Seminar Series on Graph Neural Networks 02

On the Representational Power of GNNs

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Before going in....

Wrap-up: Message passing all the way up
(Up-to-date comprehensive survey on GNN archtiectures)

Towards application of graph neural networks

Towards efficient graph learning

Explainable graph neural networks

Fundamental topics on graph neural networks

On the representational power of graph neural networks (Current session)

A graph signal processing viewpoint of graph neural networks

On the problem of oversmoothing and oversquashing

Introduction to graph mining and graph neural networks
(Basic overview to kick things off)

(Some of the topics may change in the future for a better alternative)

* Presentation slides are available at:
(jordan7186.github.io/presentations/)

Objectives

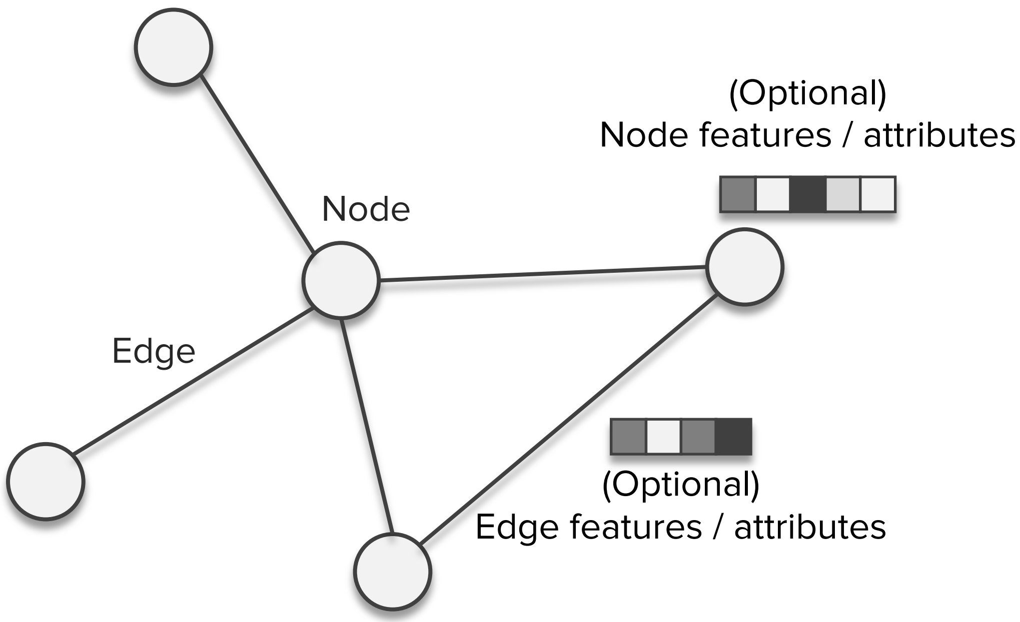
1. Understanding of **what makes two graphs the 'same'**
2. Understanding of the **Weisfeiler-Lehman isomorphism test**
3. Understanding the **connection** between the WL test and message-passing
4. In-depth understanding of (Xu et al., ICLR 2019) and (Morris et al., AAAI 2019)

*Today's topic is more relevant on chemical datasets, where the model needs to extract as much information as possible from the given graph structure.

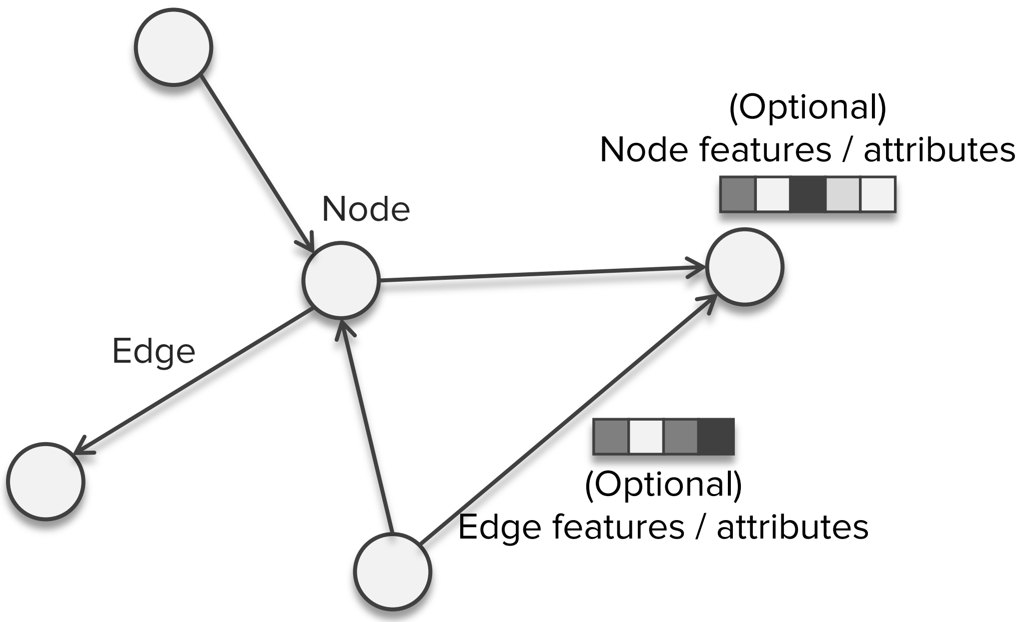
What makes two graphs the ‘same’?

(Revisit) Graphs as an abstract datatype

Graphs are an abstract type of data where nodes (entities) are **connected** by edges (connections)



Undirected graph

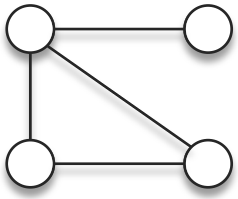


Directed graph

For now, let's assume we do not consider node / edge features.

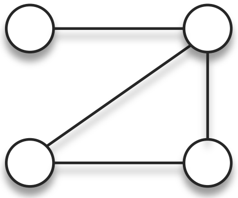
Only looking at the 'graph structure' (roughly speaking, connection patterns), how do we determine whether two graphs are the same?

Example 1



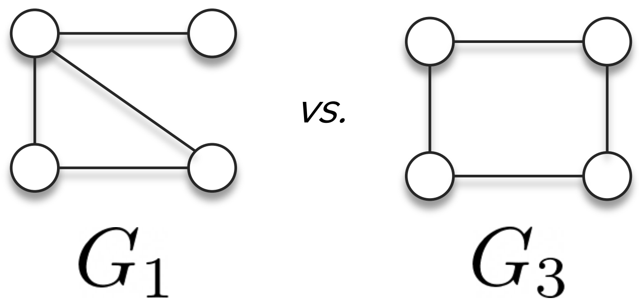
G_1

vs.

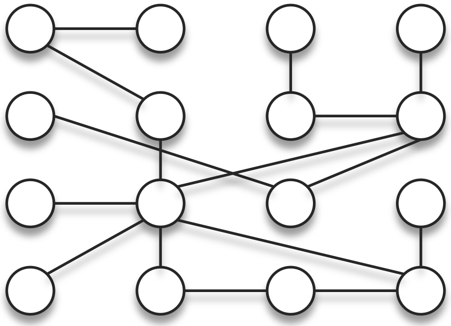


G_2

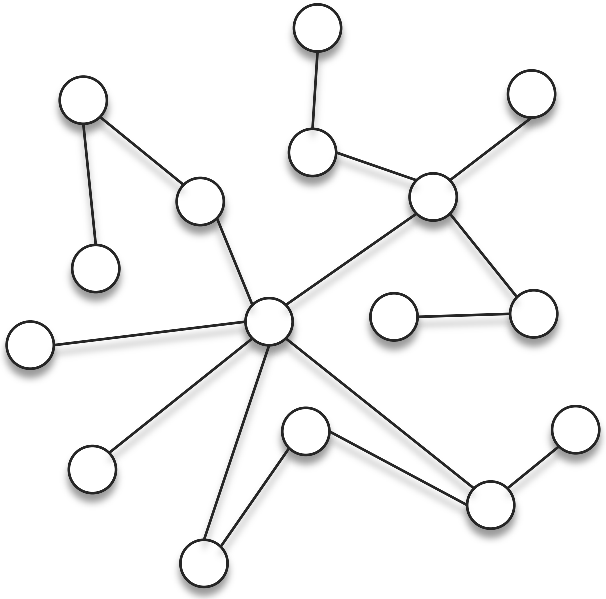
Example 2



Example 3

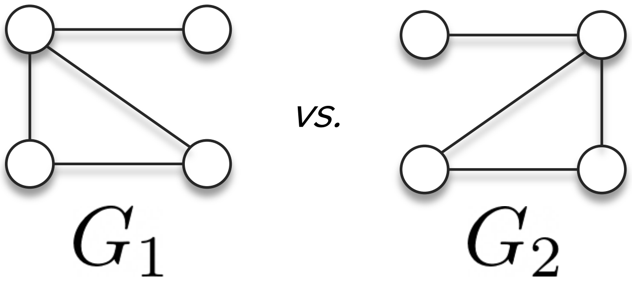


vs.

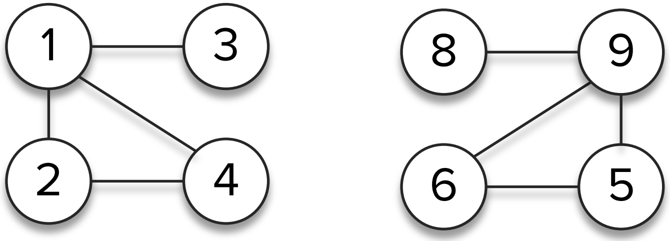


G_4 G_5

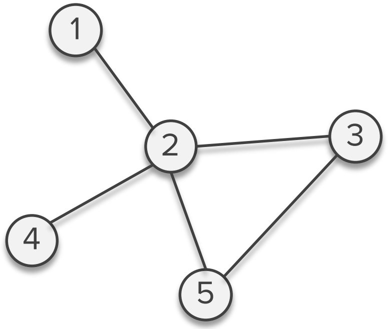
Isomorphism (a fancy word for identical graphs)



Whatever the definition of 'isomorphism' is,
it must not care aboud node orderings



We say that two graphs G and H are *isomorphic* if there exists an edge preserving bijection $\varphi : V(G) \to V(H)$, i.e., (u, v) is in $E(G)$ if and only if $(\varphi(u), \varphi(v))$ is in $E(H)$.



Assign arbitrary node ordering

- **Graphs with canonical node ordering is not common**
- Related research topic: Positional encoding of nodes
  (As an example, see [1])

Remember, there are no 'correct' node ordering.

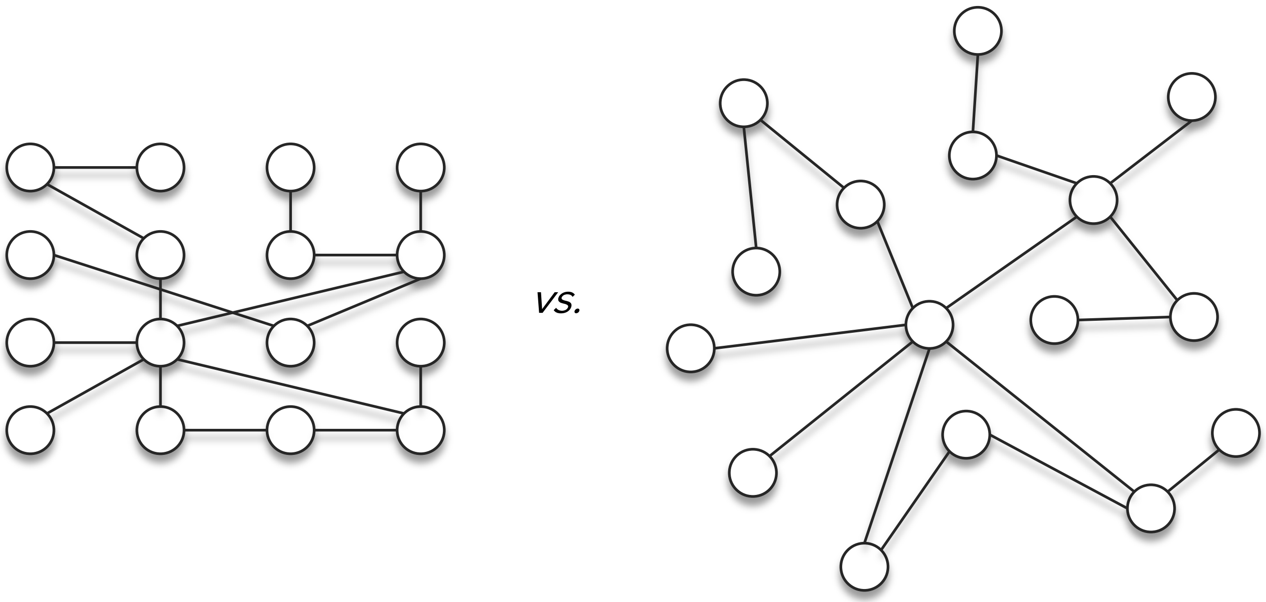
This means, G1 and G2 are **isomorphic** since we can find a bijection of:

3 – 8
1 – 9
4 – 6
2 – 5

and according to this node mapping, the edge set from G1 exactly translates to G2.

[1] (Definition) Morris et al., Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks, AAAI 2019

The practical problem of graph isomorphism test



G_4 G_5

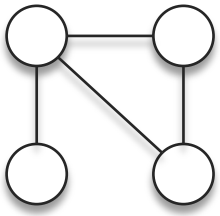
*The problem of graph isomorphism testing is suspected to be *NP-hard [2], [3]*

- Probably no exact (deterministic) polynomial-time algorithmic solutions
- **WL isomorphism test**: A heuristic algorithm to test isomorphism

[2] Huang & Villar, “A short tutorial on the Weisfeiler-Lehman test and its variants”, ICASSP 2021
[3] David Bieber, “The Weisfeiler-Lehman Isomorphism Test” (Blog post)

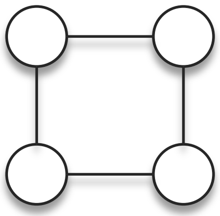
Understanding the WL-isomorphism test

One iteration of the WL-isomorphism test [1], [2]



Graph 1

Q. Is there a systematic (heuristic) method that can "mostly" identify isomorphic graphs?



Graph 2

[4] Shervashidze et al., "Weisfeiler-Lehman Graph Kernels", J. Mach. Learn. Res. (2011)
[5] Morris et al,. "Weisfeiler and Leman go Machine Learning: The Story so far", arXiv (2021)

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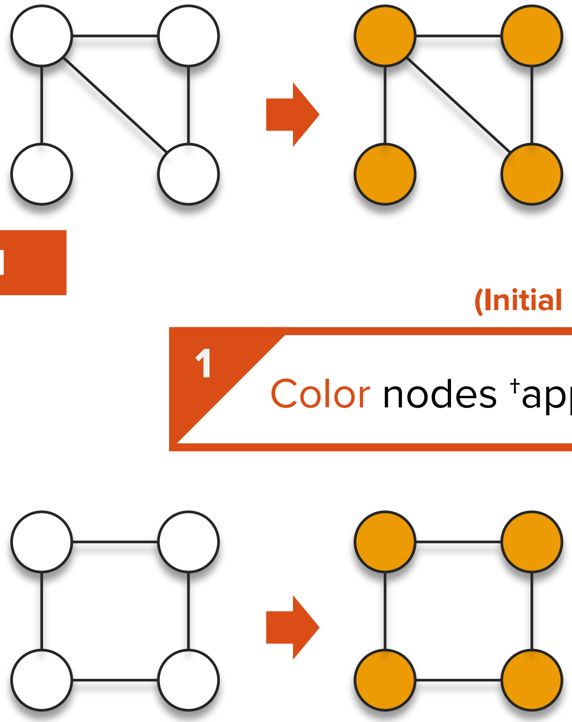
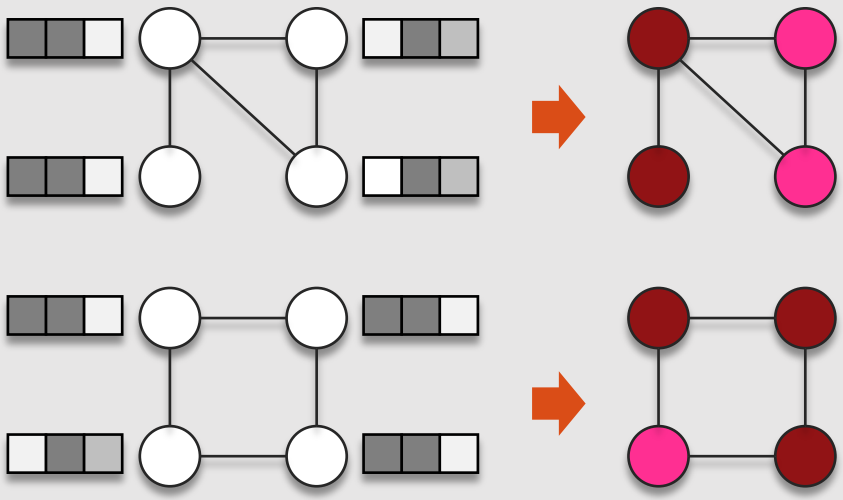


Graph 1

(Initial iteration only)

1 Color nodes †appropriately

Graph 2



Graphs with node features: Also appropriately

†As suggested by [4], color node according to the node degree. Or just start with a uniform coloring

[4] Shervashidze et al., “Weisfeiler-Lehman Graph Kernels”, J. Mach. Learn. Res. (2011)
[5] Morris et al,. “Weisfeiler and Leman go Machine Learning: The Story so far”, arXiv (2021)

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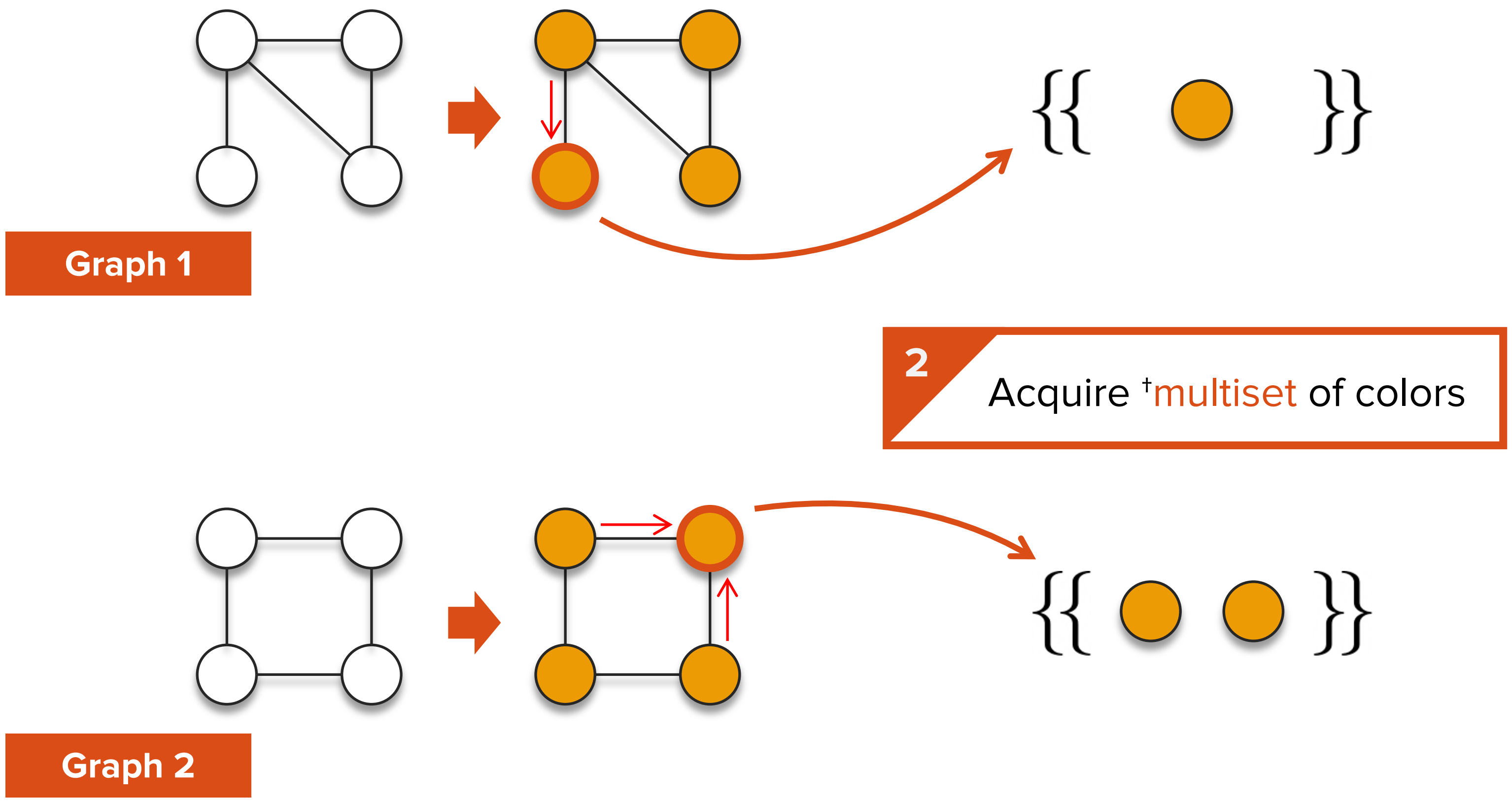

†Multiset is a set that allows multiple duplicates of elements

[4] Shervashidze et al., “Weisfeiler-Lehman Graph Kernels”, J. Mach. Learn. Res. (2011)
[5] Morris et al,. “Weisfeiler and Leman go Machine Learning: The Story so far”, arXiv (2021)

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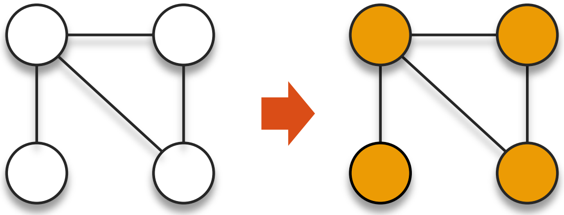
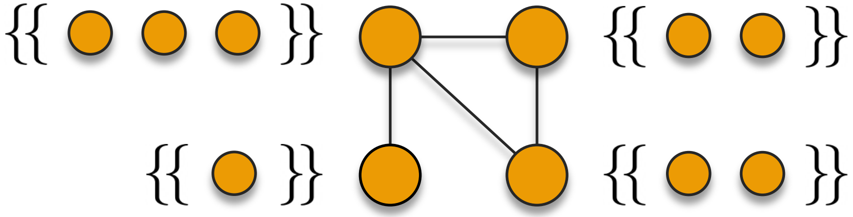
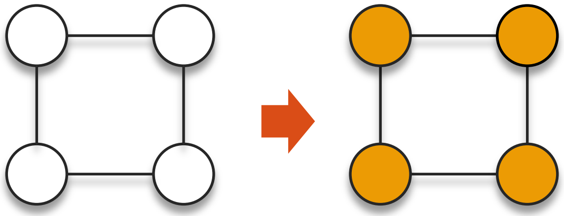
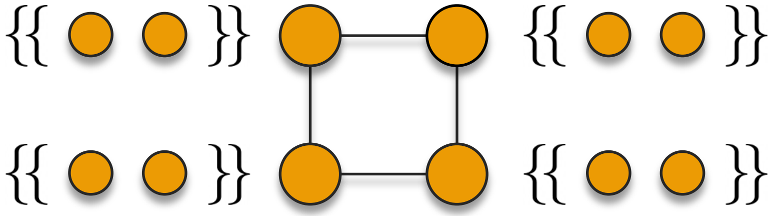




Graph 1

2 Acquire †multiset of colors





Graph 2

†Multiset is a set that allows multiple duplicates of elements

[4] Shervashidze et al., “Weisfeiler-Lehman Graph Kernels”, J. Mach. Learn. Res. (2011)
[5] Morris et al,. “Weisfeiler and Leman go Machine Learning: The Story so far”, arXiv (2021)

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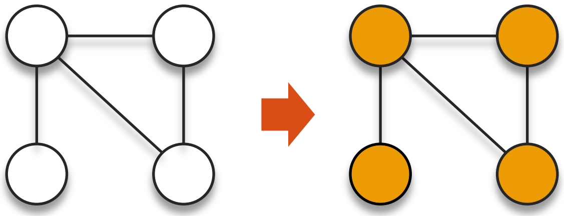
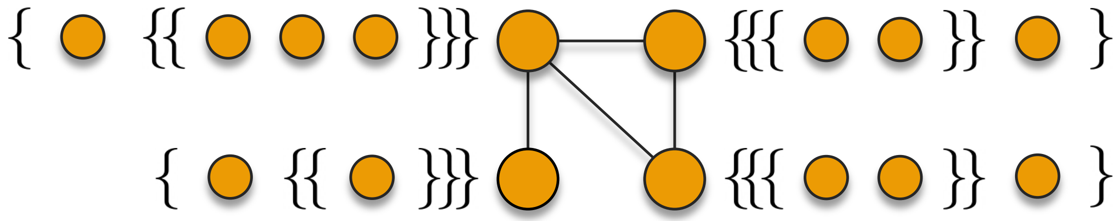
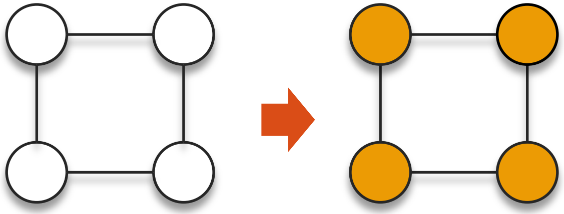
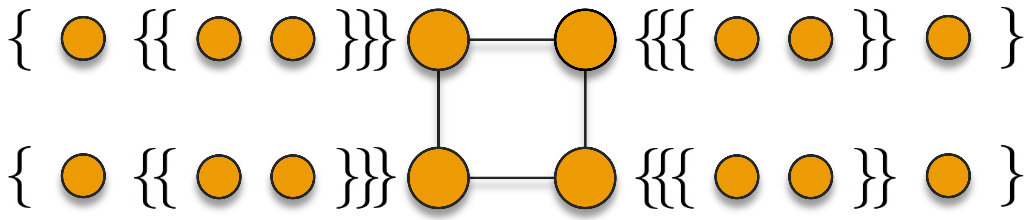




Graph 1

3 Make a set by including self





Graph 2

†Multiset is a set that allows multiple duplicates of elements

[4] Shervashidze et al., “Weisfeiler-Lehman Graph Kernels”, J. Mach. Learn. Res. (2011)
[5] Morris et al,. “Weisfeiler and Leman go Machine Learning: The Story so far”, arXiv (2021)

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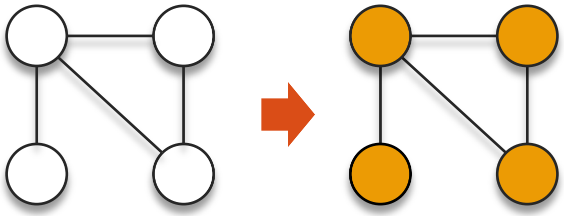
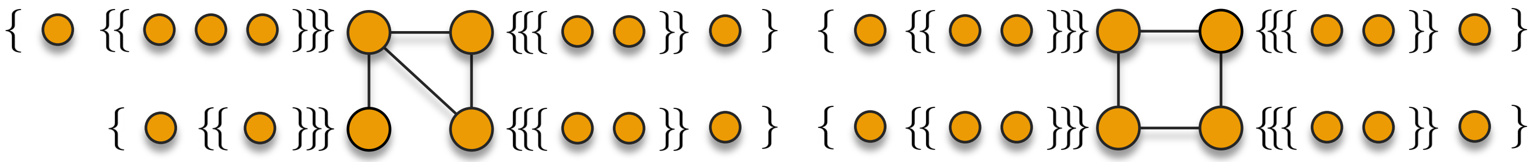
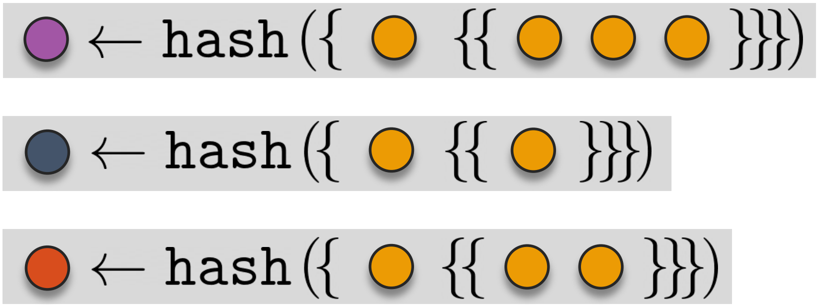
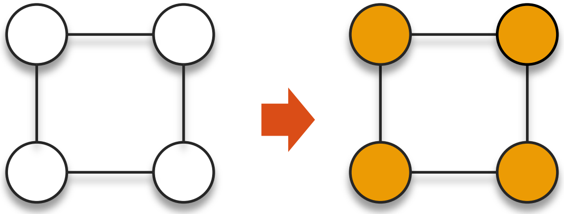


Graph 1



4 Map each set to a new color by a †bijective function



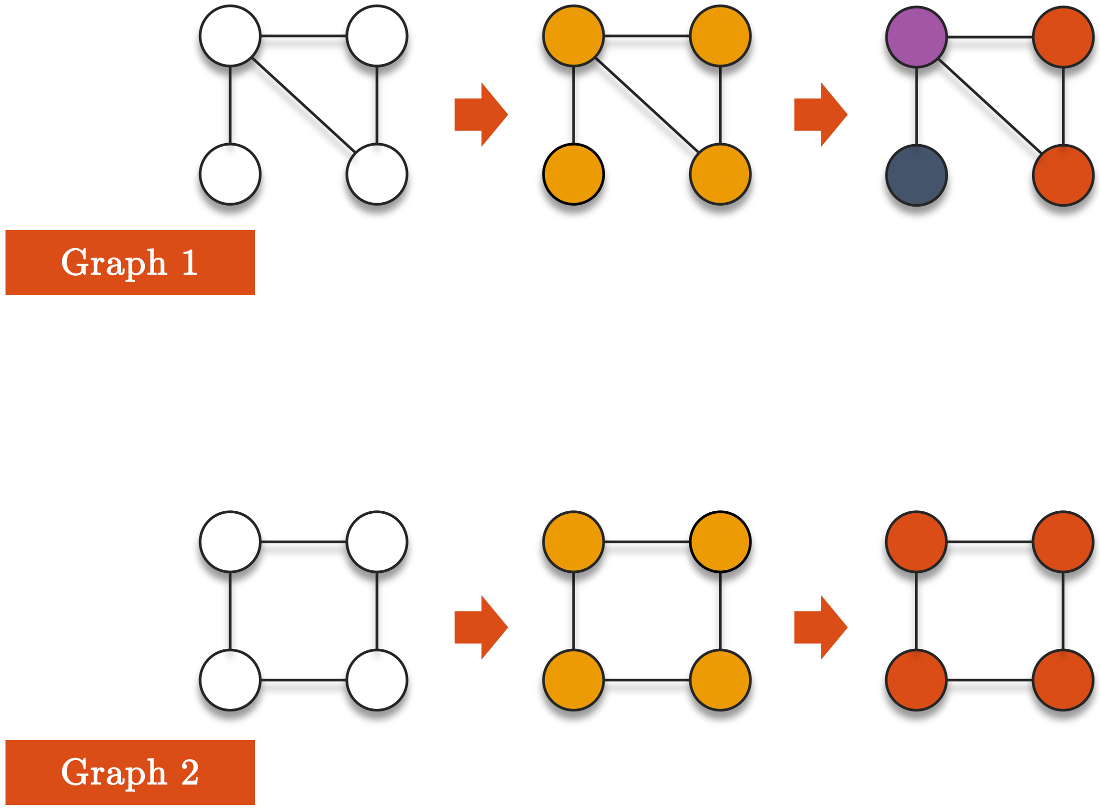


Graph 2

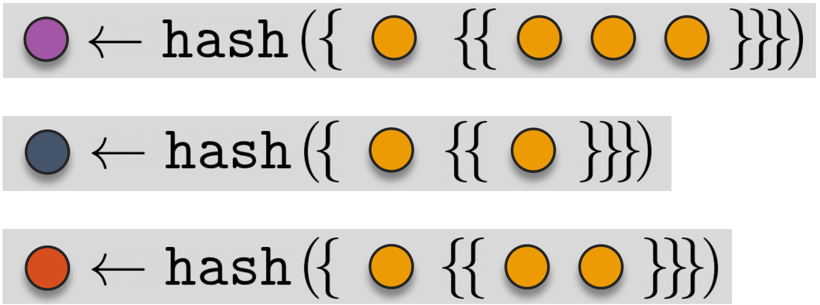
† At least injective. The function has multiple names, such as hashing functions, relabeling functions, etc.

[4] Shervashidze et al., “Weisfeiler-Lehman Graph Kernels”, J. Mach. Learn. Res. (2011)
[5] Morris et al,. “Weisfeiler and Leman go Machine Learning: The Story so far”, arXiv (2021)

One iteration of the WL-isomorphism test [1], [2]



5 Get the colors of the next iteration



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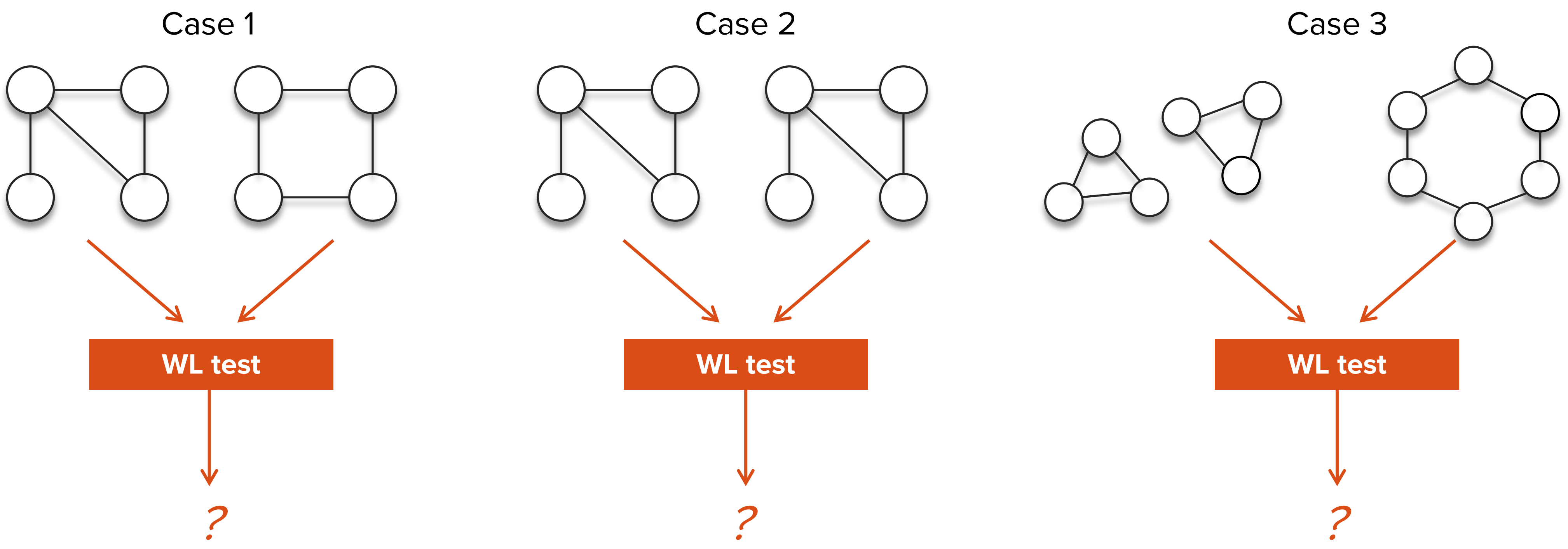
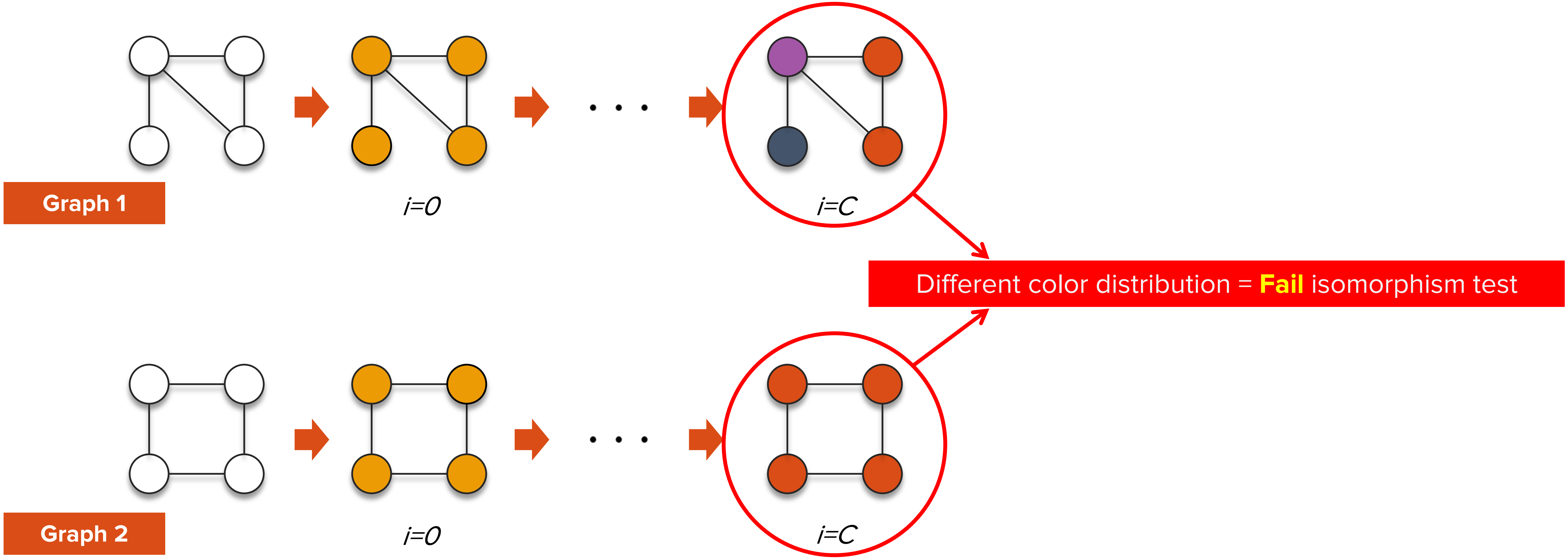
WL-isomorphism test: Three example cases



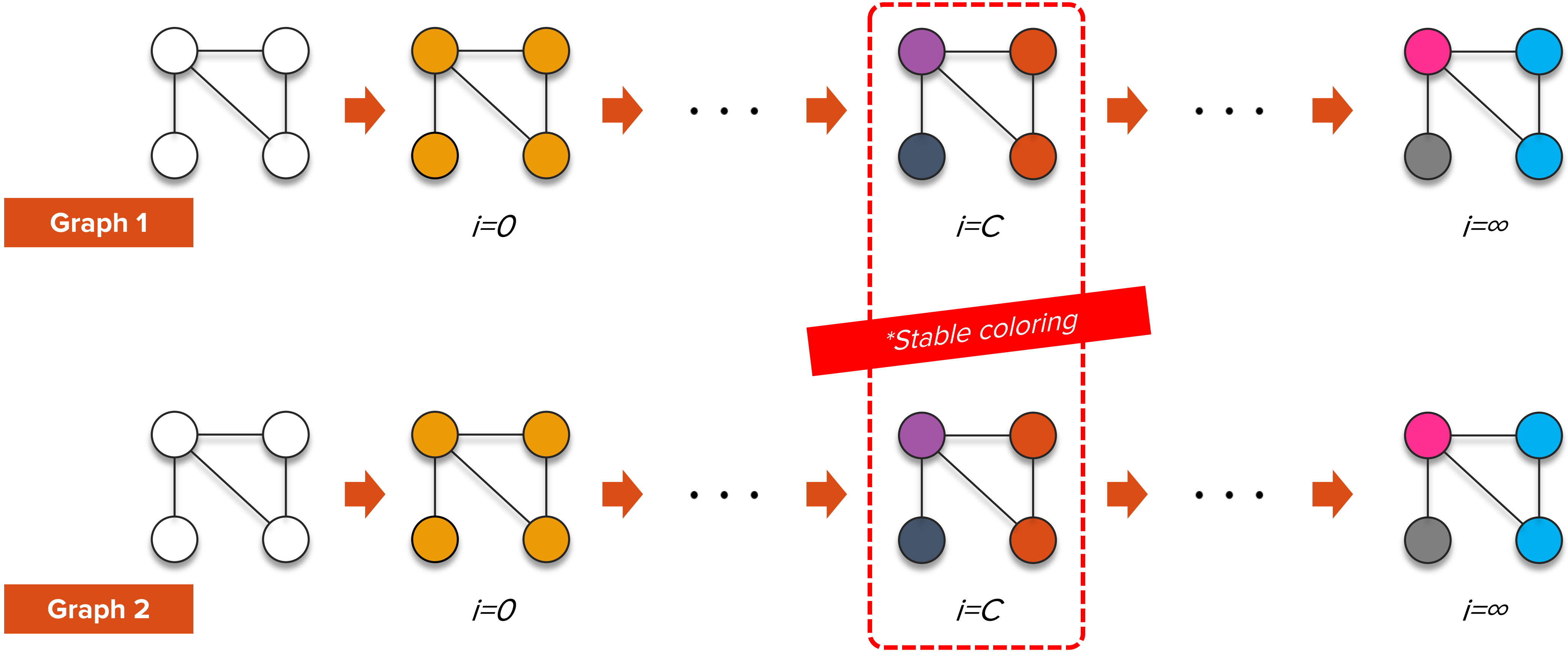
WL-isomorphism test: Three example cases

Counclusion of case 1



WL-isomorphism test: Three example cases

Counclusion of case 2

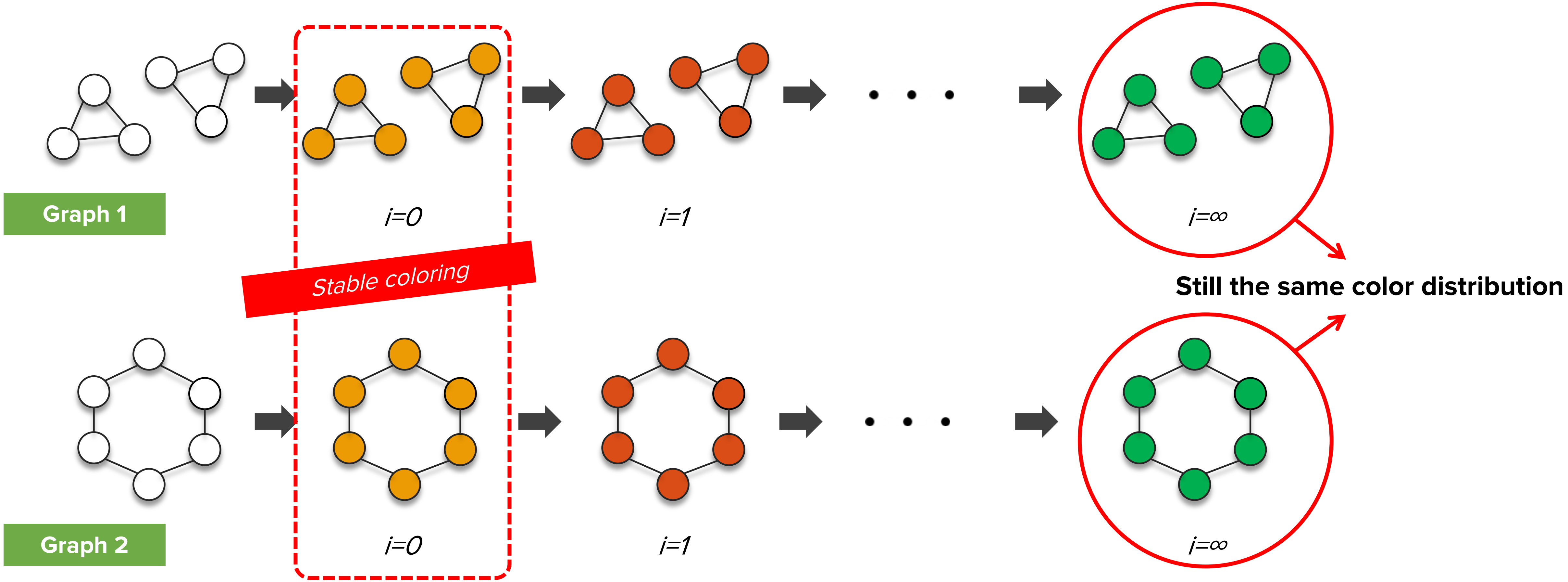


Conclusion: Two graphs are isomorphic ..?

* We do not actually need to run the iteration to the end of time: If color distributions remain unchanged for two consecutive iterations, you already reached stable coloring (hint: Use induction). Also, *C* is bounded by *max*(|Graph 1|, |Graph 2|) (see [5]).

WL-isomorphism test: Three example cases

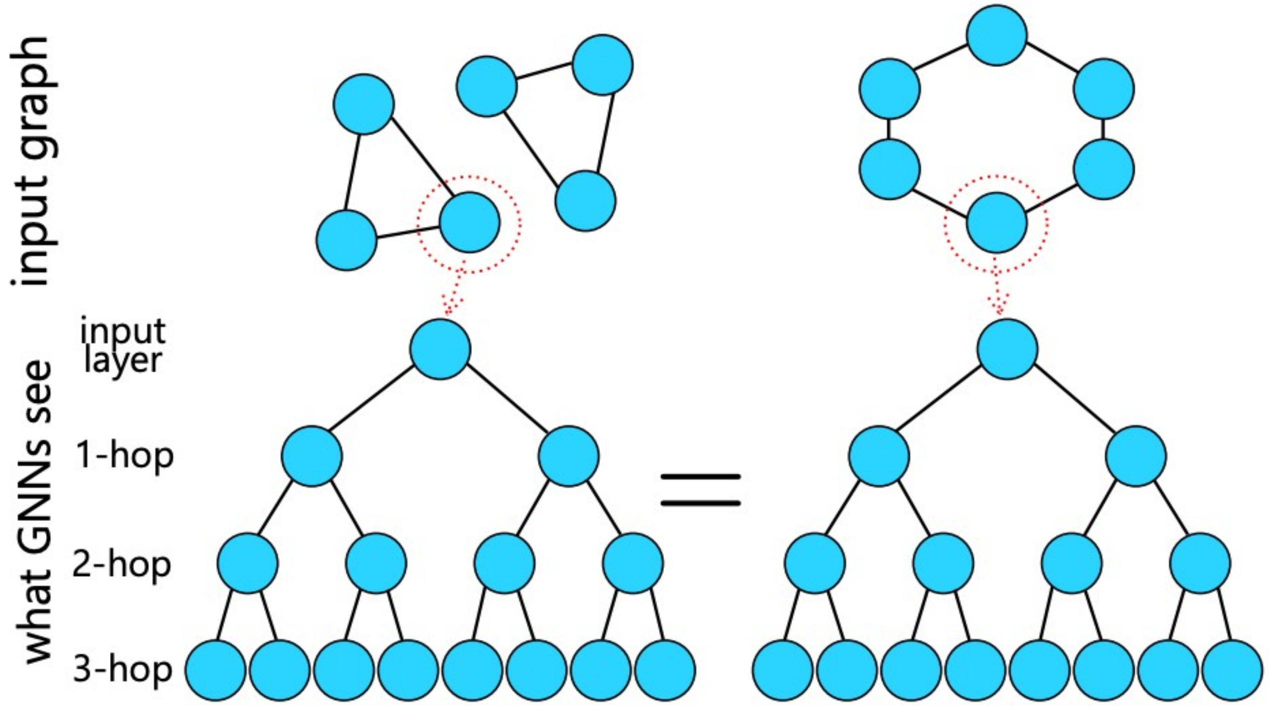
Counclusion of case 3



Conclusion: ~~Two graphs are isomorphic~~ **Cannot determine**

WL-isomorphism test: Three example cases

Counclusion of case 3

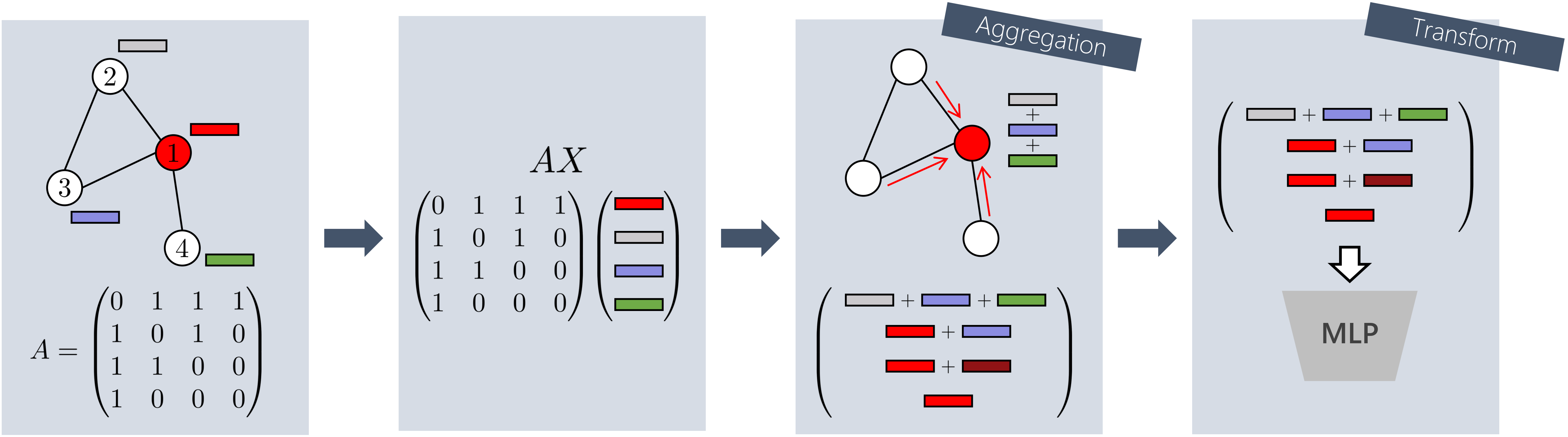


The same intuition can also be derived from the “computational tree” point of view.

Understanding the connection between the WL test and message-passing

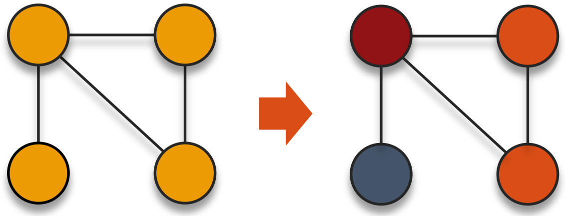
(Recap) Message-passing framework in GNNs

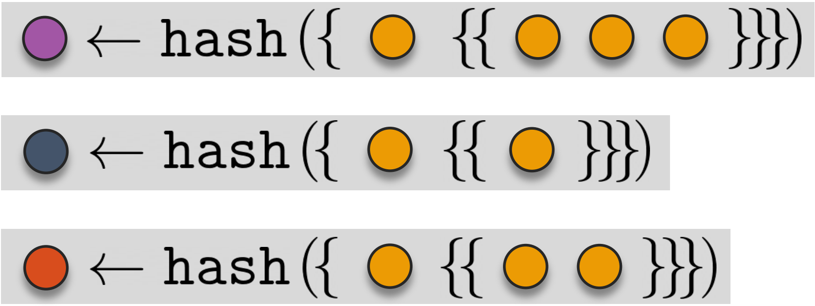
Aggregate and Transform



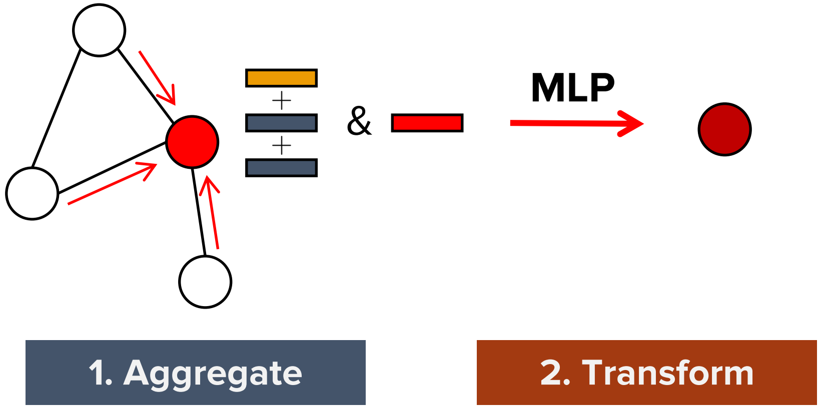
Relation between WL and GNNs

“Color refinement” in WL





Message passing in GNNs

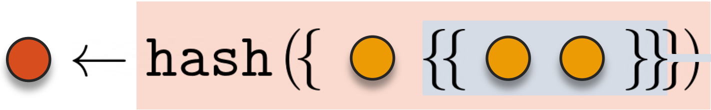


$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

Can you see the similarity?

Relation between WL and GNNs

Color refinement in WL



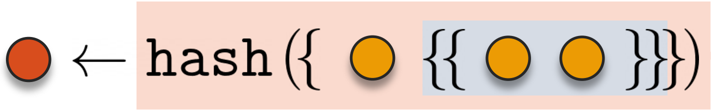
Collect neighbor information

Message passing in GNNs

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

Relation between WL and GNNs

Color refinement in WL



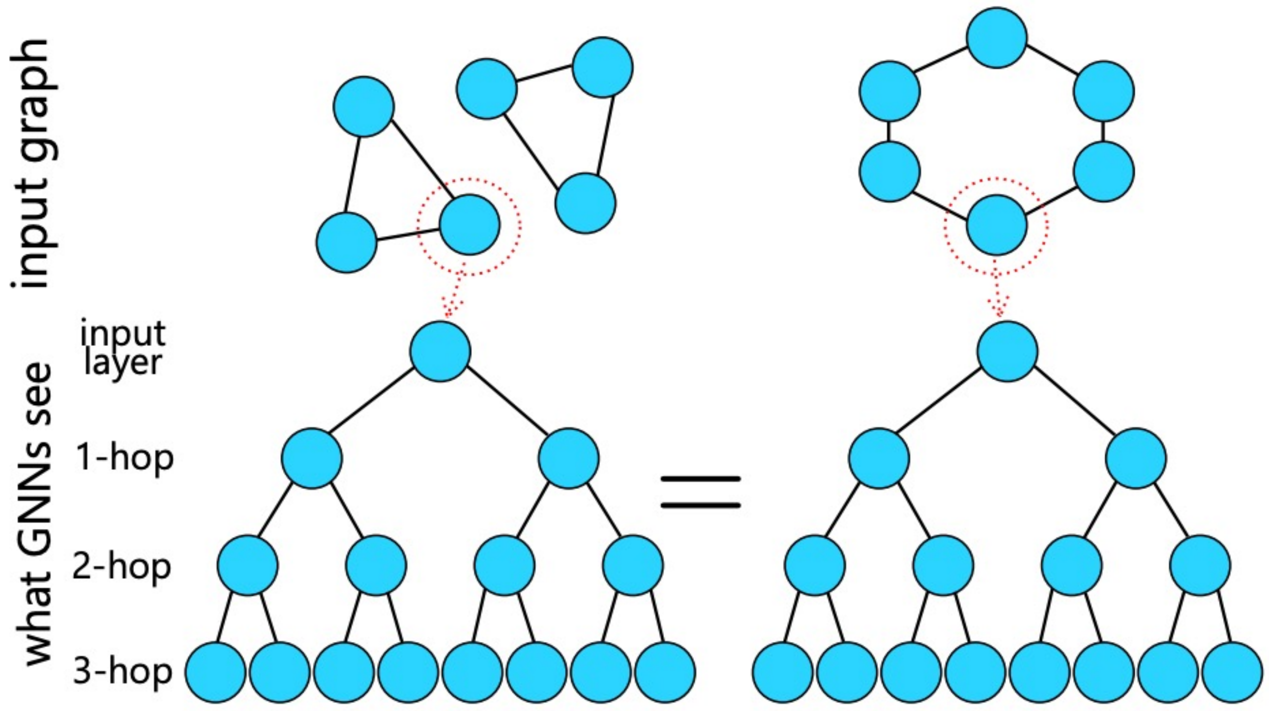
Message passing in GNNs

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

Map self & neighbor information to next iteration

Revisiting the WL-isomorphism test: Computation tree point of view

Revisiting Case 3



The same intuition can also be derived from the “computational tree” point of view [6].

[6] Sato et al., “Random Features Strengthen Graph Neural Networks”, SDM 2021

Consequences of GNN's ability to differentiate graphs

Color refinement in WL

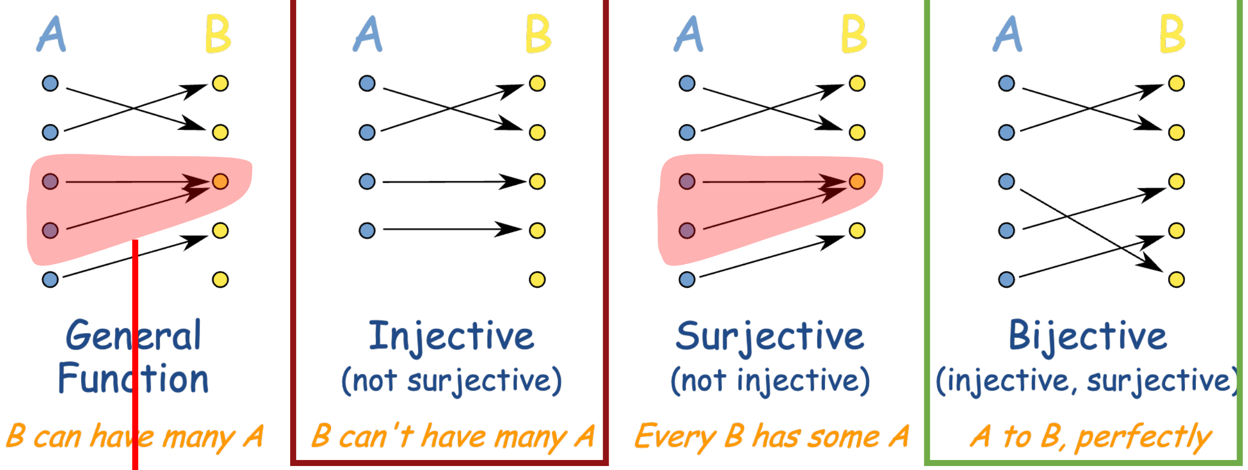
$$\bullet \leftarrow \mathtt{hash}(\{\bullet\ \{\{\bullet\ \bullet\}\}\})$$

- $\mathtt{hash}$: Fixed **bijective** function (at least **injective**)

Message passing in GNNs

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

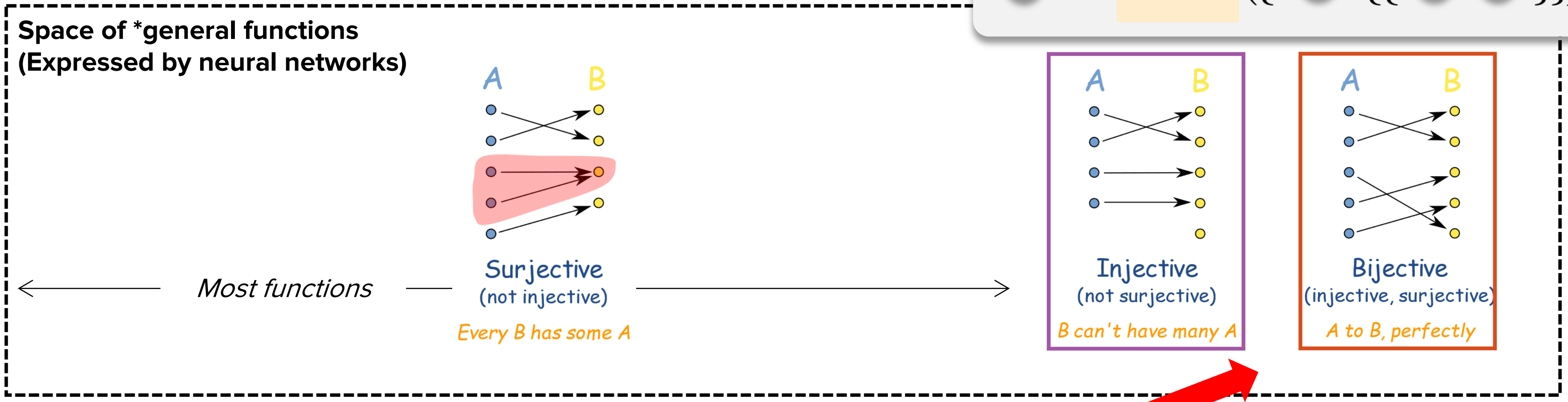
- ϕ, ψ*A neural network (Learned from data)
- (Probably) *Not* **bijective** *nor* **injective**



Loss of expressive power: Cannot distinguish some elements

Consequences of GNN's ability to differentiate graphs

Color refinement in WL



Message passing in GNNs

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v\in\mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

GNNs are *at best* 1-WL

In-depth understanding of (Xu et al., ICLR 2019) and (Morris et al., AAAI 2019)

GNNs cannot exceed WL in terms of its expressivity

Theorem [Morris et al., 2019, Xu et al., 2019] (informal)

If the 1-WL test cannot distinguish two graphs, then any GNNs also cannot distinguish them.

If GNNs can distinguish two graphs, the 1-WL test can also distinguish them.

In other words, the expressive power of GNNs is capped by 1-WL.

Color refinement in 1-WL

$$\bullet \leftarrow \texttt{hash}(\{\ \bullet\ \{\{\ \bullet\ \bullet\ \}\}\})$$

$$\geq$$

Message passing in GNNs

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

GNNs cannot exceed WL in terms of its expressivity

Proof of existence

Theorem (informal)
There exists weight parameters of GNN such that, expressivity of GNNs **exactly match** 1-WL test.

How to go beyond?

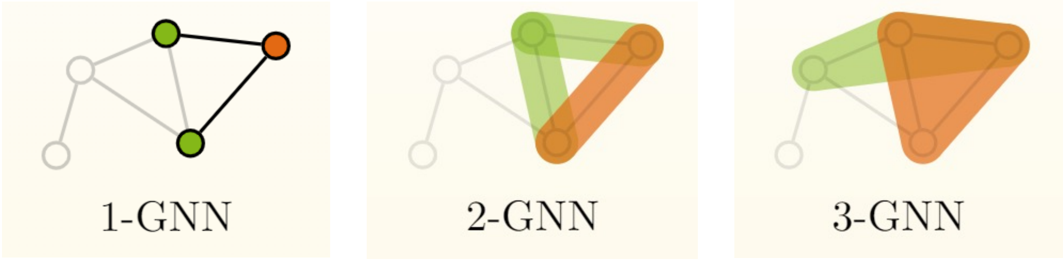
Problem: GNNs are bound by 1-dim WL-test

Solution: Make GNNs based on k-dim WL-test ($k > 1$)

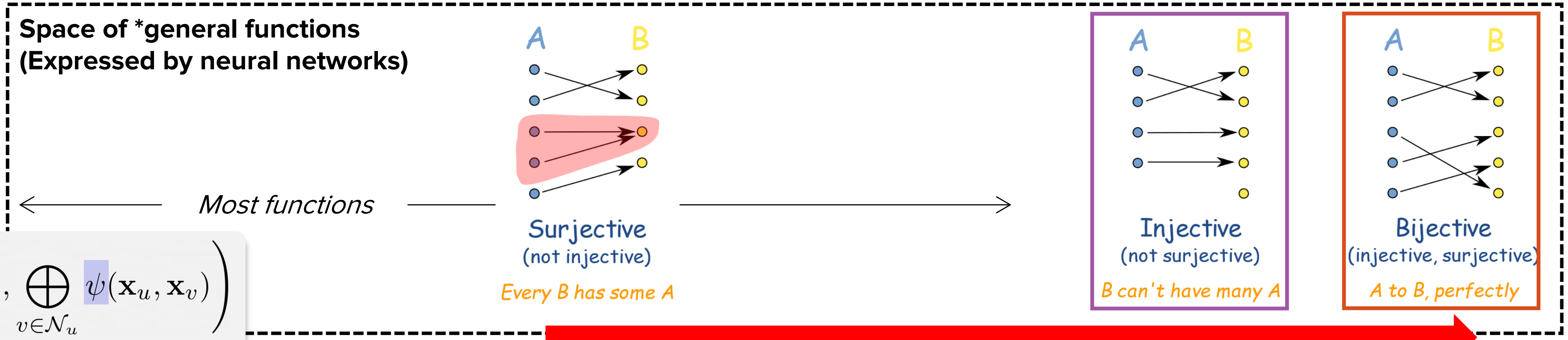
Theorem 2. Let (G, l) be a labeled graph. Then for all $t \geq 0$ there exists a sequence of weights $\mathbf{W}^{(t)}$, and a 1-GNN architecture such that

$$c_l^{(t)} \equiv f^{(t)} .$$

Hence, in the light of the above results, 1-GNNs may viewed as an extension of the 1-WL which in principle have the same power but are more flexible in their ability to adapt to the learning task at hand and are able to handle continuous node features.



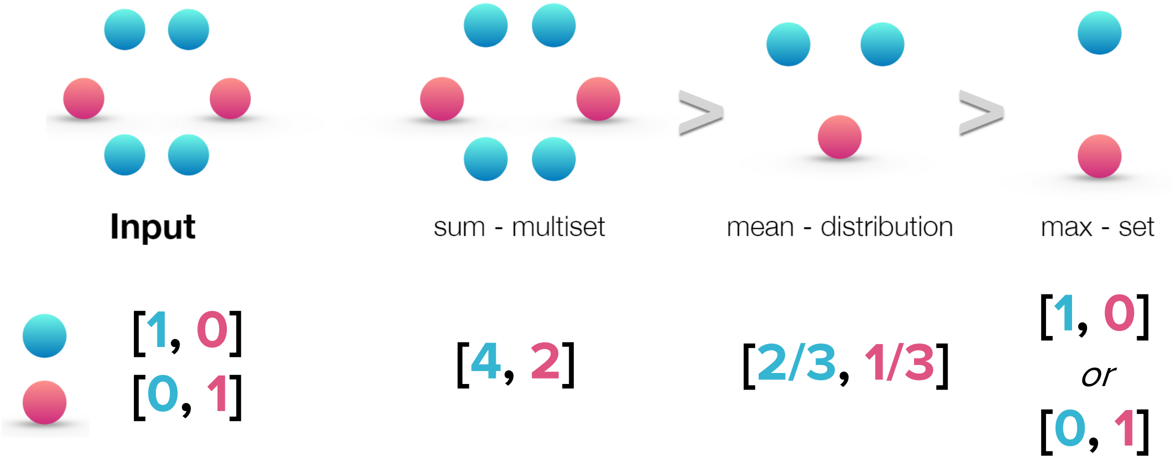
GNNs cannot exceed WL in terms of its expressivity



$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

Q. What design choices are needed to make the function *injective as possible?

1. Use summation for aggregation



Input | sum - multiset | mean - distribution | max - set

[1, 0]
[0, 1]

[4, 2]

[2/3, 1/3]

[1, 0] *or* [0, 1]

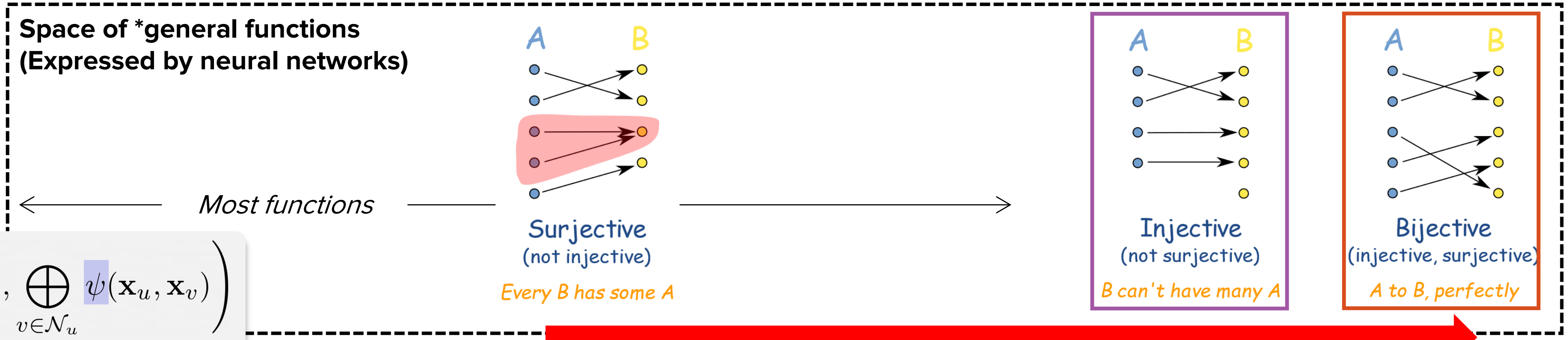
2. Use at least 2 layers of MLP

Theorem [Xu et al., 2019] (informal)

One-layer ReLU MLPs are *not* injective.

* Does not necessarily mean the resulting neural network is injective.
For injectivity in neural networks, see Puthawala et al., "Globally Injective ReLU Networks", J. Mach. Learn. Res. (2020)

GNNs cannot exceed WL in terms of its expressivity



$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

Q. What design choices are needed to make the function *injective as possible?

Graph Isomorphism Networks (GIN)

$$h_v^{(k)} = \mathrm{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right) \cdot h_v^{(k-1)} + \sum\nolimits_{u \in \mathcal{N}(v)} h_u^{(k-1)}\right)$$

*In my experience, just setting epsilon as a non-learnable pararmeter with 0 value works fine

Takeaways

1. Defining graphs being ‘identical’ = isomorphism test
2. WL-isomorphism test: Heuristic that can be used for isomorphism, but not 100% work
3. Connections: GNN’s message-passing and WL test, and GNN’s limitations

Thank you!

Please feel free to ask any questions :)

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