NEURAL INFORMATION PROCESSING SYSTEMS

UNIVERSITY OF HELSINKI

YaiYai

Going Beyond Persistent Homology Using Persistent Homology

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Persistent homology (PH)

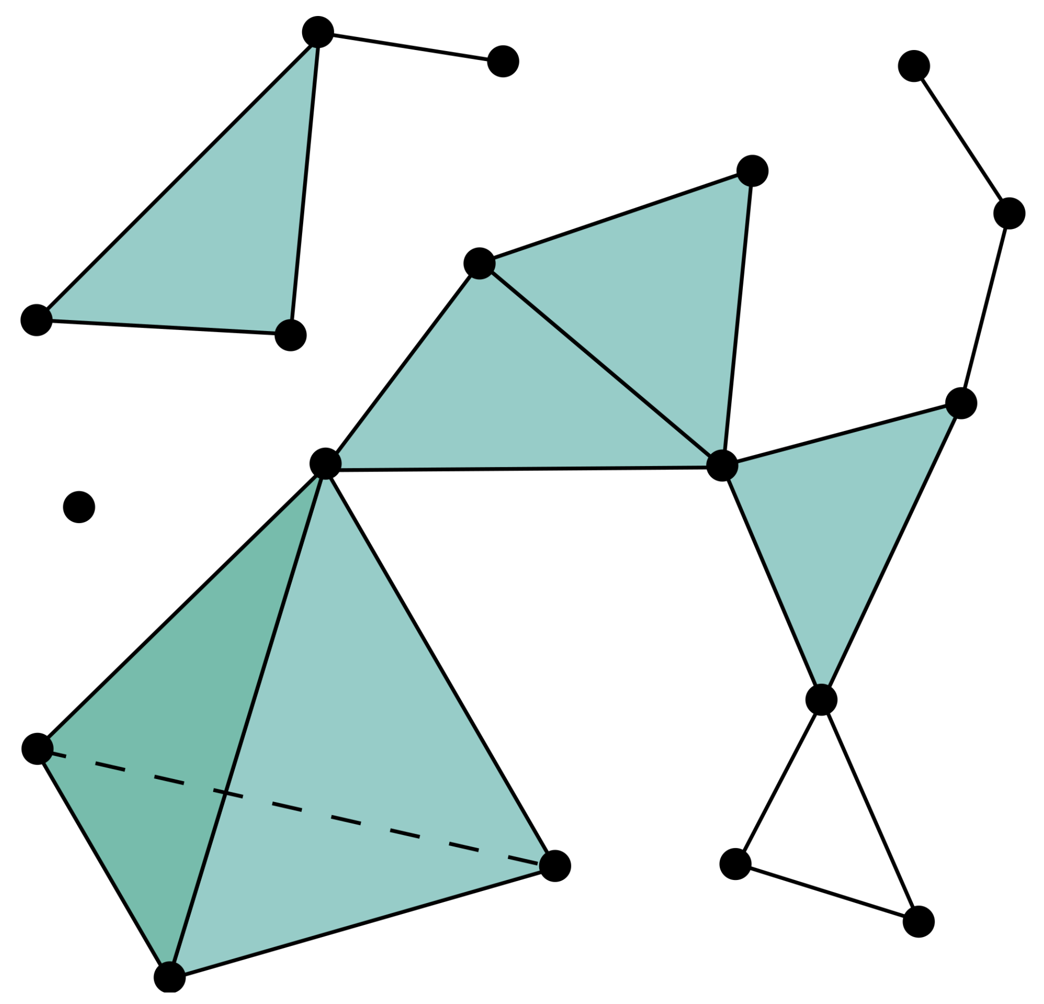
An approach to extract detailed **topological features** (e.g., persistence of connected components or cycles) of simplicial complexes (e.g., **graphs**).

Basic idea:

1) Obtain a **filtration** (i.e., sequence of sub-complexes) by applying a filtering function on simplices (elements of the original complex);
2) Keep track of the appearance (birth) and disappearance (death) of topological features, obtaining the so-called **persistence diagrams**.

Among other applications, PH has been successfully employed as a feature extractor in many disciplines, such as Astrophysics, Computer Vision, and Bioinformatics.

A simplicial complex.



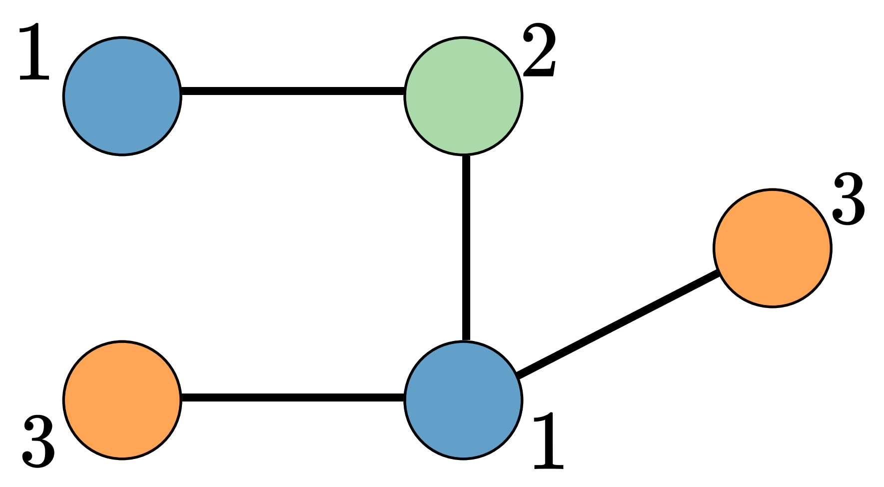
Source: Wikipedia

Persistent homology on graphs

Colors/features

Vertex-color Filtrations: Nested sequence of subgraphs $\varnothing = G^{(0)} \subseteq G^{(1)} \subseteq \ldots \subseteq G$ induced by $f : X \rightarrow (0,\infty)$

Attributed graph



Persistent homology on graphs

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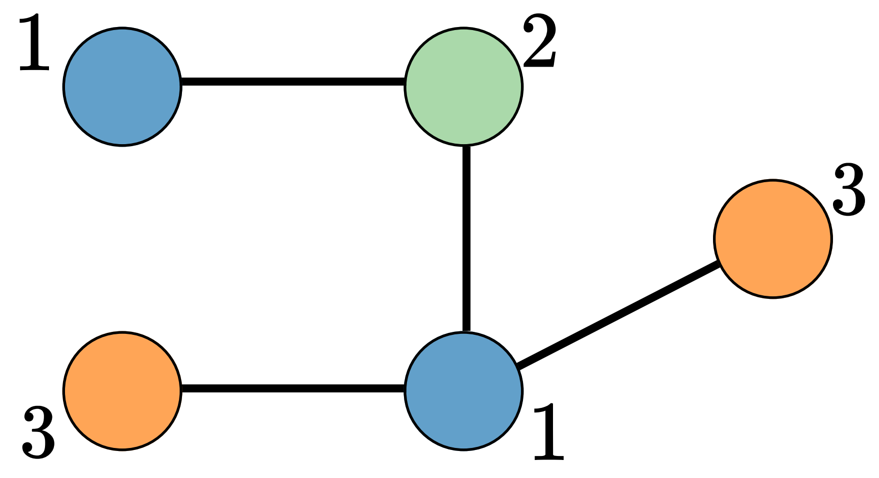
Filtration induced by: $\mapsto 1$ $\mapsto 2$ $\mapsto 3$

Attributed graph



Persistent homology on graphs

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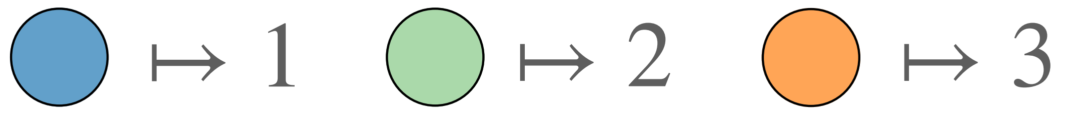
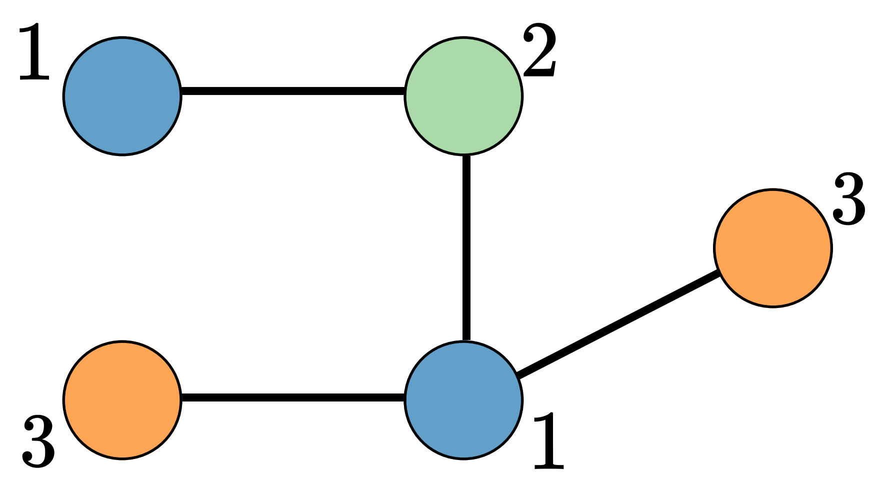
Filtration induced by: 

Attributed graph



Persistent homology on graphs

Colors/features

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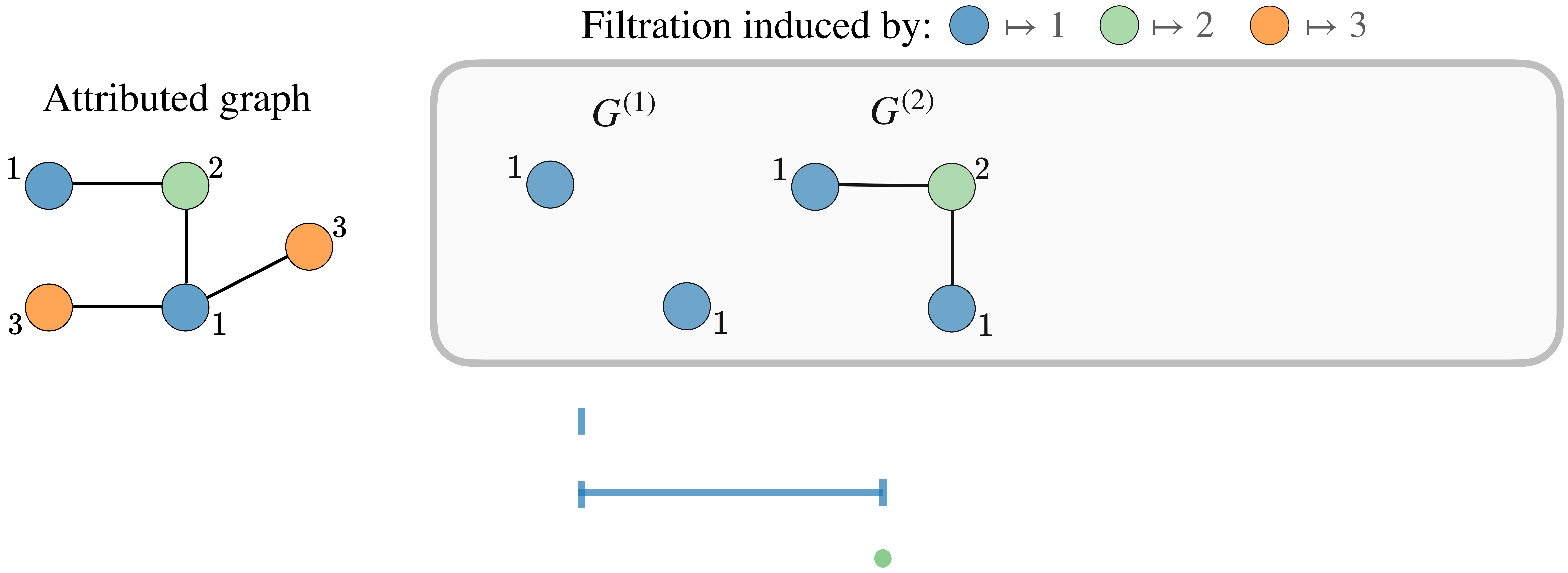

Persistent homology on graphs

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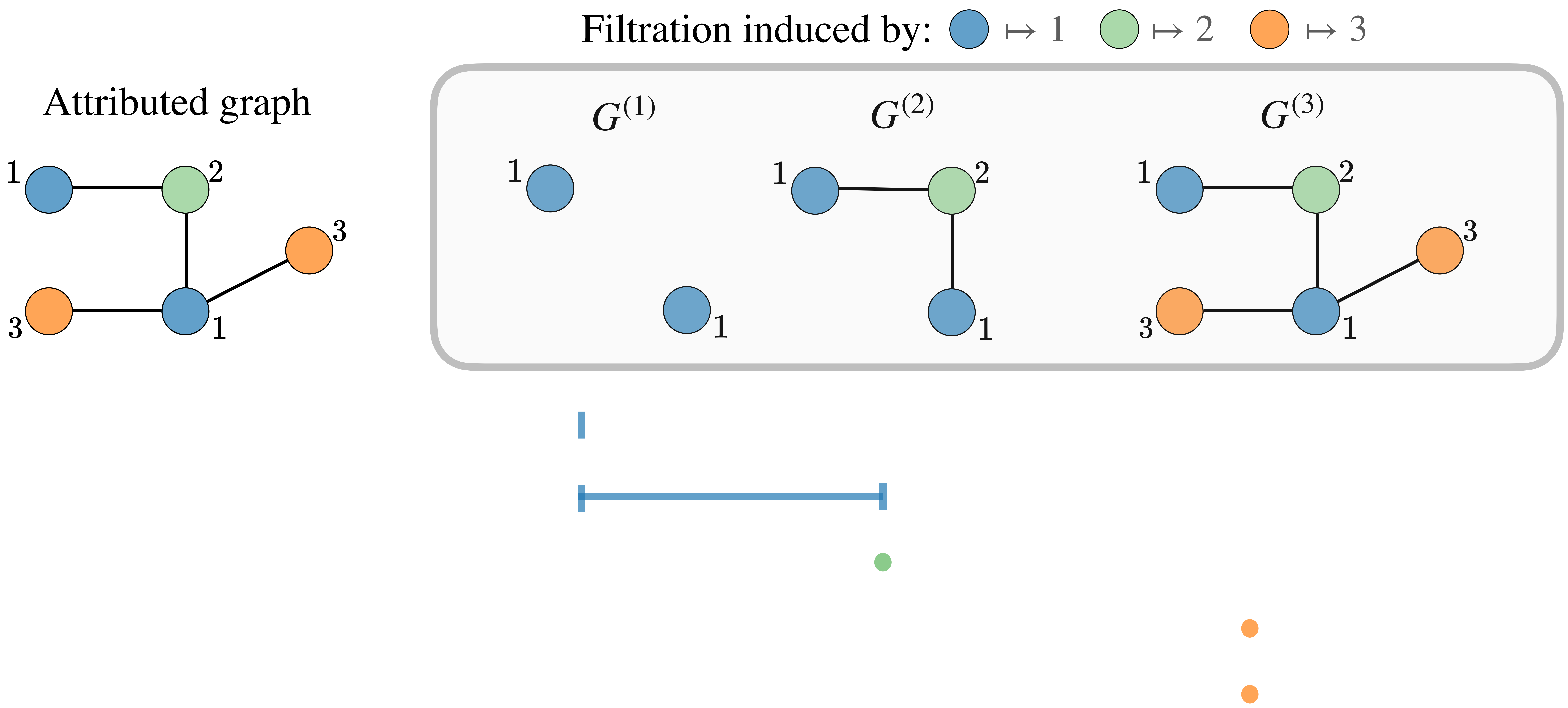


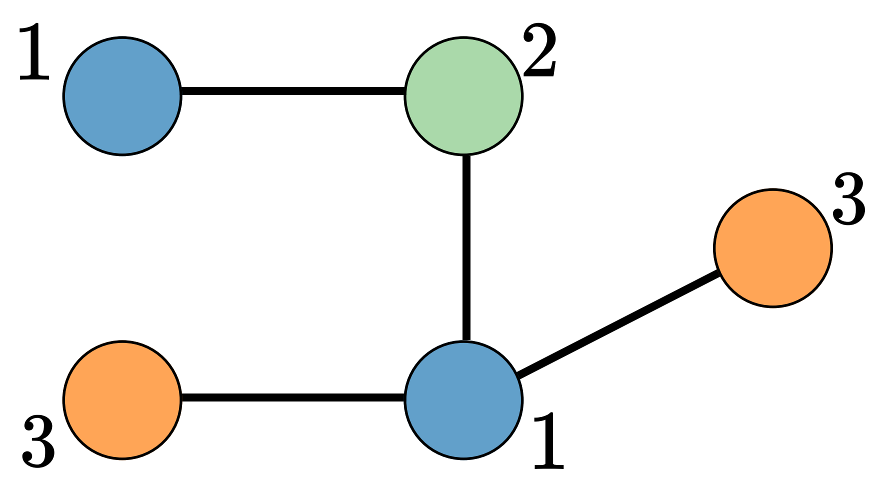
Persistent homology on graphs

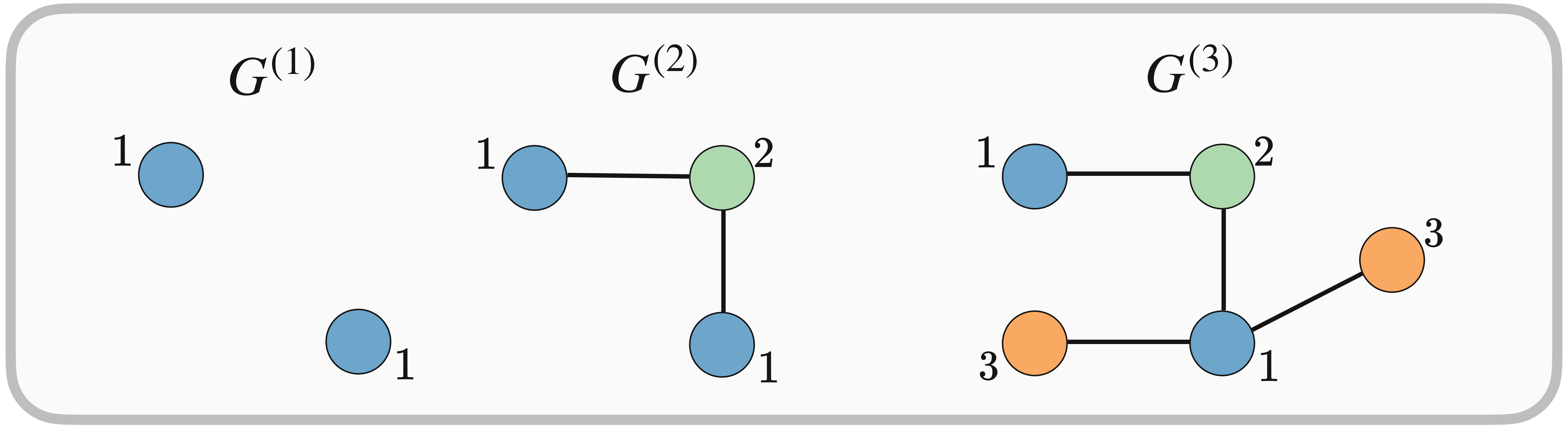
Colors/features

Vertex-color Filtrations: Nested sequence of subgraphs $\varnothing = G^{(0)} \subseteq G^{(1)} \subseteq \ldots \subseteq G$ induced by $f : X \to (0,\infty)$

Filtration induced by: (blue) $\mapsto 1$ (green) $\mapsto 2$ (orange) $\mapsto 3$

Attributed graph





$(1,\infty)$

$(1,2)$

$(2,2)$

$(3,3)$

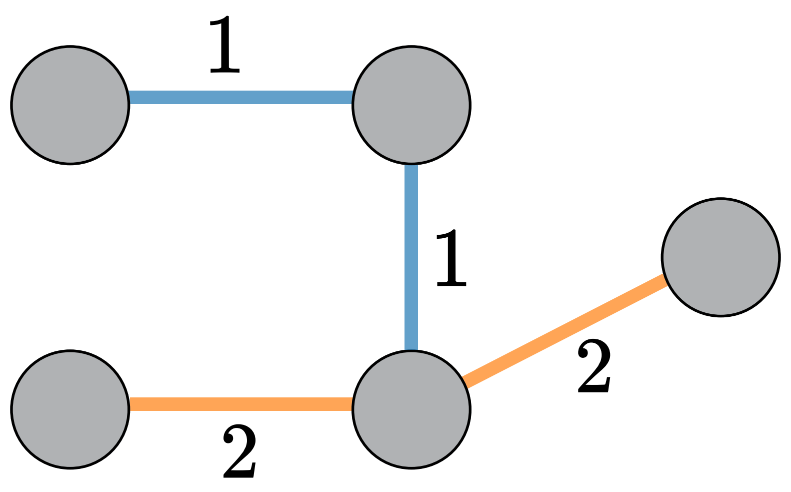
$(3,3)$

Persistence diagram (0-dim)

Persistent homology on graphs (cont.)

Edge-color Filtrations

Edge-colored graph

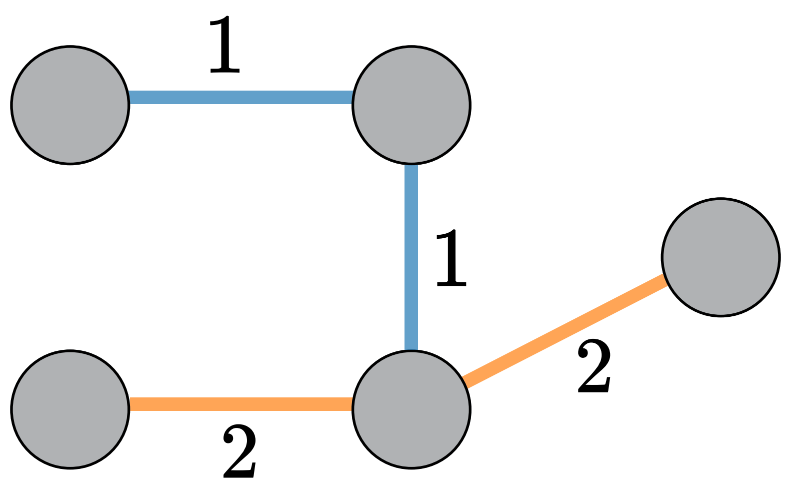


Persistent homology on graphs (cont.)

Edge-color Filtrations

Filtration induced by: ↦ 1 ↦ 2

Edge-colored graph

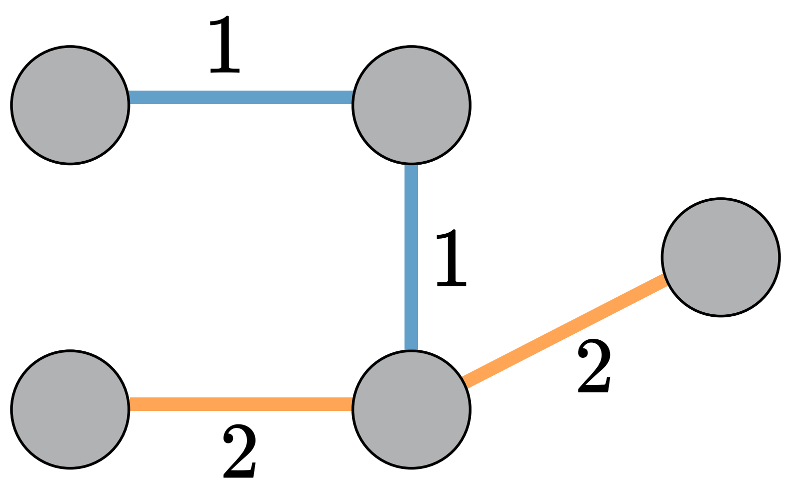


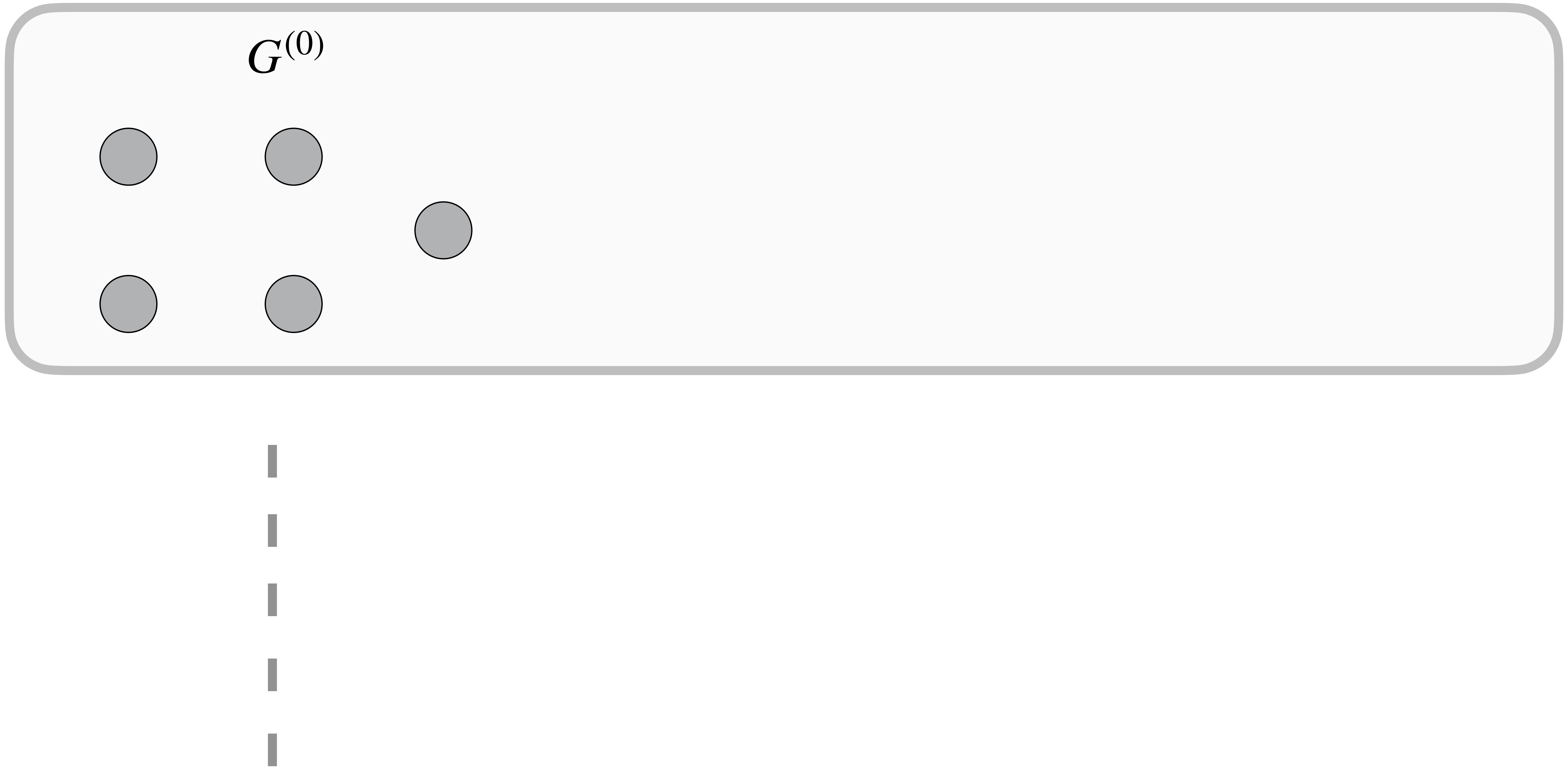
Persistent homology on graphs (cont.)

Edge-color Filtrations

Filtration induced by: $\mapsto 1$ $\mapsto 2$

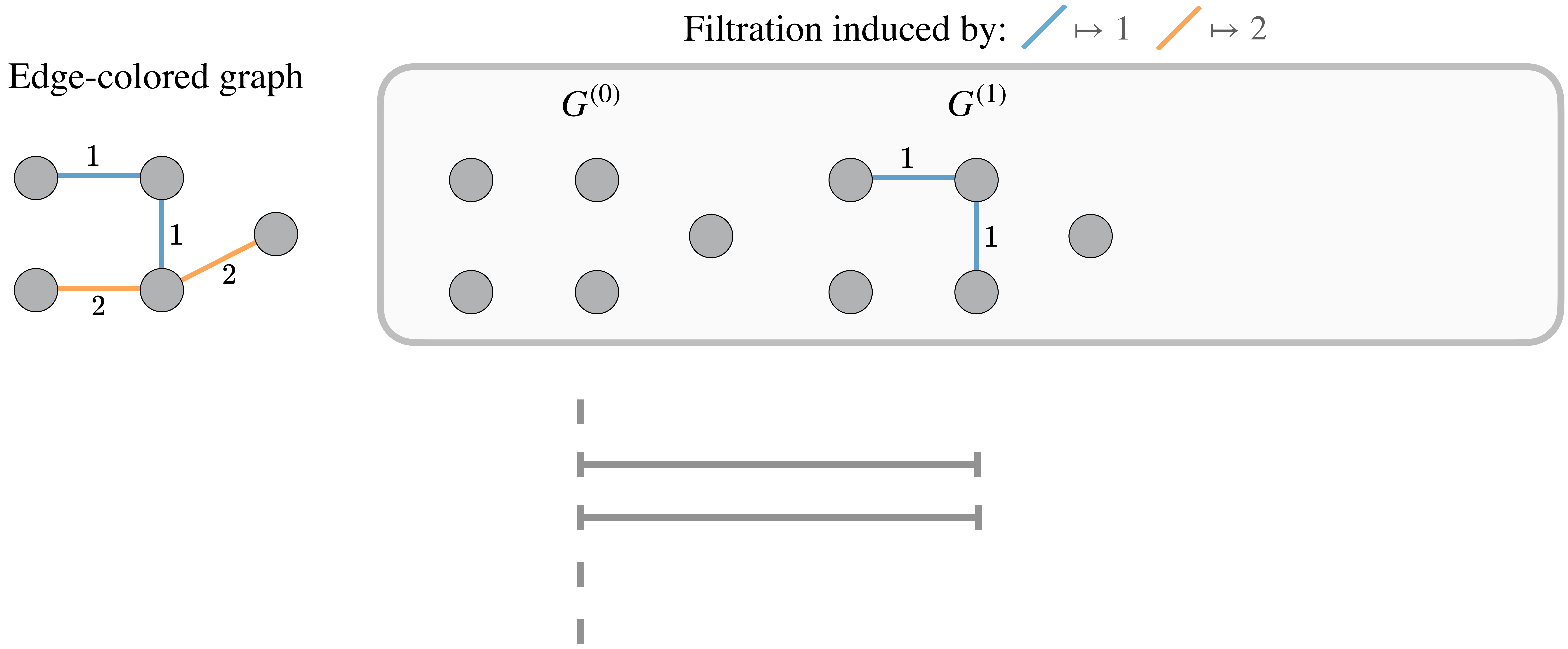
Edge-colored graph





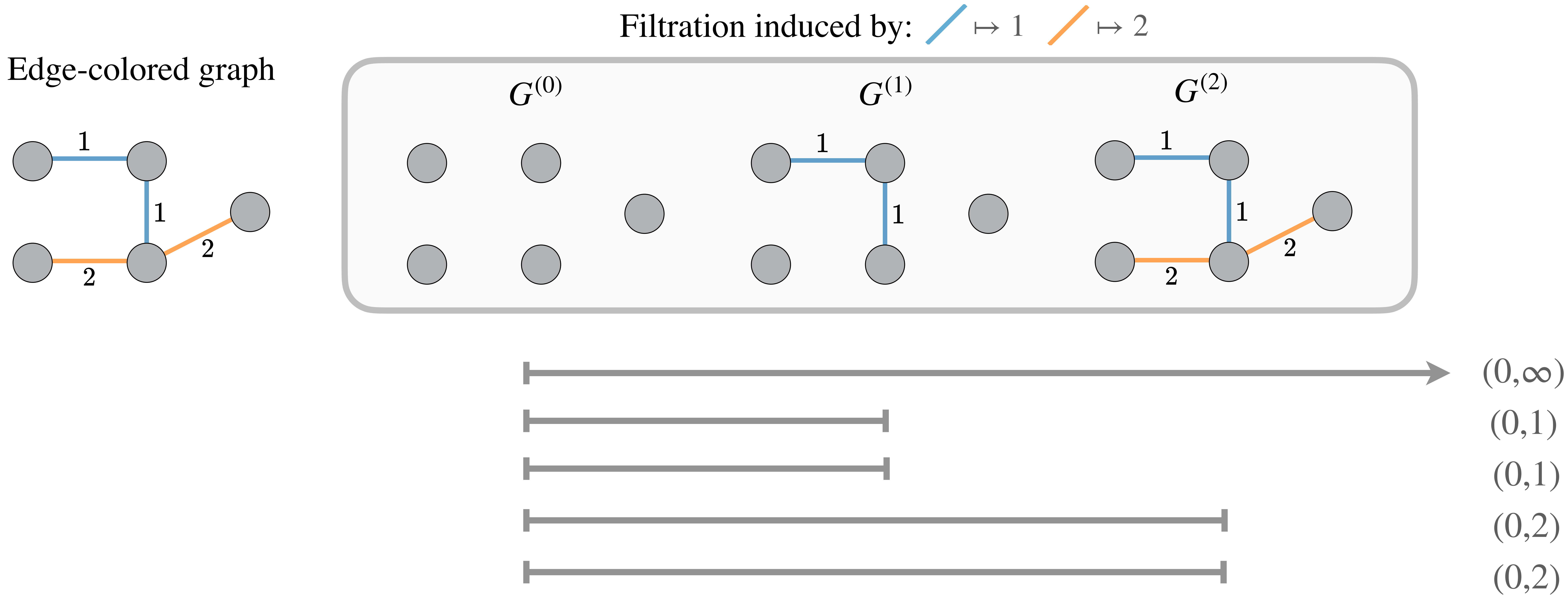
Persistent homology on graphs (cont.)

Edge-color Filtrations



Persistent homology on graphs (cont.)

Edge-color Filtrations



Motivation

Persistent homology has been used to **boost the predictive capabilities of** graph neural networks (**GNNs**).

However, while the expressivity of GNNs is well-understood (e.g., in terms of the Weisfeiler-Leman test), **the theoretical underpinnings of PH on graphs is less explored**.

In this work, we want to answer two fundamental **open questions**:

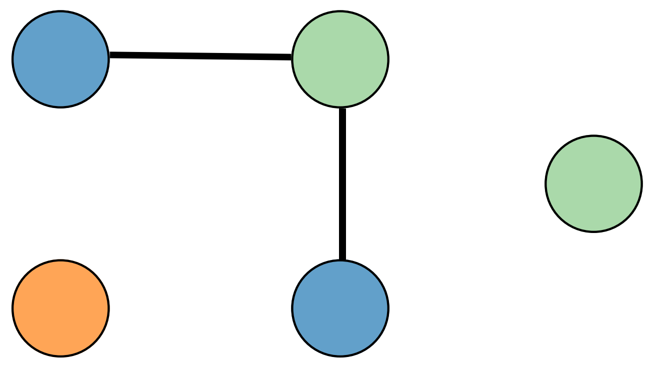
Q1: What is the expressive power of persistent homology (from vertex-color filtrations) on graphs?

Q2: Can we design more expressive persistence diagrams?

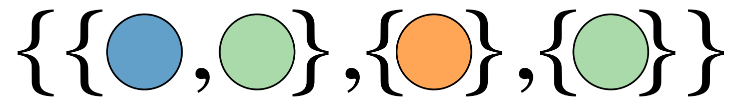
What is the expressive power of persistent homology on graphs?

An important notion: **color-separating sets**

Component-wise colors: The multiset comprising the set of colors of each connected component.

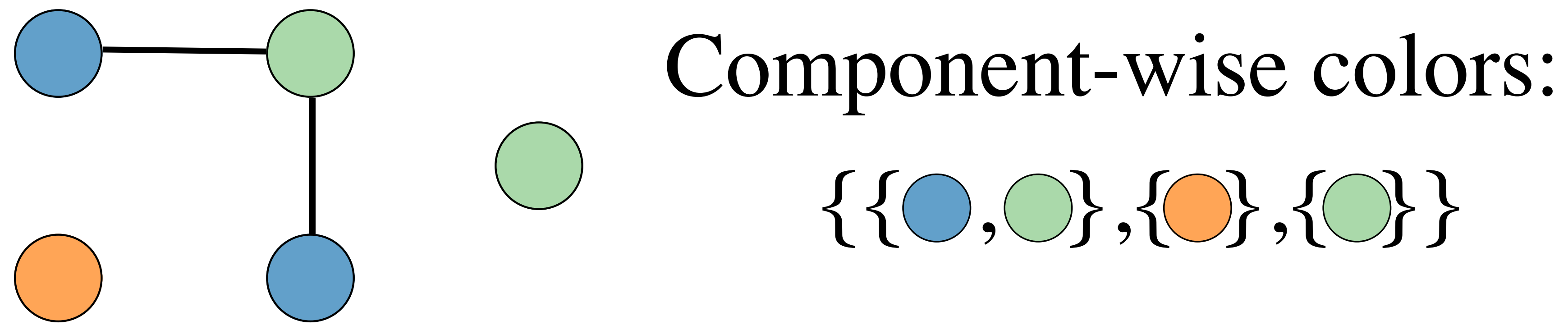


Component-wise colors:

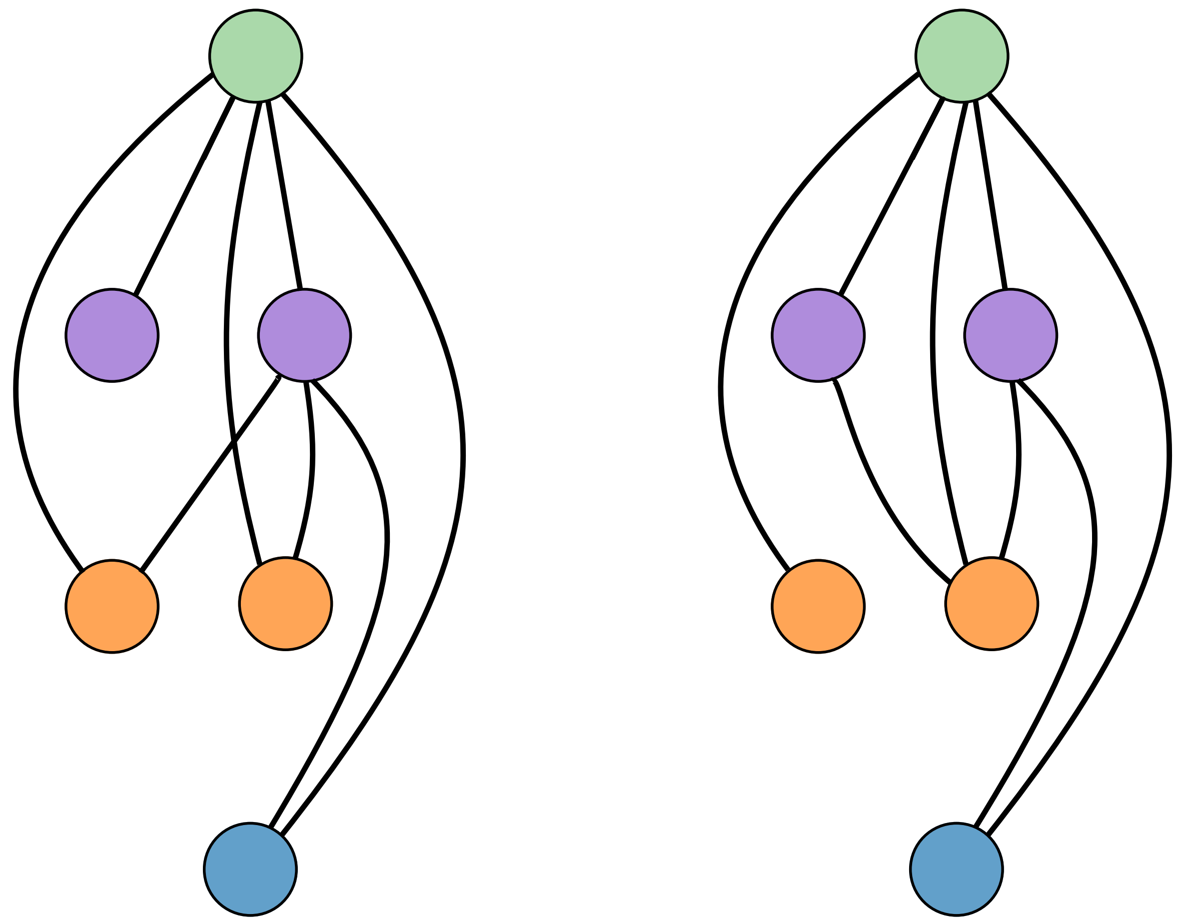


An important notion: **color-separating sets**

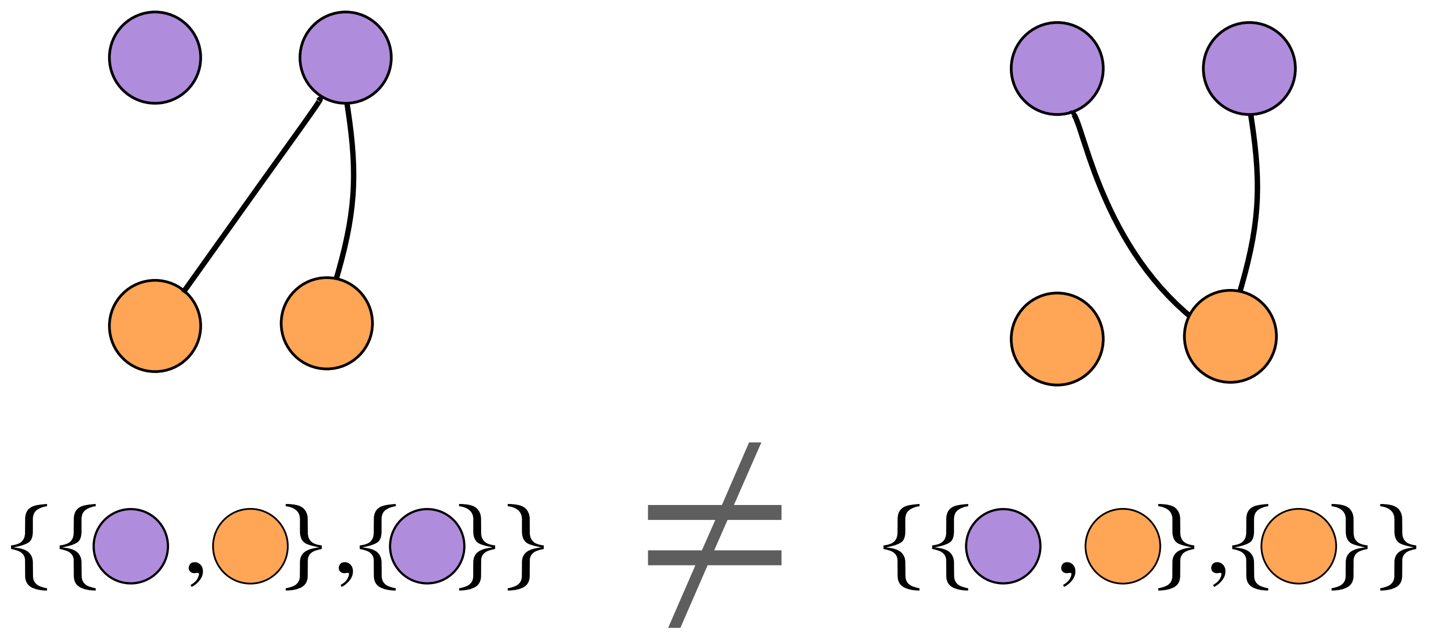
Component-wise colors: The multiset comprising the set of colors of each connected component.

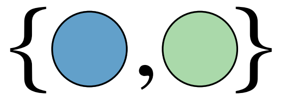


A **color-separating set** for a pair of graphs (G, G') is a set of colors Q such that, if we remove Q from G and G', we obtain subgraphs with **distinct component-wise colors**.



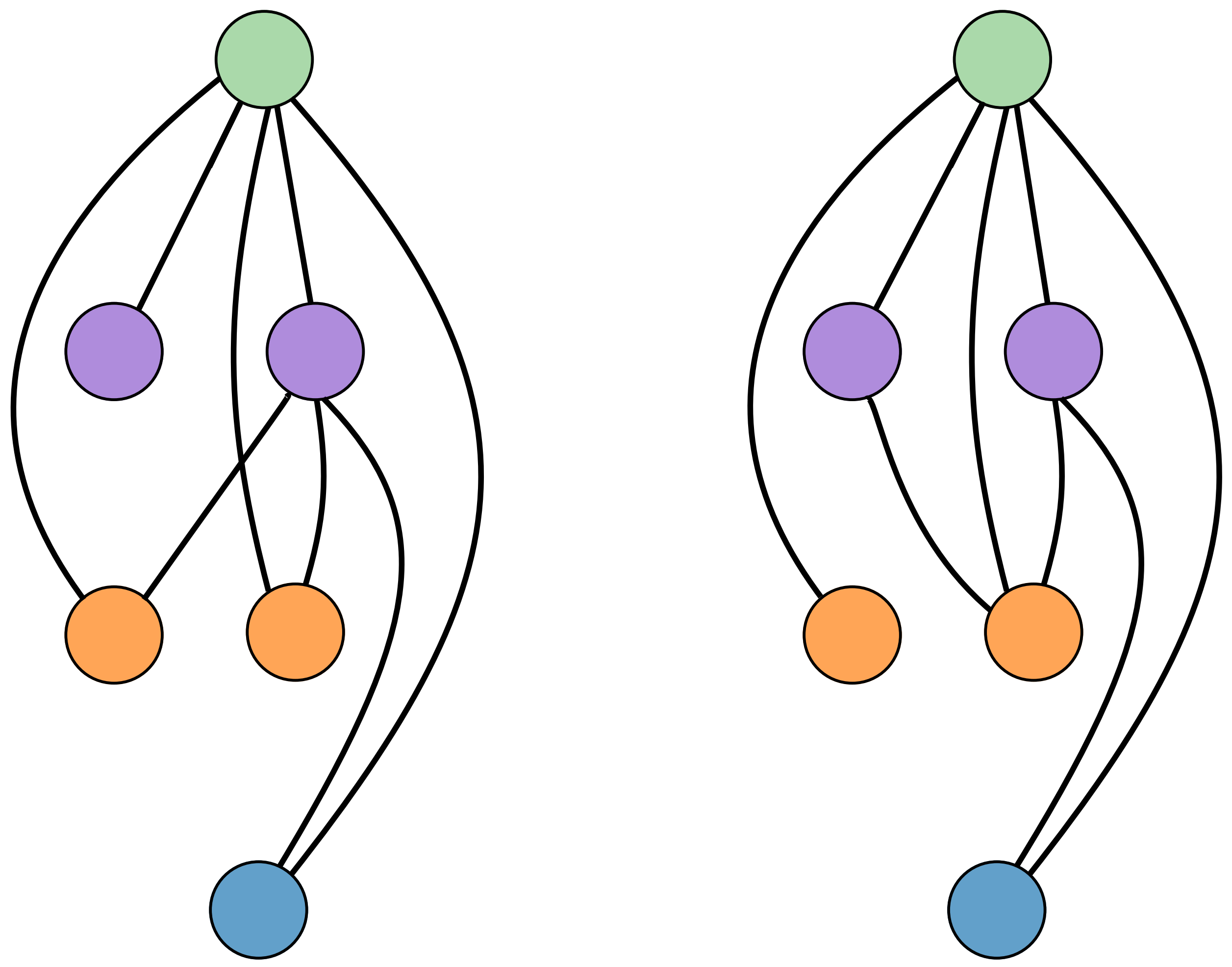
Removing blue and green, we obtain…



Thus,  is a color-separating set!

Theorem 1: On the power of vertex-color filtrations

We can obtain different vertex-color (0-dim) diagrams if and only if there is a color-separating set.

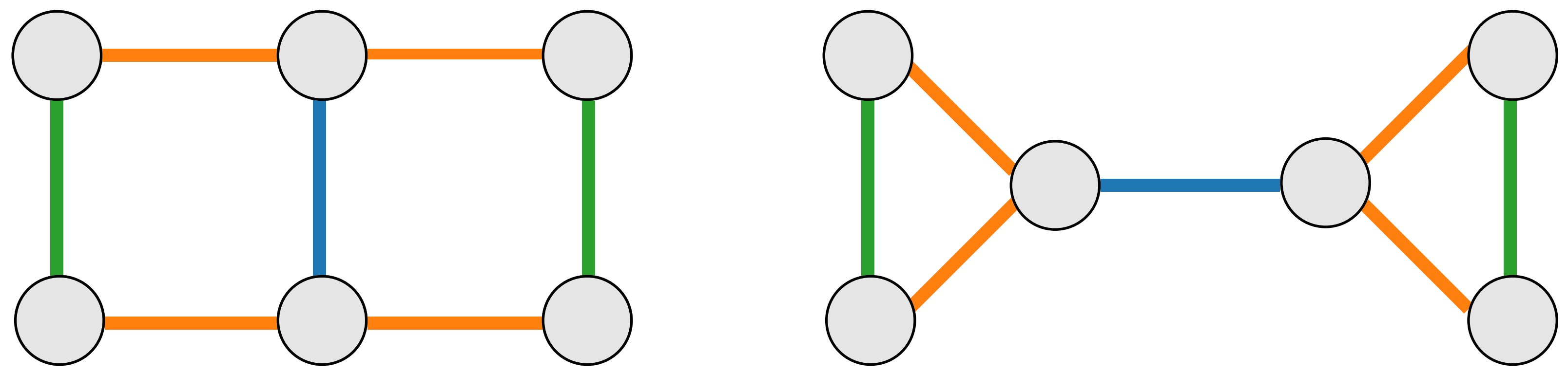


Can PH based on vertex-color filtrations distinguish these graphs?

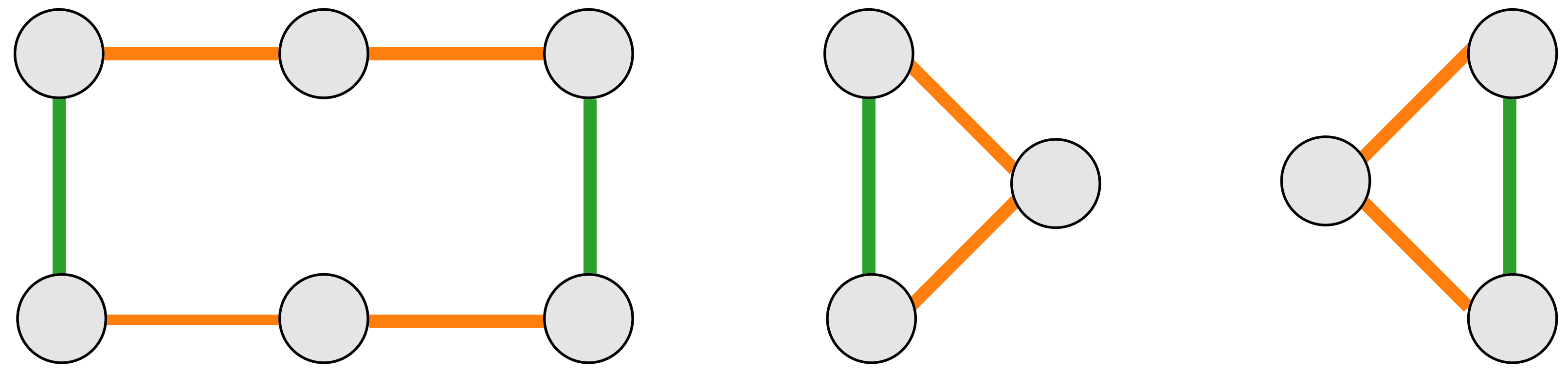
Yes!!{ , } is a color-separating set!

Another important notion: **color-disconnecting sets**

A **color-disconnecting set** for a pair of graphs (G, G') is a set of colors Q such that, if we remove edges of colors Q from G and G', we obtain subgraphs with **different number of connected components**.



Removing **blue**, we obtain…

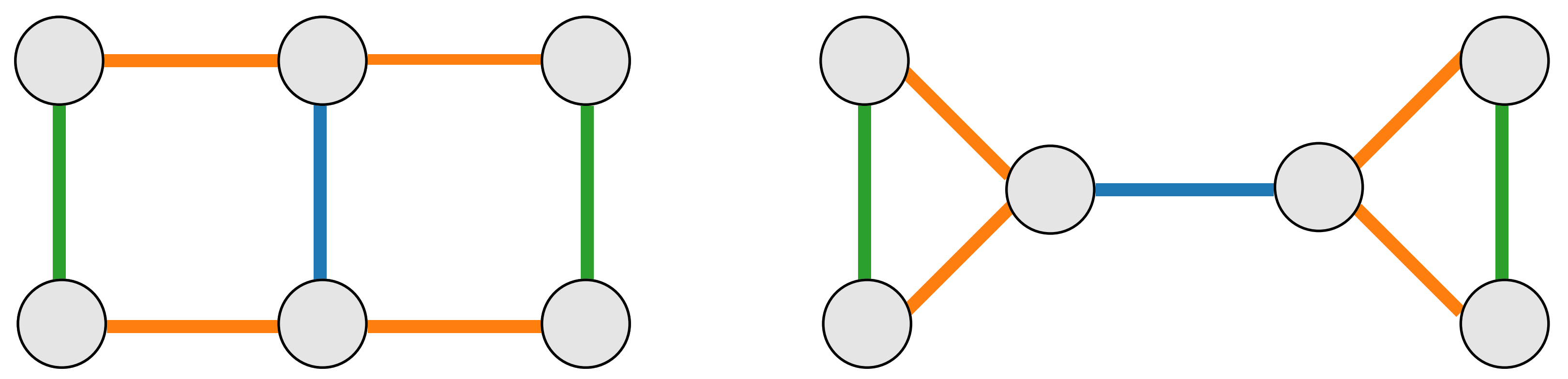


1 component   2 components

Thus, $Q = \{$**blue**$\}$ is a color-disconnecting set!

Theorem 2: On the power of edge-color filtrations

We can obtain different edge-color (0-dim) diagrams if and only if there is a color-disconnecting set.

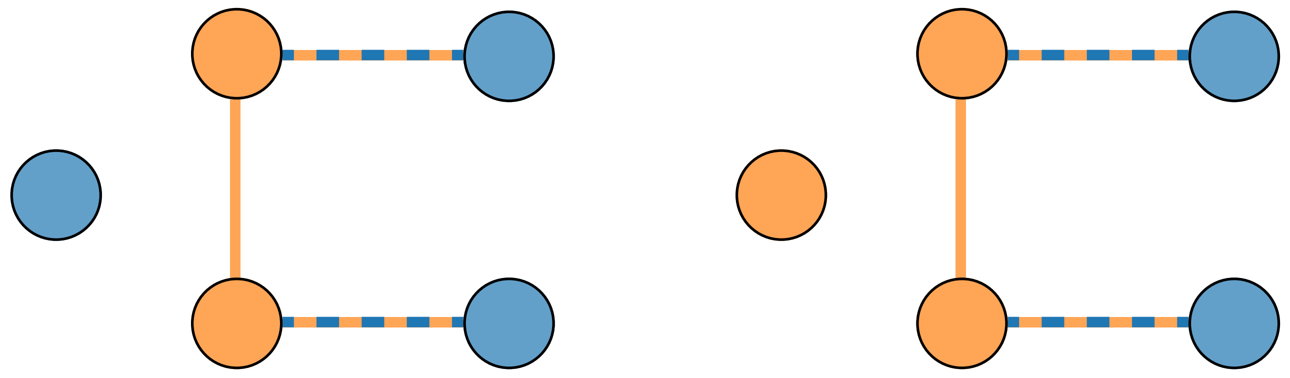


Can PH based on edge-color filtrations distinguish these graphs?

Yes!! $Q = \{\mathbf{blue}\}$ is a color-disconnecting set!

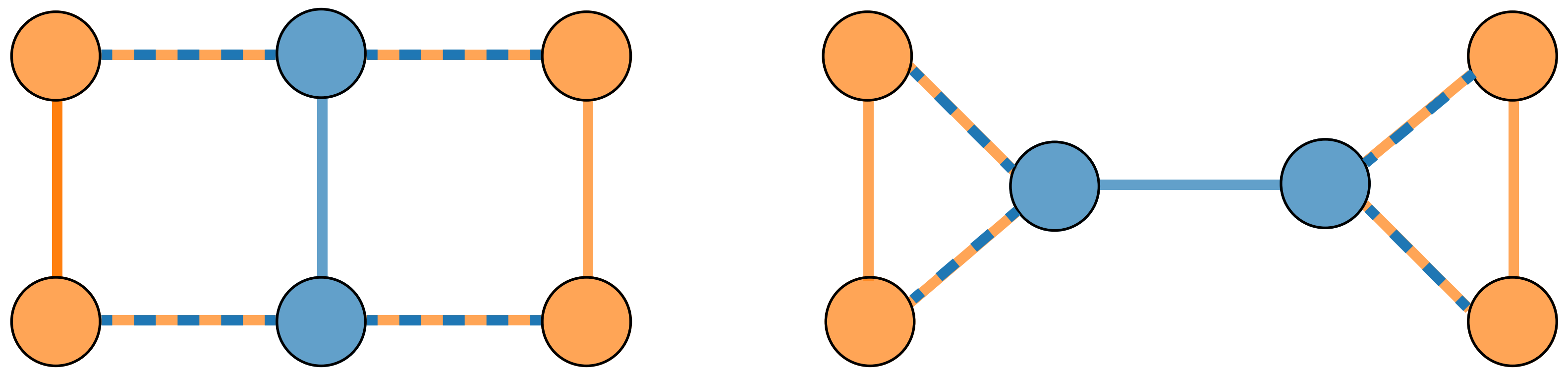
Theorem 3: Vertex-color vs. edge-color filtrations

There exist non-isomorphic graphs that vertex-color filtrations can distinguish but edge-color filtrations cannot, and vice-versa.



Vertex-color **succeeds**

Edge-color **fails**



Vertex-color **fails**

Edge-color **succeeds**

Can we design more expressive persistence diagrams?

RePHINE (**Re**fining **PH** by **I**ncorporating **N**ode-color into **E**dge-based filtration)

Idea: Given independent vertex- and edge-color filtration functions (f_v, f_e), we augment persistence diagrams from edge-color filtrations with vertex-color information.

Original birth and death time (from edge-color filtration)

Color of node u

$$w : \left(b, d, f_v(c(w)), \min_{u \in \mathcal{N}(w)} f_e(\{\{c(u), c(w)\}\}) \right)$$

Independent vertex-color filtration function.

Edge-color filtration function.

Building RePHINE diagrams

Original birth and death time (from edge-color filtration)

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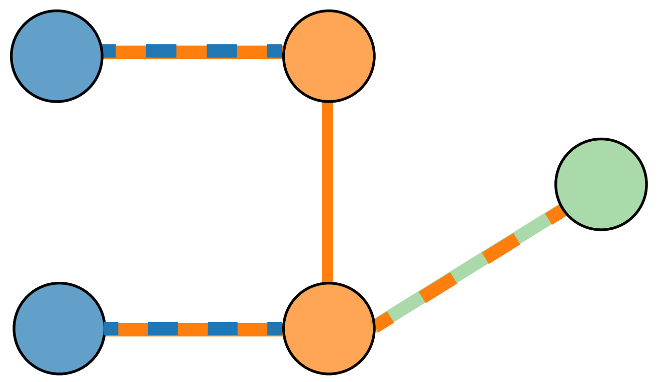

Building RePHINE diagrams

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Independent vertex-color filtration function.

Edge-color filtration function.

(0, ,1,)

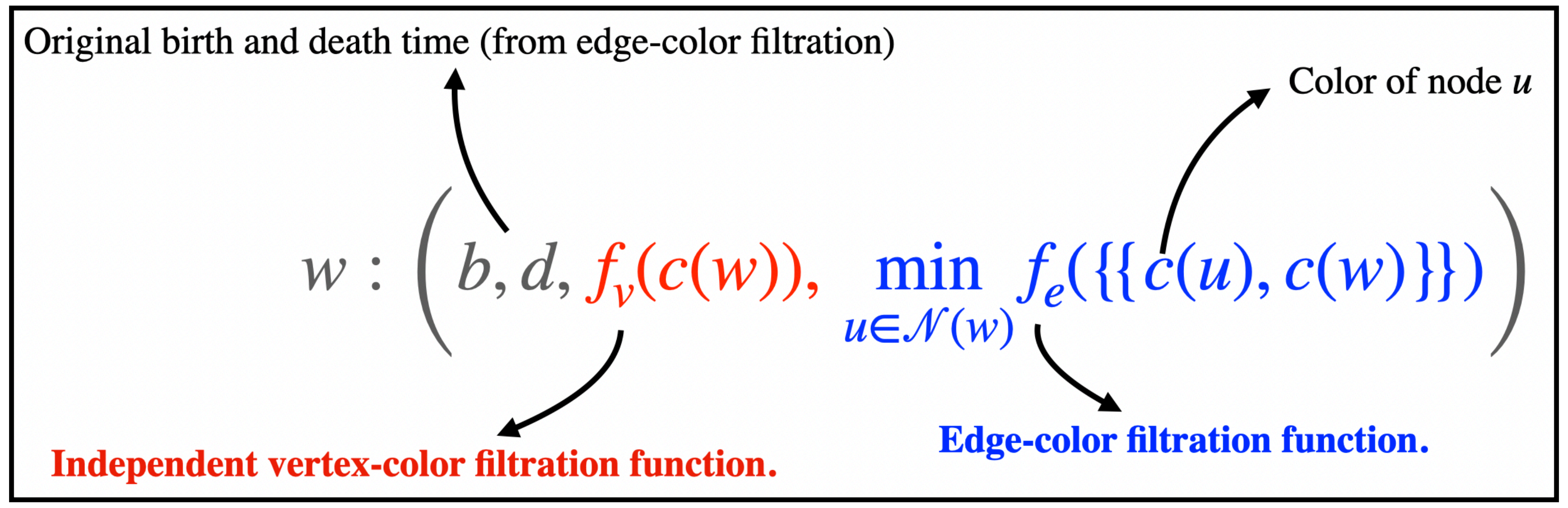
(0, ,1,)

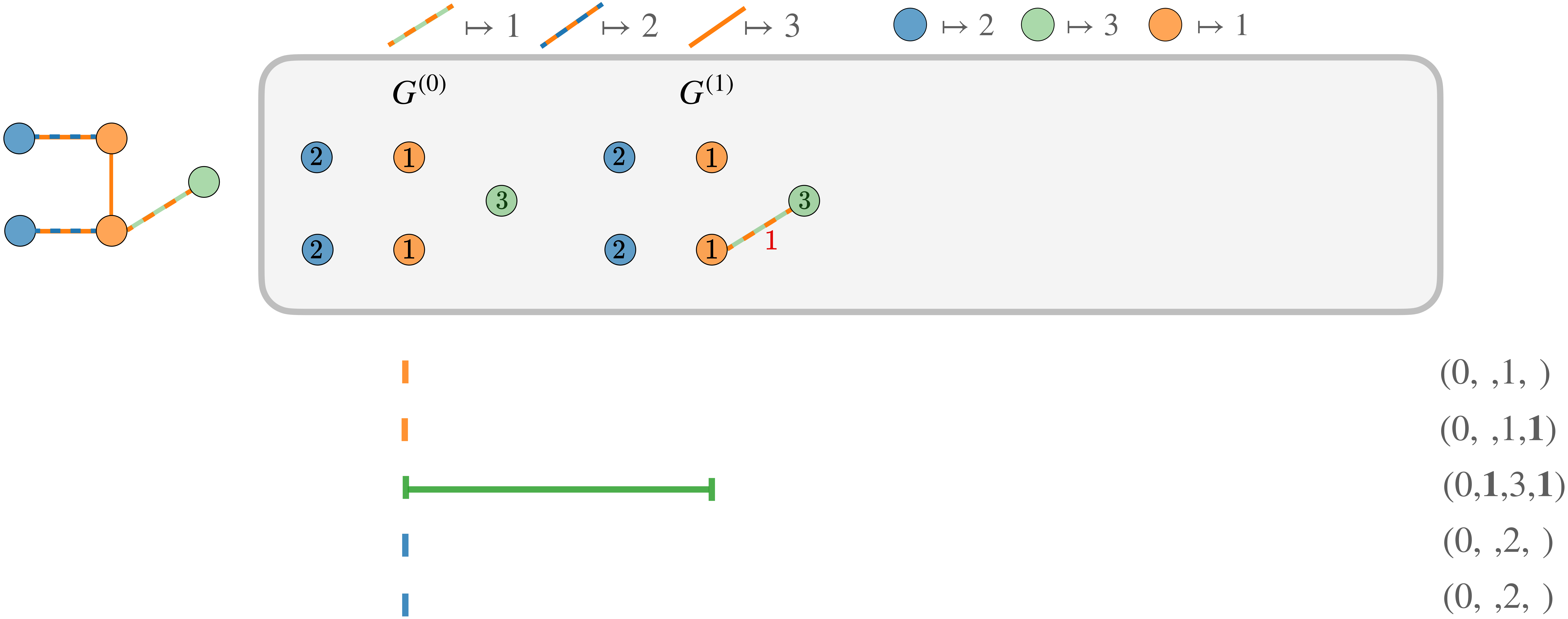
(0, ,3,)

(0, ,2,)

(0, ,2,)

Building RePHINE diagrams





Building RePHINE diagrams

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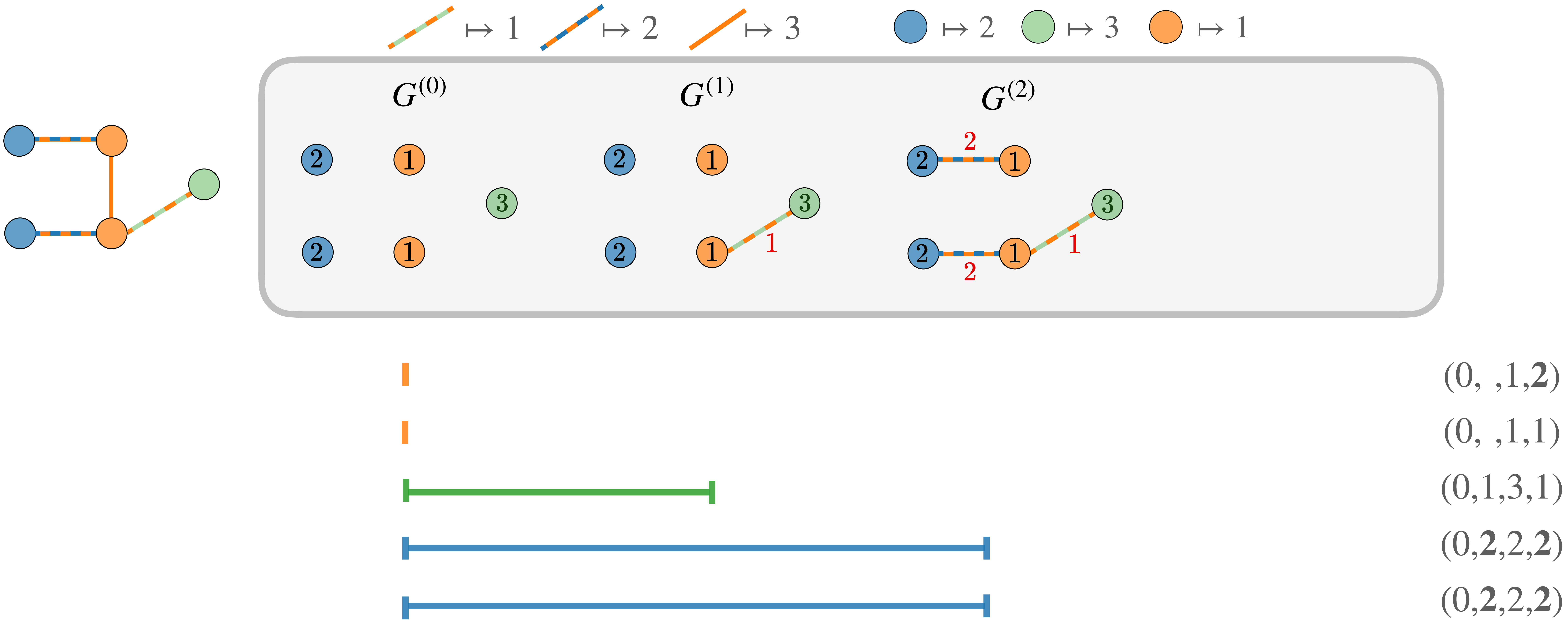
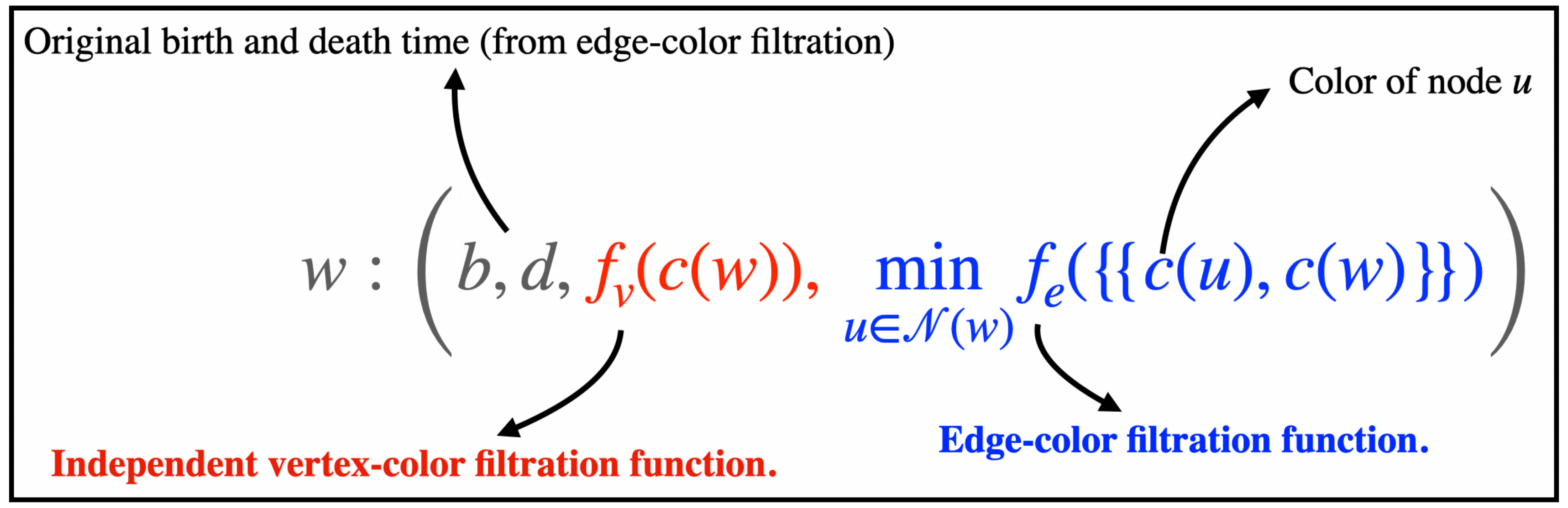
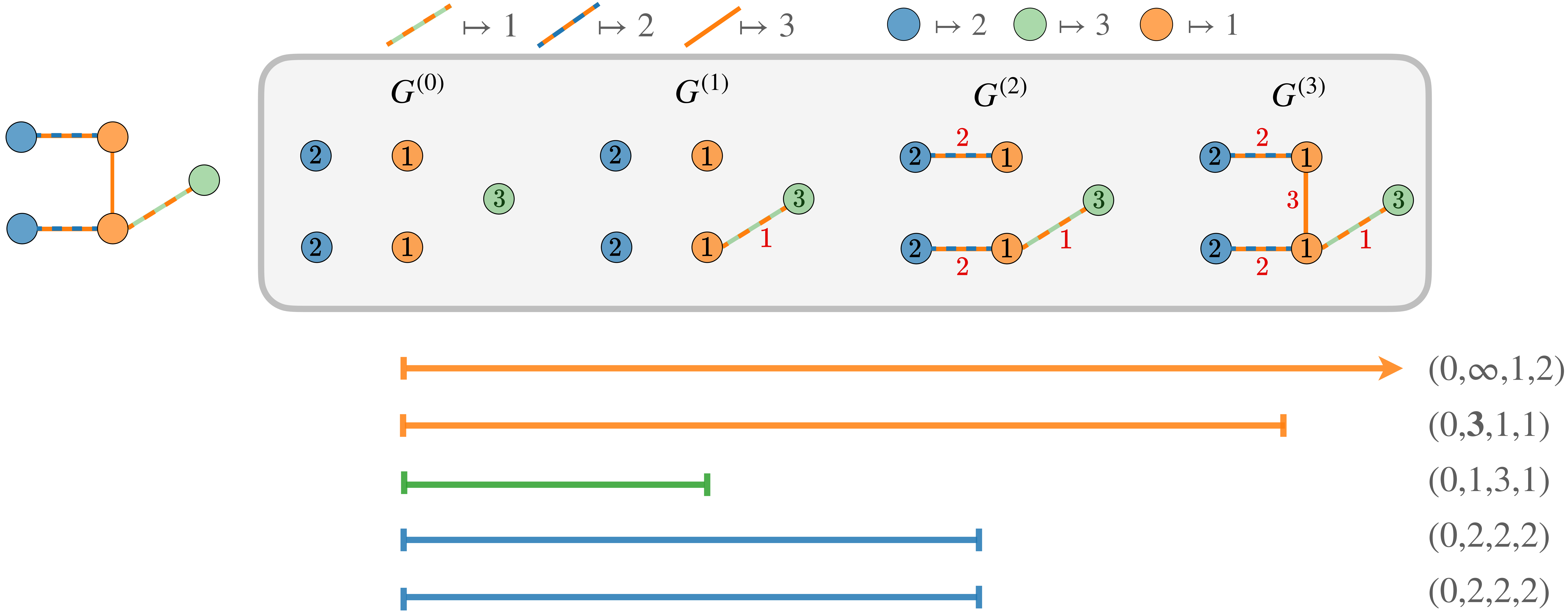


Building RePHINE diagrams

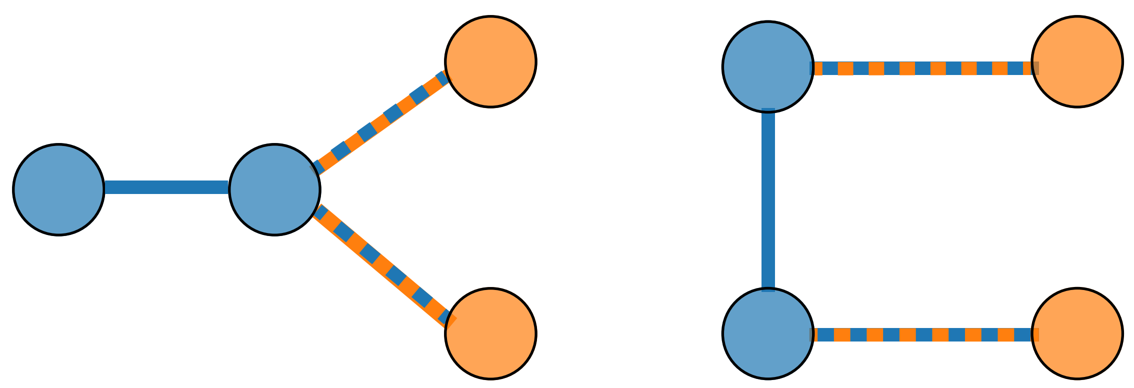




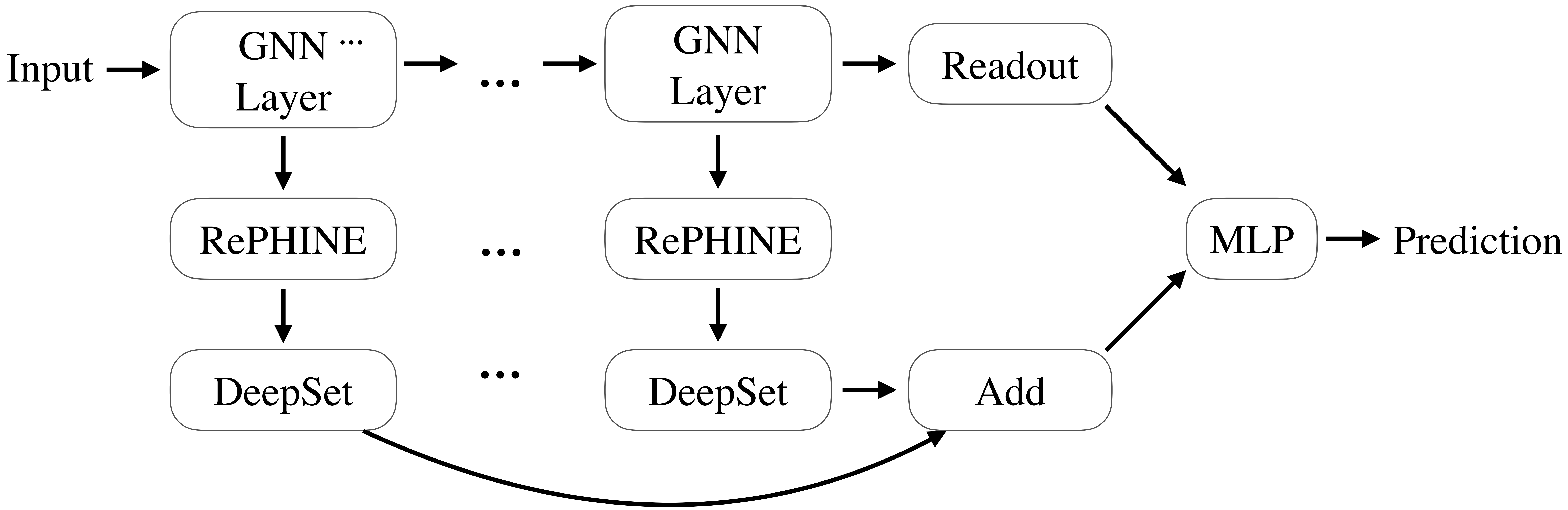
Theorem 4: RePHINE vs color-based diagrams

RePHINE is isomorphism invariant and is strictly more expressive than color-based PH.

Two graphs that color-based **PH cannot distinguish**, but **RePHINE can**.



Combining RePHINE and GNNs



Results on real-world data

We process the persistence diagrams using DeepSets and combine the resulting vectors with GNN embeddings.

Table 1: Predictive performance on graph classification. We denote in bold the best results. For ZINC, lower is better. For most datasets, RePHINE is the best-performing method.

GNN	Diagram	NCI109 ↑	PROTEINS ↑	IMDB-B ↑	NCI1 ↑	MOLHIV ↑	ZINC ↓
GCN	-	76.46 ± 1.03	70.18 ± 1.35	64.20 ± 1.30	74.45 ± 1.05	74.99 ± 1.09	0.875 ± 0.009
	PH	77.92 ± 1.89	69.46 ± 1.83	64.80 ± 1.30	79.08 ± 1.06	73.64 ± 1.29	0.513 ± 0.014
	RePHINE	**79.18** ± 1.97	**71.25** ± 1.60	**69.40** ± 3.78	**80.44** ± 0.94	**75.98** ± 1.80	**0.468** ± 0.011
GIN	-	76.90 ± 0.80	**72.50** ± 2.31	**74.20** ± 1.30	76.89 ± 1.75	70.76 ± 2.46	0.621 ± 0.015
	PH	78.35 ± 0.68	69.46 ± 2.48	69.80 ± 0.84	79.12 ± 1.23	73.37 ± 4.36	0.440 ± 0.019
	RePHINE	**79.23** ± 1.67	72.32 ± 1.89	72.80 ± 2.95	**80.92** ± 1.92	**73.71** ± 0.91	**0.411** ± 0.015

Wanna know more?

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Thu 14 Dec 10:45 a.m. CST

Code: www.github.com/Aalto-QuML/rephine

Theoretical contributions of this work	
On vertex-level filtrations (Section 2 and Section 3.1):	
Inconsistency issues due to injective vertex filtrations	Lemma 1
Real holes ($d = \infty$) $\cong$ Component-wise colors	Lemma 2
Almost holes ($b \neq d, d \neq \infty$) $\cong$ Separating sets	Lemma 3
Distinct almost holes $\Rightarrow$ Color-separating set	Lemma 4
Birth time of persistence tuples $\cong$ Vertex color	Lemma 5
The expressive power of vertex-color filtrations	Theorem 1
On edge-level filtrations (Section 3.2):	
Almost holes $\cong$ Disconnecting sets	Lemma 6
Reconstruction of disconnecting sets	Lemma 7
The expressive power of edge-color filtrations	Theorem 2
Vertex-level vs. edge-level filtrations (Section 3.3):	
Vertex-level persistence $\not\succ$ edge-level persistence, and vice-versa	Theorem 3
New method (RePHINE) (Section 4):	
RePHINE is isomorphism invariant	Theorem 4
RePHINE $\succ$ vertex-, edge-, and vertex- $\cup$ edge-level diagrams	Theorem 5

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