Topological Stability and Preconditioning of Higher-Order **Laplacian Operators on Simplicial Complexes**

Anton Savostianov¹

Gran Sasso Science Institute, viale F.Crispi 7, L'Aquila, Italy, 67100, email: anton.savostianov@ gssi.it

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Keywords: NNs, condition number

I. Introduction

II. From Graphs to Simplicial Complex

II.I Simplicial Complexes

Let $V = \{v_1, v_2, \dots, v_n\}$ be a set of nodes; as discussed above, such set may refer to various interacting entities and agents in the system, e.g. neurons, genes, traffic stops, online actors, publication authors, etc. Then:

(Simplicial Complex) The collection of subsets \mathcal{K} of the nodal set V is a (abstract) Def. 1 simplicial complex if for each subset $\sigma \in \mathcal{K}$, referred as a simplex, all its subsets σ' , $\sigma' \subseteq \sigma$, referred as faces, enter \mathcal{K} as well, $\sigma' \in \mathcal{K}$.

addition of the word "abstract" to the term is more common in the topological setting

A simplex $\sigma \in \mathcal{K}$ on k+1 vertices is said to be of the order k, ord $(\sigma) = k$. Let $\mathcal{V}_k(\mathcal{K})$ be a set of all k-order simplices in \mathcal{K} and m_k is the cardinality of $\mathcal{V}_k(\mathcal{K})$, $m_k = |\mathcal{V}_k(\mathcal{K})|$; then $\mathcal{V}_0(\mathcal{K})$ is the set of nodes in the simplicial complex \mathcal{K} , $\mathcal{V}_1(\mathcal{K})$ — the set of edges, $\mathcal{V}_2(\mathcal{K})$ — the set of triangles, or 3-cliques, and so on, with $\mathcal{K}=$ $\{\mathcal{V}_0(\mathcal{K}), \mathcal{V}_1(\mathcal{K}), \mathcal{V}_2(\mathcal{K}) \dots\}$. Note that due to the inclusion rule in Definition 1, the number of non-empty $\mathcal{V}_k(\mathcal{K})$ is finite and, moreover, uninterupted in a sense of the order: if $\mathcal{V}_k(\mathcal{K}) = \emptyset$, then $\mathcal{V}_{k+1}(\mathcal{K})$ is also necessarily empty.

Example (Simplicial Complex) 123

Def. 2

II.II Hodge's Theory

which is equivalent to im $B \subseteq \ker A$.

Two linear operators A and B are said to satisfy Hodge's theory if and only if their composition is a null operator,

$$AB = 0 (Eqn. 1)$$

For a pair of operators A and B satisfying Hodge's theory, the quotient space $\mathcal H$ is defined as follows:

$$\mathcal{H} = \frac{\ker A}{\lim B}$$
 (Eqn. 2)

where each element of \mathcal{H} is a manifold $\mathbf{x} + \operatorname{im} B = \{\mathbf{x} + \mathbf{y} \mid \forall \mathbf{y} \in \operatorname{im} B\}$ for $\mathbf{x} \in \ker A$. It follows directly from the definition that ${\cal H}$ is an abelian group under addition.

By Definition 2, the quotient space \mathcal{H} is a collection of equivalence classes $\mathbf{x} + \text{im } B$. $\mathbf{x} + \text{im } B$. Then, each class $\mathbf{x} + \operatorname{im} B = \mathbf{x}_H + \operatorname{im} B$ for some $\mathbf{x}_H \perp \operatorname{im} B$ (both $\mathbf{x}, \mathbf{x}_H \in \ker A$); indeed, since the orthogonal component \mathbf{x}_H (referred as harmonic representative) of \mathbf{x} with

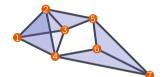


Figure II.1: Example of a simplicial complex

respect to im B is unique, the map $\mathbf{x}_H \leftrightarrow \mathbf{x} + \text{im } B$ is bijectional.

Theorem 1

([Lim20, Thm 5.3]) Let A and B be linear operators, AB = 0. Then the homology group \mathcal{H} satisfies:

$$\mathcal{H} = \ker A /_{\text{im } B} \cong \ker A \cap \ker B^{\top}, \tag{Eqn. 3}$$

where \cong denotes the isomorphism.

Proof One builds the isomorphism through the harmonic representative, as discussed above. It sufficient to note that $\mathbf{x}_H \perp \text{im } B \Leftrightarrow \mathbf{x}_H \in \text{ker } B^\top$ in order to complete the proof.

Lemma 1

[([Lim20, Thm 5.2]) Let A and B be linear operators, AB = 0. Then:

$$\ker A \cap \ker B^{\top} = \ker \left(A^{\top} A + B B^{\top} \right)$$
 (Eqn. 4)

Note that if $\mathbf{x} \in \ker A \cap \ker B^{\top}$, then $\mathbf{x} \in \ker A$ and $\mathbf{x} \ker B^{\top}$, so $\mathbf{x} \in \mathbb{R}$ $\ker (A^{\top}A + BB^{\top})$. As a result, $\ker A \cap \ker B^{\top} \subset \ker (A^{\top}A + BB^{\top})$. On the other hand, let $\mathbf{x} \in \ker (A^{\top}A + BB^{\top})$, then

$$A^{\mathsf{T}}A\mathbf{x} + BB^{\mathsf{T}}\mathbf{x} = 0 \tag{Eqn. 5}$$

Exploiting AB = 0 and multiplying the equation above by B^{\top} and A one gets the following:

$$B^{\mathsf{T}}BB^{\mathsf{T}}\mathbf{x} = 0$$

$$AA^{\mathsf{T}}A\mathbf{x} = 0$$
(Eqn. 6)

Note that $AA^{\top}A\mathbf{x} = 0 \Leftrightarrow A^{\top}A\mathbf{x} \in \ker A$, but $A^{\top}A\mathbf{x} \in \operatorname{im} A^{\top}$, so by Fredholm alternative, $A^{\top}A\mathbf{x} = 0$. Finally, for $A^{\top}A\mathbf{x} = 0$:

$$A^{\top}A\mathbf{x} = 0 \Longrightarrow \mathbf{x}^{\top}A^{\top}A\mathbf{x} = 0 \iff \|A\mathbf{x}\|^2 = 0 \Longrightarrow \mathbf{x} \in \ker A \pmod{\mathbb{F}}$$

Similarly, for the second equation, $\mathbf{x} \in \ker B^{\top}$ which completes the proof.

Here we need some words about the transitions.

Since AB = 0, $B^{T}A^{T} = 0$ or im $A^{T} \subset \ker B^{T}$. Then, exploiting $\mathbb{R}^{n} = \ker A \oplus$ im A^{\top} :

$$\ker B^{\top} = \ker B^{\top} \cap \mathbb{R}^{n} = \ker B^{\top} \cap \left(\ker A \oplus \operatorname{im} A^{\top}\right) =$$

$$= \left(\ker A \cap \ker B^{\top}\right) \oplus \left(\operatorname{im} A^{\top} \cap \ker B^{\top}\right)$$
(Eqn. 8)

Given Lemma 1, $\ker A \cap \ker B^{\top} = \ker (A^{\top}A + BB^{\top})$ and, since $\operatorname{im} A^{\top} \subset \ker B^{\top}$, $\operatorname{im} A^{\top} \cap \ker B^{\top} = \operatorname{im} A^{\top}$, yeilding:

Theorem 2

(Hodge Decomposition) Let A and B be linear operators, AB = 0. Then:

$$\mathbb{R}^{n} = \underbrace{\operatorname{im} A^{\top} \oplus \ker \left(A^{\top} A + B B^{\top} \right) \oplus \operatorname{im} B}_{\ker A}$$
 (Eqn. 9)

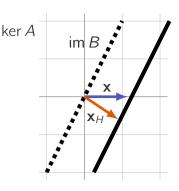


Figure II.2: Illustration of a harmonic representative for an equivalence class

II.III Boundary and Laplacian Operators

II.III.I Boundary operators

Each simplicial complex \mathcal{K} has a nested structure of simplicies: indeed, if σ is a simplex of order k, $\sigma \in \mathcal{V}_k(\mathcal{K})$, then all of (k-1)-th order faces forming the boundary of σ also belong to \mathcal{K} : for instance, for the triangle $\{1,2,3\}$ all the border edges $\{1,2\}$, $\{1,3\}$ and $\{2,3\}$ are also in the simplicial complex, Figure II.1.

This nested property implies that one can build a formal map from a simplex to its boundary enclosed inside the simplicial complex.

Def. 3 (Chain spaces) Let \mathcal{K} be a simplicial complex; then the space C_k of formal sums of simplices from $\mathcal{V}_k(\mathcal{K})$ over real numbers is called a k-th chain space.

Chain spaces on its own are naturally present in the majority of the network models: C_0 is a space of states of vertices (e.g. in the dynamical system $\dot{\mathbf{x}} = A\mathbf{x}$ the evoloving vector $\mathbf{x} \in C_0$), C_1 — is a space of (unrestricted) flows on graphs edges, and so on.

refs?

Since C_k is a linear space, versor vectors corresponding to the elements of $\mathcal{V}_k(\mathcal{K})$ is a natural basis of C_k ; in order to proceed with the boundary maps, one needs to fix an order of the simplices inside $\mathcal{V}_k(\mathcal{K})$ (alas one fixes the order of vertices in the graph to form an adjacency matrix) as a matter of bookkeeping. Additionally, since C_k is a space over \mathbb{R} , chains σ and $-\sigma$ naturally introduce the notion of orientation of the simplex.

III. Matrix nearness problems

III.I 101 on MNP

Generally speaking, for a given matrix A a matrix nearness problem consists of finding the closest possible matrix X among the admissible set with a number of desired properties.

IV. Topological Stability of Simplicial Complexes

V. Preconditioning

TMP

Here we need to say general words about how we need an efficient preconditioning scheme.

V.I Iterative methods for Positive Definite Systems

V.II Preconditioning 101

V.III Cholesky preconditioning for classical graphs

V.IV Classical collapsibility

In this section we borrow the terminology from [Whi39]; additionally, let us assume that considered simplicial complex $\mathcal K$ is restricted to its 2-skeleton, so $\mathcal K$ consists only of nodes, edges, and triangles, $\mathcal K = \mathcal V_0(\mathcal K) \cup \mathcal V_1(\mathcal K) \cup \mathcal V_2(\mathcal K)$.

Simplex $\tau \in \mathcal{K}$ is called an (inlusion-wise) maximal face of simplex $\sigma \in \mathcal{K}$ if τ is maximal by inlusion simplex such that $\sigma \subseteq \tau$ and ord $(\sigma) < \text{ord } (\tau)$. For instance, in Figure V.1 the edge $\{1,2\}$ and nodes $\{1\}$ and $\{2\}$ have two maximal faces, $\{1,2,3\}$ and $\{1,2,4\}$, while all the other edges and nodes have unique maximal faces — their corresponding triangles. Note that in the case of the node $\{1\}$, there are bigger simplices containing it besides the triangles (e.g. the edge $\{1,2\}$), but they are not maximal by inclusion.

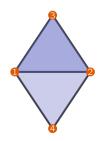


Figure V.1: Example of a simplicial complex: free simplices and maximal faces.

Def. 4 **(Free simplex)** The simplex $\sigma \in \mathcal{K}$ is free if it has exactly one maximal face τ , $\tau = \tau(\sigma)$. F.i. edges $\{1,3\}$, $\{1,4\}$, $\{2,3\}$ and $\{2,4\}$ are all free in Figure V.1.

The collapse $\mathcal{K}\setminus\{\sigma\}$ of \mathcal{K} at a free simplex σ is the transition from the original simplicial complex \mathcal{K} to a smaller simplicial complex \mathcal{L} without the free simplex σ and the corresponding maximal face τ , $\mathcal{K}\to\mathcal{K}'=\mathcal{K}-\sigma-\tau$; namely, one can eliminate a simplex τ if it has an accessible (not included in another simplex) face σ .

Naturally, one can perform several consequent collapses at $\Sigma = \{\sigma_1, \sigma_2, \ldots\}$ assuming σ_i is free in collapse simplicial complex from the previous stage; Σ is called the collapsing sequence. Formally:

Def. 5 (Collapsing sequence) Let $\mathcal K$ be a simplicial complex. $\Sigma = \{\sigma_1, \sigma_2, \ldots\}$ is a collapsing sequence if σ_1 is free in $\mathcal K$ and each σ_i , i > 1, is free at $\mathcal K^{(i)} = \mathcal K^{(i-1)} \setminus \{\sigma_i\}$, $\mathcal K^{(1)} = \mathcal K$. The collapse of $\mathcal K$ to a new complex $\mathcal L$ at Σ is denoted by $\mathcal L = \mathcal K \setminus \Sigma$.

By the definition, every collapsing sequence Σ has a corresponding sequence $\mathbb{T} = \{\tau(\sigma_1), \tau(\sigma_2), \ldots\}$ of maximal faces being collapsed at every step.

Def. 6 (Collapsible simplicial complex, [Whi39]) The simplicial complex $\mathcal K$ is collapsible if there exists a collapsing sequence Σ such that $\mathcal K$ collapses to a single vertex at Σ , $\mathcal K \setminus \Sigma = \{v\}$.

Determining whether the complex is collapsible is in general NP-complete, [Tan16], but can be almost linear for a set of specific families of \mathcal{K} , e.g. if the simplex can be embeded into the triangulation of the d-dimensional unit sphere, [CFM $^+$ 14]. Naturally restricting the collapses to the case of d-collapses (such that ord $(\sigma)_i \leq d-1$), one arrive at the notion of d-collapsibility, [Tan09].

Def. 7 (*d*-Core) A *d*-Core is a subcomplex of \mathcal{K} such that every simplex of order d-1 belongs to at least 2 simplices of order d. E.g. 2-Core is such a subcomplex of the original 2-skeleton \mathcal{K} that every edge from $\mathcal{V}_1(\mathcal{K})$ belong to at least 2 triangles from $\mathcal{V}_2(\mathcal{K})$.

Lemma 2 ([LN21]) \mathcal{K} is d-collapsible if and only if it does not contain a d-core.

Proof The proof of the lemma above naturally follows from the definition of the core. Assume Σ is a d-collapsing sequence, and $\mathcal{K}\backslash\Sigma$ consists of more than a single vertex and has no free simplices of order d-1 ("collapsing sequence gets stuck"). Then, each simplex of order d-1 is no free but belongs to at least 2 simplices of order d, so $\mathcal{K}\backslash\Sigma$ is a d-Core.

Conversely if a d-Core exists in the complex, the collapsing sequence should necessarily include its simplices of order d-1 which can not become free during as a result of a sequence of collapses. Indeed, for σ from d-Core, ord $(\sigma) = d-1$, to become free, one needs to collapse at least one of σ 's maximal faces for d-Core , all of whose faces are, in turn, contained in the d-Core (since d-Core is a simplicial complex). As a result one necessarily needs a prior collapse inside the d-Core to perform the first collapse in the d-Core, which is impossible.

In the case of the classical graph model, the 1-Core is a subgraph where each vertex has a degree at least 2; in other words, 1-Core cannot be a tree and necessarily contains a simple cycle. Hence, the collapsibility of a classical graph coincides with the acyclicity. The d-Core is the generalization of the cycle for the case of 1-collapsibility of the classical graph; additionally, the d-Core is very dense due to its definition. In the case of 2-Core, we provide simple exemplary structures on Figure V.2 which imply various possible configurations for a

d-Core, $d \geq 2$, hence a search for *d*-Core inside \mathcal{K} is neither trivial, no computationally cheap.

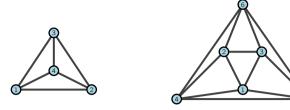


Figure V.2: 2-Core, examples.

Additionally, we demonstrate that an arbitrary simplicial complex $\mathcal K$ tends to contain 2-Cores as long as $\mathcal K$ is denser than a trivially collapsible case. Assume the complex formed by triangulation of m_0 random points on the unit square with a sparsity pattern ν ; the triangulation itself with the corresponding ν_{Δ} is collapsible, but a reasonably small addition of edges already creates a 2-Core (since it is local), Figure V.3, left. Similarly, sampled sensor networks, where $\exists \sigma \in \mathcal V_1(\mathcal K): \sigma = [v_1, v_2] \iff \|v_1 - v_2\|_2 < \varepsilon$ for a chosen percolation parameter $\varepsilon > 0$, quickly form a 2-Core upon the densifying of the network.

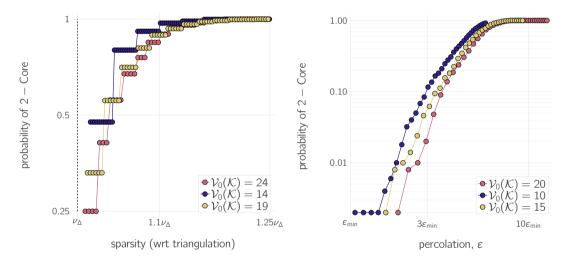


Figure V.3: The probability of the 2-Core in richer-than-triangulation simplicial complexes: triangulation of random points modified to have $\left[\nu^{\frac{|\mathcal{V}_0(\mathcal{K})|\cdot(|\mathcal{V}_0(\mathcal{K})|-1)}{2}}\right]$ edges on the left; random sensor networks with ε -percolation on the right. ν_{Δ} defines the initial sparsity of the triangulated network; $\varepsilon_{\min} = \mathbb{E}\min_{\mathbf{x}, \mathbf{y} \in [0,1]^2} \|\mathbf{x} - \mathbf{y}\|_2$ is the minimal possible percolation parameter.

However, in the following, we observe that a weaker condition is enough to efficiently design a preconditioner for any "sparse enough" simplicial complex.

V.V Weak collapsibility

Let the complex $\mathcal K$ be restricted up to its 2-skeleton, $\mathcal K=\mathcal V_0(\mathcal K)\cup\mathcal V_1(\mathcal K)\cup\mathcal V_2(\mathcal K)$, and $\mathcal K$ is collapsible. Then the collapsing sequence Σ necessarily involves collapses at simplices σ_i of different orders: at edges (eliminating edges and triangles) and at vertices (eliminating vertices and edges). One can show that for a given collapsing sequence Σ there is a reordering $\tilde \Sigma$ such that $\dim \tilde \sigma_i$ are non-increasing, [CFM+14, Lemma 2.5]. Namely, if such a complex is collapsible, then there is a collapsible sequence $\Sigma=\{\Sigma_1,\Sigma_0\}$ where Σ_1 contains all the collapses at edges first and Σ_0 is composed of collapses at vertices. Note that the partial collapse $\mathcal K\backslash\Sigma_1=\mathcal L$ eliminates all the triangles in the complex, $\mathcal V_2(\mathcal L)=\varnothing$; otherwise, the whole sequence Σ is not collapsing $\mathcal K$ to a single vertex. Since $\mathcal V_2(\mathcal L)=\varnothing$, the associated up-Laplacian $\mathcal L_1^\uparrow(\mathcal L)=0$.

Def. 8 **(Weakly collapsible complex)** Simplicial complex $\mathcal K$ restricted to its 2-skeleton is called weakly collapsible, if there exists a collapsing sequence Σ_1 such that the simplicial complex $\mathcal L = \mathcal K \backslash \Sigma_1$ has no simplices of order 2, $\mathcal V_2(\mathcal L) = \varnothing$ and $\mathcal L_1^{\uparrow}(\mathcal L) = 0$.

Example

Note that a collapsible complex is necessarily weakly collapsible; the opposite does not hold. Consider the following example in Figure V.4: the initial complex is weakly collapsible either by a collapse at [3, 4] or at [2, 4]. After this, the only available collapse is at the vertex [4] leaving the uncollapsible 3-vertex structure.

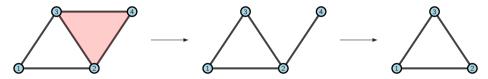


Figure V.4: Example of weakly collapsible but not collapsible simplicial complex

Theorem 3 Weak collapsibility of 2-skeleton \mathcal{K} is polynomially solvable.

Proof

The greedy algorithm for the collapsing sequence intuitively operates as follows: at each iteration perform any of possible collapses; in the absence of free edges, the complex should be considered not collapsible, Algorithm 1. Clearly, such an algorithm runs polynomially with respect to the number of simplexes in \mathcal{K} .

The failure of the greedy algorithm indicates the existence of a weakly collapsible complex $\mathcal K$ such that the greedy algorithm gets stuck at a 2-Core, which is avoidable for another possible order of collapses. Among all the counter exemplary complexes, let $\mathcal K$ be a minimal one with respect to the number of triangles m_2 . Then there exist a free edge $\sigma \in \mathcal V_1(\mathcal K)$ such that $\mathcal K \setminus \{\sigma\}$ is collapsible and another $\sigma' \in \mathcal V_2(\mathcal K)$ such that $\mathcal K \setminus \{\sigma'\}$ is not collapsible.

Note that if \mathcal{K} is minimal then for any pair of free edges σ_1 and σ_2 belong to the same triangle: $\tau(\sigma_1) = \tau(\sigma_2)$. Indeed, for any $\tau(\sigma_1) \neq \tau(\sigma_2)$, $\mathcal{K}\setminus \{\sigma_1,\sigma_2\} = \mathcal{K}\setminus \{\sigma_2,\sigma_1\}$. Let $\tau(\sigma_1) \neq \tau(\sigma_2)$ for at least one pair of σ_1 and σ_2 ; in our assumption, either both $\mathcal{K}\setminus \{\sigma_1\}$ and $\mathcal{K}\setminus \{\sigma_2\}$, only $\mathcal{K}\setminus \{\sigma_1\}$ or none are collapsible. In the former case either $\mathcal{K}\setminus \{\sigma_1\}$ or $\mathcal{K}\setminus \{\sigma_2\}$ is a smaller example of the complex satisfying the assumption, hence, violating the minimality. If only $\mathcal{K}\setminus \{\sigma_1\}$ is collapsible, then $\mathcal{K}\setminus \{\sigma_2,\sigma_1\}$ is not collapsible; hence, $\mathcal{K}\setminus \{\sigma_1,\sigma_2\}$ is not collapsible, so $\mathcal{K}\setminus \{\sigma_1\}$ and $\mathcal{K}\setminus \{\sigma_2\}$ are collapsible, then for known σ' such that $\mathcal{K}\setminus \{\sigma'\}$ is not collapsible, $\tau(\sigma') \neq \tau(\sigma_1)$ or $\tau(\sigma') \neq \tau(\sigma_2)$, which revisits the previous point.

As a result, for σ ($\mathcal{K}\setminus\{\sigma\}$ is collapsible) and for σ' ($\mathcal{K}\setminus\{\sigma'\}$ is not collapsible) it holds that $\tau(\sigma) = \tau(\sigma') \Rightarrow \sigma \cap \sigma' = \{v\}$, so after collapses $\mathcal{K}\{\sigma\}$ and $\mathcal{K}\setminus\{\sigma'\}$ we arrive at two identical simplicial complexes modulo the hanging vertex irrelevant for the weak collapsibility. A simplicial complex can not be simultaneously collapsible and not collapsible, so the question of weak collapsibility can always be resolved by the greedy algorithm which has polynomial complexity.

V.VI Computational cost of the greedy algorithm

Let \mathcal{K} be a 2-skeleton; let Δ_{σ} be a set of triangles of \mathcal{K} containing the edge σ , $\Delta_{\sigma}=\{t\mid t\in\mathcal{V}_2(\mathcal{K}) \text{ and } \sigma\in t\}$. Then the edge σ is free iff $|\Delta_{\sigma}|=1$ and $F=\{\sigma\mid |\Delta_e|=1\}$ is a set of all free edges. Note that $|\Delta_e|\leq m_0-2=\mathcal{O}(m_0)$.

The complexity of Algorithm 1 rests upon the precomputed $\sigma \mapsto \Delta_{\sigma}$ structure that defacto coincides with the boundary operator B_2 (assuming B_2 is stored as a sparse matrix, the adjacency structure describes its non-zero entries). Similarly, the initial F set can be

Algorithm 1 GREEDY_COLLAPSE(\mathcal{K}): greedy algorithm for the weak collapsibility

computed alongside the construction of B_2 matrix. Another concession is needed for the complexity of the removal of elements from Δ_{σ_i} and F, which may vary from $\mathcal{O}(1)$ on average up to guaranteed $\log(|\Delta_{\sigma_i}|)$. As a result, given a pre-existing B_2 operator, Algorithm 1 runs linearly, $\mathcal{O}(m_1)$, or almost linearly depending on the realisation, $\mathcal{O}(m_1 \log m_1)$.

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V. Glossary

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collapse transition to a smaller simplicial complex without a free simplex and its maximal face . 4
collapsible simplex that can be collapsed to a single vertex . 4
collapsing sequence several consequent collapses . 4
face subsimplex of a given simplex . 1
free wrt a simplex: having exactly one facet . 4
maximal face a maximal simplex of higher-order containing given simplex . 3
simplex elements of the simplicial complex; subset of vertex set. 1
simplicial complex higher-order network model; hypergraph closed for edge inclusion. 1
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