Q_0, Q_1) : G \simeq G'$ is an isomorphism given in permutation matrix terms between G and G', then the map $[q]_{\mathcal{H}} : \mathcal{H}_*(G) \to \mathcal{H}(G')$ generated as before is the desired chain isomorphism. □

Analogous results can be established for the free and torsion homologies.

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