Alma Mater Studiorum · Università di Bologna

SCUOLA DI SCIENZE
Corso di Laurea Magistrale in Matematica

SIMPLICIAL COMPLEXES FROM GRAPHS TOWARDS GRAPH PERSISTENCE

Tesi di Laurea Magistrale in Topologia Algebrica

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Contents

Introduzione

Lo scopo di questo elaborato è di esplorare diversi metodi attraverso i quali ottenere complessi simpliciali a partire da un grafo, suggerendo alcuni risultati originali in tal senso. L'obiettivo è introdurre, in un articolo di prossima pubblicazione, una generalizzazione della teoria dell'omologia persistente [9] in un contesto di teoria dei grafi.

La teoria dei grafi, disciplina a cavallo tra matematica e informatica, si occupa di studiare i grafi, oggetti combinatori costituiti da vertici e da spigoli che collegano i vertici tra loro. La scelta di tale ambito, così pervasivo della matematica e di tutte le scienze applicate, è motivata dalla volontà di introdurre in questa disciplina alcune potenti tecniche di analisi fornite dalla topologia algebrica.

L'*omologia persistente* è una di queste tecniche ed è quella su cui ci siamo concentrati. Serve per calcolare proprietà topologiche e geometriche di spazi topologici su cui siano definite *funzioni filtranti* che convogliano determinate qualità d'interesse per l'osservatore. L'omologia persistente, tra l'altro, ha la capacità di distinguere quantitativamente tra caratteristiche essenziali dello spazio e caratteristiche transitorie, classificabili come "rumore topologico". È stata introdotta con il nome di Teoria della Taglia [12] e ha trovato applicazione in svariati campi (*shape analysis* [2], neuroscienze [20], diagnostica [11] e altri).

Nel nostro lavoro useremo l'omologia persistente per studiare le caratteristiche geometriche e topologiche di alcuni complessi simpliciali. L'omologia persistente prevede che tale complesso simpliciale venga studiato progressivamente lungo una successione non decrescente di suoi sottocomplessi (questa successione è detta *filtrazione*).

Il nostro punto di partenza è un grafo $G = (V, E)$ e nostro il primo problema consiste nel ricavare da esso un complesso simpliciale.

Ottenere un complesso simpliciale da un grafo è un argomento ben noto in letteratura (si vedano per esempio [15], [8], [3]) ed è un risultato che può essere ottenuto con una grande quantità di metodi. Alcuni di questi metodi sono molto studiati, come ad esempio il complesso delle cricche (section 1.2) o il complesso dei vicini (section 1.4).

Una volta fissato il metodo, il secondo problema consiste nella costruzione della filtrazione sul complesso simpliciale ottenuto. Per far dipendere la filtrazione dal grafo di partenza supponiamo di ordinare gli spigoli del grafo attraverso una biiezione $w : E \longrightarrow \{1, 2, \dots, |E|\}$. In questo modo definiamo due famiglie di sottografi di G:

$$G_k = (V, w^{-1}(\{1, 2, \dots, k\})$$
$$\tilde{G}_k = \big(\{v \in V | \; \{v, \cdot\} \in w^{-1}(\{1 \dots, k\})\}, w^{-1}(\{1, \dots, k\})\big)$$

In pratica, G_k contiene i primi k spigoli (ordinati secondo w) e tutti i vertici di G, mentre $\tilde{G}_k$ contiene i primi k spigoli e i vertici che sono alle estremità degli spigoli considerati.

I complessi simpliciali costruiti da questi sottografi forniscono le nostre filtrazioni per lo studio dell'omologia persistente. I risultati ottenuti in questo studio vanno poi interpretati e ricondotti al grafo G da cui eravamo partiti.

Le idee che stanno alla base della teoria persistenza sono molto potenti e proficuamente esportabili in nuovi contesti matematici. In particolare la teoria dei grafi è un buon ambito tentare questo approccio. Dunque abbiamo cercato di applicare sui grafi tecniche simili a quelle che vengono utilizzate nell'omologia persistente sui complessi simpliciali. Le direzioni in cui è possibile sviluppare questa intuizione sono molte e degne di indagine: noi in questo lavoro abbiamo svolto uno studio sulla persistenza di blocchi e di edge-blocchi lungo una filtrazione di sottografi (section 2.3).

Struttura della tesi. La tesi si apre con alcune definizioni introduttive su grafi, complessi simpliciali e omologia simpliciale.

Il primo capitolo descrive i principali metodi che abbiamo considerato per costruire complessi simpliciali a partire da un grafo. Alcuni di questi sono già ampiamente presenti in letteratura (come il complesso delle cricche, degli insiemi indipendenti e dei vicini, studiati in misura minore sono invece i complessi derivanti da sottografi aciclici), mentre per quanto riguarda il complesso degli *enclaveless* non abbiamo trovato riferimenti nella letteratura precedente. In questo capitolo vengono fatte osservazioni basilari sulla natura del complesso simpliciale a partire dal grafo di partenza e si indaga quali complessi simpliciali siano costruibili a partire da un grafo qualunque.

Il secodo capitolo si occupa invece di persistenza. Vengono richiamate rapidamente le nozioni di omologia persistente, e si applicano queste osservazioni alle filtrazioni dei sottografi, attraverso un caso-studio su K_4 (filtrazione su G_i) e un altro dettagliato esempio su un grafo su 6 vertici (filtrazione su $\tilde{G}_i$). L'ultima parte del capitolo è dedicata all'indagine sui diagrammi persistenti di blocchi ed edge-blocchi lungo una filtrazione. Anche qui viene mostrato un esempio dettagliato.

Il terzo capitolo tratta di altri due metodi, proposti per la costruzione di complessi simpliciali a partire da un grafo: il complesso dei k-cicli e il complesso delle cricche connesse.

In appendice è riportata parte del codice utilizzato durante il lavoro di tesi.

Introduction

The aim of this work is to explore various methods to build simplicial complexes from a graph, and suggest some novel results in this filed. The purpose is to introduce in a forthcoming paper a generalisation of persistent homology [9] in the graph theory context.

Graph theory is a field ranging from mathematics to information theory, that studies graphs, combinatorial objects made of vertices and edges connecting those vertices. We choose this discipline, that is so pervasive of mathematics and all applied sciences, because we want to introduce some powerful algebraic topology techniques into this discipline.

Persistent homology is one of those techniques and is the one we focus on. It is useful to analyse topological spaces, of which it is capable to compute topological and geometrical properties. Moreover, persistent homology enables us to distinguish between meaningful features and "topological noise". It was introduced under the name of Size Theory [12] and it has been applied in various fields ever since (*shape analysis* [2], neuroscience [20], diagnostics [11] and others).

In our work we use persistent homology to examine geometrical and topological features of a simplicial complexes. Persistent homology examines the simplicial complex progressively, along a non-decreasing sequence of subcomplexes. This sequence is called a *filtration*.

Our starting point is a graph $G = (V, E)$ and our fist problem is to associate a simplicial complex to G.

Obtaining a simplicial complex out of a graph is a well-known subject in the literature (see for example [15], [8], [3]). This result can be archived with a multitude of methods. Some of those methods are well studied, as for example the complex of cliques (section 1.2), either or the complex of neighbours (section 1.4).

Once we set the method, our second problem is to search for a filtration. To do this we sort the edges of the graph through a bijection $w : E \longrightarrow \{1, 2, \dots, |E|\}$. This way we define two families of subgraphs of G:

$$G_k = (V, w^{-1}(\{1, 2, \dots, k\})$$

$$\tilde{G}_k = \big(\{v \in V \mid \{v, \cdot\} \in w^{-1}(\{1 \dots, k\})\}, w^{-1}(\{1, \dots, k\})\big)$$

Essentially G_k contains the first k edges (sorted thanks to w), and all vertices of G, while $\tilde{G}_k$ contains the first k edges, and their end-points as vertices.

The simplicial complexes built from these subgraphs form our filtrations to study persistent homology. The results obtained through this process will be interpreted and reconsidered toward the graph G from where we started.

Core ideas of persistence theory are very powerful and profitably applicable in new mathematical context. In particular, graph theory is a field where such an approach could be revelatory. So we tried to apply on graphs techniques akin to the ones used in persistent homology on simplicial complexes. There are multiple research paths that can be followed using this intuition. In this work we studied block persistence and edge-block persistence along a filtration of subgraphs (section 2.3).

Structure of this thesis. The first section contains some introductory definitions on graphs, simplicial complexes and simplicial homology.

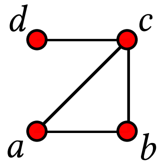
The first chapter describes the main methods we considered to build simplicial complexes from a graph. Some of those methods are well studied in the literature (such as complexes of cliques, independent sets and neighbours, other methods are less known, as the complexes from acyclic subsets), while we could not find any previous reference in the literature about the complex of enclaveless sets. In this chapter there are basic observations on the complexes, on the relationship with the original graph and on the possibility of building a given simplicial complex from any graph.

The second chapter deals with persistence. We recall the definitions at the beginning of the chapter. Then filtrations on graphs are studied through a case study on K_4 (filtrations on G_i), and a detailed example on a graph on 6 vertices (filtrations on $\tilde{G}_i$). The last part of the chapter is about persistent diagrams of blocks and edge-blocks along a filtration, featuring another detailed example.

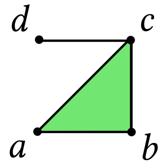
The third chapter deals with other two methods we proposed to build simplicial complexes from a graph: the complex of k-cycles and the complex of connected cliques.

In the appendix we transcribed slices of code we employed.

How to read figures. Each part of this thesis contains many examples illustrated by figures where graphs and simplicial complexes were put beside. Graphs are drawn with red points as vertices, while vertices of simplicial complexes are black, and simplices of higher dimension are colored in green.



$G=(\{a,b,c,d\},\{ab,bc,ac,dc\})$



$\Delta=<a,b,c> \cup <c,d>$

Preliminary standard definitions

Graphs

Definition 1 (Graph)**.** An (undirected, simple) graph G is an ordered pair $G = (V, E)$ where V is a set of vertices, and E is a set of edges, which are 2-element subsets of V. So every edge is a couple of two distinct unordered vertices.

Definition 2. Let $G = (V, E)$ be a graph.

- (*Adjacent vertices*) An adjacent vertex of $v \in V$ is a vertex that is connected to v by an edge.
- (*Paths and Cycles*) Let $v, w \in V$. A path from v to w is a sequence of pairwise adjacent vertices $vv_1v_2 \cdots v_n w$. The path is simple if no vertex is repeated in the sequence. The path is a cycle if $v = w$. The path has length k if it pass through k edges. The distance between v and w is the minimum length of the paths from v to w. If such a path does not exists, the distance is said to be infinite.
- (*Connected graph*) G is connected if for every couple $v, w \in V$ exists a path from v to w.
- (*Isomorphism of graphs*) Let $G = (V, E)$ and $H = (W, F)$ be two graphs. We say that G and H are isomorphic if there is a bijection $\varphi : V \longrightarrow W$ such that: $(\{v, w\} \in E \iff \{\varphi(v), \varphi(w)\} \in F)$.
- (*Induced Graph*) Let $W \subset V$ and $E(W) = \{\{i, j\} \in E : \; i, j \in W\}$. We define $G[W] = (W, E(W))$ the subgraph of G induced by W. Equivalently, $G[W]$ is the subgraph formed from the vertices in W and all of the edges in E connecting pairs of vertices in W.
- (*Tree*) A tree is an acyclic connected graph.
- (*Complementary graph*) The complementary graph of G is:

$$G^C = (V, \{\{x, y\} : \; x, y \in V, x \neq y \text{ and } \{x, y\} \notin E\}$$

Equivalently, G^C is the graph whose vertices are the vertices of G and whose edges are the edges that are not present in G.

- A set of vertices of a graph of cardinality n will be denoted V_n
- (*Complete graph on n vertices*) $K_n = (V_n, E(K_n))$, is defined as follows: for every $v_1, v_2 \in V_n \Longrightarrow \{v_1, v_2\} \in E(K_n)$
- (*Complete bipartite graph on n and m vertices*) $K_{n,m} = (V_n \cup V_m, E_{n,m})$, is defined as follows:
$$\begin{cases} V_n \cap V_m = \emptyset, \\ \forall\ v_1 \in V_n,\ \ v_2 \in V_m \Longrightarrow \{v_1, v_2\} \in E_{n,m}, \\ \forall\ v_1, v_2 \in V_n \Longrightarrow \{v_1, v_2\} \notin E_{n,m}, \\ \forall\ v_1, v_2 \in V_m \Longrightarrow \{v_1, v_2\} \notin E_{n,m} \end{cases}$$
- (*Complete m-partite graph*) $K_{n_1,n_2,\ldots,n_m}$ is a graph whose set of vertices can be partitioned in m subsets of respective cardinality $n_1, \ldots, n_m$, where an edge is present if and only if its ends are in different subsets of the partition.
- (*Chromatic number*) The chromatic number $\gamma(G)$ of a graph G is the smallest number of colors needed to color the vertices of G so that no two adjacent vertices share the same color. We say that G is *k-colorable* for every $k \leq \gamma(G)$.

Example. The graph G represented in fig. 1, along with G^C, and $G[W]$, where $W = \{1, 2, 3, 6\}$:

$$\begin{aligned} G =& (\{1,2,3,4,5,6\}, \{\{1,2\}, \{2,3\}, \{1,3\}, \{3,4\}, \{5,6\}\}) \\ G[W] =& (\{1,2,3,6\}, \{\{1,2\}, \{2,3\}, \{1,3\}\}) \\ G^C =& (\{1,2,3,4,5,6\}, \big\{\{1,4\}, \{1,6\}, \{1,5\}, \{2,4\}, \{2,5\}, \\ & \{2,6\}, \{3,5\}, \{5,6\}, \{4,5\}, \{4,6\}\big\}) \end{aligned}$$

Simplicial complexes

Definition 3 (Abstract simplicial complex)**.** A family Δ of finite subsets of a set V is an *abstract simplicial complex* if, for every $\sigma \in \Delta$, every subset $\tau \subset \sigma$ also belongs to Δ (*inheritance property*). We will call every set $\sigma \in \Delta$ of cardinality $(n+1)$ an *n-simplex*, and every $\tau \subsetneq \sigma$ a *face* of the simplex.

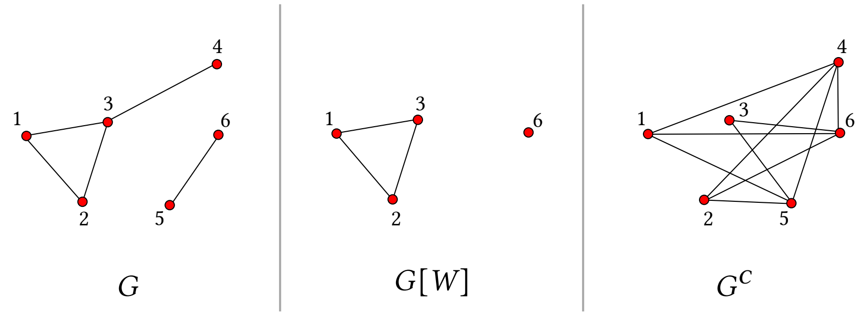


Figure 1: A simple graph G on 6 vertices and 5 edges, along with the induced graph $G[W]$ on the set of vertices $W = \{1, 2, 3, 6\}$, and the complementary graph G^C.

Notation. We will indicate the power set of the set $\{x_0, \dots, x_n\}$ as $< x_0, \dots, x_n >$. So, if σ is an n-simplex on the vertices $x_0, \dots, x_n$, the simplicial complex made of σ and all its faces will be $\Delta =< x_0, \dots, x_n >$.

Remark 4. I stick to the definition given by Jonsson in [15], including the emptyset $\emptyset$ in every simplicial complex.

Definition 5 (Barycentric subdivision)**.** The Barycentric Subdivision of a simplex Δ is the simplicial complex $\mathrm{sd}(\Delta)$ on a set V. V is in bijection with the faces of Δ and very sequence $F_0, F_1, \dots, F_n$ of faces of Δ, totally ordered by inclusion, is an n-simplex of $\mathrm{sd}(\Delta)$, with vertices $\{v_0, \dots, v_n\}$. Each vertex v_i is called the barycenter of the face F_i.

Example. The following simplicial complex (fig. 2) represent a 2-simplex and all its faces:

$$\Delta = \Big\{\emptyset, \{x\}, \{y\}, \{z\}, \{x, y\}, \{y, z\}, \{x, z\}, \{x, y, z\}\Big\} =< x, y, z >$$

And this is its first barycentric subdivision:

$$\begin{aligned}
\mathrm{sd}(\Delta) = \Big\{ &\emptyset, \{x\}, \{y\}, \{z\}, \{g_1\}\{g_2\}, \{g_3\}, \{g_4\},\\
&\{x, g_1\}, \{g_1, y\}, \{y, g_2\}, \{g_2, z\}, \{z, g_3\}, \{g_3, x\},\\
&\{g_1, g_4\}, \{g_4, z\}, \{g_2, g_4\}, \{g_4, x\}, \{g_3, g_4\}, \{g_4, y\},\\
&\{x, g_1, g_4\}, \{x, g_3, g_4\}, \{y, g_1, g_4\}, \{y, g_3, g_4\}, \{z, g_1, g_4\}, \{z, g_2, g_4\}\Big\}\\
= &< x, g_1, g_4 > \cup < x, g_3, g_4 > \cup < y, g_1, g_4 > \cup < y, g_2, g_4 > \cup\\
&\cup < z, g_2, g_4 > \cup < z, g_3, g_4 >
\end{aligned}$$

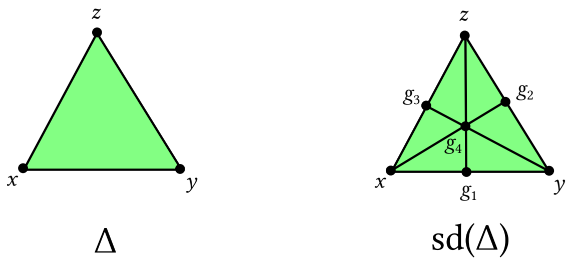


Figure 2: The simplicial complex described in the example and its first barycentric subdivision.

Definition 6 (k-skeleton of a simplicial complex)**.** Let Δ be a simplicial complex and $k \in \mathbb{N} \cup \{0\}$. The k-skeleton of Δ is the simplicial complex $\Gamma = \{\sigma \in \Delta \ : \ |\sigma| < (k+1)\}$.

For example the 1-skeleton of a simplicial complex Δ is the simplicial complex containing all 0-simplices and 1-simplices in Δ.

Definition 7 (Join)**.** The join of two non-empty families Δ and Γ (assumed to be defined on disjoint ground sets) is the family:

$$\Delta * \Gamma = \{\sigma \cup \tau \ : \ \ \sigma \in \Delta, \tau \in \Gamma\}$$

Definition 8 (Cones and Suspensions)**.** The cone of a family Δ is the join with a 0-simplex:

$$\mathrm{Cone}_x(\Delta) = \{\emptyset, \{x\}\} * \Delta$$

The suspension of Δ is the join with two 0-simplices:

$$\mathrm{Susp}_{x,y}(\Delta) = \{\emptyset, \{x\}, \{y\}\} * \Delta$$

Simplicial Homology

Homology is a standard in Algebraic Topology subject, that we will only consider in the simplicial case, although it can be described in more general settings (see for example [13],[22]). Moreover, we only consider homology on the field $\mathbb{Z}_2 = \mathbb{Z}/2\,\mathbb{Z}$, while it could be defined also on an arbitrary group, or module over a ring. Our choice allows us not to require an orientation on simplices. In addition, homology groups will not show any torsion.

Definition 9 (n-chains)**.** Let K be a simplicial complex. A simplicial n-chain ($n \in \mathbb{Z}$) is a formal sum of n-simplices of K:

$$c = \sum_{i=1}^{k} \alpha_i \sigma_i, \ \alpha_i \in \mathbb{Z}_2, \ \sigma_i \in K, |\sigma_i| = n+1$$

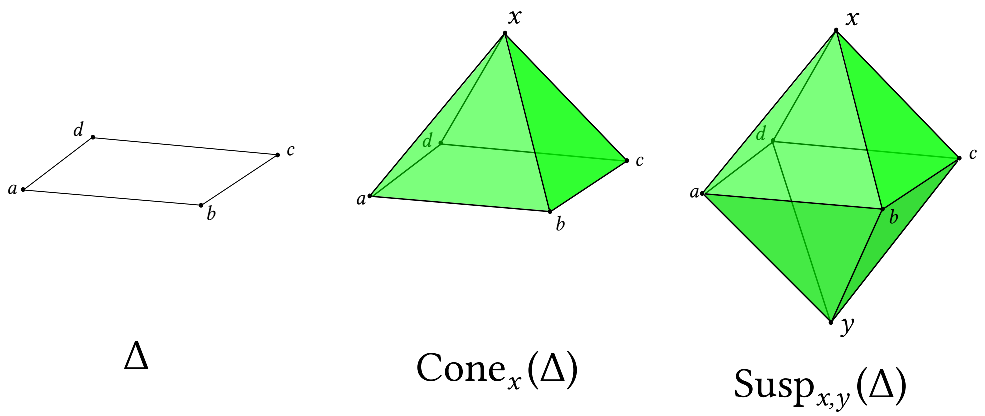


Figure 3: The Cone and the Suspension of the simplicial complex $\Delta = \{\emptyset, \{a\}, \{b\}, \{c\}, \{d\}, \{a, b\}, \{b, c\}, \{c, d\}, \{d, a\}\}$

We can assume that every n-simplex is present in each n-chain: the formal sum does not change adding any n-simplex with coefficient $\alpha_i = 0$. We define the sum of two n-chains $c_1 = \sum \alpha_i \sigma_i$, $c_2 = \sum \beta_i \sigma_i$ as: $c_1 + c_2 = \sum(\alpha_i + \beta_i)\sigma_i$.

The set of n-chains, denoted C_n or $\mathsf{C}_n(K)$, equipped with this operation of sum, is a group where the neutral element is the null chain (that is the chain with every $\alpha_i = 0$) and the opposite of $c \in \mathsf{C}_n$ is c itself, since the coefficients sum up in $\mathbb{Z}_2$. The group inherits the commutative property by $\mathbb{Z}_2$. Remark that the group of n-chains is trivial if n is less than 0 or greater than the dimension of K.

Definition 10 (Boundaries)**.** The boundary of an n-simplex $\sigma = \{v_0, \dots, v_n\}$ is defined as the chain of its $(n-1)$-faces:

$$\partial_n(\sigma) = \sum_{i=0}^{n} \{v_0, \dots, \hat{v}_i, \dots, v_n\}$$

where the hat means that the vertex was eliminated from the set:
$\{v_0, \dots, \hat{v}_i, \dots, v_n\} = \{v_0, \dots, v_{i-1}, v_{i+1}, \dots, v_n\}$. Remark that $\partial_n(\sigma) \in \mathsf{C}_{n-1}$.

The n-boundary of a simplicial complex is defined as the sum of boundaries of its n-simplices. This definition implies that $\partial_n : \mathsf{C}_n \longrightarrow \mathsf{C}_{n-1}$ is a group homomorphism: if $c_1, c_2 \in \mathsf{C}_n$ then $\partial_n(c_1 + c_2) = \partial_n(c_1) + \partial_n(c_2)$.

We have a sequence of abelian groups that we call a *chain complex*:

$$\dots \xrightarrow{\partial_{n+2}} \mathsf{C}_{n+1} \xrightarrow{\partial_{n+1}} \mathsf{C}_n \xrightarrow{\partial_n} \dots \xrightarrow{\partial_1} \mathsf{C}_0 \xrightarrow{\partial_0} 0$$

Every $c \in \mathsf{C}_n$ such that $\partial_n(c) = 0$ is called an *n-cycle*. We denote the set of n-cycles by Z_n. We observe that $\mathsf{Z}_n \subseteq \mathsf{C}_n$ is the kernel of ∂_n and thus it is a subgroup of C_n.

Any $a \in \mathsf{C}_n$ such $\partial_{n+1}(b) = a$ for some $b \in \mathsf{C}_{n+1}$ is called an *n-boundary*. We denote the set of n-boundaries as B_n. $\mathsf{B}_n \subseteq \mathsf{C}_n$ is the image of ∂_{n+1} and a subgroup of C_n.

Lemma 11 (Homology lemma)**.** $\partial_{n-1} \circ \partial_n = 0$ for every $n \in \mathbb{Z}$

Proof. For every simplex $\sigma = \{v_0, \dots, v_n\}$ we have:

$$\begin{aligned}
\partial_{n-1}(\partial_n(\sigma)) &= \partial_{n-1}\left(\sum_{i=0}^{n}\{v_0, \dots, \hat{v}_i, \dots, v_n\}\right) \\
&= \sum_{i=0}^{n} \partial_{n-1}(\{v_0, \dots, \hat{v}_i, \dots, v_n\}) \\
&= \sum_{i=0}^{n}\left(\sum_{j=0}^{i-1}\{v_0, \dots, \hat{v}_j, \dots, \hat{v}_i, \dots, v_n\} + \sum_{j=i+1}^{n}\{v_0, \dots, \hat{v}_i, \dots, \hat{v}_i \dots, v_n\}\right)
\end{aligned}$$

In the last sum we have the same chains added twice, so the result is zero. Then, for linearity, $\partial_{n-1} \circ \partial_n = 0$ holds for every simplicial complex. □

From lemma 11 follows that $\mathsf{B}_n \subset \mathsf{Z}_n$, because $b \in \mathsf{B}_n$ if $b = \partial_{n+1}(c)$ for some $c \in \mathsf{C}_{n+1}$, then $\partial_n(b) = \partial_n(\partial_{n+1}(c)) = 0$. This remark allows us to give the next definition.

Definition 12. The n^{th} *simplicial homology group* of a simplicial complex K is the quotient of abelian groups:

$$\mathsf{H}_n(K) = \mathsf{Z}_n(K) \big/ \mathsf{B}_n(K)$$

All the sets we considered so far ($\mathsf{C}_n, \mathsf{Z}_n, \mathsf{B}_n, \mathsf{H}_n$) are groups, but also $\mathbb{Z}_2$-vector spaces for every $n \in \mathbb{Z}$. Thus the following dimensional equations holds:

$$\begin{aligned}
&\pi : \mathsf{Z}_n \longrightarrow \mathsf{Z}_n/\mathsf{B}_n = \mathsf{H}_n \\
&\Longrightarrow \dim(\mathsf{Z}_n) = \dim(\ker(\pi)) + \dim(\mathrm{Im}(\pi)) = \dim(\mathsf{B}_n) + \dim(\mathsf{H}_n) \\
&\partial_n : \mathsf{C}_n \longrightarrow \mathsf{B}_{n-1} \\
&\Longrightarrow \dim(\mathsf{C}_n) = \dim(\ker(\partial_n)) + \dim(\mathrm{Im}(\partial_n)) = \dim(\mathsf{Z}_n) + \dim(\mathsf{B}_{n-1})
\end{aligned}$$

Definition 13. The n^{th} *Betti number* of a simplicial complex is the dimension of its n^{th} homology group:

$$\beta_n = \dim(\mathsf{H}_n) = \dim(\mathsf{Z}_\mathsf{n}) - \dim(\mathsf{B}_n)$$

Chapter 1

Simplicial compexes built from a graph

Contents

1.1 Abstract

When considering a graph there are several methods to analyse its topology. It is possible to tackle this problem by building an abstract simplicial complex out of the graph, in order to use algebraic topology tools. The analysis of the resulting complex could provide topological insights about the original graph.

There are many well-studied methods to associate simplicial complexes out of a graph. In the literature the approach is twofold: on the one hand, there is the study of a family of simplicial complexes derived from graphs, where simplicial complexes

are studied with an interest in their own right (see [15], [4]). On the other hand, the study of a simplicial complex coming from a specific graph, in order to grasp additional information from the simplicial interpretation of the graph (see, e. g., [17], [21], [1]). This work mainly focuses on the latter approach: we want to find topological properties of the simplicial complex that could describe the original graph.

The following list provides a summary the methods described to build an abstract simplicial complex out of a graph. We also give here the references of various authors who use those methods to build simplicial complexes. In particular in [15] it is possible to find an encompassing description of several methods we do not consider in this work.

1. **The complex of Cliques:** consider every $(n + 1)$-clique of the graph as an abstract n-simplex (see for example: [15],[17], [21]);

2. **The complex of Independent Sets:** consider every $(n + 1)$-independent set of the graph as an abstract n-simplex (see for example: [15]);

3. **The complex of neighbours:** for every vertex $v \in V$ consider the simplices given by every subset of the set $\{v\} \cup \{w \in V \ : \ w \text{ is adjacent to } v\}$ (see for example: [15] [16], [17]);

4. **Complexes built from acyclic subsets**:

   - The complex of induced acyclic subsets: a set of vertices is a simplex if its induced graph is acyclic;
   - The complex of acyclic subsets of the edge set: every edge is a 0-simplex and n-simplices are given by $(n + 1)$ edges forming an acyclic graph;
   - The complex of removable acyclic subsets: simplices are given by non-disconnecting acyclic subsets of edges of a connected graph;

   (Even though some references for these complexes can be found in [15], the attempts we made to explore these methods are due to professor Fabrizio Caselli's suggestions.)

5. **The complex of enclaveless sets:** consider every enclaveless set of cardinality $(n + 1)$ as an n-simplex (we could not find any reference for this method in the literature).

1.2 Complex of Cliques

Definition 14 (Clique)**.** Let $G = (V, E)$ be a simple graph. A set of vertices is a clique in G if the induced subgraph is complete. Formally, a subset $C \subset V$ is a clique of G if for every pair $v, w \in C$, $v \neq w$, the edge $\{v, w\}$ is in E.

Definition 15 (Complex of Cliques)**.** The abstract simplicial complex of cliques of a graph $G = (V, E)$ is the abstract simplicial complex whose n-simplices are the cliques of G of cardinality $(n + 1)$. This complex will be denoted as Cl_G.

Remark 16. Since every subset of a clique is still a clique, Cl_G is well-defined.

This is the simplest way to build a simplicial complex out of a graph. In fact, the 1-skeleton of the complex is isomorphic to the graph, and where the graph is "dense" enough the complex is "filled" with simplices of higher dimension.

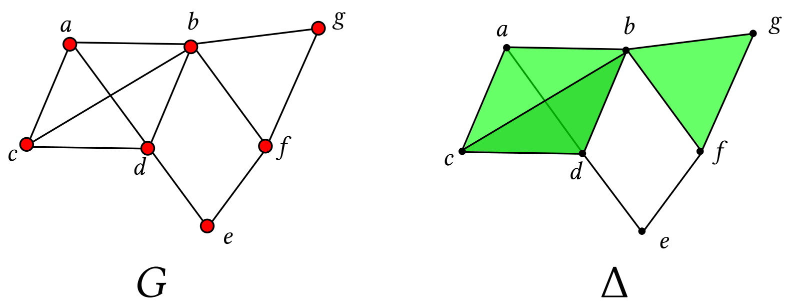


Figure 1.1: Example of a graph G and its complex of cliques $\Delta =< a, b, c, d > \cup < b, f, g > \cup < d, e > \cup < f, e >$

Observable simplicial complexes

Remark 17. Given a simplicial complex Δ, it is not possible to find a graph $G = (V, E)$ such that $\mathsf{Cl}_G = \Delta$. As a counterexample see fig. 1.2.

The problem is that there is no graph $G = (V, E)$ such that $\mathsf{Cl}_G = 2^V \setminus \{V\}$. However, if we accept to subdivide the simplicial complex we want to be represented, we can find a suitable G, as stated in the proposition 18.

Proposition 18. Let Δ be a simplicial complex and let $\mathrm{sd}(\Delta)$ be its first barycentric subdivison. If we consider the 1-skeleton of $\mathrm{sd}(\Delta)$ as a graph $G = (V, E)$, then we have $\mathsf{Cl}_G = \mathrm{sd}(\Delta)$.

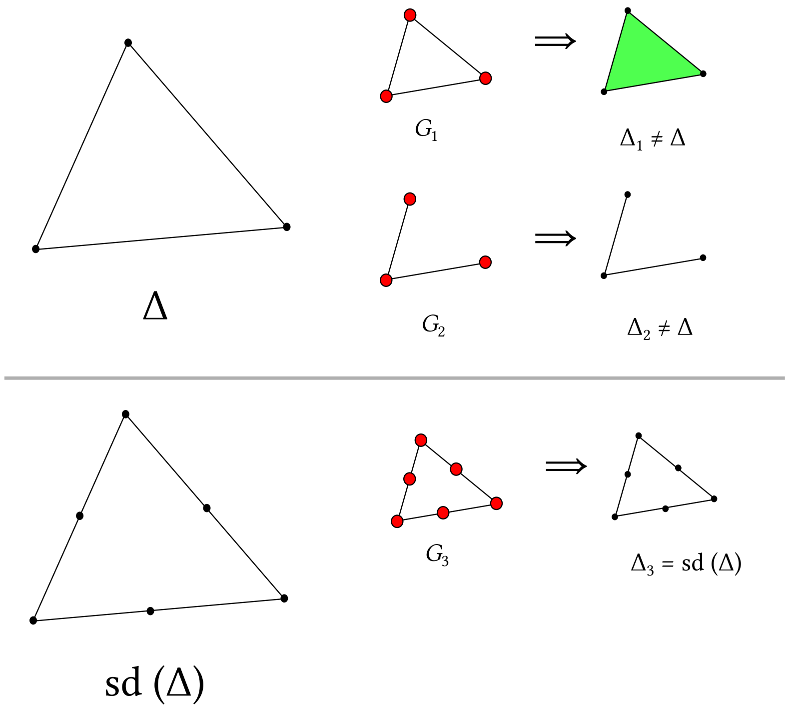


Figure 1.2: It is impossible to find a graph G such that its complex of cliques is the simplicial complex Δ (boundary of the 2-simplex), but it is possible to find a graph such that its complex of cliques is $\mathrm{sd}(\Delta)$.

Proof. We show that $\mathrm{sd}(\Delta)$ is both a subset and a superset of Cl_G.

$\sigma \in \mathrm{sd}(\Delta) \Rightarrow \sigma \in \mathsf{Cl}_G$:
this is straightforward, since every simplex in $\mathrm{sd}(\Delta)$ is necessarily a clique in G, thus a simplex in Cl_G.

$\sigma \in \mathsf{Cl}_G \Rightarrow \sigma \in \mathrm{sd}(\Delta)$:
$\sigma \in \mathsf{Cl}_G$ means that σ is a clique of the 1-skeleton of $\mathrm{sd}(\Delta)$.
By induction on $n = |\sigma|$ we are going to show:

> $P(n)$: *for every clique σ in G, its vertices are barycenters of simplices forming a chain of faces of the same simplex.*

This will prove the claim, since $P(n)$ is precisely the definition of a simplex σ in $\mathrm{sd}(\Delta)$.
For $n = 1$, $P(1)$ is trivial.
$P(n-1) \Rightarrow P(n)$: in a barycentric subdivision every barycenter belongs to a simplex of dimension different from the adjacent barycenters. For every clique σ we consider the vertex barycenter of the simplex $\tau \in \Delta$ of maximal dimension (with respect to that

clique). Thus the $(n-1)$ adjacent vertices are barycenters of faces of τ, and, by the induction hypothesis, they all belong to the same face. This proves $P(n)$. $\square$

Homology of the complex of cliques

Proposition 19 (Suspensions)**.** Let $G = (V, E)$ be a graph, let Cl_G be its complex of cliques, and $x, y \notin V$. Let CSusp(G) be the graph:

$$\mathrm{CSusp}(G) := \Big(V \cup \{x, y\}, E \cup \Big\{\{v, x\}, \{v, y\} \ : \ v \in V\Big\}\Big)$$

Then the complex of cliques of CSusp(G) is $\mathrm{Susp}_{x,y}(\mathsf{Cl}_G)$.

Proof. By definition of suspension: $\sigma \in \mathrm{Susp}_{x,y}(\mathsf{Cl}_G)$ if and only if one of the following conditions holds:

1. $\sigma \in \mathsf{Cl}_G$;
2. $(\sigma \setminus x) \in \mathsf{Cl}_G$;
3. $(\sigma \setminus y) \in \mathsf{Cl}_G$.

In each of the three cases, the definition of CSusp guarantees that σ is a clique in CSusp(G). In fact every subgraph of G is still a subgraph of CSusp(G), thus the first case is proved. As for the second and the third case: consider $(\sigma \setminus x) \in \mathsf{Cl}_G$, then, by construction, each element of the clique $(\sigma \setminus x)$ is connected to the vertex x in the graph CSusp(G). So σ is a clique in CSusp(G). $\square$

Remark 20. By definition CSusp(G) is obtained from G by adding two vertices completely connected to the other vertices of G, but not with each other. If we iterate n times the suspension of the graph $G = (\{x, y\}, \emptyset)$ we obtain graphs that are represented by a simplicial complex of cliques whose euclidean embedding is homeomorphic to the sphere S^n (see fig. 1.3). Thus the reduced homology groups of that simplicial complex are all trivial, except the n-th.

1.3 Complex of Independent sets

Definition 21 (Independent set)**.** Let $G = (V, E)$ be a simple graph. A set of vertices is an independent set in G if the induced subgraph does not contain any edge. Formally, a subset $I \subset V$ is an independent set of G, if every pair $v, w \in I$ is such that $\{v, w\} \notin E$.

Definition 22 (Complex of Independent sets)**.** The abstract simplicial complex of independent sets of a graph $G = (V, E)$ is the one whose n-simplices are the independent sets of G of cardinality $(n + 1)$. This complex will be denoted as I_G.

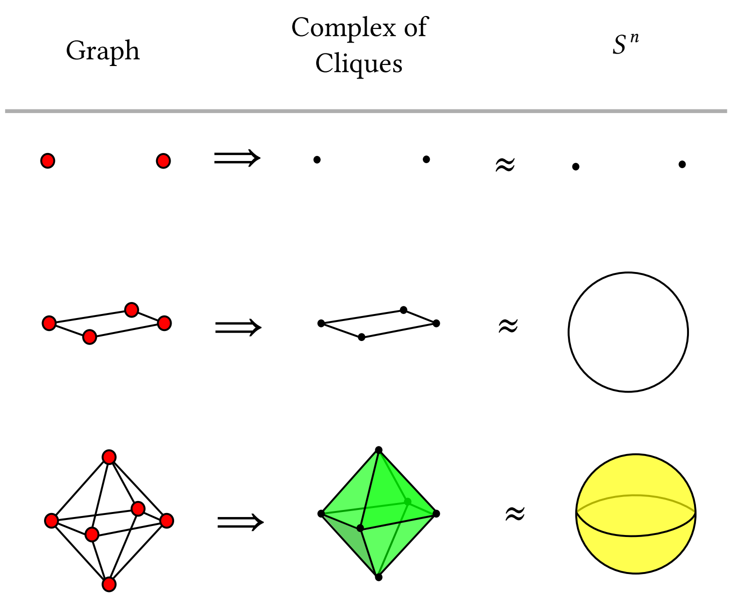


Figure 1.3: The first two suspensions of the graph $G = (\{x, y\}, \emptyset)$

Lemma 23 (Complex of cliques is the complex of independent sets of the complementary)**.** Let $G = (V, E)$ be a graph. Then $\mathsf{Cl}_G = \mathsf{I}_{G^C}$.

Proof. To prove the lemma it suffices to remark that, by definition of complementary graph, a clique in G is an independent set of G^C. □

Remark 24. lemma 23 implies that everything we previously stated about the complex of cliques holds also for the complex of independent sets of the complementary graph. By the way we will briefly recall those results in the following propositions.

Proposition 25. Let Δ be a simplicial complex and let $\mathrm{sd}(\Delta)$ be its first barycentric subdivison. If we consider the 1-skeleton of $\mathrm{sd}(\Delta)$ as a graph $G = (V, E)$, then $\mathsf{I}_{G^C} = \mathrm{sd}(\Delta)$.

Proposition 26 (Suspensions)**.** Let $G = (V, E)$ be a graph, and let $x, y \notin V$. Let $\mathrm{ISusp}(G)$ be the graph:

$$\mathrm{ISusp}(G) := \left(V \cup \{x, y\}, E \cup \left\{\{x, y\}\right\}\right)$$

Then the complex of independent sets of $\mathrm{ISusp}(G)$ is $\mathrm{Susp}_{x,y}(\mathsf{I}_G)$.

Remark 27. By definition $\mathrm{ISusp}(G)$ $\mathrm{ISusp}(G)$ is Gobtained with the addition of two vertices connected with each other only to the graph G. If we iterate n times the suspension of the graph $G = (\{x, y\}, \{x, y\})$ we obtain graphs that are represented by a simplicial complex of independent sets that is homeomorphic to the sphere S^n (see fig. 1.4. Thus the reduced homology groups of that simplicial complex are all trivial, except the n-th.

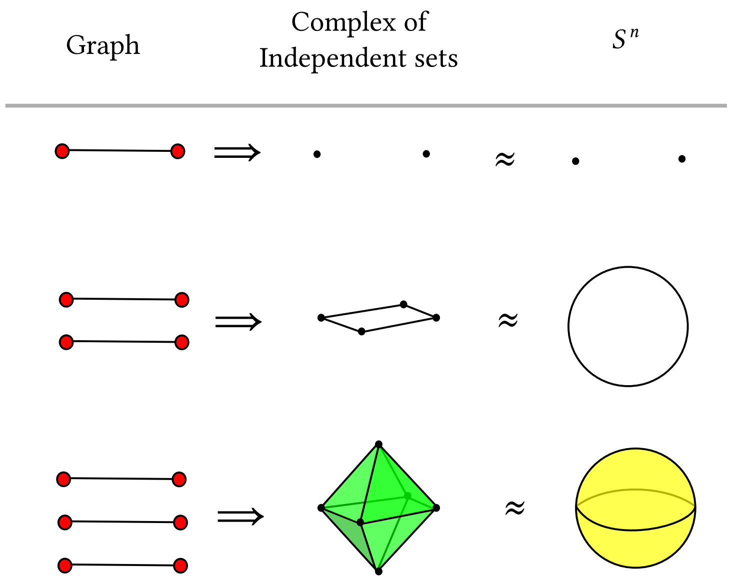


Figure 1.4: The first two suspensions of the graph $G = (\{x, y\}, \{x, y\})$

1.4 Complex of Neighbours

Definition 28 (neighbours)**.** Let $G = (V, E)$ be a graph and let $v \in V$. The set of neighbours of v is

$$N(v) = \left\{ w \in V \ : \ \{v, w\} \in E \right\}$$

Definition 29 (Complex of neighbours)**.** Simplices of the abstract simplicial complex of neighbours of a graph $G = (V, E)$ are all the subsets of $\{v\} \cup N(v)$, for every $v \in V$. This complex will be denoted Nb_G.

Remark 30. The inheritance property is included in the definition, so the simplicial complex is well-defined.

We have various obvious straightforward relations between the *degree of the vertices* and the simplicial complex of neighbours. In particular: the maximum degree of G

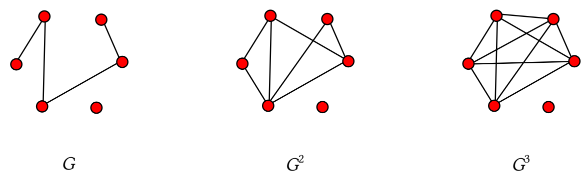


Figure 1.5: An example of graph and its powergraphs.

is equal to the greatest dimension of the simplices of the complex of neighbours. Moreover if G is a regular graph (every vertex has the same degree) Nb_G is a homogeneous simplicial complex.

Observable simplicial complexes

Definition 31 (Power graph)**.** Let $G = (V, E)$. For $k \in \mathbb{N}$ we define the power graph G^k as the graph that has V as a set of vertices and where two vertices are adjacent if their distance in G is at most k.

Lemma 32 (Complex of neighbours is subcomplex of the complex of cliques of the power graph)**.** Let $G = (V, E)$ be a graph. Then $\mathsf{Nb}_G \subset \mathsf{Cl}_{G^2}$.

Proof. Let $\sigma \in \mathsf{Nb}_G$, then there is a vertex $v \in \sigma$ such that $\sigma \subseteq \{v\} \cup N(v)$. Thus the distance among the vertices of σ is at most 2 (they all have a common neighbour) and this implies that the set of vertices σ is a clique in G^2. □

Remark 33. The converse ($\mathsf{Cl}_{G^2} \subseteq \mathsf{Nb}_G$) is not true. For example fig. 1.6 is a counterexample.

Remark 34. Not all simplicial complexes are observable. For example there is not such a graph whose simplicial complex is an empty triangle: it is sufficient to observe that if the graph has maximum degree bigger than 1, then we have at least a 2-simplex.

Moreover the first barycentric subdivision does not provide the homeomorphism of the bodies (as the complex of cliques provided), but probably we could have homotopic equivalence (see fig. 1.7).

Homology and Homotopy of the complex of neighbours

The complex of neighbours, as stated in lemma 32, is a super-complex of the complex of cliques of G, and a sub-complex of the complex of cliques of G^2. This fact prevents us from giving easy proofs about suspensions and homology type.

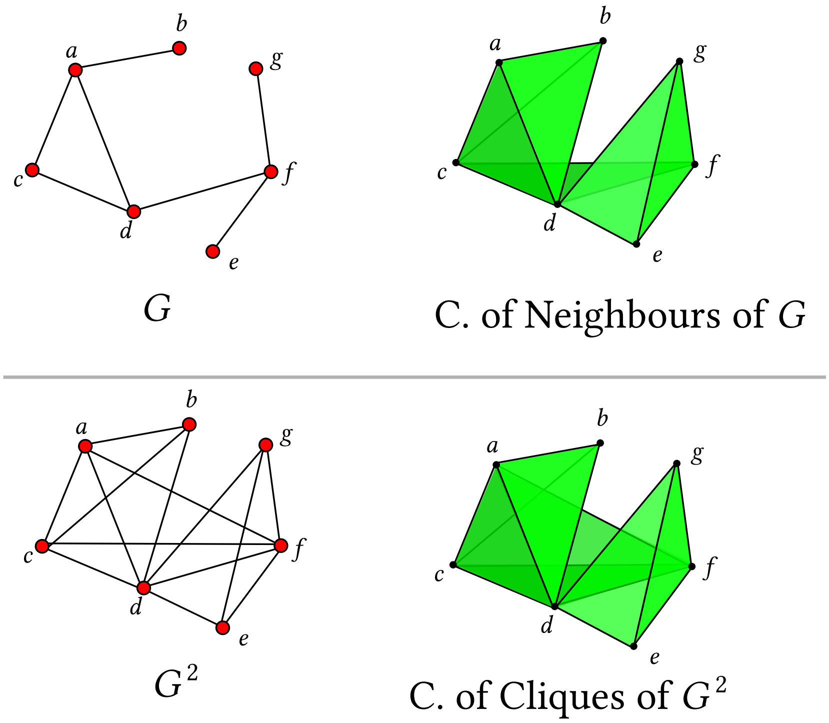


Figure 1.6: Example of the complex of neighbours of a graph G: $\mathsf{Nb}_G =< a, b, c, d > \cup < d, e, f, g > \cup < c, d, f >$. Moreover we have: $\mathsf{Cl}_{G^2} =< a, b, c, d > \cup < d, e, f, g > \cup < a, c, d, f >$, so $\mathsf{Nb}_G \subsetneq \mathsf{Cl}_{G^2}$

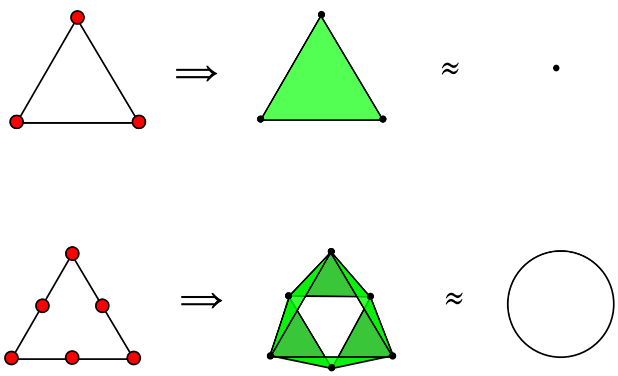


Figure 1.7: Refining a triangle does not give a complex of neighbours PL-equivalent to an empty triangle, but at least provide homotopical equivalence

The main preserved information about the original graph is the connectedness. To each connected component of the graph corresponds a connected component of the simplicial complex, and connected components of a graph are preserved via the power graph.

Definition 35 (Chordless cycle)**.** A chordless cycle in a graph G is a cycle such that no two vertices of the cycle are connected by an edge that does not itself belong to the cycle.

Remark 36 (n-cycles)**.** Let $G = (V, E)$ be a chordless cycle on n vertices and let Nb_G be its complex of neighbours.

- if $n = 3$, then $\mathsf{Nb}_G = 2^V$ is a 2-simplex.
- if $n = 4$, then $\mathsf{Nb}_G = 2^V \setminus V$. That is: Nb_G is the complex containing the faces of a 3-simplex but not the 3-simplex itself (i.e. is an empty tetrahedron). So it is simply connected and has the homotopy type of the 2-sphere S^2.
- if $n \geq 5$, Nb_G is homotopically equivalent to S^1. [In particular is not simply connected, and a representant of the fundamental group is the loop given by the simplexes forming the cycle in G.]

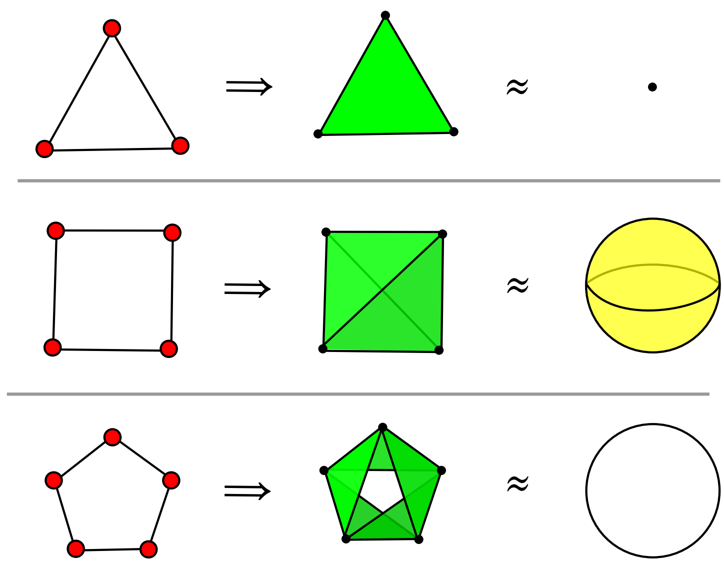


Figure 1.8: Illustration of the graphs and the simplicial complexes of neighbours considered in remark 36

We state now a result form Lovász [16], which relates the connectedness of the complex of neighbours with the chromatic number of the original graph. A topological space T is called *n-connected* if each continuous mapping of the surface S^r of the $(r+1)$-dimensional ball into T extends continuously to the whole ball, for $r \in \{0, 1, \dots, n\}$.

Theorem 37. If the complex of neighbours of G is $(k+2)$-connected, then G is not k-colorable.

1.5 Acyclic subsets

We acknowledge professor Fabrizio Caselli[1], for his valuable contribution to this section, in which we describe three methods to build simplicial complexes from acyclic subgraphs.

1.5.1 Complex of induced acyclic subgraphs

Definition 38. Let $G = (V, E)$ be a simple graph. The simplicial complex of induced acyclic subgraphs of G is the simplicial complex Δ such that $\sigma \subset V$ is a simplex in Δ if the induced subgraph $G[\sigma]$ is acyclic.

Remark 39. The simplicial complex is well-defined since if $\tau \subset \sigma$ then $G[\tau] \subset G[\sigma]$, and every subgraph of an acyclic graph is still acyclic.

The 1-skeleton of the complex of induced acyclic subgraphs of every graph $G = (V, E)$ is always isomorphic to the complete graph on $|V|$ vertices. In fact, let $x, y \in V$. Then $G[x, y]$ is acyclic in any case: both if $G[x, y] = (\{x, y\}, \emptyset)$, either or if $G[x, y] = (\{x, y\}, \{x, y\})$.

Moreover this complex preserves very little topological information of the original graph: every acyclic induced subgraph on $(n+1)$-vertices is represented by an n-simplex, regardless of the structure of the subgraph (see fig. 1.9).

1.5.2 Complex of acyclic subsets of the edge set

Definition 40. Let $G = (V, E)$ be a graph and let $\varphi : I \longrightarrow E$ be a bijection. The simplicial complex of acyclic subsets of the edge set is the simplicial complex on I such that $\sigma \subset I$ is a simplex if $\varphi(\sigma)$ is an acyclic subgraph of G.

Remark 41. In the simplicial complex of acyclic subsets of the edge set 0-simplices are represented by the edges of the graph, while in the previous methods 0-simplices were represented by the vertices of the graph. The complex is well-defined since every subgraph of an acyclic graph is still acyclic.

[1] University of Bologna, fabrizio.caselli@unibo.it

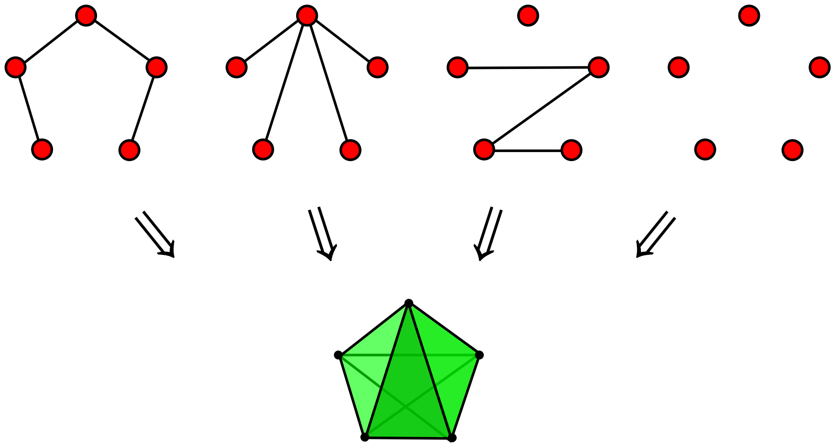


Figure 1.9: Every acyclic graph on 5 vertices is represented (as a complex of induced acyclic subgraphs) by a simplicial complex containing a 4-simplex and all its faces.

We lose much topological information about the original graph: every acyclic subgraph on $n+1$ edges is represented by an n-simplex,while the pieces of information about inner structure, connected components, degree of the vertices of the acyclic subgraph is lost (see fig. 1.10).

Remark 42. A special case of subcomplex of the acyclic subsets of the edge set is the well studied *matching complex* (see [8] and [3]), where the vertex set of this complex is the set of edges of G and its faces are sets of edges of G with no two edges meeting at a vertex.

1.5.3 Complex of removable acyclic subgraphs

Definition 43. Let $G = (V, E)$ be a connected graph and let $\varphi : I \longrightarrow E$ be a bijection. The simplicial complex of removable acyclic subgraphs is the simplicial complex on I such that $\sigma \subset I$ is a simplex if $\varphi(\sigma)$ is an acyclic subgraph of G and $G' = (V, E \setminus \varphi(\sigma))$ is still connected.

Remark 44. This graph is well-defined because, as usual, a subgraph of an acyclic graph is still acyclic, and if we remove a smaller number of edges the graph is still connected.

As in remark 39 and remark 41 the structure of the removed subgraph is not significant. n-simplices are generated by sets of $(n+1)$ edges, regardlessly of the connectedness either or the degree of the vertices.

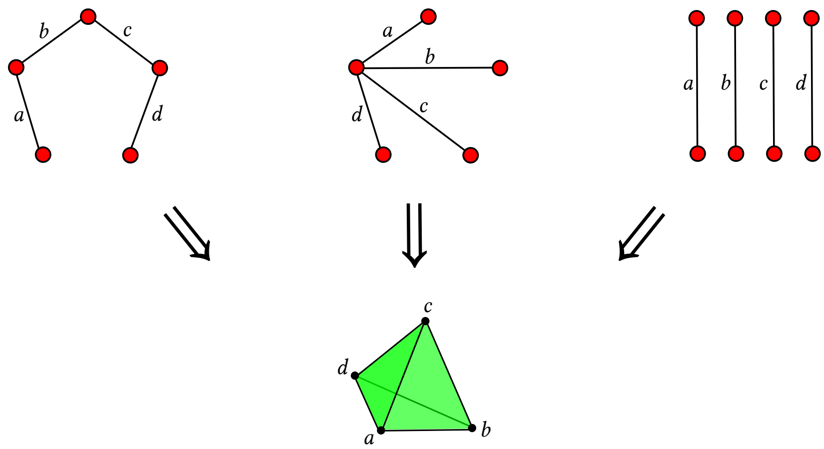


Figure 1.10: Every acyclic graph on 4 edges is represented (as a complex of acyclic subgraphs of the edge set) by a simplicial complex containing a 3-simplex and all its faces.

Proposition 45. In the complete graph on n vertices K_n, the complex of removable acyclic subgraphs is homogeneous of dimension $(n-2)$ and the simplices of maximal dimension are $n^{n-2} - n$.

Proof. The dimension of the complex comes from two standard graph theory theorems about trees and spanning trees: every tree has exactly as much vertices as the number of edges minus one, and every graph is connected if and only if it has a spanning tree (see [6, theorem 4.3, theorem 4.6]).

As for the number of simplices: in K_n there are n^{n-2} spanning trees (Cayley's formula, see [6, theorem 4.8]). We are now going to show that, if we remove from K_n the edges of one of these trees, the resulting graph is disconnected only in n cases. This will prove that the simplices of maximal dimension are $n^{n-2} - n$.

In order to disconnect K_n it is necessary to divide at least one vertex from the others, that is: we have to remove each of the $n-1$ edges starting from that vertex.

Another possibility, for example, is to disconnect a couple of vertices from the others: this can be achieved removing $n - 2$ edges from the first vertex and $n - 2$ from the second vertex, while the edge connecting the two vertices can be preserved. Thus we removed $2(n-2)$ edges overall.

Similarly, to disconnect a clique of k vertices from the rest of the graph we have to remove at least $k(n-k)$ edges.

Moreover, those edges must belong to an acyclic subgraph of K_n, so their number must be smaller than $n-1$.

Hence, to disconnect K_n removing the edges of an acyclic subset, we have the following constraint on the number of the removed edges:

$$k(n-k) \leq n-1 \quad n \in \mathbb{N}, n \geq 2$$
$$-k^2 + kn - n + 1 \leq 0$$

This second degree inequality is solved for $k \leq 1$ or $k \geq n-1$. Both the acceptable solutions $k = 1$ and $k = n-1$ mean are separating one of the n vertices from K_n by removing its $n-1$ incident edges. So there are only n spanning trees whose edges disconnect K_n. □

1.6 Complex of enclaveless sets

We did not find any reference in the literature that used this method to build simplicial complexes out of a graph. The definition of enclaveless set and further results in domination in graphs can be found in[14].

Definition 46 (Enclaves and Enclaveless sets)**.** Let $G = (V, E)$ be a simple graph. For $S \subset V$ a vertex $v \in S$ is an enclave if $N(v) \subset S$. A set is said to be enclaveless if it does not contain any enclaves.

Definition 47 (Dominating set)**.** Let $G = (V, E)$ be a simple graph. A set of vertices D is dominating in G if for every $v \in V$, $v \in D$ or exist $w \in D$ such that $\{v, w\} \in E$. That is: a set of vertices D is dominating if every vertex in V is either in D or adjacent to a vertex in D.

Remark 48. It is possible to characterize an enclaveless set as complementary of a dominating set. In fact, if D is a dominating set, then every $v \in V \setminus D$ adjacent to a vertex in D, so $N(v)$ is not a subset of $V \setminus D$. Thus $V \setminus D$ is enclaveless for every dominating set D. Vice versa, if $S \subset V$ is enclaveless, then every $v \in V$ is either in $V \setminus S$ or adjacent to it, because $N(v)$ is not a subset of S.

Definition 49 (Complex of enclaveless sets)**.** The abstract simplicial complex of enclaveless sets of a graph $G = (V, E)$ is the one whose n-simplices are the enclaveless sets of G of cardinality $(n+1)$. We will denote this complex with El_G.

Remark 50. This complex is well defined. The inheritance property comes from the fact that every superset of a dominating set is still a dominating set, thus a subset of an enclaveless set is still an enclaveless set.

Remark 51. There are many restrictions when we try to find a specific graph to build a given simplicial complex. For example it is not possible to build a simplicial complex of enclaveless sets made by an n-simplex alone. Every time we have an n-simplex, there is always a further 0-simplex in the complex, and this is due to the topological structure of a graph containing an enclaveless set of cardinality $n+1$ (see fig. 1.11).

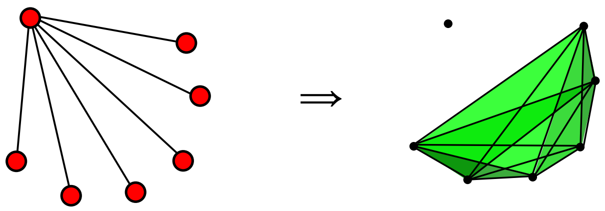


Figure 1.11: On the left, the smallest graph with an enclaveless set of cardinality 6. On the left, its complex of enclaveless sets, made of a 5-simplex and a 0-simplex. In general, the smallest graph with an enclaveless set of cardinality n has the same structure: acyclic on $n+1$ vertices with a vertex of degree n. Analogously its complex of enclaveless sets is composed by an n-simplex (generated by the enclaveless set of vertices of degree 1) and a 0-simplex (generated by the vertex of degree n).

Homology of the complex of enclaveless sets

Proposition 52. The body of the geometric complex El_{K_n} is homeomorphic to S^{n-2}.

Proof. Minimal dominating sets of K_n are the singletons, thus maximal enclaveless sets of K_n are subsets of vertices of cardinality $(n-1)$. So, in the complex of enclaveless sets there are all the $(n-2)$-simplices on n vertices, and this is the geometric representation of the boundary of an $(n-1)$-simplex, and the body of this boundary is homeomorphic to S^{n-2}. □

Proposition 53 (Suspensions)**.** Let $G = (V, E)$ be a graph, and let $x, y \notin V$. Let $\mathrm{ESusp}(G)$ be the graph:

$$\mathrm{ESusp}(G) := \Big(V \cup \{x, y\}, E \cup \Big\{\{x, y\}\Big\}\Big)$$

Then the complex of enclaveless sets of $\mathrm{ESusp}(G)$ is $\mathrm{Susp}_{x,y}(\mathsf{El}_G)$.

Remark 54. The definition of the graph $\mathrm{ESusp}(G)$ and $\mathrm{ISusp}(G)$ (see proposition 26) is the same: the addition of two vertices connected with each other only. As in the case of the complex of independent sets, if we iterate n times the suspension of the graph $G = (\{x, y\}, \{x, y\})$ we obtain graphs that are represented by a simplicial complex of independent sets that is homeomorphic to the sphere S^n (the figure is identical to fig. 1.4). Thus the reduced homology groups of that simplicial complex are all trivial, except the n-th.

1.6.1 Enclaveless sets implementations

Looking for minimal dominating sets. We adapted the method designed to find minimal covering used in [5, sec. 8.6].

We define a symbolic way to refer to the subsets of the power set of V. Let $v, w \in V$, then $v+w$ is the set $\{\{v\}, \{w\}\}$ and $v \cdot w$ is the set $\{\{v, w\}\}$. These are logic operations: we define the sum of two vertices to be "the first vertex *either or* the second vertex" and the product of vertices to be "the first vertex *and* the second". Those definitions are generalizable to represent elements of the power set 2^V (products) and subsets of the power set (additions of products). Using the distributive and associative properties we can exploit symbolic computations to manipulate the sets. It is possible to find all the minimal dominating sets of a graph G following this procedure:

S = $\emptyset$
for $v \in V$ **do**
  Nv =$\{\{$v$\}\}$
  for $w \in N(v)$ **do**
    Nv = Nv + w
  end
  S = S $\cdot$ Nv
end

The main idea is that in every dominating set D, every vertex of V must be either in D or at least have a neighbour contained in D. So in the end we have:

$$2^V \supset S = \prod_{v \in V} \left(v + \sum_{w \in N(v)} w \right)$$

Once performed all the calculations, each product of vertices is a minimal dominating set.

Simplifications. There are a couple useful simplifications for the computation:

1. duplicates of every vertex that appears more than once in a product are removable (e.g.: $vwxv$ becomes vwx).

2. if in a sum there are a couple of addends such that one is contained in the other, then the bigger addend is removable (e.g. $vwx + vwxy$ becomes vwx).

3. let p_i be products of vertices and v_k be vertices. Then we can simplify the product $(p_1 + \dots + p_s)(v_1 + \dots + v_r)$. Let $p'_1, \dots, p'_h$ be the products containing at least one of the vertices $v_1, \dots, v_r$ and let $p''_1, \dots, p''_k$ be the products not containing any of the vertices $v_1, \dots, v_r$. Then the product can be simplified in:

$$p'_1 + \dots + p'_h + (p''_1 + \dots + p''_k)(v_1 + \dots + v_r)$$

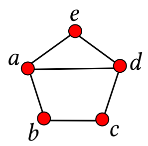


Figure 1.12: Example of a graph. The first step in the computation of minimal dominating sets for the graph above is the following: $(a+b+d+e)(b+a+c)(c+b+d)(d+c+a+e)(e+a+d)$.

Implementation. We tried to implement this strategy using the following idea: every vertex is associated to a prime number and then computations are made with arrays: every element of the array is an addend of the sum and every element is a product of prime numbers. This way simplifications are easily performed: for simplification 1 it suffices to reduce every element of the array to a product of primes raised to the first power; for simplification 2, if an element of the array divides the other, then the divisible element is deleted (see appendix).

This solution is an elegant one, but the evidence shows that numbers grow steadily while the number of vertices grows and computations becomes challenging and the elaboration time slows down. So it is advisable to find another implementation strategy.

Chapter 2

Graph persistence

Contents

2.1 Persistent homology: a brief introduction

Persistent homology is a useful method for computing topological features of a space. It was introduced by Patrizio Frosini and collaborators under the name of Size Theory [12] and used for shape recognition. This theory was also independently developed by Edelsbrunner et al. [9]. We consider only the case of persitent homology on simplicial complexes, but the general setting of the theory refers to topological spaces.

Let K be a finite simplicial complex. We want to define a nested sequence of increasing subcomplexes of K called a filtration. So, let $f : K \longrightarrow \mathbb{R}$ be a real valued function such that f is non-decreasing on increasing sequences of faces. That is: if $\sigma, \tau \in K$ and $\sigma \subset \tau$, then $f(\sigma) \leq f(\tau)$.

For every $a \in \mathbb{R}$ the *sublevel set* $K(a) = f^{-1}((-\infty, a])$ is a subcomplex of K. The hypothesis on f ensure that the ordering of the simplices provided by the values of f induces a *filtration*, that is an ordering on the sublevel complexes:

$$\emptyset = K_0 \subsetneq K_1 \subsetneq \cdots \subsetneq K_p = K$$

Where $K_i = K(\alpha_i)$ and $\alpha_i \in [a_i, a_{i+1})$ for some $a_i \in \mathbb{R}$.

For every couple of i, j such that $0 \leq i \leq j \leq p$, the inclusion $K_i \hookrightarrow K_j$ induces a homomorphism on the simplicial homology groups for each dimension n:

$$f_n^{i,j} : \mathsf{H}_n(K_i) \longrightarrow \mathsf{H}_n(K_j)$$

For every $n \in \{0, \ldots, p\}$ the n^{th} *persistent homology groups* are the images of these homomorphisms and the n^{th} *persistent Betti number* are the ranks of those groups:

$$\beta_n^{i,j} = \dim\left(\operatorname{Im} f_n^{i,j}\right)$$

Persistent Betti numbers count how many homology classes of dimension n survive the passage from K_i to K_j. We say that a homology class $\alpha \in \mathsf{H}_n(K_i)$ *is born entering* in K_i if α does not come from a previous subcomplex, that is $\alpha \notin \operatorname{Im} f_n^{i-1,i}$. Similarly, if α is born in K_i, it *dies entering* K_j if the image of the map induced by $K_{i-1} \subset K_{j-1}$ does not contain the image of α but the image of the map induced by $K_{i-1} \subset K_j$ does. In this case the *persistence* of α is $j - i$.

We can draw the *persistence diagram* where we represent the points (i, j) where i is the birth of an homological class and j is its death. If the class does not die we represent a vertical line called *cornerline*, starting from the diagonal in correspondence of the moment of its birth. In the diagram we usually draw the diagonal of the first and third quadrant.

This pairing of homology classes generalizes the pairing that Edelsbrunner calls “the elder rule”. The reason for this name is easily understood in the study of persistence for single variable functions $g : \mathbb{R} \longrightarrow \mathbb{R}$. When a new component is introduced (a local minimum is found) in $g^{-1}(-\infty, t]$ we say that the local minimum represent the component (birth of the component at time t). When passing a local maximum and merging two components, we pair the maximum with the “younger” of two local minima that represent the two components, and the other minimum is now the representative of the component resulting from the merger [9]. This is the same strategy we will use to define other persistent properties of a graph in section 2.3.

Example. We show now a simple example of a simplicial complex and its zero-persistence diagram, that is the story of its connected components along the filtration.

Let the filtration be the following sequence of nested simplicial complexes (see fig. 2.1):

$$
\begin{aligned}
K_0 &= \quad \emptyset \\
K_1 &= \{\{a,b\},\{a\},\{b\},\emptyset\} \\
K_2 &= \{\{c,d\},\{c\},\{d\},\{a,b\},\{a\},\{b\},\emptyset\} \\
K_3 &= \{\{e,f\},\{e\},\{f\},\{c,d\},\{c\},\{d\},\{a,b\},\{a\},\{b\},\emptyset\} \\
K_4 &= \{\{a,b,c\},\{a,c\},\{b,c\},\{e,f\},\{e\},\{f\},\{c,d\},\{c\},\{d\},\{a,b\},\{a\},\{b\},\emptyset\} \\
K_5 &= \{\{a,c,d\},\{a,d,f\},\{f,d,c\},\{a,d\},\{a,f\},\{f,d\},\{d,e\},\{a,b,c\},\{a,c\}, \\
&\quad\ \{b,c\},\{e,f\},\{e\},\{f\},\{c,d\},\{c\},\{d\},\{a,b\},\{a\},\{b\},\emptyset\}
\end{aligned}
$$

This example shows how to build a persistence diagram according to the definition above.

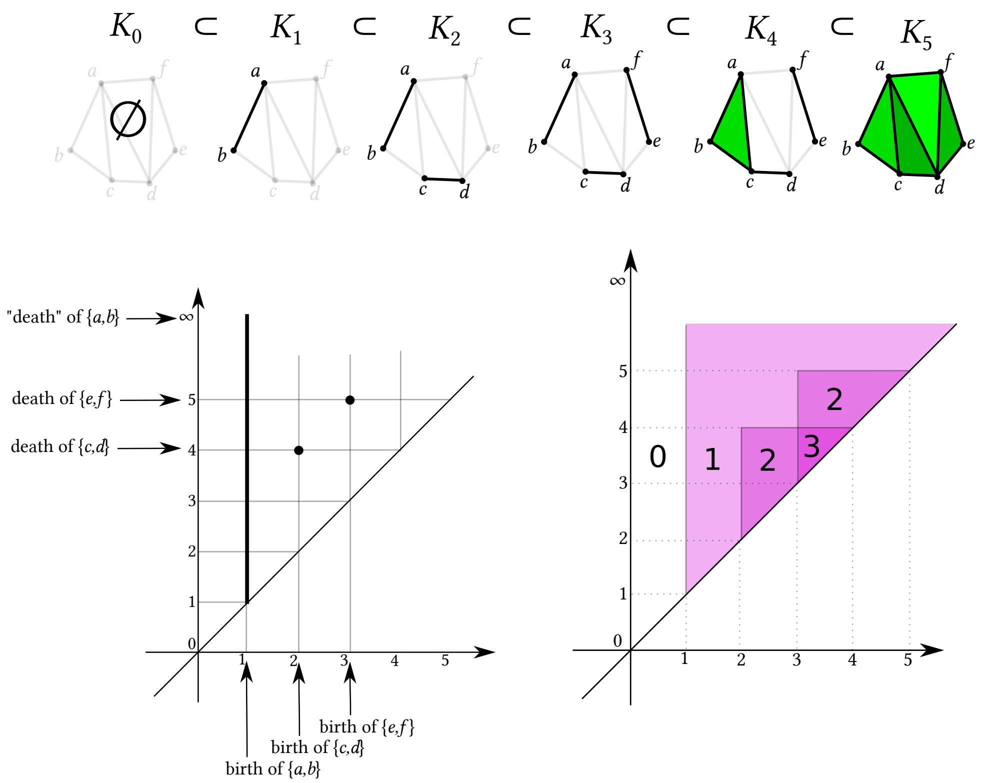


Figure 2.1: Example of a filtration (on top), its zero-persistence diagram (on the left), and the persistent betti number function (on the right)

2.2 Persistent homologic properties for simplicial complexes from a graph

Definition 55. A *weighted graph* $G = (V, E, w)$ is a graph $G = (V, E)$ where the *weight* function w is a bijection $w : E \longrightarrow \{1, 2, \dots, |E|\}$. On $G = (V, E, w)$ we define the subgraph $G_i = (V, w^{-1}(\{1, 2, \dots, i\})$.

Our *filtration* will be the sequence of complexes associated to each G_i (see for example fig. 2.2)

This setting allows us to study the persistence of the simplicial complexes described in chapter 1 (built from the various stages of the filtration of the edges).

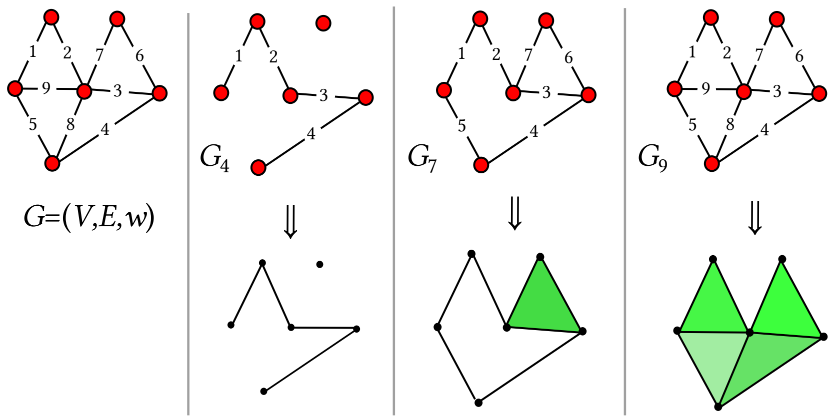


Figure 2.2: The weighted graph $G = (V, E, w)$ and some subgraphs in the filtration: $G_4 = (V, w^{-1}(\{1, \dots, 4\}))$, $G_7 = (V, w^{-1}(\{1, \dots, 7\}))$, $G_9 = (V, w^{-1}(\{1, \dots, 9\}))$ and their complexes of cliques

Notation warnings. According to our definition, when we refer to weighted graphs, we are talking about graphs with a relation of total order on the edge set.

By contrast, in the literature weighted graphs are usually defined with a weight function $\bar{w} : E \longrightarrow \mathbb{R}$ where every edge is associated to a real number. This induces a filtration as well, where $G_a = (V, \bar{w}^{-1}((-\infty, a]))$ for all $a \in \mathbb{R}$.

Our definition is less general, but gives us a complete sorting of the edges of G, while in the general case two edges with the same weight (i.e. $\bar{w}(e_1) = \bar{w}(e_2)$) would appear at the same time.

Weights could also be associated to vertices, but in this work we will only consider weights on edges.

2.2.1 Case study: edge filtrations on K_4

In this section we are going to deal with a simple example to show some features of the persistent homology for simplicial complexes from graphs. We suppose that in the step 0 of the filtration all vertices are added, then edges are added one by one. This choice leads to "monodimensional" zero-persistence diagrams (see fig. 2.9), that is: all the information of the diagram is contained in the leftmost cornerline and its internal cornerpoints. See section 2.2.2 for a different initial step in the filtration.

First, we present some notations that is going to be standard in the remainder of this section.

Notations. There are 10 classes of isomorphic graphs on 4 vertices (seefig. 2.3 on page 41). The notation for each equivalence class is a letter ranging from *(a)* to *(k)*. Here we present a representative for each equivalence class (the bigger graph of each class in fig. 2.3), and the number of elements in each class.

Equivalence classes of graphs up to isomorphism:

(a) $\ni (\{v, w, x, y\}, \emptyset)$, 1 element.

(b) $\ni (\{v, w, x, y\}, \{\{v, y\}\})$, 6 elements.

(c) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}\})$, 12 elements.

(d) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{w, x\}\})$, 3 elements.

(e) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, v\}\})$, 4 elements.

(f) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{y, w\}\})$, 4 elements.

(g) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, w\}\})$, 12 elements.

(h) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, v\}, \{v, w\}\})$, 12 elements.

(i) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, w\}, \{v, w\}\})$, 3 elements.

(j) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, v\}, \{v, w\}, \{w, x\}\})$, 6 elements.

(k) $\ni (\{v, w, x, y\}, \{\{v, y\}, \{y, x\}, \{x, v\}, \{v, w\}, \{w, x\}, \{w, y\}\})$, 1 element.

The directed graph D (see fig. 2.4 on page 42), represents the filtrations on K_4: each node is a class of equivalence of isomorphic graphs on 4 vertices, while each arrow represent the insertion of an edge. Figure 2.5 on page 43 explains the route of each filtration.

Possible filtrations (in each step an edge is added) along the classes are all the possible paths in D starting from the node (a):

1 : $(a) \longrightarrow (b) \longrightarrow (c) \longrightarrow (e) \longrightarrow (h) \longrightarrow (j) \longrightarrow (k)$

2 : $(a) \longrightarrow (b) \longrightarrow (c) \longrightarrow (f) \longrightarrow (h) \longrightarrow (j) \longrightarrow (k)$

3 : $(a) \longrightarrow (b) \longrightarrow (c) \longrightarrow (g) \longrightarrow (h) \longrightarrow (j) \longrightarrow (k)$

4 : $(a) \longrightarrow (b) \longrightarrow (c) \longrightarrow (g) \longrightarrow (i) \longrightarrow (j) \longrightarrow (k)$

5 : $(a) \longrightarrow (b) \longrightarrow (d) \longrightarrow (g) \longrightarrow (h) \longrightarrow (j) \longrightarrow (k)$

6 : $(a) \longrightarrow (b) \longrightarrow (d) \longrightarrow (g) \longrightarrow (i) \longrightarrow (j) \longrightarrow (k)$

Weights of the digraph of filtrations: the graph D in fig. 2.4 can be equipped with weights on the arrows. In fact, a filtration is the sorting of the edge set. We can suppose that the sorting is made through a stochastic process where each edge is picked out at random with homogeneous probability among the edges still to be chosen. Then every arrow weight is the inherited probability of transition from the two classes, according to the defined stochastic process.

We can see that in our digraph most weights are obviously equal to 1. The weight is equal to 1 in the cases where, no matter the choice of the next edge, the resulting graphs after the any insertion are all isomorphic. This is the case for the oriented edges *(a)(b), (d)(g), (e)(h), (f)(h), (h)(j), (i)(j),* and *(j)(k).*

Consider now the class *(c).* For each representative there are 4 possible edges to be added. The insertion of one of them would result in a graph isomorphic to a 3-cycle and an external vertex (that is, a graph in *(e)*), the insertion of another edge would result in a graph with a vertex of degree 3 and the other vertices of degree 1 (a graph in *(f)*). The insertion of one of the other two possible edges would result in a graph that is a path of 3 adjacent edges (a graph in *(g)*). So the transition probabilities from the class *(c)* give the following weights: $\frac{1}{4}$ for *(c)(e)*, $\frac{1}{4}$ for *(c)(f)* and $\frac{2}{4}$ for *(c)(g).*

Similar arguments give the weights: $\frac{4}{5}$ for *(b)(c)*, $\frac{1}{5}$ for *(b)(d)*, $\frac{2}{3}$ for *(g)(h)*, and $\frac{1}{3}$ for *(g)(i).*

This allows us to compute how probable is a filtration with respect to the sorting of the edges done through a uniform random choice.

1 : $1 \cdot \frac{4}{5} \cdot \frac{1}{4} \cdot 1 \cdot 1 \cdot 1 = \dfrac{3}{15}$

2 : $1 \cdot \frac{4}{5} \cdot \frac{1}{4} \cdot 1 \cdot 1 \cdot 1 = \dfrac{3}{15}$

3 : $1 \cdot \frac{4}{5} \cdot \frac{2}{4} \cdot \frac{2}{3} \cdot 1 \cdot 1 = \dfrac{4}{15}$

4 : $1 \cdot \frac{4}{5} \cdot \frac{2}{4} \cdot \frac{1}{3} \cdot 1 \cdot 1 = \dfrac{2}{15}$

5 : $1 \cdot \frac{1}{5} \cdot 1 \cdot \frac{2}{3} \cdot 1 \cdot 1 = \dfrac{2}{15}$

6 : $1 \cdot \frac{1}{5} \cdot 1 \cdot \frac{1}{3} \cdot 1 \cdot 1 = \dfrac{1}{15}$

Remark 56. The weighted graph D is a Markov Chain and could be considered as such in the analysis of the persistence. We did not investigate this aspect, but this could be an interesting topic for further research on filtrations on a graph. For a definition of Markov Chain and some applications on graphs see for example [7].

We depict in fig. 2.6 on page 44 a summary table of the simplicial complexes derived from the classes of graphs on 4 vertices: the complex of cliques Cl_G, the complex of independent sets I_G, the complex of neighbours Nb_G and the complex of enclaveless sets El_G. The complexes built from acyclic subsets are not represented in this table, since those methods mostly build simplicial complexes out of edges, and not vertices, so they are not easily comparable (for further clarification see section 2.2.3). In our comparison we will not consider the complex of independent sets either for two reasons:

1. the inclusion of the complexes runs backward with respect to the filtration: the filtration is not non-decreasing as required in the definition of persistence, but *non-increasing*. This does not prevent us from defining persistent Betti numbers simply reversing birth and death of the classes, but the comparison with other methods is not possibile.

2. for lemma 23 we have that all the information provided in the complex of independent sets can be retrieved from the complex of cliques of the complementary graph.

Zero-persistence diagrams. Now we consider all the filtrations and their features in the complexes of cliques, neighbours and enclaveless.

The sequences of simplicial complexes along the filtrations are represented in fig. 2.7 and fig. 2.8 on pages 45 and 46. The zero-persistence diagrams of those filtrations are represented in fig. 2.9 on page 47.

Correspondences are the following: Cl_G and Nb_G have always the same zero- persistence diagram in each filtration. In particular 2, 3, 4, 5, 6 have I as persistence diagram, while the filtration 1 has II. El_G shows III as a persistence diagram for filtrations 3, 5 and 6, IV for 1 and 4, and V for the filtration 2.

Cl_G and Nb_G zero-persistence diagrams give only information about the connection of the subgraph considered. The number of connected components at the beginning of the filtration is exactly equal to the number of vertices of G. This number decrease along the filtration down to 1, reached at the j^{th} step, when the graph G_j is connected. This number j is equal to 3 for every filtration except 2, where j is 4.

Since the only information retrieved from the zero-persistence of the simplicial complexes of Cl_G and Nb_G is only about connected components of the original graph, the zero-persistence diagrams of Cl_G and Nb_G are always equal (in fact the connected components in Cl_G and Nb_G are made of the same vertices). This is not the case for the one-persistence diagrams: the first homology group of the complex of cliques and of the complex of neighbours may be different. For example, consider the class of isomorphic graphs (*i*) in fig. 2.6: the complex of cliques is a 4-cycle (thus H_1 is non-trivial), while the complex of neighbours is a hollow tetrahedron (thus H_1 is trivial, but, H_2 is not).

As for the enclaveless, isolated vertices of G do not represent a connected component in El_G. So the persistence diagram is different: at the beginning G_0 is made of isolated vertices and thus El_{G_0} is the empty complex; two connected components arise together with the first edge of the filtration (this way there are two dominant set whose complementary has at least one element).

In particular that first edge determines the first two connected components that will eventually merge to a single connected component. This merging occurs in different steps of the three filtrations: second step in diagram III, third step in diagram IV, and fourth step in diagram V.

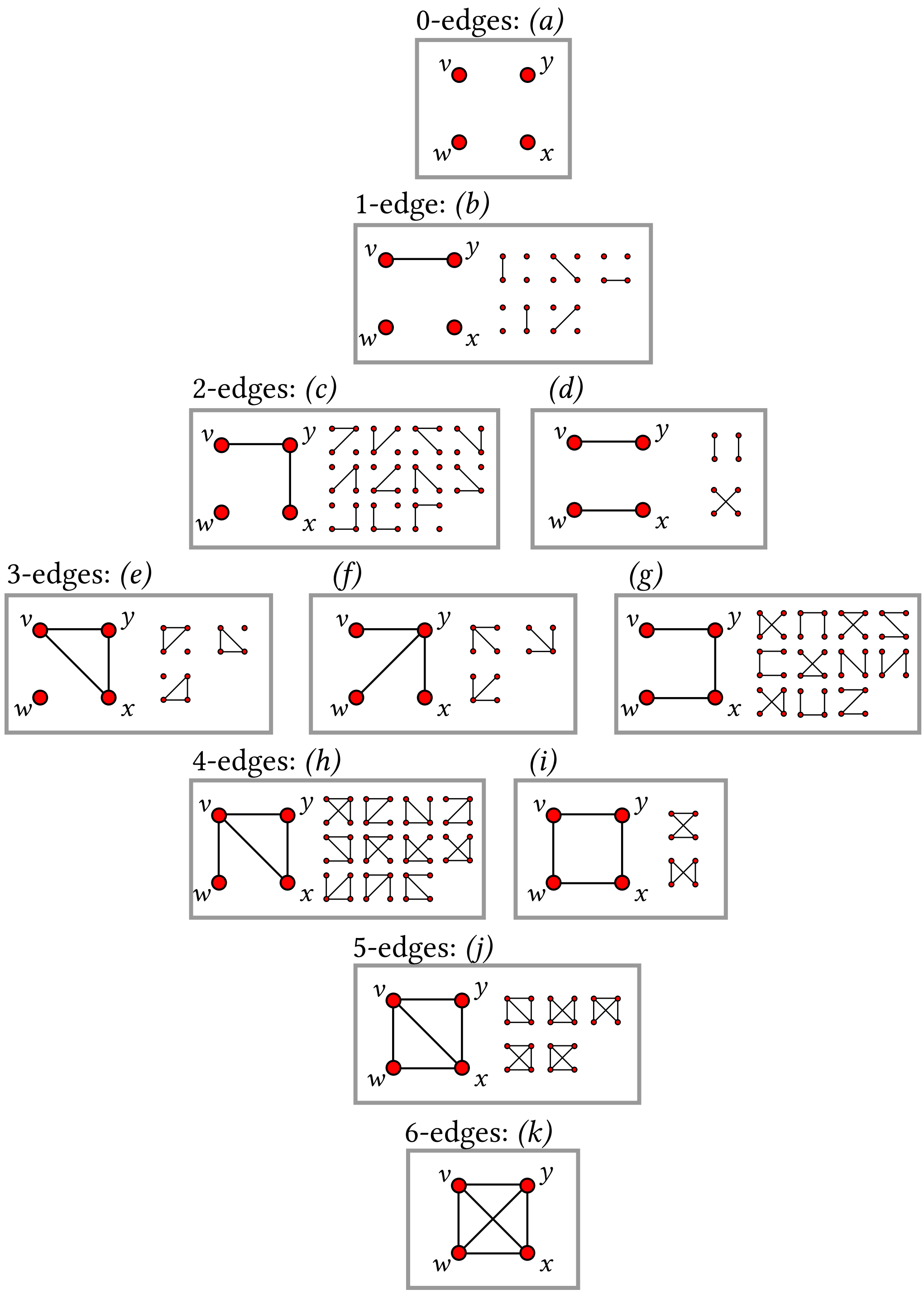


Figure 2.3: The 11 equivalence classes of isomorphic graphs on 4 vertices. The representative we will refer to is the biggest.

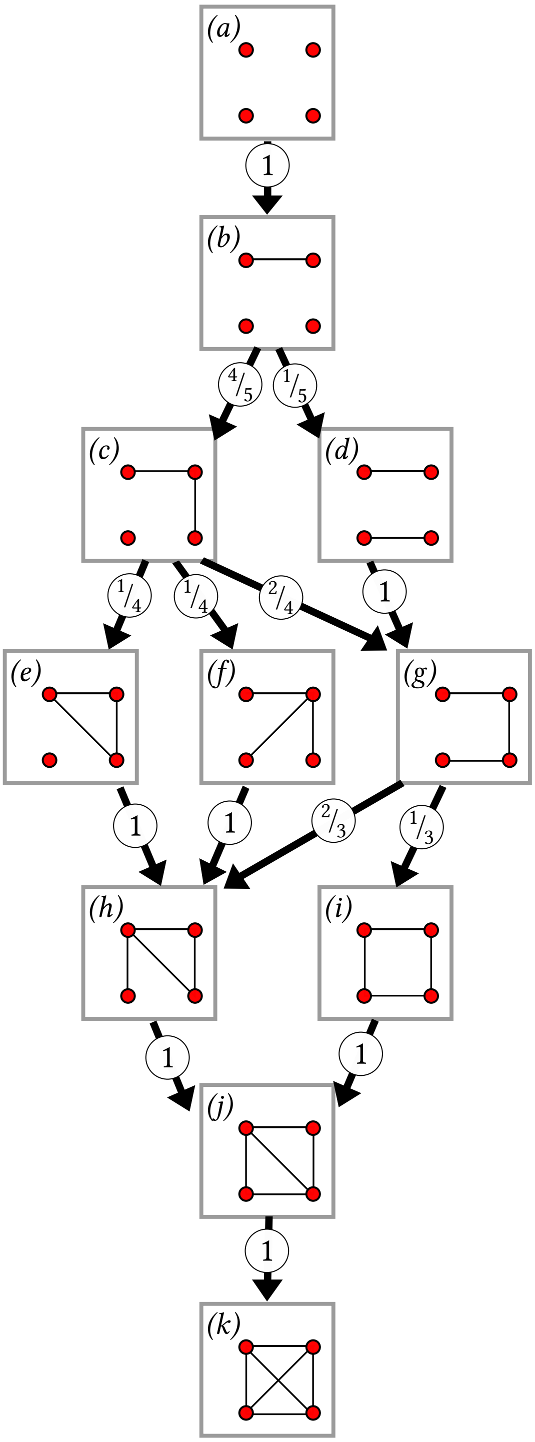


Figure 2.4: The oriented graph D. Vertices are the equivalence classes of graphs on 4 vertices, while arrows represent the insertion of an edge in the graph. Arrows are labelled with their probabilities.

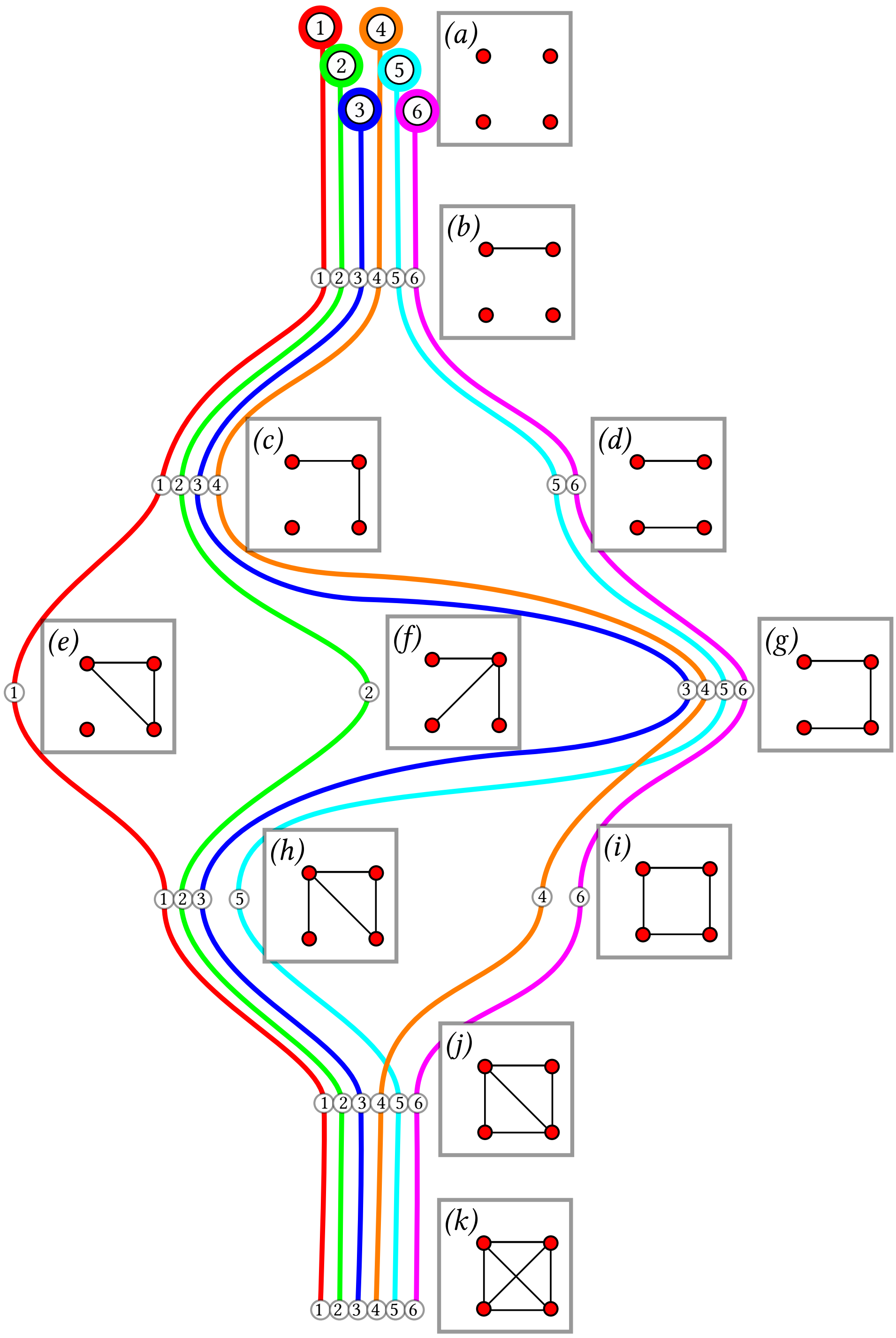


Figure 2.5: The 6 filtrations on the edges of K_4, or, equivalently, paths from (a) to (k) in D.

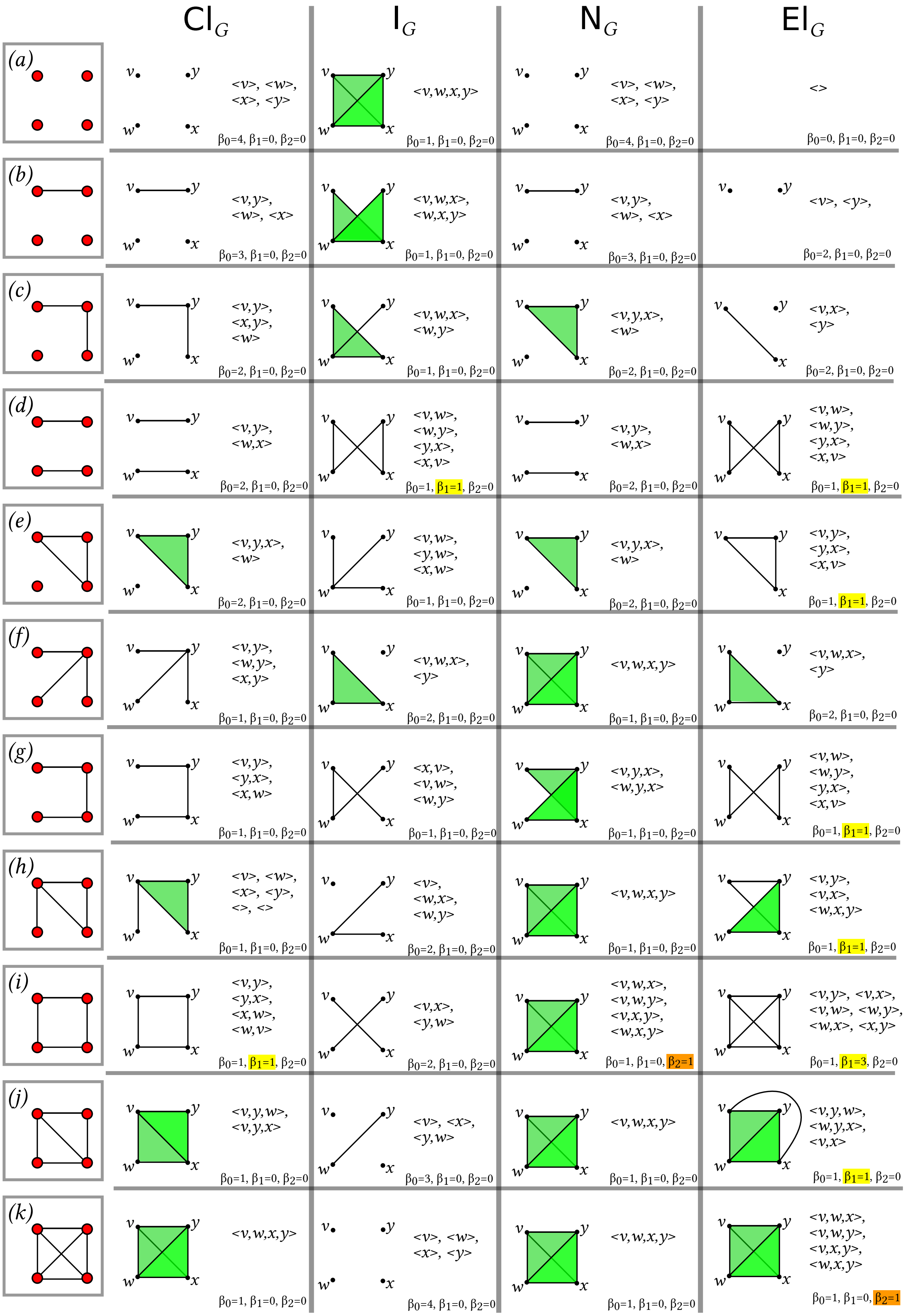

Cl_G
I_G
N_G
El_G
(a)
<v>, <w>, <x>, <y>
β0=4, β1=0, β2=0
<v,w,x,y>
β0=1, β1=0, β2=0
<v>, <w>, <x>, <y>
β0=4, β1=0, β2=0
<>
β0=0, β1=0, β2=0
(b)
<v,y>, <w>, <x>
β0=3, β1=0, β2=0
<v,w,x>, <w,x,y>
β0=1, β1=0, β2=0
<v,y>, <w>, <x>
β0=3, β1=0, β2=0
<v>, <y>,
β0=2, β1=0, β2=0
(c)
<v,y>, <x,y>, <w>
β0=2, β1=0, β2=0
<v,w,x>, <w,y>
β0=1, β1=0, β2=0
<v,y,x>, <w>
β0=2, β1=0, β2=0
<v,x>, <y>
β0=2, β1=0, β2=0
(d)
<v,y>, <w,x>
β0=2, β1=0, β2=0
<v,w>, <w,y>, <y,x>, <x,v>
β0=1, β1=1, β2=0
<v,y>, <w,x>
β0=2, β1=0, β2=0
<v,w>, <w,y>, <y,x>, <x,v>
β0=1, β1=1, β2=0
(e)
<v,y,x>, <w>
β0=2, β1=0, β2=0
<v,w>, <y,w>, <x,w>
β0=1, β1=0, β2=0
<v,y,x>, <w>
β0=2, β1=0, β2=0
<v,y>, <y,x>, <x,v>
β0=1, β1=1, β2=0
(f)
<v,y>, <w,y>, <x,y>
β0=1, β1=0, β2=0
<v,w,x>, <y>
β0=2, β1=0, β2=0
<v,w,x,y>
β0=1, β1=0, β2=0
<v,w,x>, <y>
β0=2, β1=0, β2=0
(g)
<v,y>, <y,x>, <x,w>
β0=1, β1=0, β2=0
<x,v>, <v,w>, <w,y>
β0=1, β1=0, β2=0
<v,y,x>, <w,y,x>
β0=1, β1=0, β2=0
<v,w>, <w,y>, <y,x>, <x,v>
β0=1, β1=1, β2=0
(h)
<v>, <w>, <x>, <y>, <>, <>
β0=1, β1=0, β2=0
<v>, <w,x>, <w,y>
β0=2, β1=0, β2=0
<v,w,x,y>
β0=1, β1=0, β2=0
<v,y>, <v,x>, <w,x,y>
β0=1, β1=1, β2=0
(i)
<v,y>, <y,x>, <x,w>, <w,v>
β0=1, β1=1, β2=0
<v,x>, <y,w>
β0=2, β1=0, β2=0
<v,w,x>, <v,w,y>, <v,x,y>, <w,x,y>
β0=1, β1=0, β2=1
<v,y>, <v,x>, <v,w>, <w,y>, <w,x>, <x,y>
β0=1, β1=3, β2=0
(j)
<v,y,w>, <v,y,x>
β0=1, β1=0, β2=0
<v>, <x>, <y,w>
β0=3, β1=0, β2=0
<v,w,x,y>
β0=1, β1=0, β2=0
<v,y,w>, <w,y,x>, <v,x>
β0=1, β1=1, β2=0
(k)
<v,w,x,y>
β0=1, β1=0, β2=0
<v>, <w>, <x>, <y>
β0=4, β1=0, β2=0
<v,w,x,y>
β0=1, β1=0, β2=0
<v,w,x>, <v,w,y>, <v,x,y>, <w,x,y>
β0=1, β1=0, β2=1

Figure 2.6:

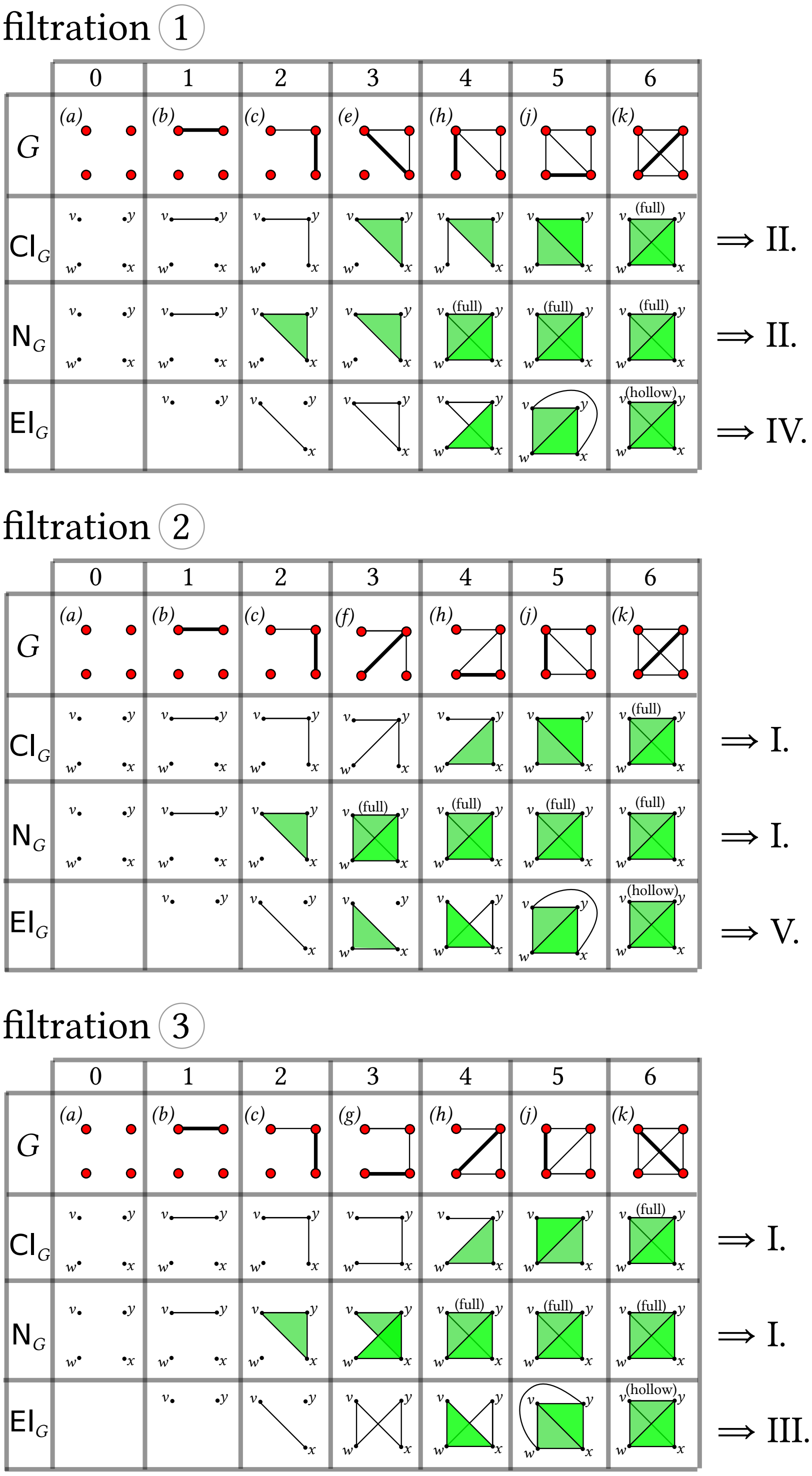


Figure 2.7: Three filtrations on the graph K_4 and the respective sequences of simplicial complexes Cl_G, Nb_G and El_G. The edge added in each step to the graph is highlighted by a thicker line. The roman numbers indicate which zero-persistence diagram in fig. 2.9 correspond to the sequence of simplicial complexes.

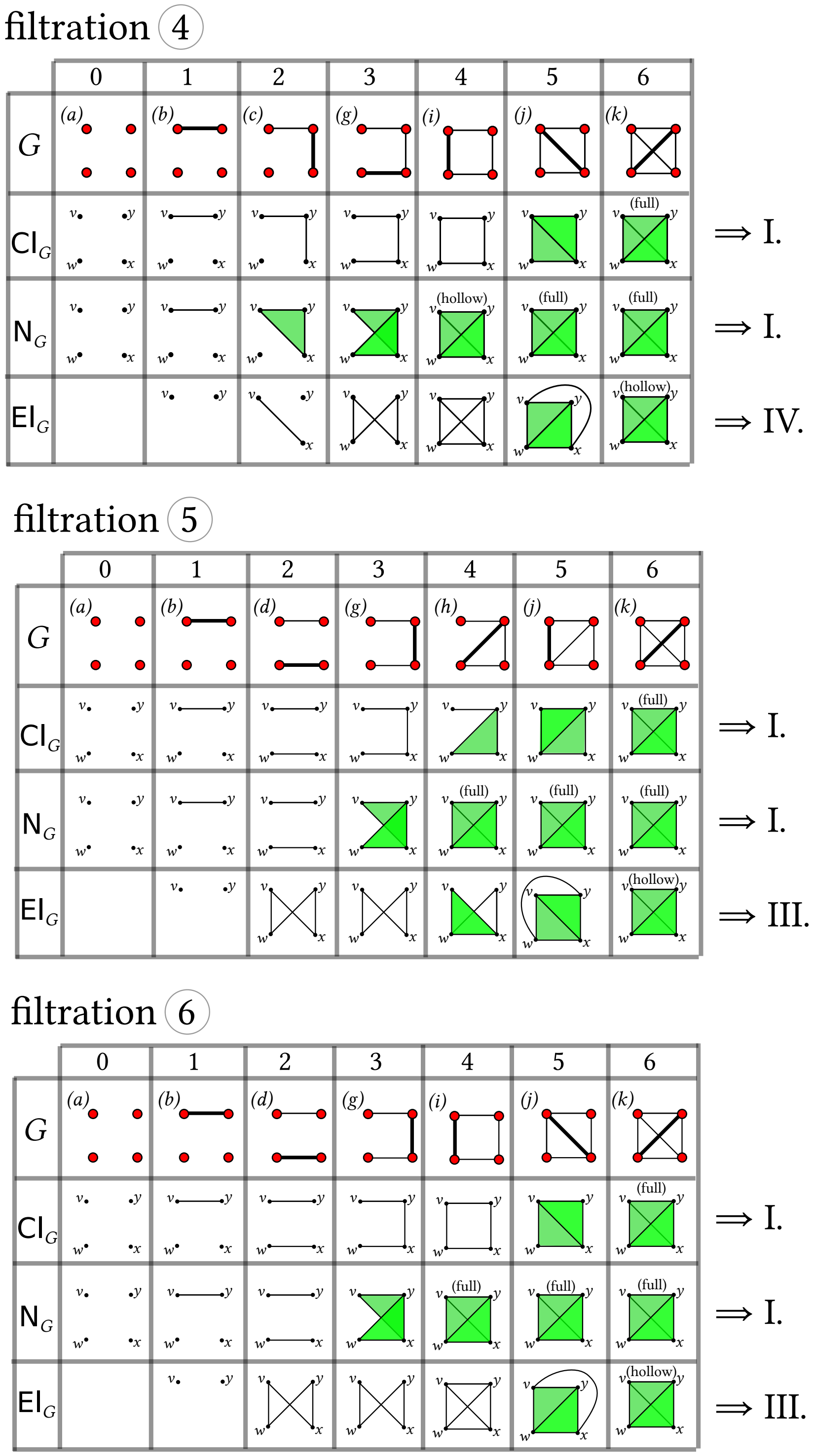


Figure 2.8: Three filtrations on the graph K_4 and the respective sequences of simplicial complexes Cl_G, Nb_G and El_G. The edge added in each step to the graph is highlighted by a thicker line. The roman numbers indicate which zero-persistence diagram in fig. 2.9 correspond to the sequence of simplicial complexes.

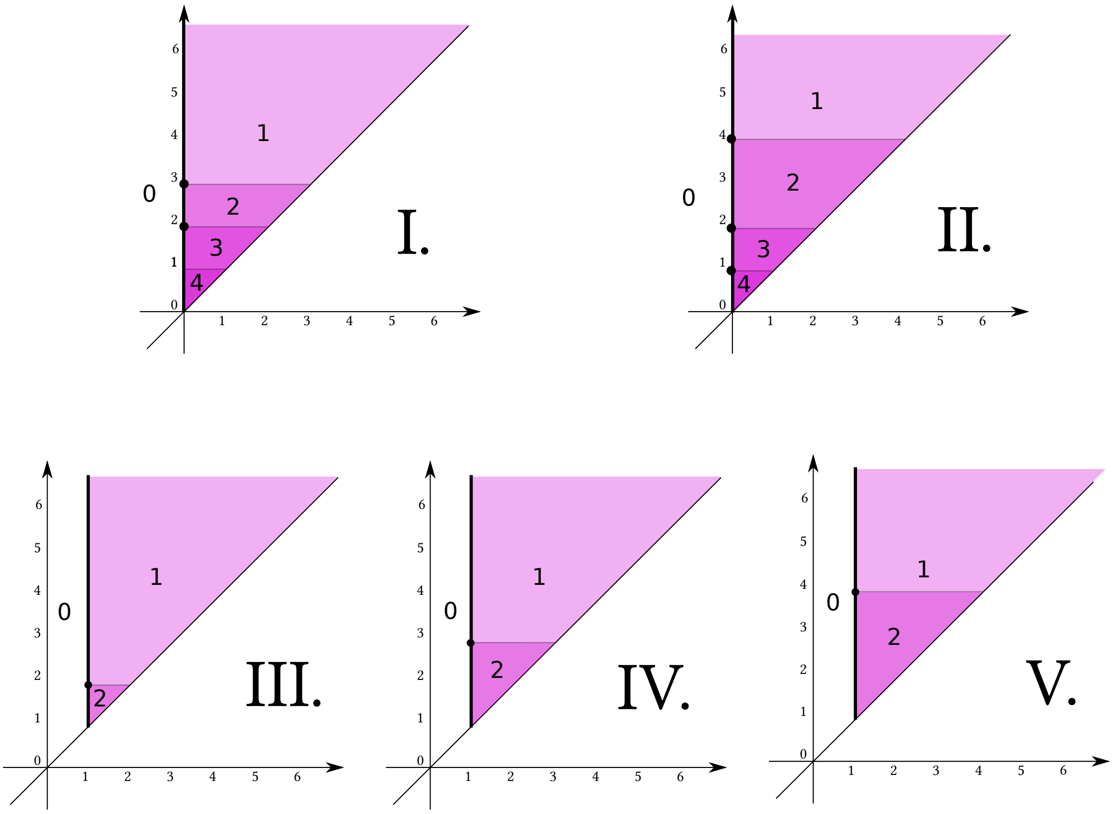


Figure 2.9: Zero-persistence diagrams for the filtrations on K_4 showed in fig. 2.7 and fig. 2.8. (I): this persistence diagram is the result of the filtrations ②, ③, ④, ⑤ and ⑥ on the complexes Cl_{G_i} and Nb_{G_i}. (II): this persistence diagram is the result of the filtration ① on the complexes Cl_{G_i} and Nb_{G_i}. (III): this persistence diagram is the result of the filtrations ③, ⑤ and ⑥ on the complex El_{G_i}. (IV): this persistence diagram is the result of the filtrations ① and ④ on the complex El_{G_i}. (V): this persistence diagram is the result of the filtration ② on the complex El_{G_i}.

2.2.2 Filtration on edge-induced subgraphs: a simple example

In order to show persistence diagrams with more interesting features we define a new kind of filtration. In this filtration we consider only the graph induced by the edges considered so far. Formally:

$$\tilde{G}_i = \left(\{v \in V | v \in e \in w^{-1}(\{1 \dots, i\})\}, w^{-1}(\{1, \dots, i\})\right)$$

In practice the difference with the previous filtration G_i is only on isolated vertices, that are not considered as vertices of G_i any more. This allows, once we consider the birth of connected components in $\mathsf{Cl}_{\tilde{G}_i}$, $\mathsf{Nb}_{\tilde{G}_i}$ and $\mathsf{El}_{\tilde{G}_i}$ to be spread over time, while the birth of all the connected components of Cl_{G_i}, Nb_{G_i} was at the 0-th step of the filtration.

We provide a couple examples of two such filtrations on a particular graph. See fig. 2.10 and fig. 2.11.

2.2.3 Complexes from acyclic subsets and persistent homology

These simplicial complexes are not very well suited for persistence studies via a filtration of edges. Here are some reasons.

The complex of induced acyclic subgraphs. This complex is not stable under the addition of edges. The problem is that if we add a further edge to the graph that edge could be part of a cycle. So a set of vertices that previously induced an acyclic set may not induce an acyclic set any more. To study the persistence of a complex we must show a filtration (a sequence of nested simplicial complexes) and the complex of induced acyclic subgraphs does not provide one if we progressively add edges.

The complex of acyclic edge subsets To study a filtration on this complex means that in every step a new 0-simplex is added to the simplicial complex. This means that our simplicial complex may be much more complicated than the graph we started from.
For example: K_n has n vertices and $\binom{n}{2}$ edges (growing like n^2 asymptotically), while its complex of acyclic edge subsets have $\binom{n}{2}$ 0-simplices and $\binom{\binom{n}{2}}{2}$ 1-simplices (growing like n^4 asymptotically).

The complex of removable acyclic subgraphs. The biggest drawback for the study of persistence of this complex is that we can not build this simplicial complex unless this graph is connected. And this is not the case at the beginning of a filtration of the edges of a graph. So we should start the filtration by already providing a connected subgraph.

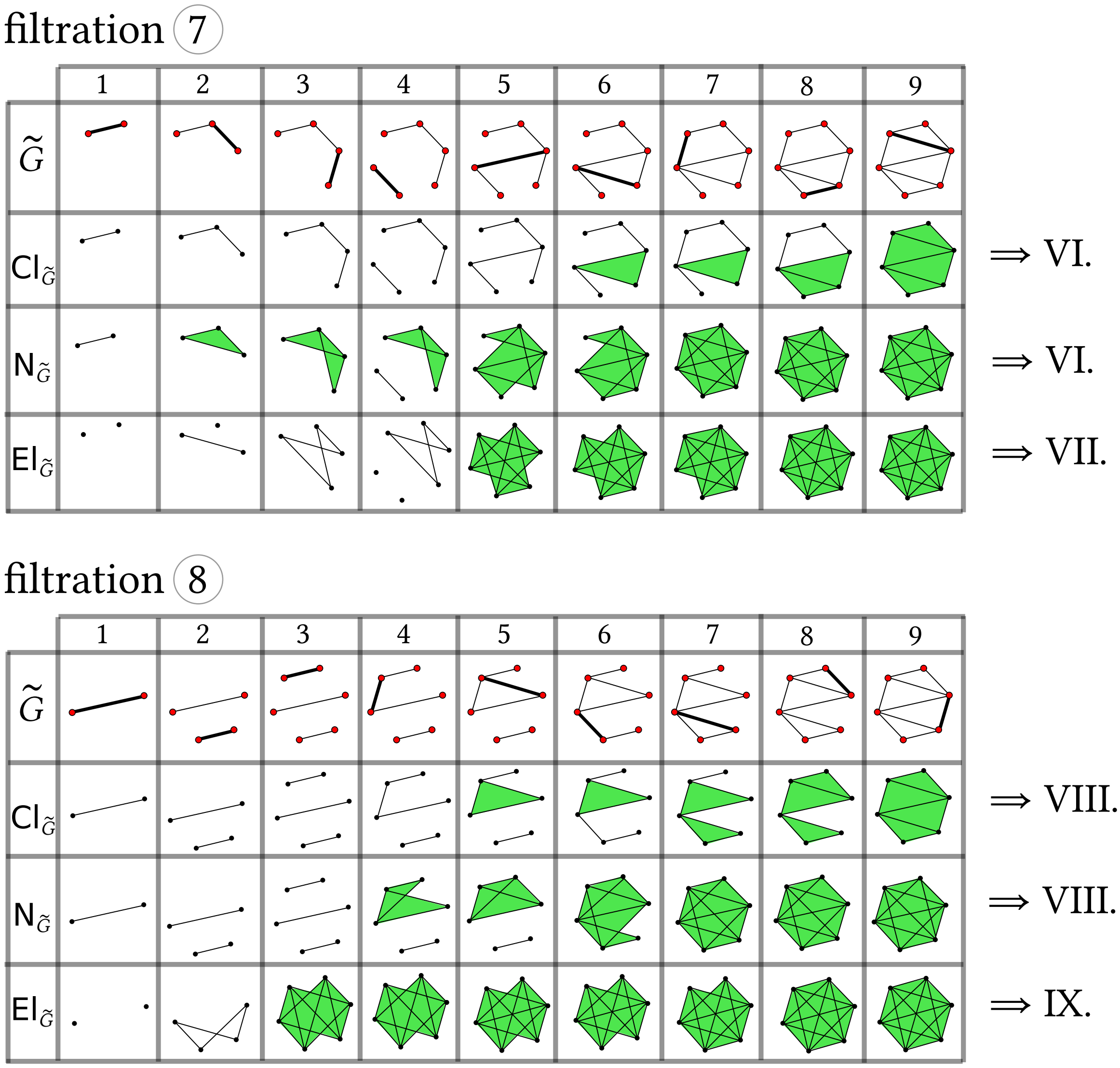


Figure 2.10: Two filtrations on a graph on six vertices, and the respective sequences of simplicial complexes Cl_G, Nb_G and El_G. The edge added in each step is highlighted by a thicker line. The roman numbers indicate which zero-persistence diagram in fig. 2.11 correspond to the sequence of simplicial complexes.

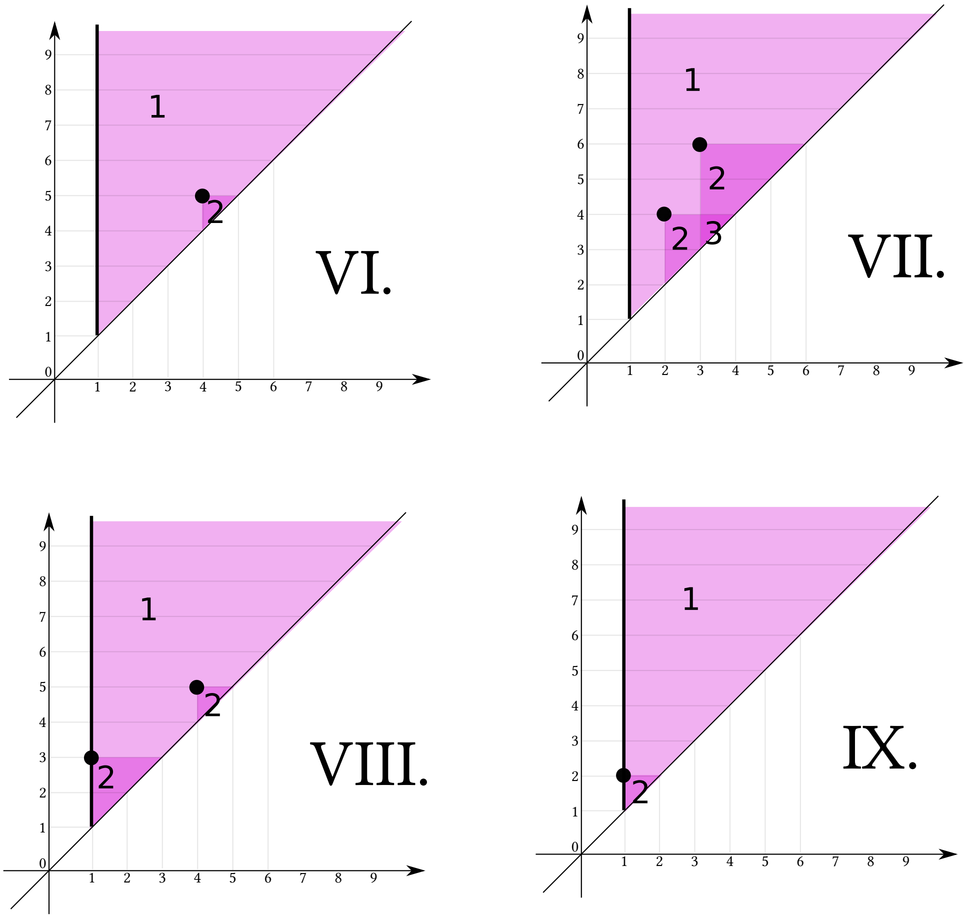


Figure 2.11: Zero-persistence diagrams for the filtrations of fig. 2.10. (VI): this persistence diagram is the result of the filtration ⑦ on the complexes $\mathsf{Cl}_{\tilde{G}_i}$ and $\mathsf{Nb}_{\tilde{G}_i}$. (VII): this persistence diagram is the result of the filtration ⑦ on the complex $\mathsf{El}_{\tilde{G}_i}$. (VIII): this persistence diagram is the result of the filtration ⑧ on the complexes $\mathsf{Cl}_{\tilde{G}_i}$ and $\mathsf{Nb}_{\tilde{G}_i}$. (XI): this persistence diagram is the result of the filtration ⑧ on the complex $\mathsf{El}_{\tilde{G}_i}$

2.3 Other Persistent properties: blocks and edge-blocks

In this section we are going to consider new persistent properties of the weighted graph $G = (V, E, w)$. Now we do not consider any simplicial complex or persistent homology features. We would like to consider a more general setting to talk about "persistence" which preserves the core idea: we have a filtration on the considered object and we observe specific features that *are born* and *die* in a specific step of the filtration, where we consider more informative the features that last longer along the filtration.

We start with some useful definitions.

Definition 57. Let $G = (V, E)$ be graph.

- If every subgraph of G obtained deleting any $k - 1$ vertices (and incident edges) is connected, then G is a *k-connected graph* (or: k-vertex connected). For equivalent characterisation in terms of paths between vertices see [6, theorem 5.1, theorem 9.7].

- A *cut vertex* is a vertex $v \in V$ whose deletion (along with incident edges) increase the number of connected components of G.

- A *block* is a connected graph which does not contain any cut vertex. A block of a graph G is a maximal subgraph H such that H is a block.

- A connected graph with at least one cut vertex is called a *separable graph.*

- If every subgraph $G' = (V, E \setminus X)$ is connected for all $X \subset E$ where $|X| < K$, then G is a *k-edge-connected graph.* For equivalent characterisation in terms of cycles and paths between vertices see [6, proposition 3.2, theorem 9.7].

- A *bridge* (or *cut edge*) is a edge $e \in E$ whose deletion increase the number of connected components of G.

- An *edge-block* is a connected graph which does not contain any bridge (*bridgeless component* in the literature.

Cut edges deletion increase the number of connected components by 1. Cut vertices deletion instead can raise the number of connected components by n for every $n \in \mathbb{N}$.

Blocks are of two kind: $K_2 = (\{a, b\}, \{a, b\})$ (called the *trivial block*), or a connected graph where every edge is contained in at least one cycle.

2.3.1 The persistent block number

Lemma 58. Let $G = (V, E)$. The relation $\sim$ on the edge set:

$$\begin{aligned} e \sim f \iff & \text{ there exists a simple cycle in } G \text{ containing both } e \text{ and } f\text{, or } e = f \\ \iff & \text{ there exist two distinct paths in } G \text{ from } e \text{ to } f\text{, or } e = f \end{aligned}$$

is an equivalence relation on E and the subgraphs formed by the edges in each equivalence class are the blocks of G.

Proof. The equivalence between the two definitions given for the relation is straightforward. The relation is reflexive and symmetric. Moreover it is transitive: if there exist a simple cycle containing e and f and a simple cycle containing f and g, then it is possible to combine those cycles (deleting the common edges) in a simple cycle containing e and g. □

Remark 59. The lemma 58 implies that the blocks of a graph $G = (V, E)$ induce a partition on the edge set, but vertices can be shared among the blocks. Those vertices are exactly the cut vertices of G.

Let $G = (V, E)$ be a graph and let $B_1, \dots, B_p$ be the partition of E induced by the blocks in G. There are three possibilities when we add a further edge e, obtaining the graph $G' = (V, E \cup \{e\})$:

- e is not part of any cycle in G', and thus e becomes the only representative of a new block B_{p+1};
- e becomes part of cycles whose other edges are all in the same class B_i. In this case e is added to the class B_i.
- e becomes part of one or more cycles whose other edges range in a number of other classes $\{B_i\}_{i\in I}$, where $I \subset \{1, \dots, p\}$. In this case those classes of edges are merged in a new block $\bar{B} = \{e\} \cup \bigcup_{i\in I} B_i$

In particular, notice that two edges that were in the same class before adding e, are still in the same class after the insertion.

This means that we can track when a block was born or died along the filtration of a graph the same way we did for cycles along a filtration of a simplicial complex in persistent homology. Here when we say that a certain block “die” we mean that after the insertion of e the block joins another elder block.

Let us now consider a weighted graph $G = (V, E, w)$ and the induced subgraphs filtration. For every $a \in \mathbb{R}$, $E_a = w^{-1}((-\infty, a])$, the edge set of G_a, is partitioned in the blocks of G_a. In particular we have that, for $a < b$, if e_1, e_2 belong to the same block in E_a, they are still in the same block of E_b.

Example. We provide an example of a filtration on a graph and its block persistence diagram (see fig. 2.12). Note that we only considered the blocks of the subgraph induced by the already filtered edges. The reason we did not consider isolated vertices as blocks is due to the fact that blocks induce an equivalent relation on the edge set, not on the vertex set. In fact each vertex could belong to distinct blocks at the same time.

2.3.2 The persistent edge-block number

This case is very similar to the persistent block number, only speaking of vertices instead of edges, with some small differences.

Lemma 60. Let $G = (V, E)$. The relation $\dot{\sim}$ on the vertex set:

$$\begin{aligned} v \dot{\sim} w &\iff \text{there exist a simple cycle in } G \text{ containing both } v \text{ and } w\text{, or } v = w \\ &\iff \text{there exist two distinct paths in } G \text{ from } v \text{ to } w\text{, or } v = w \end{aligned}$$

is an equivalence relation on V and the subgraphs formed by the vertices in each equivalence class are the edge-blocks of G.

Proof. Equivalent to the proof given for lemma 58 □

Let $G = (V, E)$ be a graph and $V_1, \dots, V_p$ is the partition of V induced by the edge-blocks in G. There are three possibilities when we add a further edge e, obtaining the graph $G' = (V, E \cup \{e\})$:

- e is not part of any cycle in G', or e becomes part of cycles whose vertices are all in the same class V_i: in this case the partition of V does not essentially change;

- e becomes part of one or more cycles whose vertices range in a set of classes $\{V_i\}_{i \in I}$, where $I \subset \{1, \dots, p\}$. In this case those classes of vertices are merged in a new edge-block $\bar{V} = \bigcup_{i \in I} V_i$

If two vertices were in the same class before adding e, then they are still in the same class after the insertion.

Let us now consider a weighted graph $G = (V, E, w)$ and the induced subgraphs filtration. For every $a \in \mathbb{R}$, $E_a = w^{-1}((-\infty, a])$, the vertex set of G_a, is partitioned in the edge-blocks of G_a. In particular we have that, for $a < b$, if v_1, v_2 belong to the same edge-blocks in G_a, they are still in the same edge-blocks of G_b.

Example. We provide an example of persistence edge-blocks diagram (see fig. 2.13) based on the same graph and the same filtration of fig. 2.12. In this case we could use both the persistence methods of section 2.2.2 and section 2.2.1. In fact the equivalence relation $\dot{\sim}$ induced by the edge-blocks is on the vertices. So we can consider each vertex at the beginning of the filtration as an edge-block (diagram XI) either or we can consider only the subgraph induced by the already filtered edges (diagram XII).

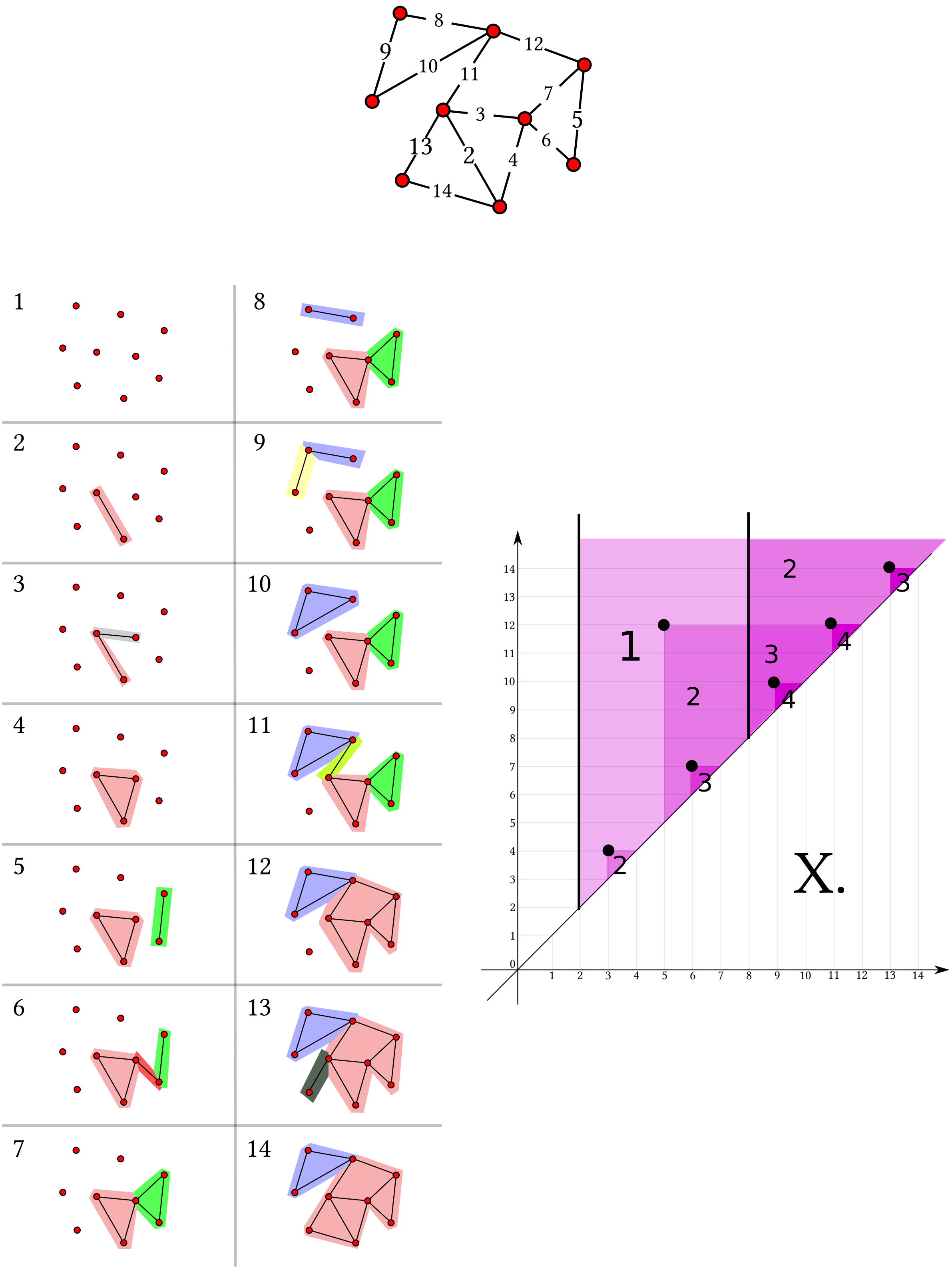


Figure 2.12: Example of a filtration on a graph, where the equivalence classes for the relation ~ on the the edge set are highlighted in different colors throughout the filtration. (X): this is the persistence block diagram based on the subgraphs $\tilde{G}_i$, so isolated vertices are not considered as blocks.

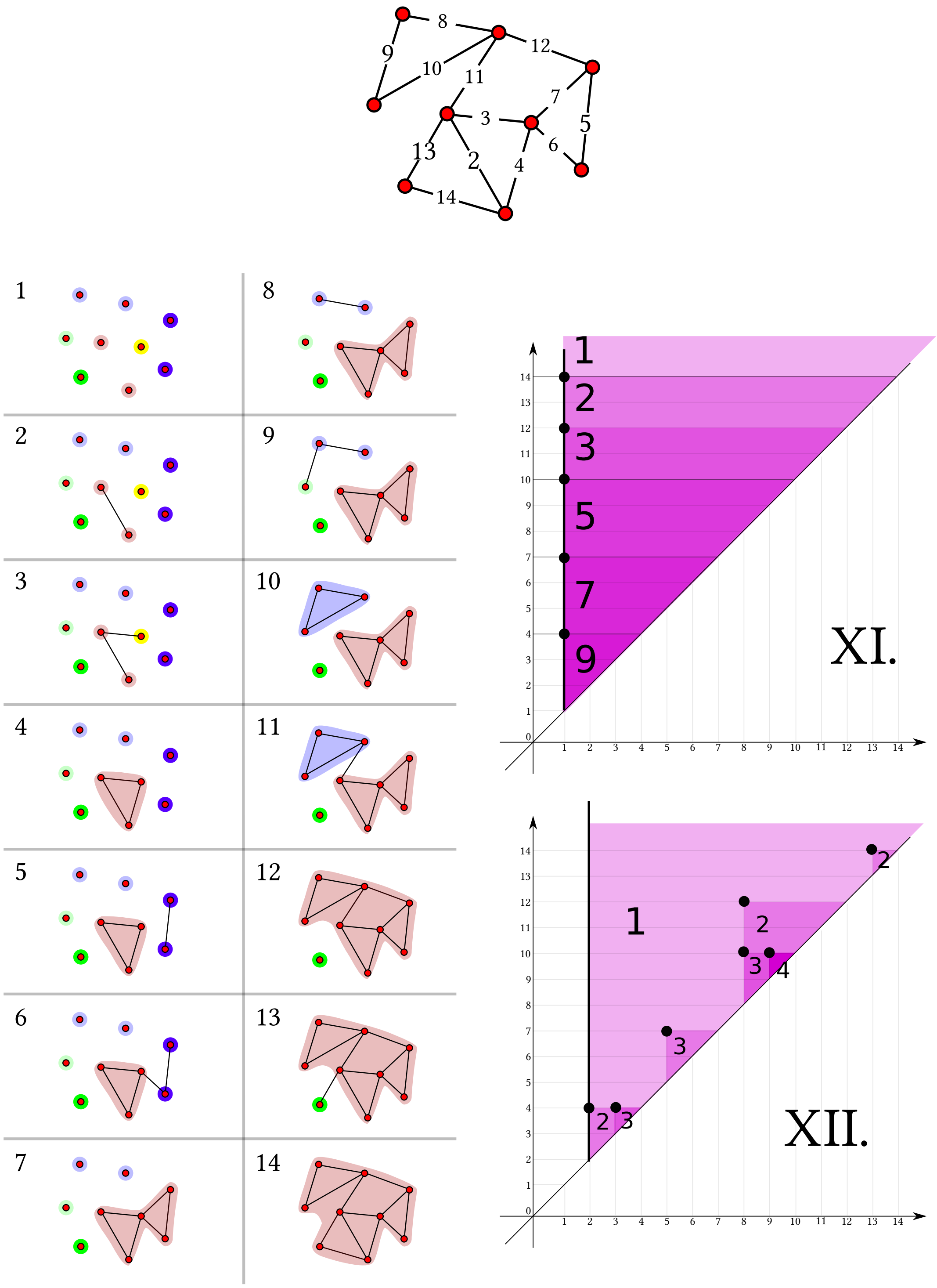


Figure 2.13: Example of a filtration on a graph, where the equivalence classes for the relation $\dot{\sim}$ on the vertex set are highlighted in different colors throughout the filtration. (XI): this is the persistence edge-block diagram based on the subgraphs G_i, so isolated vertices were considered as edge-blocks. (XII): this is the persistence edge block diagram based on the subgraphs $\tilde{G}_i$, so isolated vertices where not considered as edge-blocks.

Chapter 3

Other methods to build simplicial complexes

Contents

In many of the methods we analysed so far we lose much topological information. For this reason this chapter is dedicated to two other methods to build simplicial complexes from a graph. The features of those simplicial complexes are useful to retrieve some topological properties of the original graph.

3.1 The complex of k-cycles $\mathsf{Cy}_{j,k}(G)$

Definition 61. Let $G = (V, E)$ be a graph and j, k be integers such that $j \geq 1$, $k \geq 3$. We define the complex of j-woven k-cycles $\mathsf{Cy}_{j,k}(G)$ as follows:

- Every cycle of length k in G represents a 0-simplex of $\mathsf{Cy}_{j,k}(G)$.
- Let σ be a set of k-cycles. σ represents a simplex if all the cycles in σ share at least j vertices.

We note that $\mathsf{Cy}_{j,k}(G)$ does not contain any information about any part of G that is not included in a certain cycle of lenght k. In particular, if G is acyclic, $\mathsf{Cy}_{j,k}(G) = \emptyset$ for every j and k.

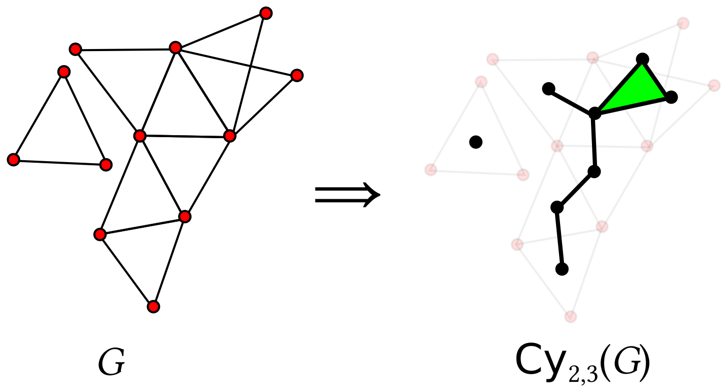


Figure 3.1:

The analysis of $\mathsf{Cy}_{j,k}(G)$ provides some local informations about G. Here we list some examples.

- If exists an odd k such that $\mathsf{Cy}_{j,k}(G) \neq \emptyset$, then G is not bipartite.
- Let $j = 1$. Then every n-simplex in $\mathsf{Cy}_{1,k}(G)$ with $n \geq 1$ represents a vertex shared by two or more k-cycles. So we can label every n-simplex σ with the names of the vertices that σ is representing. Letting k vary and detecting the simplices labelled with a given vertex name, we have a measure on how much that vertex affect the connectivity of the cyclic part of G.
- Analogously let j be fixed. Then every n-simplex in $\mathsf{Cy}_{j,k}(G)$ with $n \geq 1$ represents a specific set of j vertices shared by two or more k-cycles. Labelling every n-simplex σ with the names of the sets that σ is representing and letting k vary provides information about how much a certain set of vertices affect the connectivity of the cyclic part of G.

Persistent homology. This complex is suitable to the study of persistent homology along a filtration on the edges of G, either or studying the persistence letting the index j decrease (the index j represents the interconnection among cycles). In fact, if k is fixed and j decreases, we have that a set of 0-simplices (representing a set of k-cycles) is a simplex in $\mathsf{Cy}_{j+1,k}(G)$ if those cycles share at least $j + 1$ vertices pairwise. So they obviously share at least j vertices pairwise. Thus $\mathsf{Cy}_{j+1,k}(G) \subset \mathsf{Cy}_{j,k}(G)$ and this induces a filtration on the simplicial complex $\mathsf{Cy}_{1,k}(G)$.

On the other hand variations of k are not suitable to the study of persistence. In fact, changing the length of cycles k, the 0-skeleton of the complex changes completely every time we change k, and we are not able to compare simplicial complexes is k is different.

Remark 62. There is a further generalization of this method. We built $\mathsf{Cy}_{j,k}(G)$ with a graph (that is a simplicial complex of dimension 1) as a starting point and searching for sequences of edges forming a cycle (those are one dimensional homologic cycles). Analogously we could start from a simplicial complex K, search for n-dimensional homologic cycles of size k and arrange them in the simplicial complex $\mathsf{Cy}_{n,j,k}(K)$. n-dimensional homologic cycles of size k are the 0-simplices, while a set of cardinality $(m + 1)$ of those 0-simplices is a m-simplex if those cycles share at least j simplices of dimension n pairwise.

3.2 The complex of connected cliques

This simplicial complex may be useful to "lower" the resolution of the graph: every maximal clique is replaced with a 0-simplex and connected to the other cliques according to the number of shared vertices.

Definition 63. We say that a set C is a *maximal clique* in the graph G, if there is no other clique in G that strictly contains C.

The complex of *connected cliques sharing j vertices* of a graph G is the complex $\mathsf{CCl}_j(G)$ where every maximal clique is a weighted 0-simplex with weight equals to the order of the clique. A set of maximal cliques generates a simplex if those cliques share at least j vertices pairwise.

- We have inhomogeneity among the 0-simplices of the complex, since each of them could represent a clique of different dimension. This could lead to a big disparity in the representation of the original graph. According to one's purpose and to the type of graphs that must be examined, it is possible to avoid this problem in the following way: we chose $m \in \mathbb{N}$ and we only consider maximal cliques of order less than m as 0-simplices. One should be aware that, if m is small our aim of "lowering the resolution" of the graph wuold be lost, since the 1-skeleton of the complex could be even more complex than the original graph.

- this is a good method to lower the resolution of the graph if the complex is *"clique-decomposable"*, that is: if every maximal clique shares at most one vertex with any other maximal cliques of the graph, then $\mathsf{CCl}_1(G)$ is a good approximation for the topological shape of the graph (see fig. 3.2). This could be generalised to the case where all the maximal cliques share at least m vertices. In this case, $\mathsf{CCl}_m(G)$ could be the most useful complex.

Persistent homology. For our purposes this method is not stable if we want to operate through a filtration of edges, since maximal cliques (our 0-simplexes) are not preserved along the filtration.

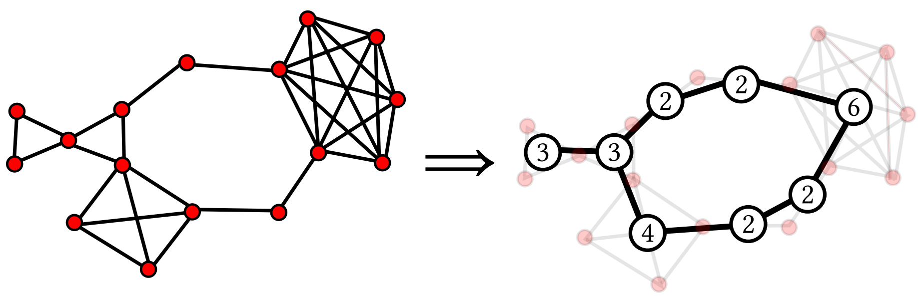


Figure 3.2: Example of a clique decomposable graph and its complex of connected cliques $\mathsf{CCl}_1(G)$

Conclusions and further developments

In this work we analysed several methods to associate simplicial complexes to graphs. In particular we focused on well studied complexes (such as the complex of cliques or the complex of neighbours), and suggested some novel methods (such as the complex of enclaveless sets).

Then we introduced a persistent homology approach to the study of weighted graphs, represented with simplicial complexes via the aforementioned methods. In particular we studied simple examples of filtrations on graphs and we represented their zero-persistence diagrams.

We applied the core ideas of persistence theory in the new context of graph theory. We suggested that the study of graph invariants along a non-decreasing sequence of graphs could be a fruitful instrument for the analysis of graphs. To this regards we defined the persistent block number and the persistent edge-block number. We applied these concepts to a simple weighted graph, to exemplify the behavior of such tools.

Finally we proposed two methods to build simplicial complexes from a graph in a way that could preserve interesting topological information.

This was an introductory work and we had to make many choices to decide where to aim our efforts. The field seems promising and there are various aspects that are worthy of a deeper study. There are some features we met in our investigation that are worth of deeper investigation.

For example the concept of graph persistence. we scratched the surface with blocks and edge-blocks persistence, but other invariants can be studied in a similar way.

In chapter 1 we narrowed down to seven the number of inquired methods. This is a very small number compared to how many ways there are to build a graph complex, and each of them could provide a specific topological insight on the features of the graph.

The fig. 2.4 represents the Markov chain which models the filtrations on the complete graph K_4. The study of filtrations with a probabilistic approach on filtrations could provide statistical models for graphs whose homologic persistence could be otherwise difficult to compute.

Finally, since there are many simplicial complexes associable to a single graph we could find interesting comparisons of persistent homology features along the filtration for pairs of complexes. For example using parallel persistence diagrams. This could be particularly interesting when simplicial complexes are somewhat mirroring each other, as in the case of cliques and independent sets.

Appendix

Python Code

In our code we employed the NetworkX software package. Documentation is avaliable at:

http://networkx.readthedocs.io/en/stable/index.html

We transcribe now part of the code implemented during our work.

Minimal dominating sets

Here is the code used to find maximal enclaveless sets as complementary of minimal dominating sets.

```
def find_min_dom_sets(G):
    import networkx as nx
    import numpy as np
    import copy

    #first 100 prime numbers:
    primes=[2, 3, 5, 7, 11, 13, 17, 19, 23, 29,
            31, 37, 41, 43, 47, 53, 59, 61, 67,
            71, 73, 79, 83, 89, 97, 101, 103, 107,
            109, 113, 127, 131, 137, 139, 149, 151, 157,
            163, 167, 173, 179, 181, 191, 193, 197, 199,
            211, 223, 227, 229, 233, 239, 241, 251, 257,
            263, 269, 271, 277, 281, 283, 293, 307, 311,
            313, 317, 331, 337, 347, 349, 353, 359, 367,
            373, 379, 383, 389, 397, 401, 409, 419, 421,
            431, 433, 439, 443, 449, 457, 461, 463, 467,
            479, 487, 491, 499, 503, 509, 521, 523, 541]
    #remapping node names in G: i --> i-th prime number
```

```
mapping=dict()
for i in G.nodes():
    mapping[i]=primes[i]

# bpi: BiggestPrimeIndex
bpi=i

H = nx.relabel_nodes(G,mapping)

#searching all dominating sets
v1=H.nodes()[0]
l=[v1]
for v2 in H.neighbors(v1):
    l.append(v2)
for v in H.nodes()[1:]:
    temp1=copy.deepcopy(l)
    temp2=[]
    temp2.append(v)
    for v2 in H.neighbors(v):
        temp2.append(v2)

    l=[]
    for i in temp1:
        for j in temp2:
            l.append(i*j)

    #deleting multiple vertices
    for m in range(len(l)):
        for n in primes[:bpi+1]:
            while(l[m]!=0 and l[m]%(n*n)==0):
                l[m] = l[m]/n
    #considering only minimal dominating sets
    for n in range(len(l)):
        for m in range(len(l)):
            if (m!=n and l[m]!=0 and l[n]%l[m]==0):
                l[n]=0
    while True:
        try:
            l.remove(0)
        except:
```

```
                break

    min_dom_sets=[]
    for i in l:
        temp=[]
        for j in G.nodes():
            if (i%primes[j]==0):
                temp.append(j)
        min_dom_sets.append(copy.deepcopy(temp))
    return min_dom_sets
```

Filtrations

```
'''
the following program describes the various possible filtrations
based on the complete graph on n vertices, draws the directed graph
associated to the filtration (nodes are class of graphs up-to-iso)
and studies the number of connected component along various filtrations
'''

import networkx as nx
import matplotlib.pyplot as plt
import Tkinter
import tkMessageBox
from Tkinter import *
import copy

def draw_graph(G):
    plt.clf()

    #possible layouts:
    pos=nx.circular_layout(G)
    #pos=nx.spring_layout(G)
    #pos=nx.spectral_layout(G)
    #pos=nx.fruchterman_reingold_layout(G)

    nx.draw(G,pos,node_size=300,picker=5.0)
    # labels
    nx.draw_networkx_labels(G,pos,font_size=10,font_family='sans-serif')
    plt.title('Possible filtrations on the complete '+str(n)+' graph')
    plt.show()
```

```
#initializer window: setting the number of nodes
start = Tkinter.Tk()
node_number = Label(start, text="Node number:").grid(row=0)
E1 = Entry(start)
E1.insert(END, 4)
E1.grid(row=0,column=1)
n=IntVar()

def nodes_init():
    global n
    n=int(E1.get()) # n = nodes of the graph
    start.destroy()

OK = Button(start, text="OK", width=10, command=nodes_init)
OK.grid(row=10,column=1)
start.mainloop()

print('Considering the '+str(n)+'-nodes graphs')

'''
from now on we dedicate to distinguish among the various filtrations
that are possible on this n-graph
'''

#number of graphs on n unlabeled nodes
#source: http://oeis.org/A000088
vertF = [1,
         1,
         2,
         4,
         11,
         34,
         156,
         1044,
         12346,
         274668,
         12005168,
         1018997864,
         165091172592,
```

```
         50502031367952,
         29054155657235488,
         31426485969804308768,
         64001015704527557894928,
         245935864153532932683719776,
         1787577725145611700547878190848,
         24637809253125004524383007491432768]


#"list" of our edges
C = nx.complete_graph(n)

#dictionary of adjacency matrices for ALL the graphs on n nodes
ad = dict()

#empty graph adjacency matrix
ad[0]= [[0 for x in range(n)] for y in range(n)]

#directed graph of possible flitrations:
F = nx.DiGraph()

#construction of the adjacency matrices
i=j=1
for e in C.edges():
    for g in range(0,j):
        ad[i]=copy.deepcopy(ad[g])
        ad[i][e[0]][e[1]]= 1
        ad[i][e[1]][e[0]]= 1
        F.add_edge(g,i)
        i+=1
    j=i


print('Number of graphs on '+str(n)+' nodes: '+str(i))

#transformation: from adjaciency matrices to graphs
Gtemp = dict() # temporary dictionary containing all graphs
for i in ad:
    l=list()
    for j in range(len(ad[i])):
```

```
        for k in range(len(ad[i][j])):
            if ad[i][j][k]==1:
                l.append([j,k])
    temp=nx.empty_graph(n)
    temp.add_edges_from(l)
    Gtemp[i]=copy.deepcopy(temp)


#reducing the number of graphs up-to-ismomorphism:
#dictionary containing only graphs on n nodes up-to-isomorphism
G = dict()
delete=False
for gtemp in Gtemp:
    for g in G:
        if (G.get(g).size() == Gtemp.get(gtemp).size()) \
           and (nx.is_isomorphic(G.get(g),Gtemp.get(gtemp))):
            delete=True
            # we modify F in order to remove gtemp
            for pred in F.predecessors(gtemp):
                F.remove_edge(pred,gtemp)
                F.add_edge(pred,g)
            for succ in F.successors(gtemp):
                F.remove_edge(gtemp,succ)
                F.add_edge(g,succ)
            F.remove_node(gtemp)
    if delete==False:
        G[gtemp]=copy.deepcopy(Gtemp.get(gtemp))
    delete=False

print('Number of graphs on '+str(n)+' nodes up to isomorphism: '
      +str(vertF[n]))

#remapping node names in G and F after the isomorphism simplifications
k=0
mapping= dict()
for i in sorted(G):
    G[k] = G.pop(i)
    mapping[i]=k
    k=k+1
F = nx.relabel_nodes(F,mapping)
```

```
print('Number of  graphs found: '+ str(k))


k=0
for path in nx.all_simple_paths(F, source=0, target=vertF[n]-1):
    k=k+1
print('number of possibile filtrations: '+str(k))

#PERSISTENCE ALONG THE FILTRATION
print('\nExample of persistence properties along the filtration:\
connected components\n')
#number connected components of the graph throughout all the flitrations
l=[[0 for x in range((n*(n-1))/2+1)] for y in range(k)]
k=0
for path in nx.all_simple_paths(F, source=0, target=vertF[n]-1):
    for i in range(len(path)):
        l[k][i]=nx.number_connected_components(G.get(path[i]))
    k=k+1

print('how many filtrations share the same number of \
connected components step by step?')
conn_comp_along_paths = dict()
for i in l:
    if tuple(i) in conn_comp_along_paths:
        conn_comp_along_paths[tuple(i)] +=1
    else:
        conn_comp_along_paths[tuple(i)]=1

for i in sorted(conn_comp_along_paths,key=conn_comp_along_paths.__getitem__):
    print(str(conn_comp_along_paths[i])+' filtration(s) show(s) exactly '+str(i)+\
          '\nconnected components step by step')

draw_graph(F)
```

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