Graph Neural Networks

Randomization & Features

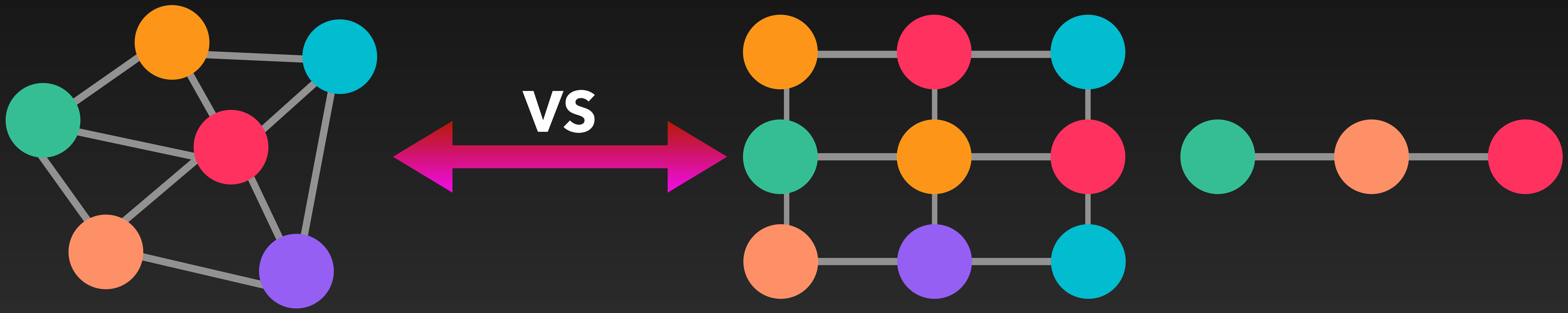
Viviane Potocnik, 15.03.22

Outline

1. **Introduction**
    i. Overview on GNNs
    ii. Limitations of GNNs
2. Motivation
3. Extensions of Classical GNNs
    i. GNNs w/ RNI
    ii. DropoutGNN
    iii. Graph with Substructure Network (GSN)
4. Discussion

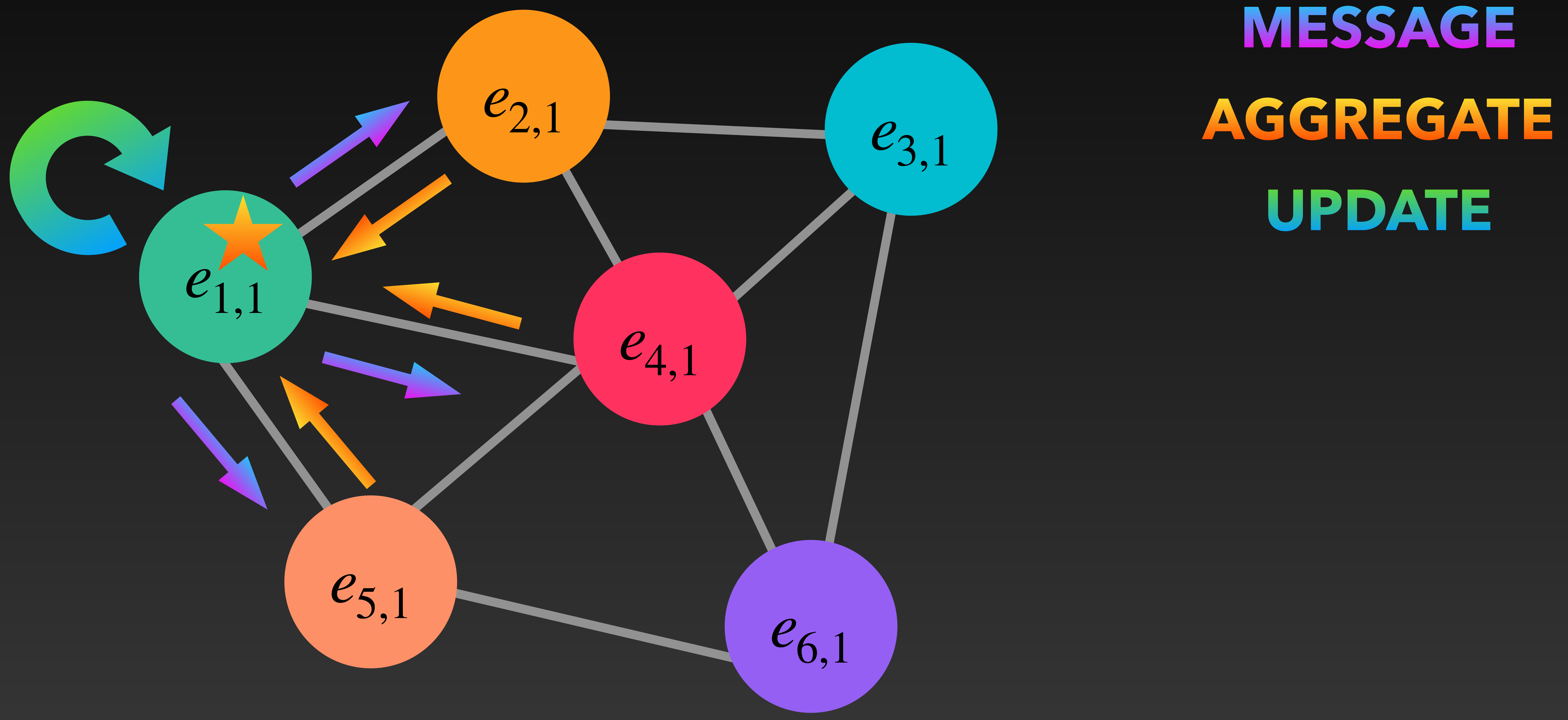
Introduction

Overview on GNNs



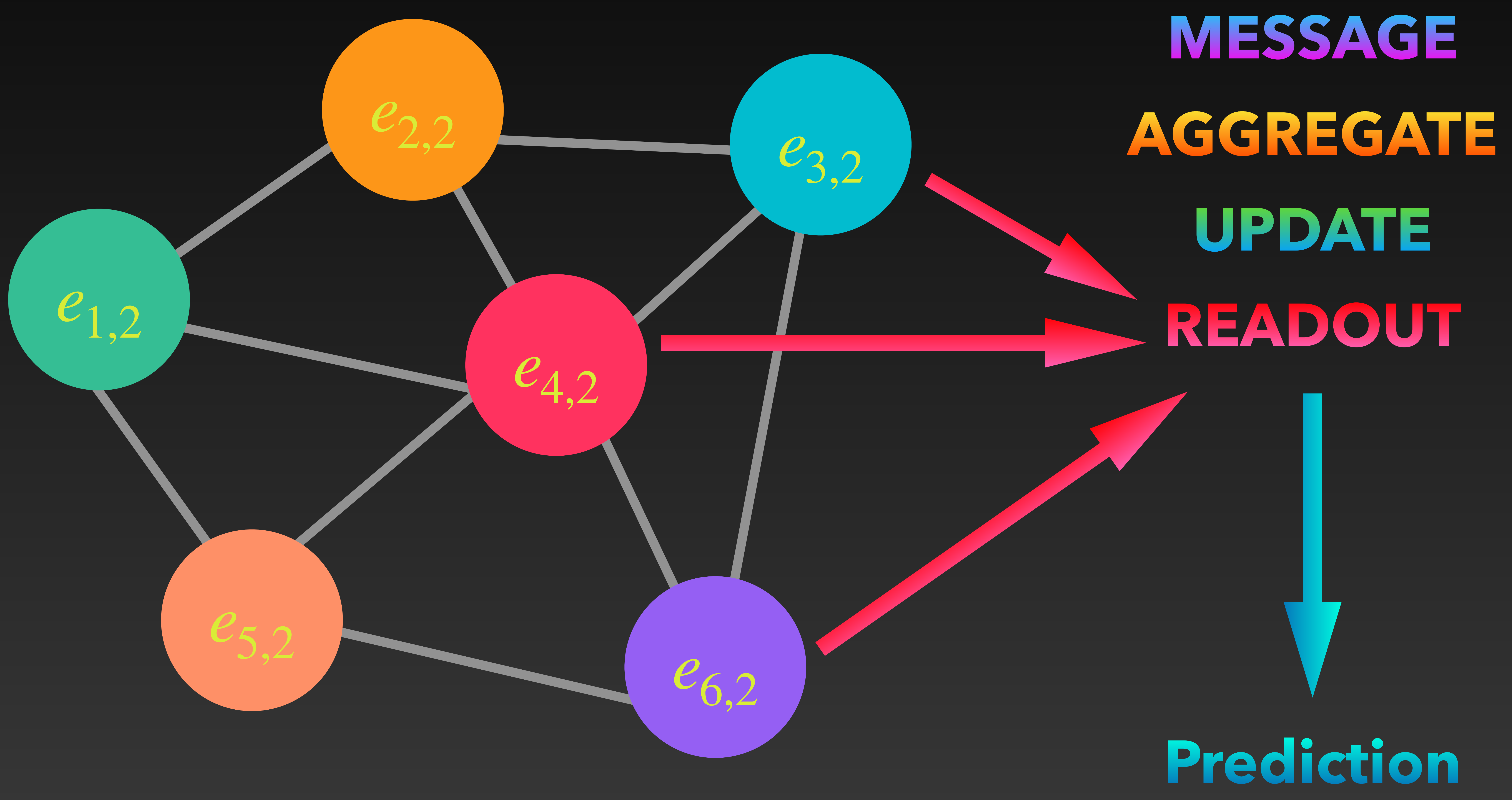
Introduction

Overview on GNNs - MPM



Introduction

Overview on GNNs - MPM



Introduction

Limitations of GNNs

1. Cannot learn simple graph algorithms
2. Cannot distinguish non-isomorphic graphs
    1. Only (at most) as powerful as 1-WL test
3. No notion of local (sub-) structures

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Motivation

1. Increase the expressive power (Universality)
2. Invariance and Equivariance (Ability to Generalize)
3. Viability (w.r.t complexity and performance)

Introduction

Example of the WL test

Introduction

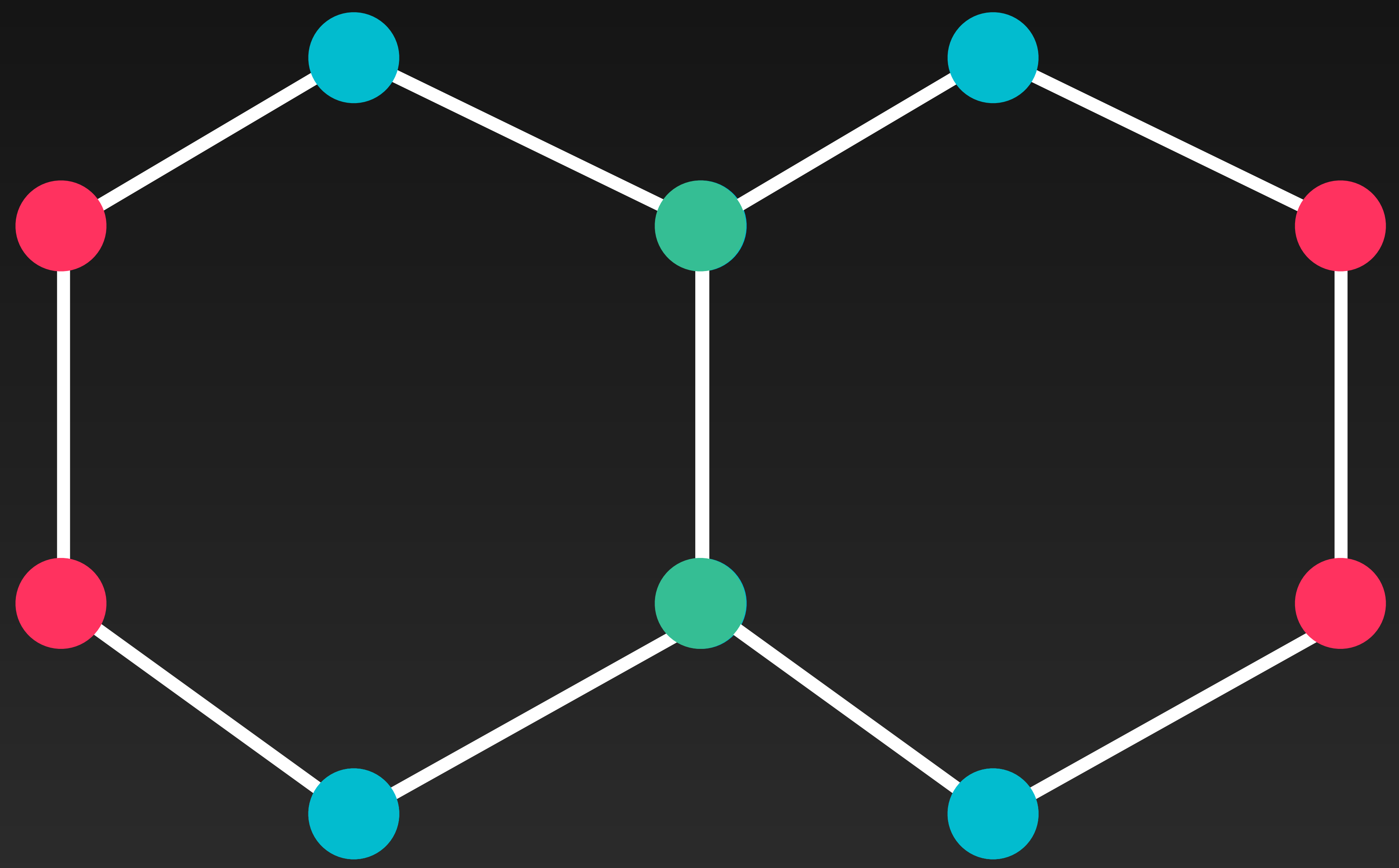
Example of the WL test

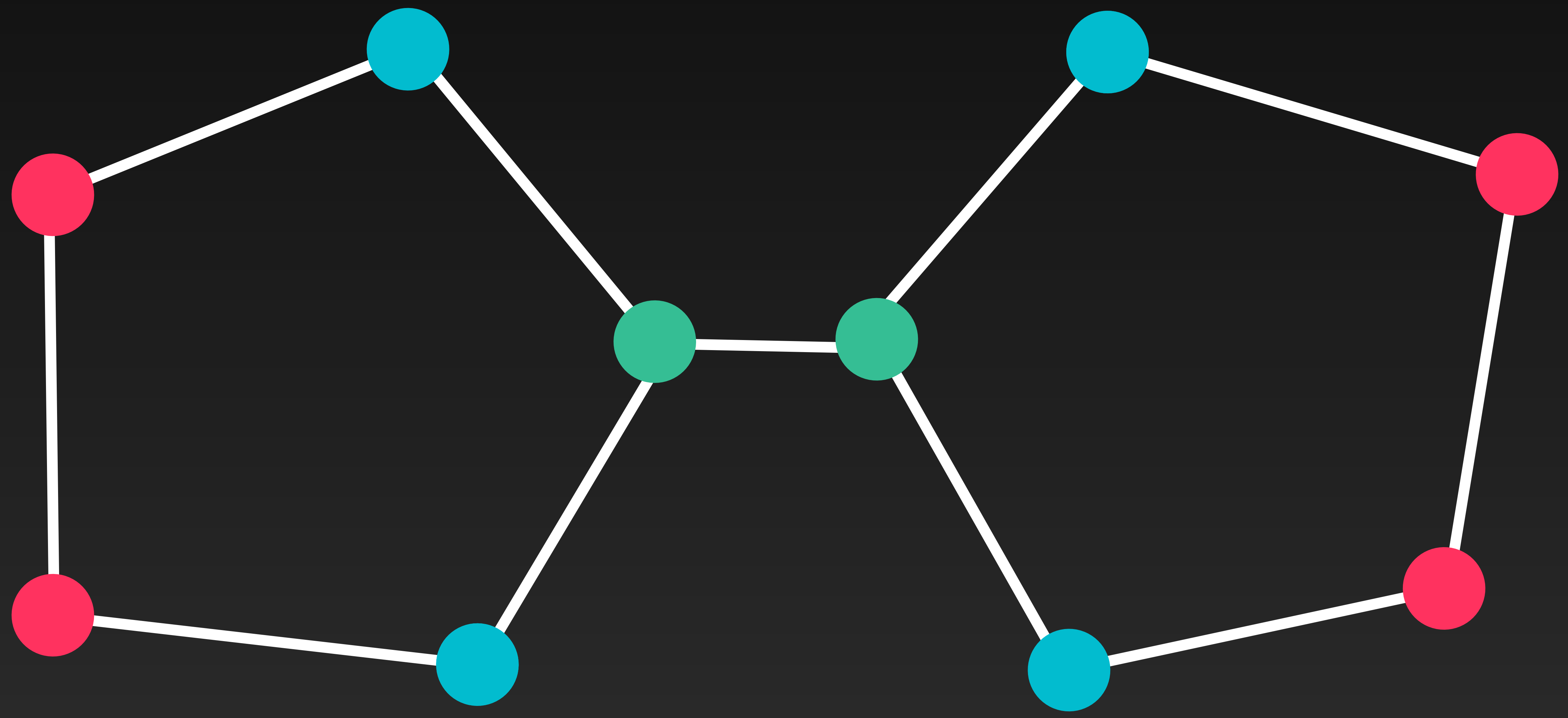
Following the WL-test we can conclude that since the histograms are equal the graphs are possibly isomorphic.

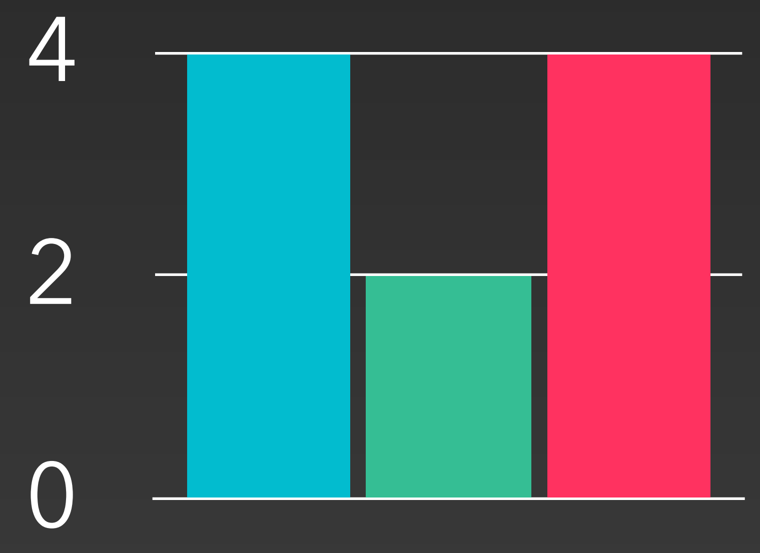
$$f : V(G) \to V(H)$$

Introduction

Example of the WL test of non-isomorphic graphs



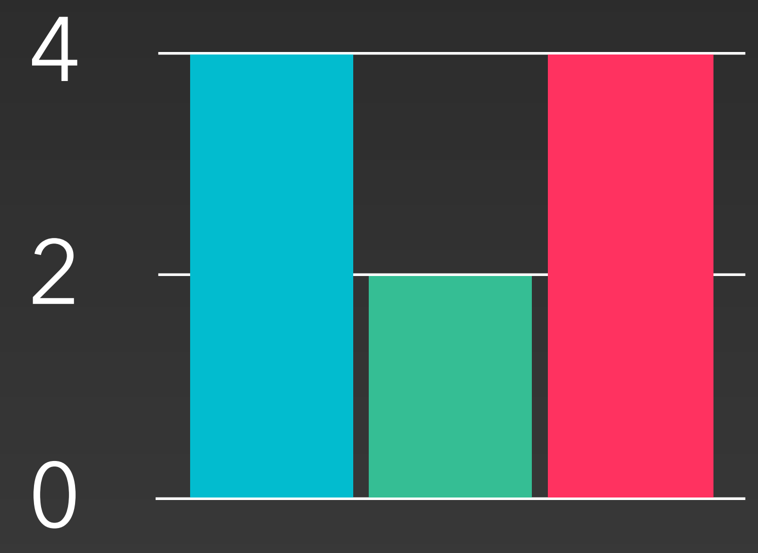




Decalin
C10H18

WL Test fails!

Bicyclopentyl
C10H18



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Extension of GNNs

GNNs w/ RNI - Introduction

Key Ideas

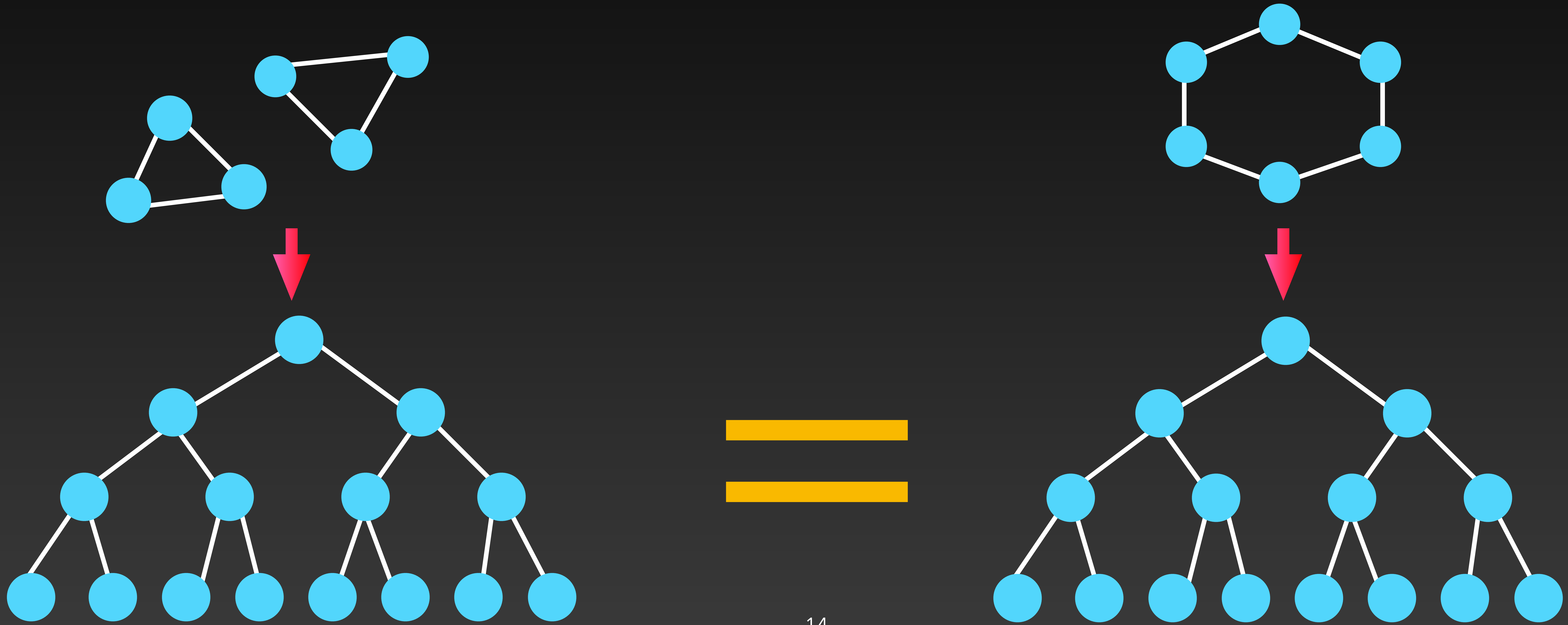
1. Randomly initialize nodes, s.t. non-isomorphic graphs become distinguishable.
2. Invariance maintained **in expectation** via randomness.

Extension of GNNs

GNNs with RNI- Illustrative Example

Problem 3: GNNs have no notion of local (sub-)structures

Problem 2: GNNs are at most powerful as the WL-test



Extension of GNNs

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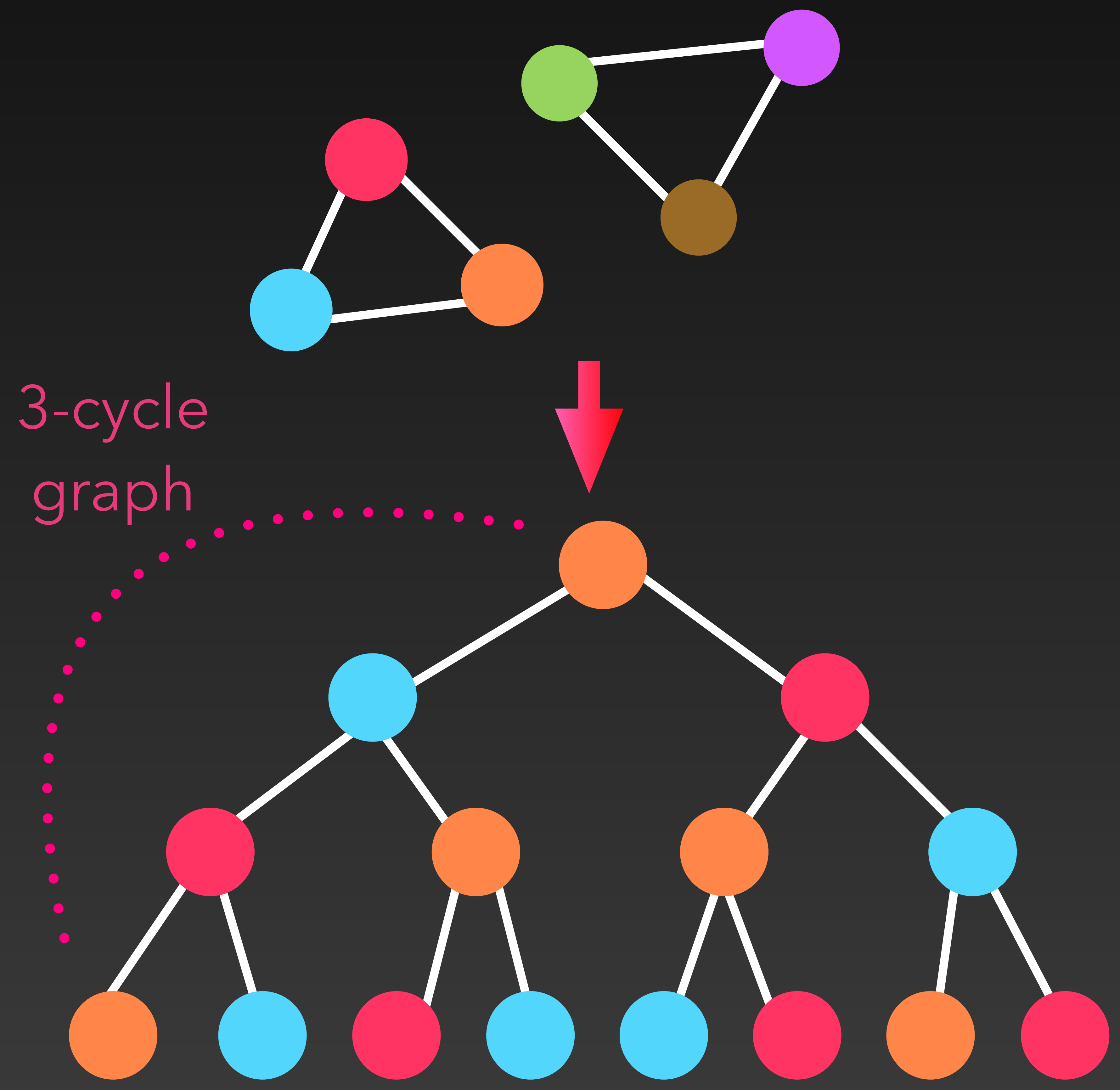

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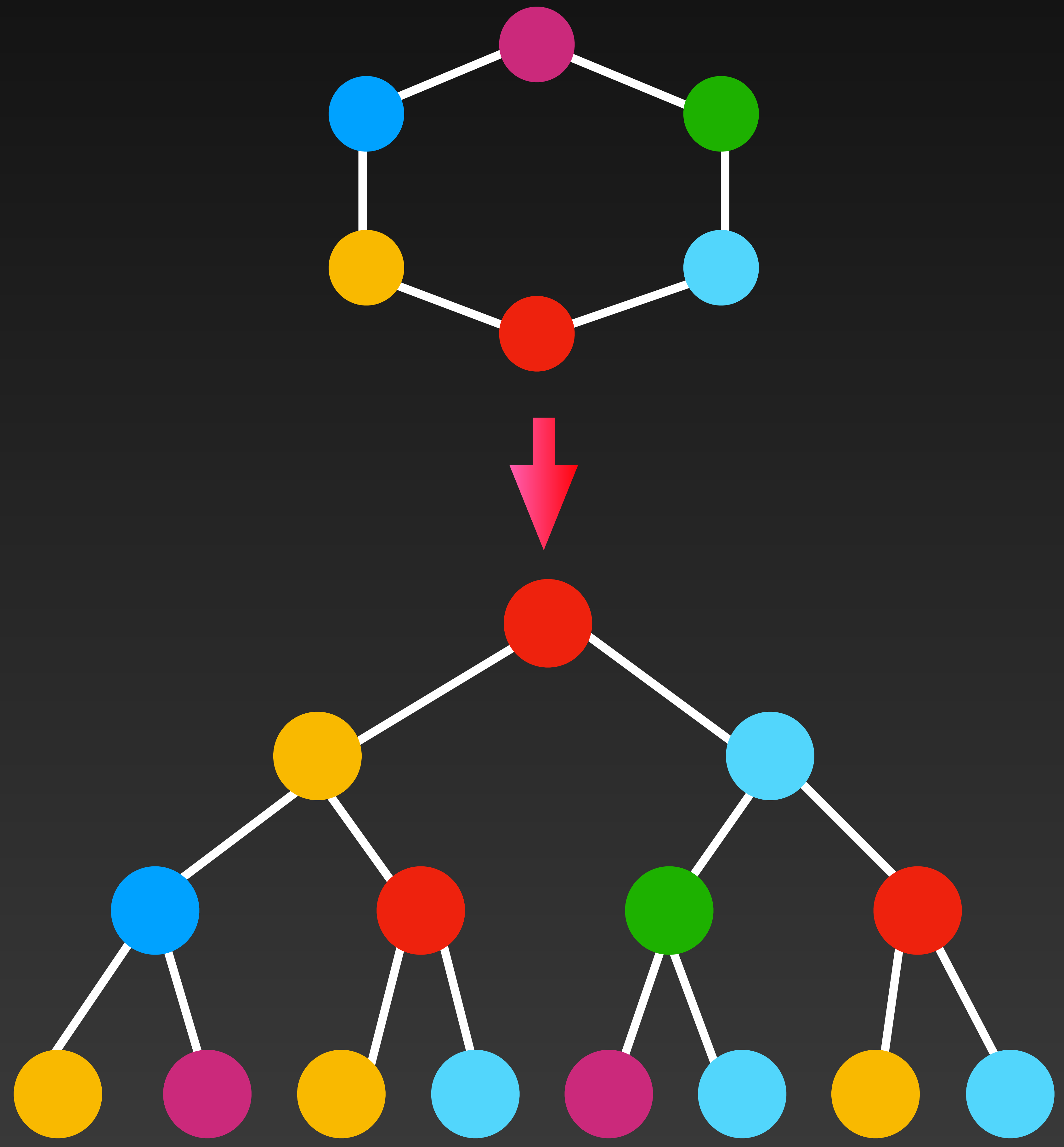
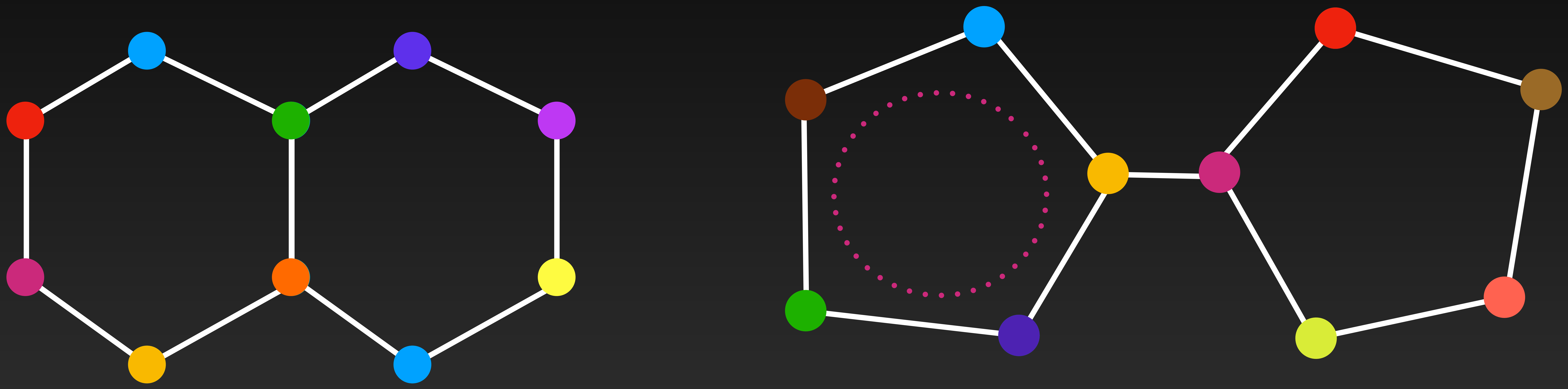


Extension of GNNs

rGIN - Back to the WL-Test

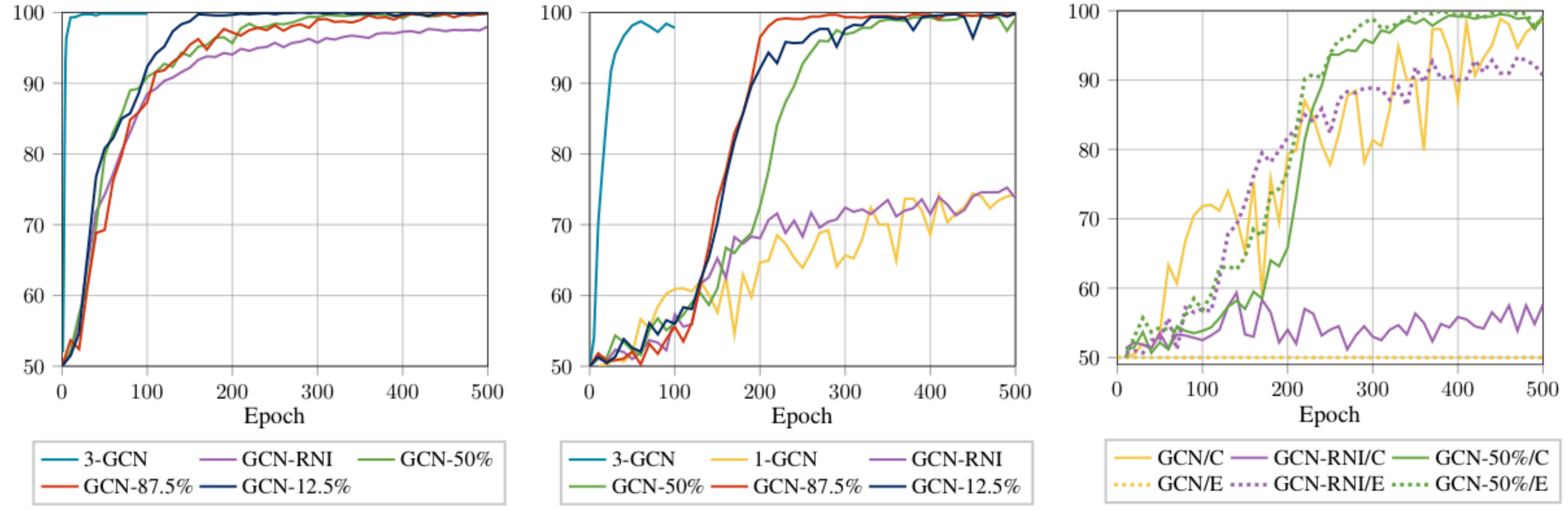
Problem 2: GNNs are at most powerful as the WL-test



GNNs w/ RNI can distinguish these molecules by the existence of cycles of length five

Extension of GNNs

GNNs w/ RNI - Results



(a) EXP. (b) CEXP. (c) $\overline{\text{EXP}}$ (/E) and CORRUPT (/C).

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Extension of GNNs

DropoutGNNs - Introduction

Key Ideas

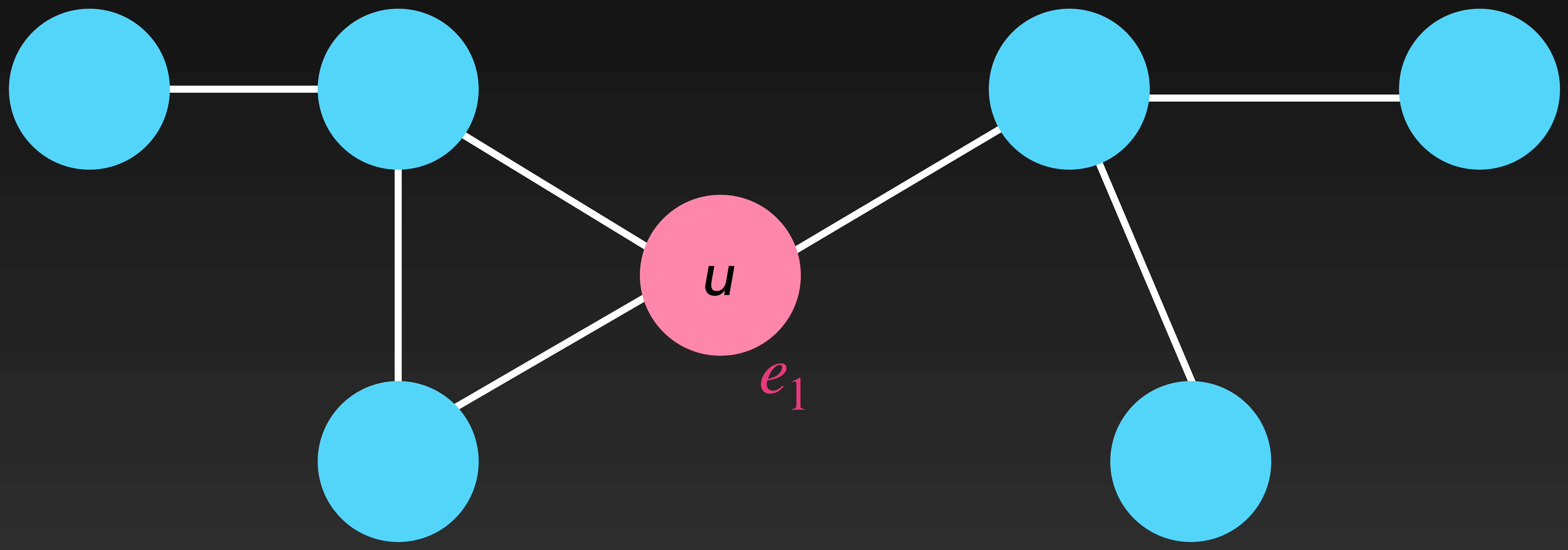
1. Multiple runs with random dropout combinations
2. Aggregate perturbed neighborhood information
3. Dropout during *testing* **and** *training*
4. Reduce randomization effect (overfitting)

Extension of GNNs

DropoutGNNs - Example

AGGREGATE

Run No. 1

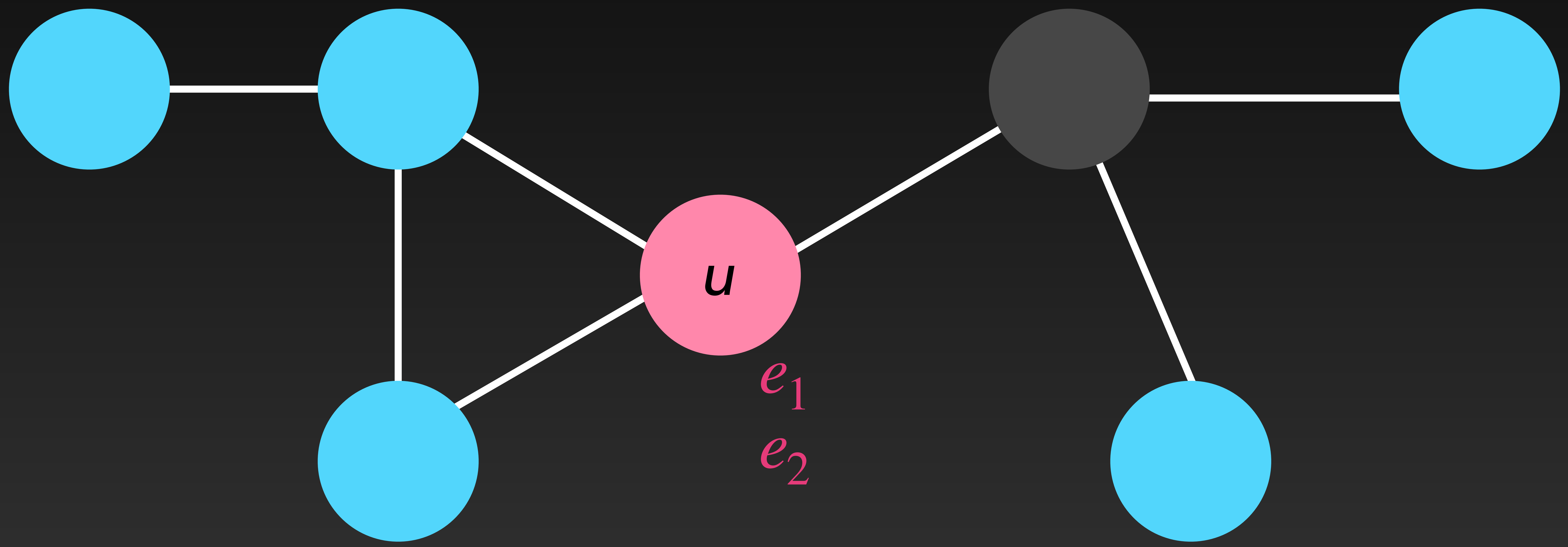


Extension of GNNs

DropoutGNNs - Example

Run No. 2

AGGREGATE

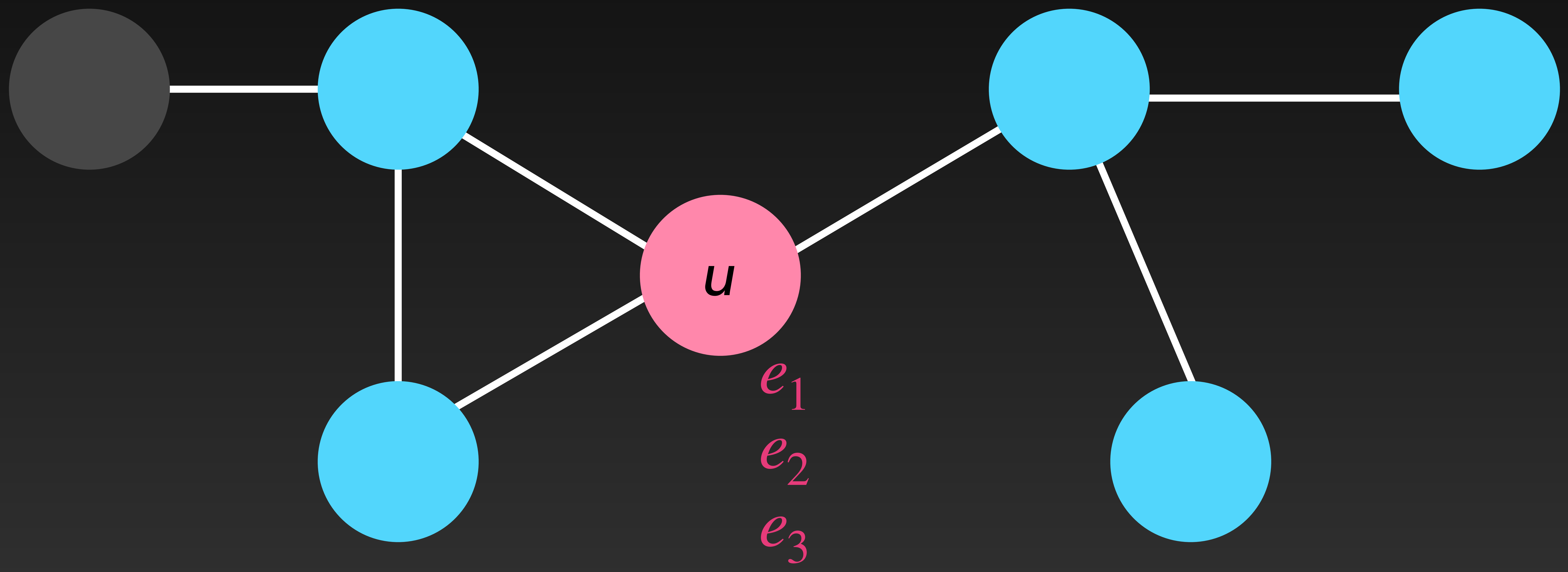


Extension of GNNs

DropoutGNNs - Example

AGGREGATE

Run No. 3

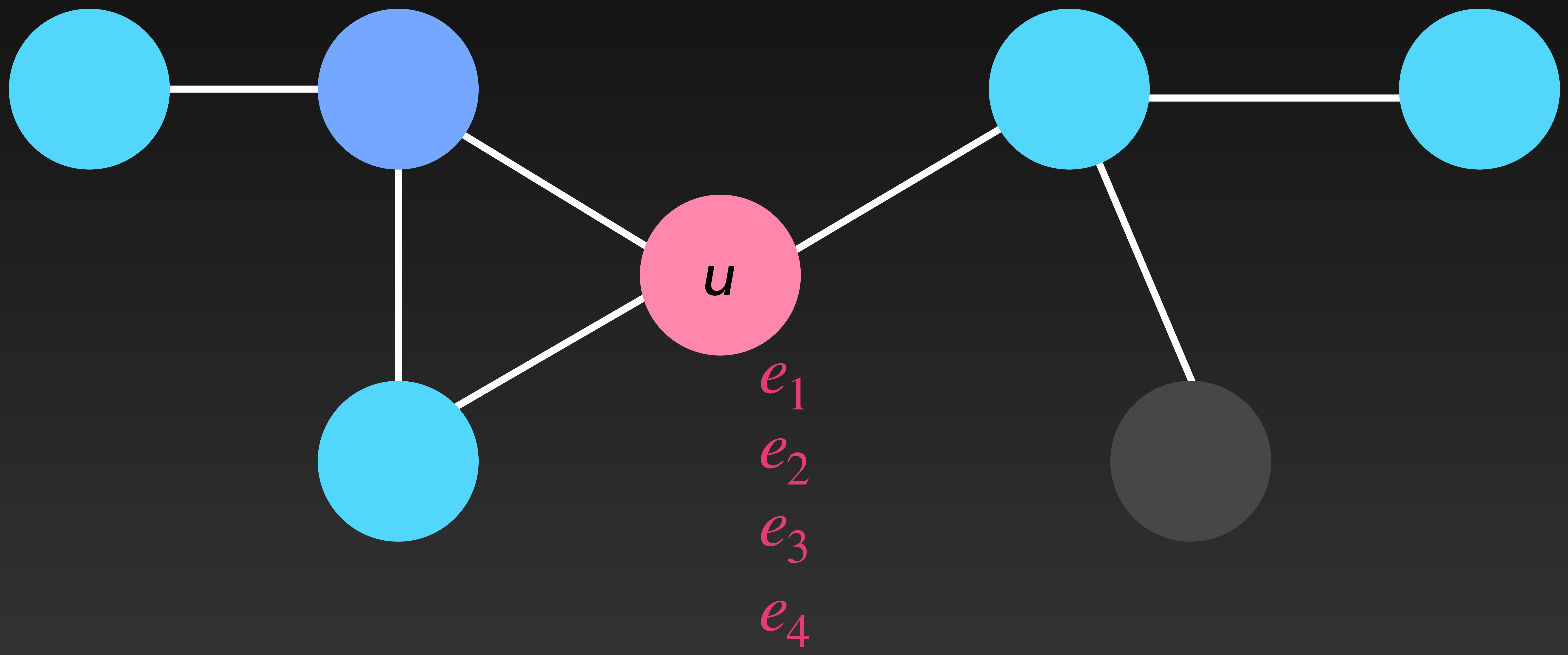


Extension of GNNs

DropoutGNNs - Example

Run No. 4

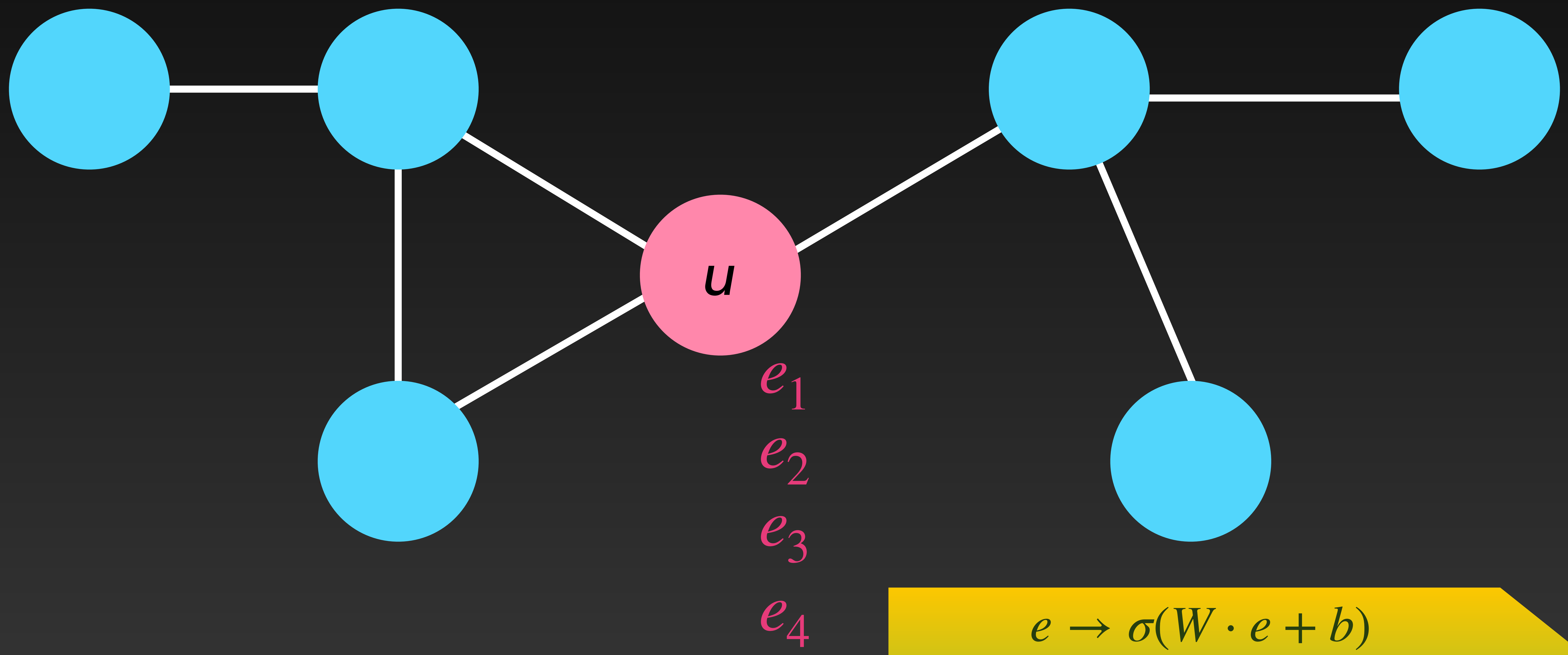
AGGREGATE



Extension of GNNs

DropoutGNNs - Example

Evaluation



$e \to \sigma(W \cdot e + b)$

RUN AGGREGATION

Extension of GNNs

DropoutGNNs - Examples

Problem 2: GNNs are at most powerful as the WL-test

1-WL fails even with angles and port numbers

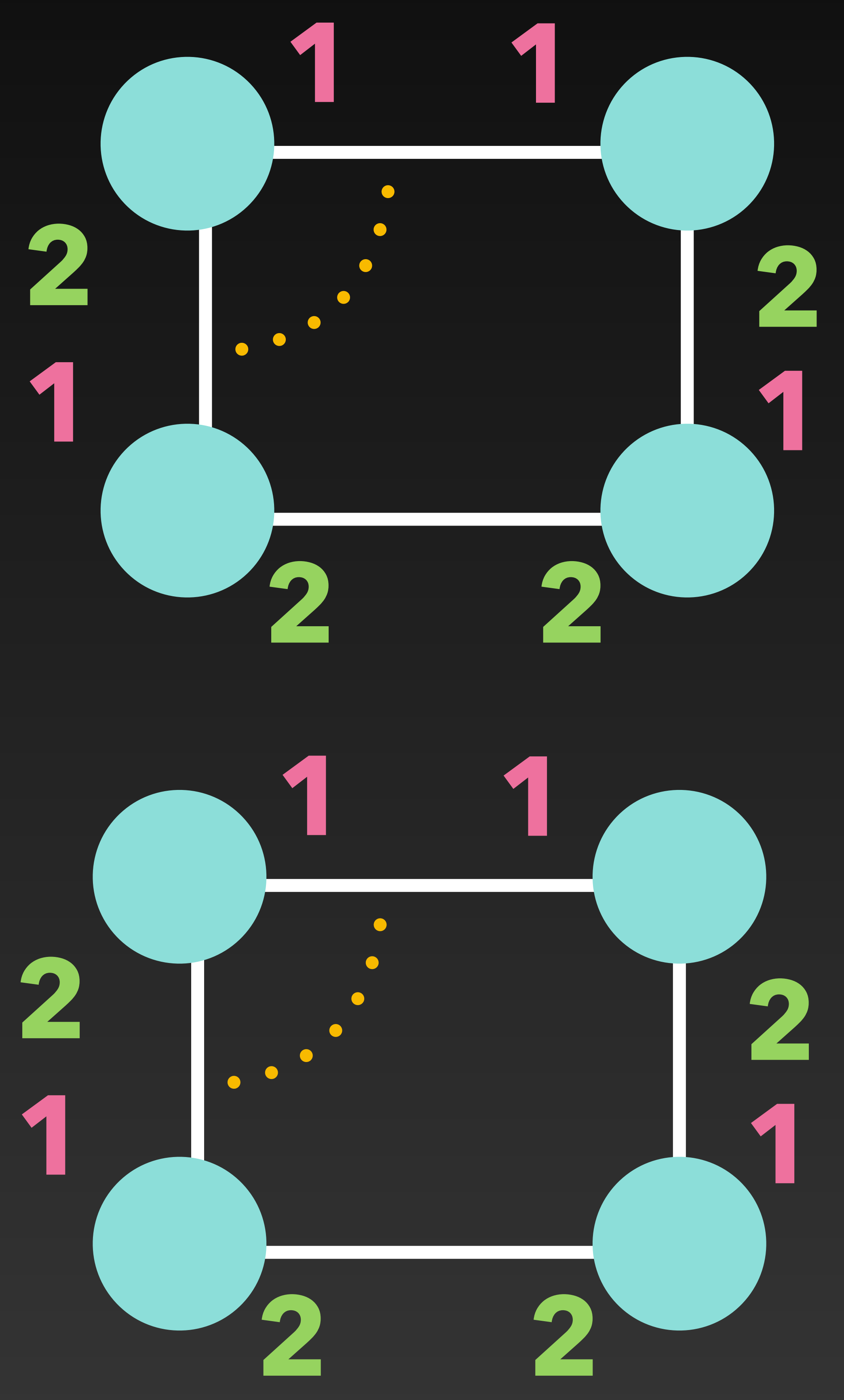


Figure 1: Graph with two 4-cycles

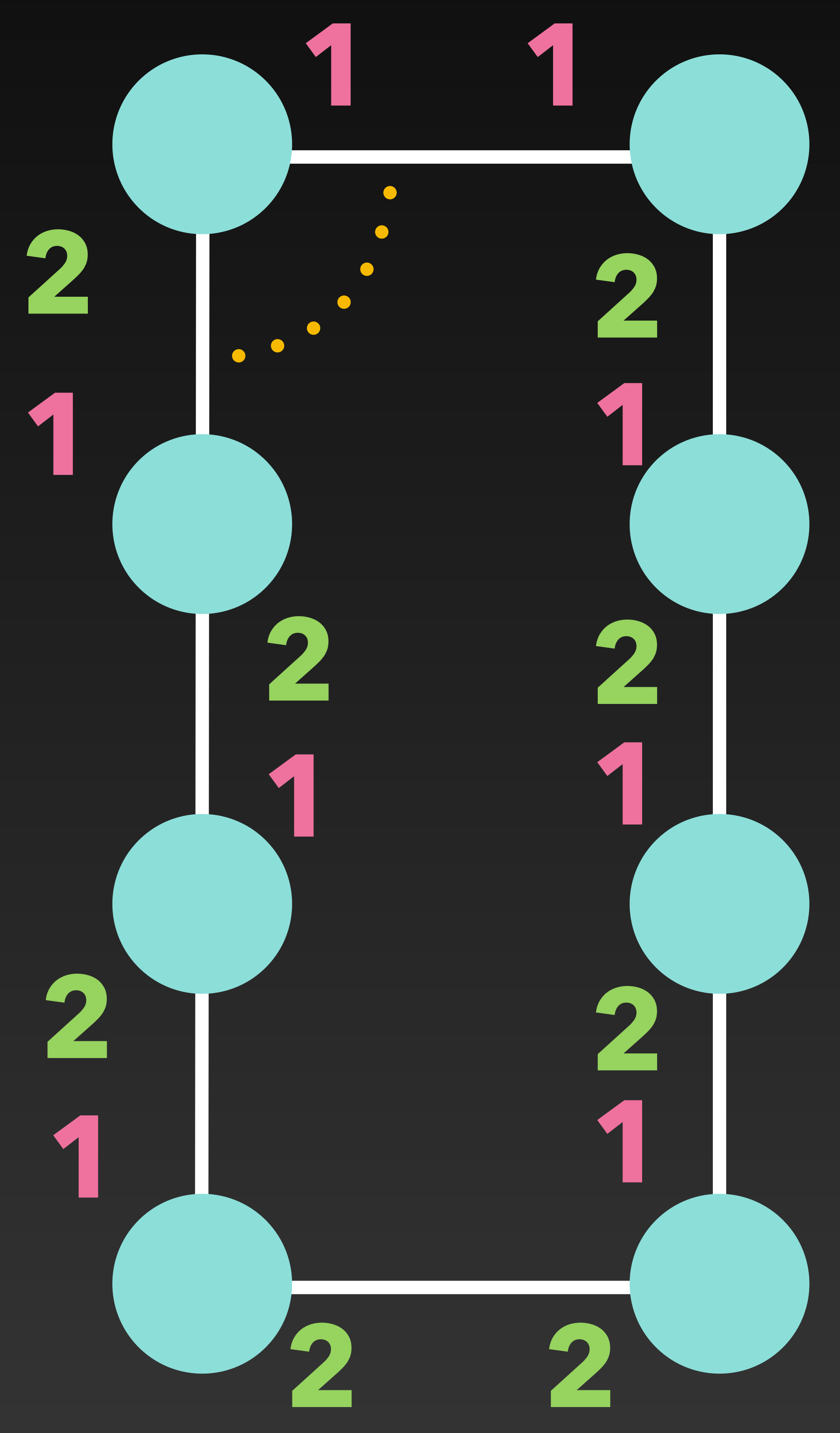


Figure 2: Graph with one 8-cycle

Extension of GNNs

DropoutGNNs - Examples

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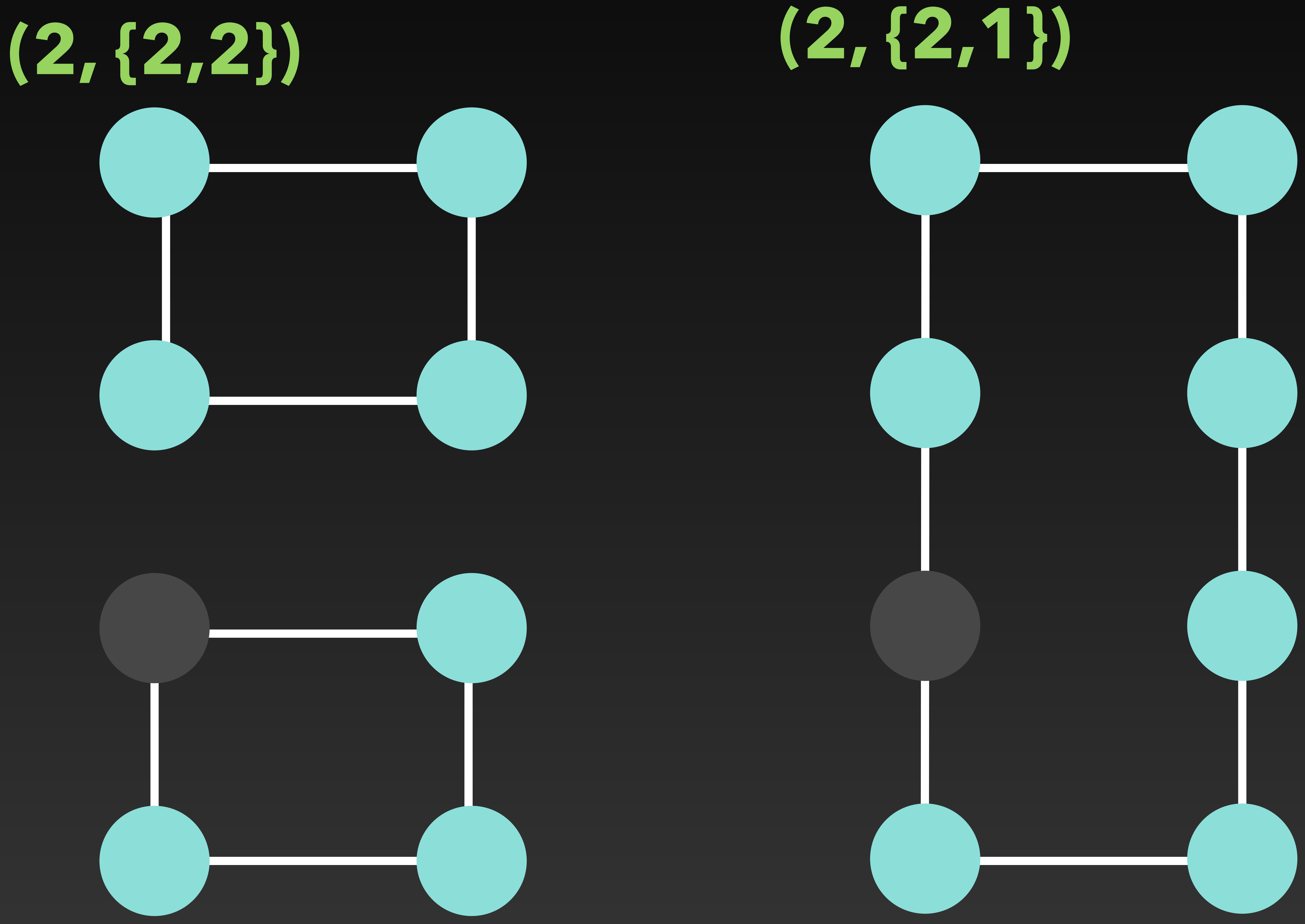
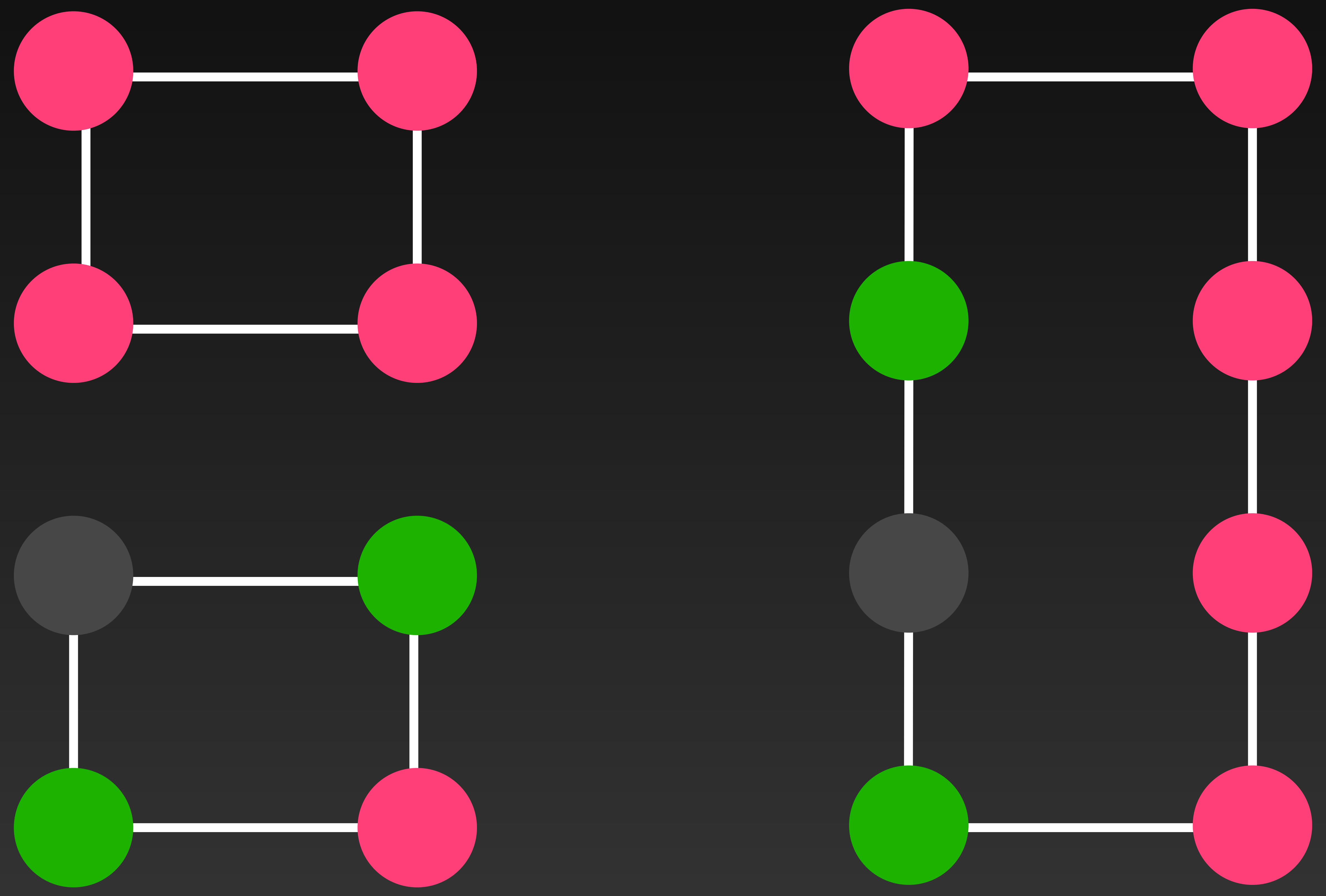


1-WL fails even with angles and port numbers

Extension of GNNs

DropoutGNNs - Examples

Problem 2: GNNs are at most powerful as the WL-test



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Extension of GNNs

DropoutGNNs - Examples

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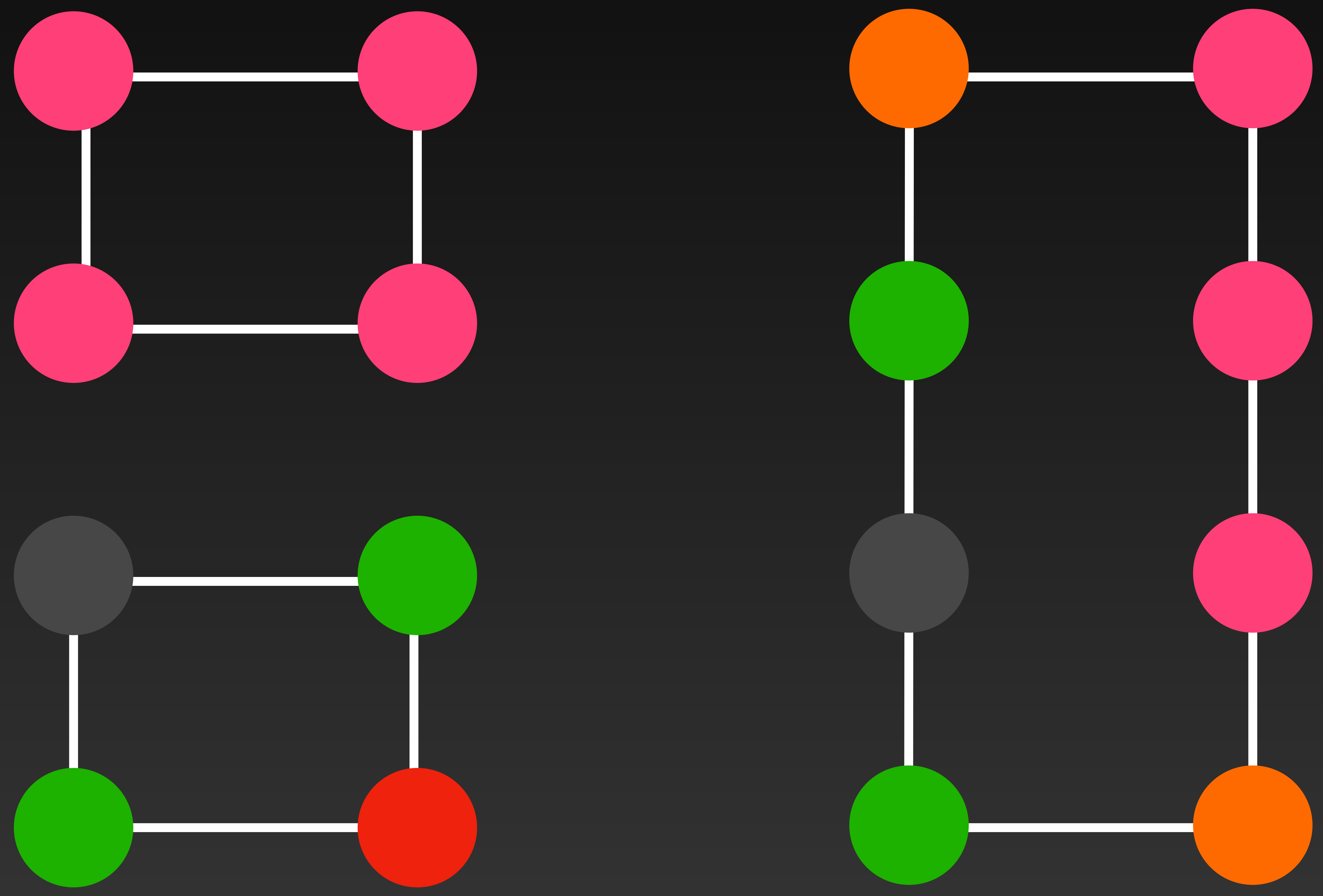

1-WL fails even with angles and port numbers

Extension of GNNs

DropoutGNNs - Examples

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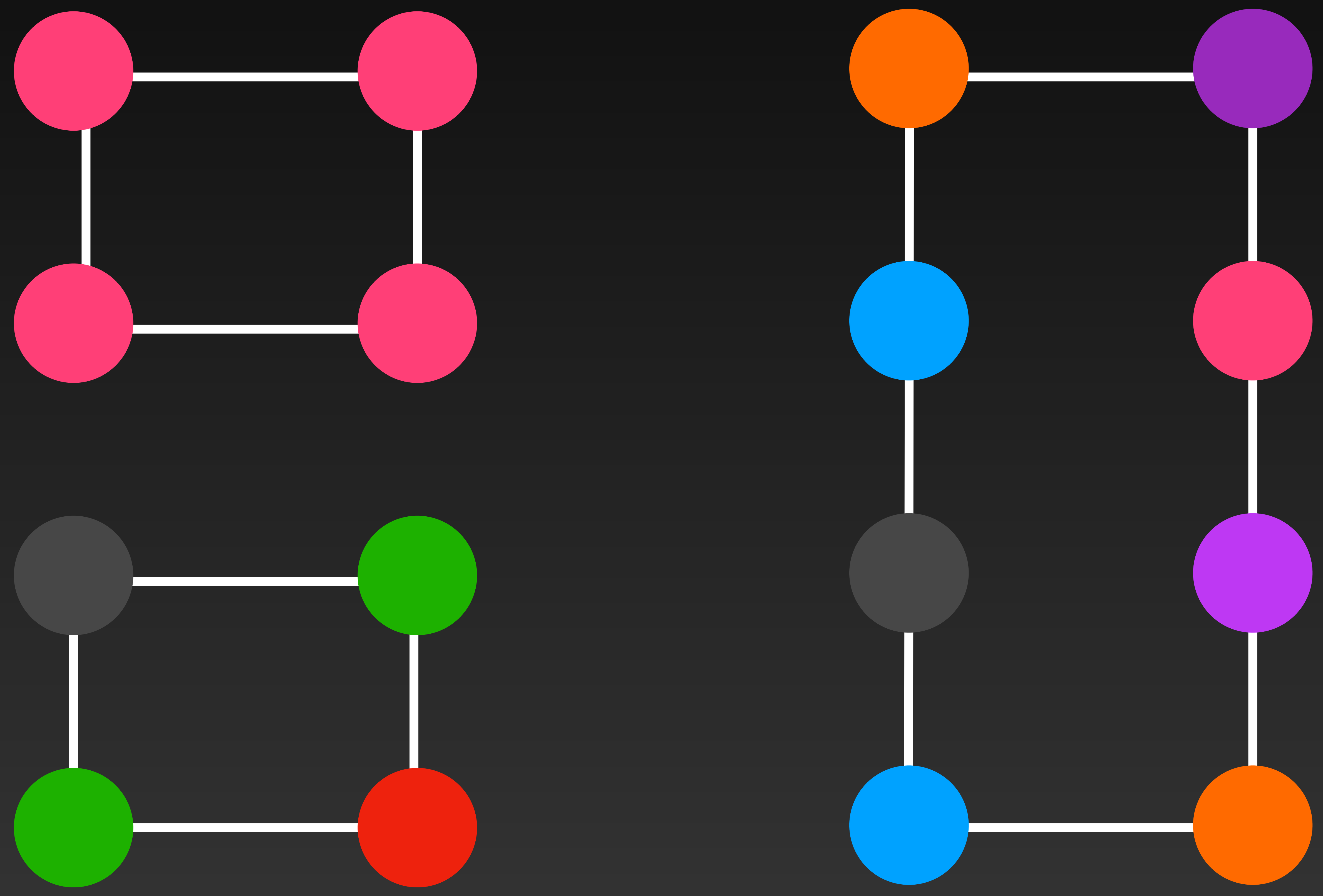


1-WL fails even with angles and port numbers

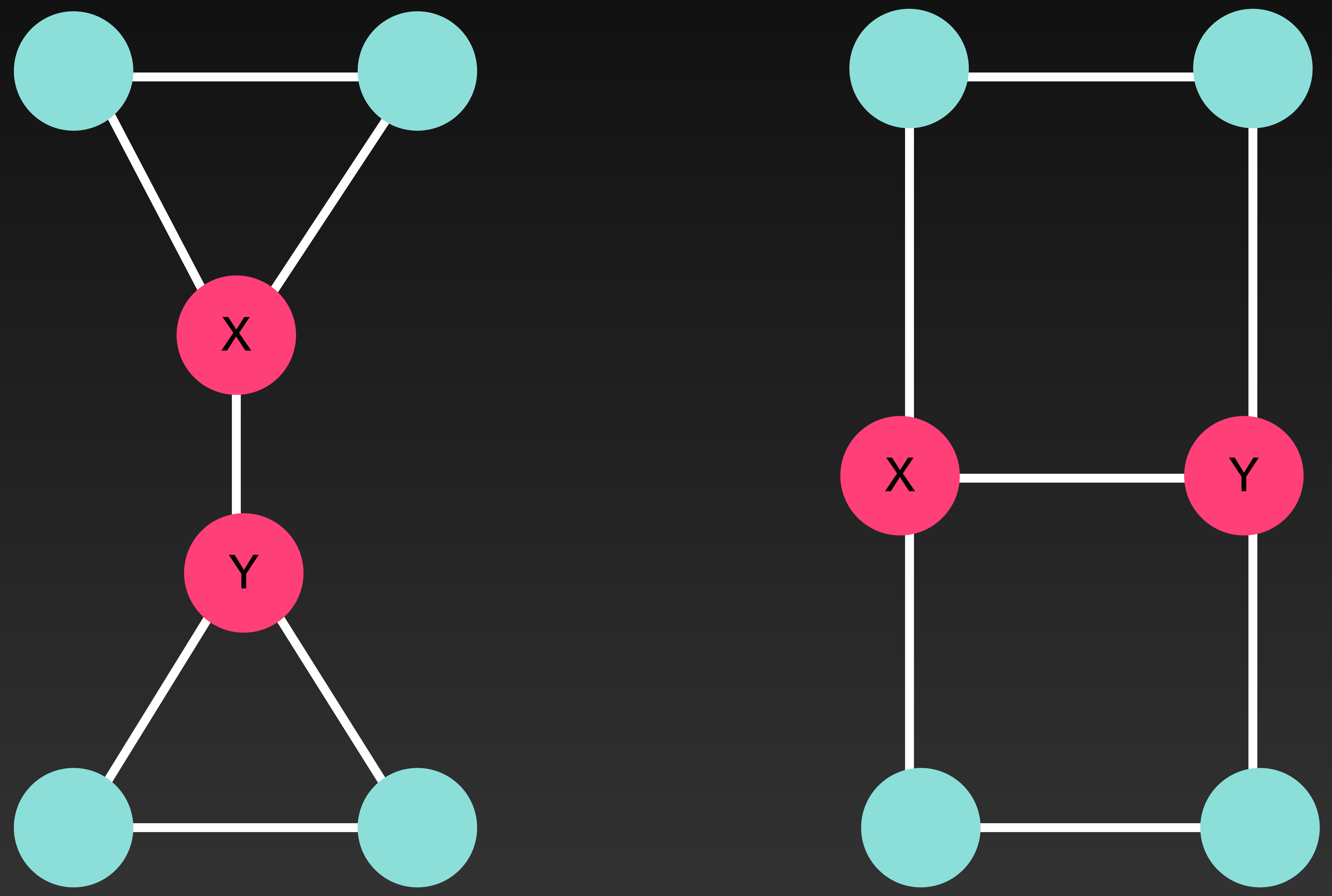
Different color distributions according to WL-test

DropGNN is able to distinguish

Extension of GNNs

DropoutGNNs - Examples

Problem 2: GNNs are at most powerful as the WL-test



1-WL fails again when determining the histogramm

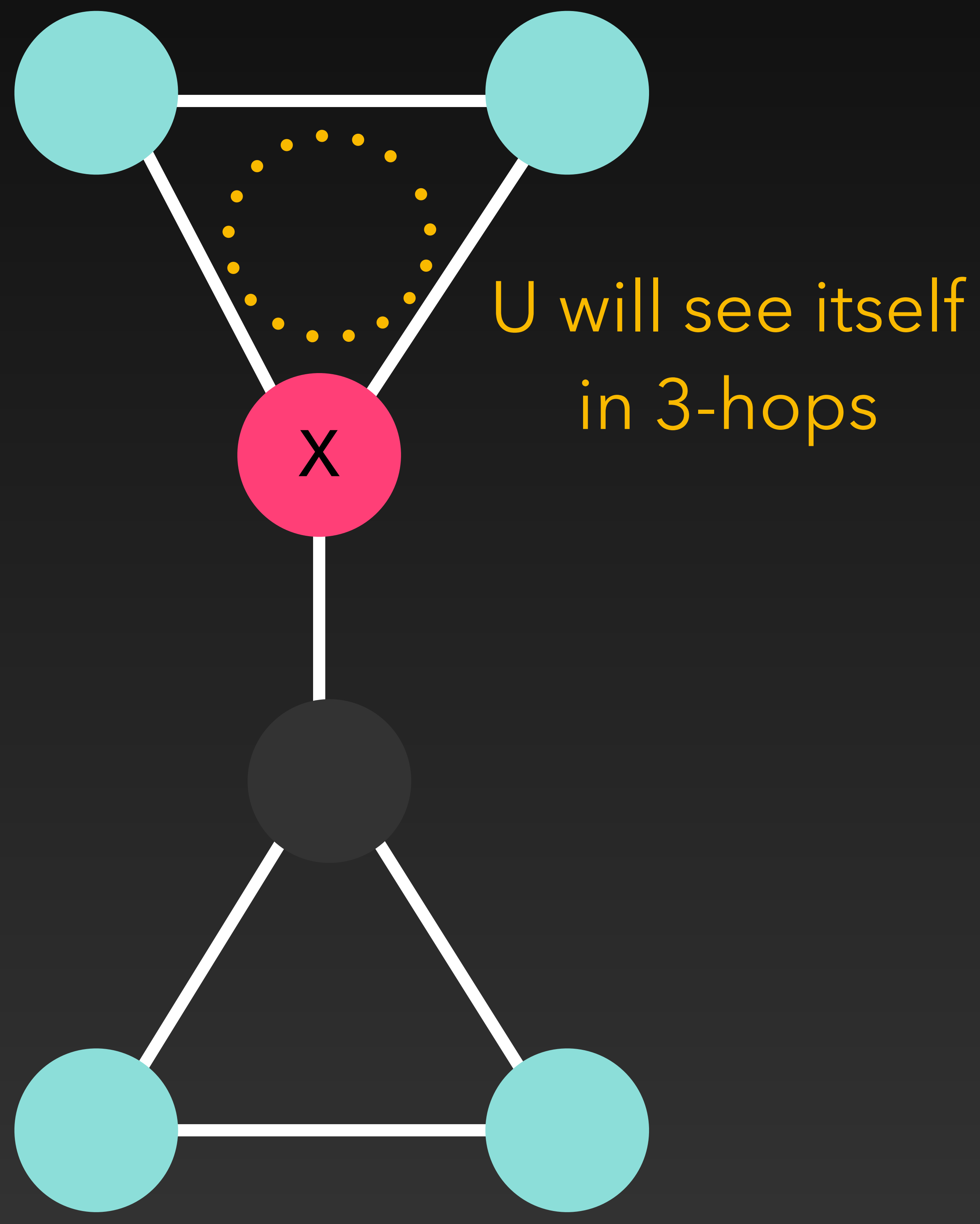
*nodes are labeled according to their degree

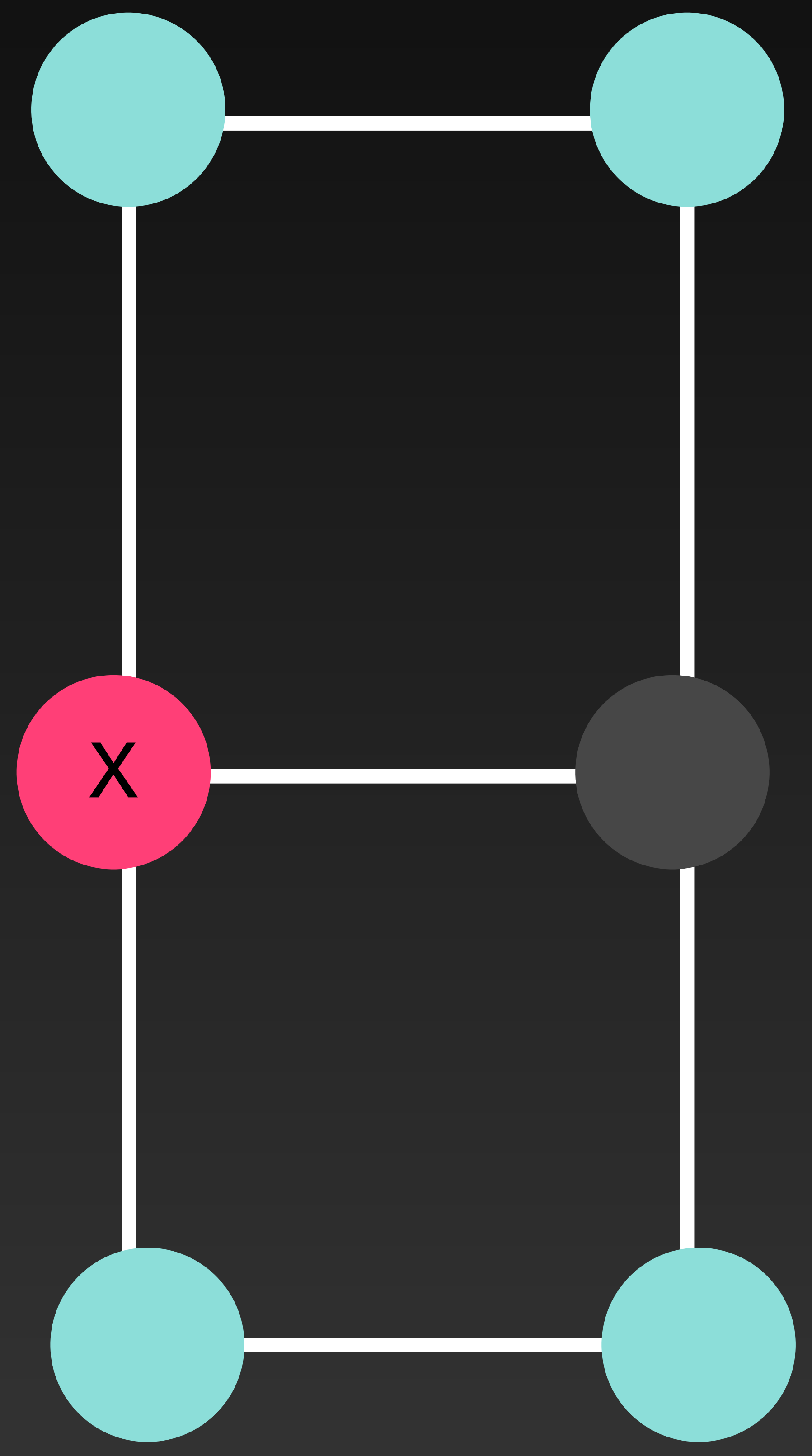
GNN not able to distinguish nodes X and Y

Extension of GNNs

DropoutGNNs - Examples

Problem 2: GNNs are at most powerful as the WL-test





1-WL fails again when determining the histogramm

Node U will recognize different neighborhoods & on the right no cycle

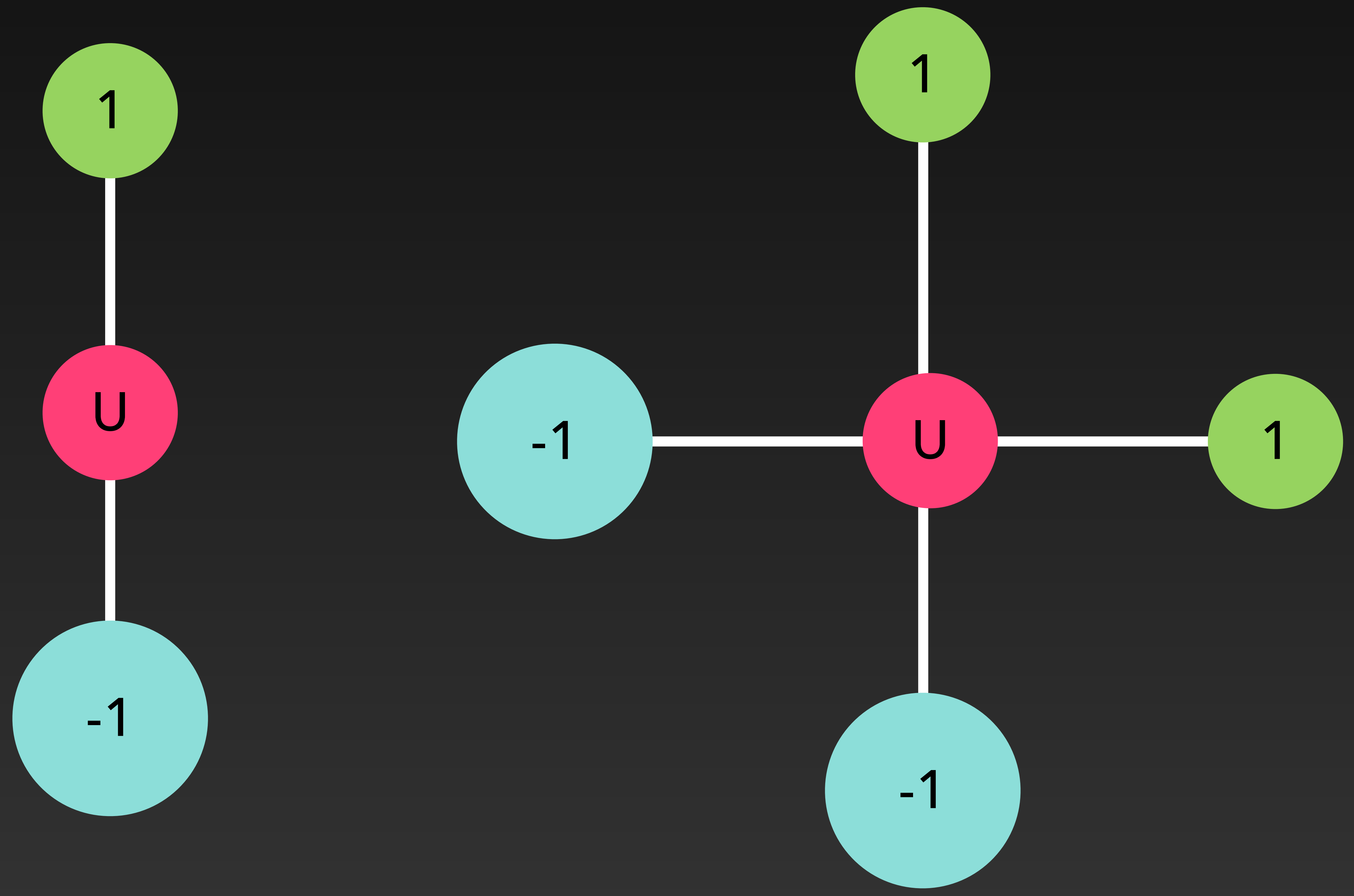
DropGNN is able to distinguish

Extension of GNNs

DropoutGNNs - Examples

Problem 2: GNNs are at most powerful as the WL-test

Naive **mean** aggregation fails



Let $p = 0.25$

Probabilities of seeing **mean = 1**:

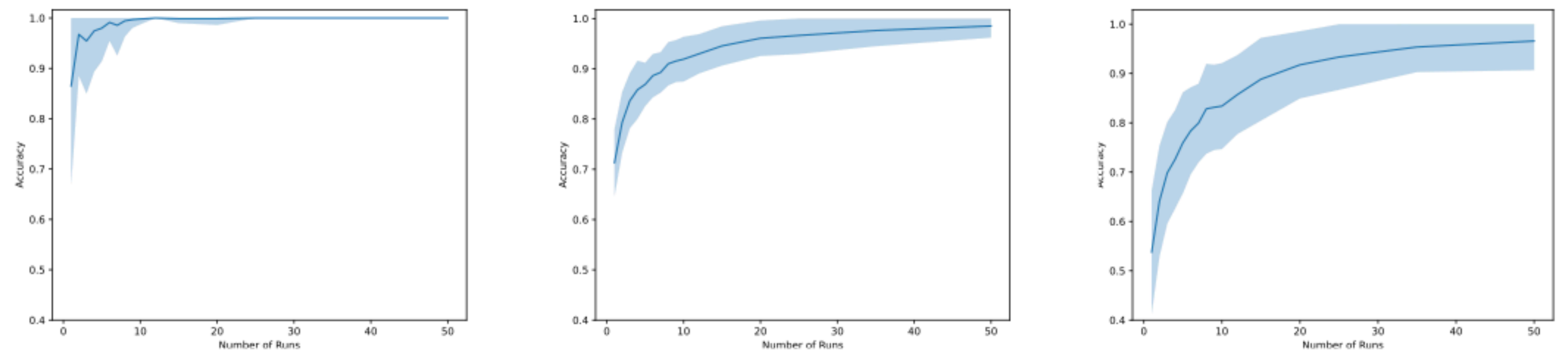
Left 0.19

Right 0.06

DropGNN is able to increase **mean** expressiveness

Extension of GNNs

DropGNNs - Results



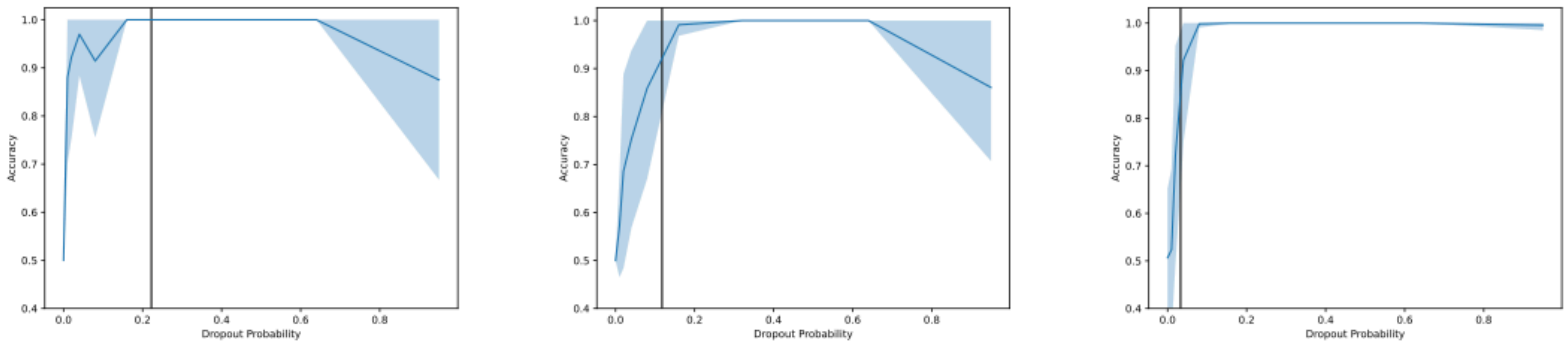
(a) LIMITS 1 (b) 4−CYCLES (c) TRIANGLES

Conclusion More runs yield higher ACC, as we observe more variants in NH

Pitfalls Requires more time, computationally expensive

Extension of GNNs

DropGNNs - Results

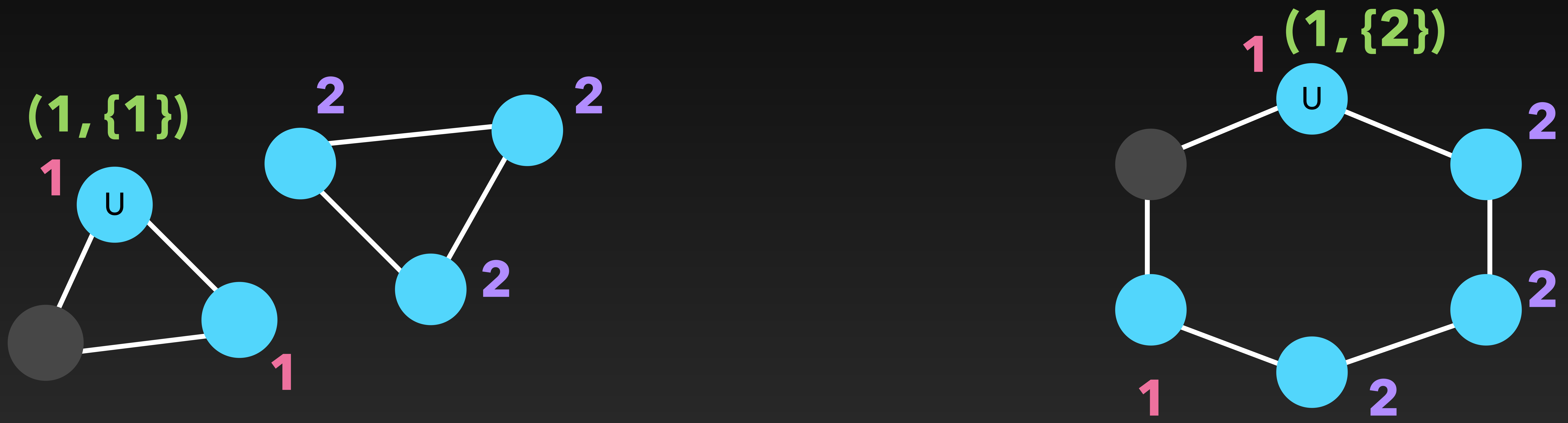


(a) LIMITS 1 (b) 4−CYCLES (c) TRIANGLES

Conclusion We can find an optimal range/value for p

Extension of GNNs

DropGNNs - Note on the dropout probability



For **1-dropouts** node *U* will receives different messages, hence the graphs are **distinguishable**.

Extension of GNNs

DropGNNs - Note on the dropout probability

For 2-**dropouts** node *U* will receive same messages, hence the graphs are **not distinguishable**.

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Extension of GNNs

Graph Structure Networks (GSNs) - Introduction

Key Ideas

1. Make model aware of local substructures in the graph
2. Node extended by structural descriptors (obtained from subgraph isomorphism counting)
3. Requires additional computing step

Extension of GNNs

GSNs - Example

Problem 3: GNNs have no notion of local (sub-)structures

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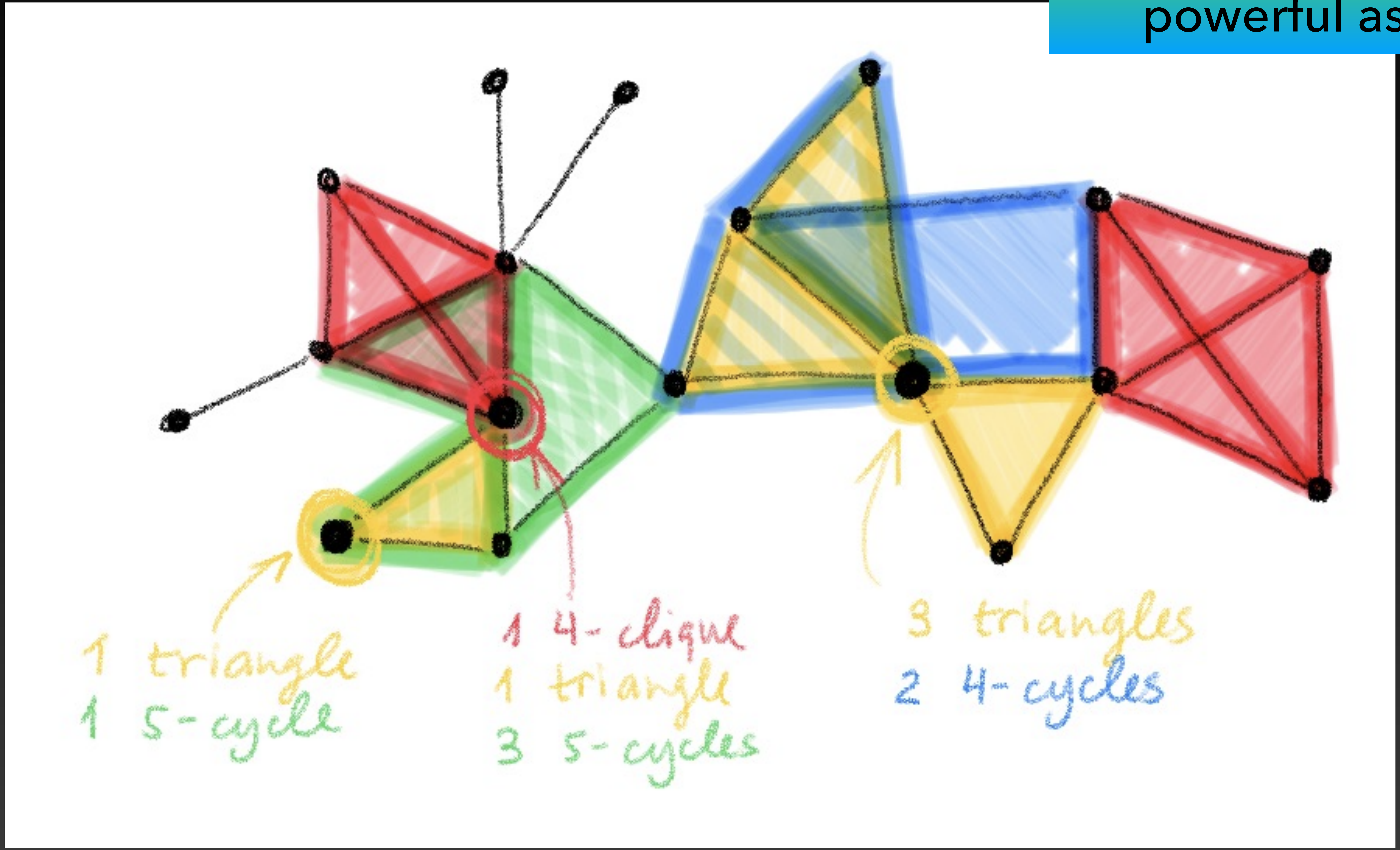
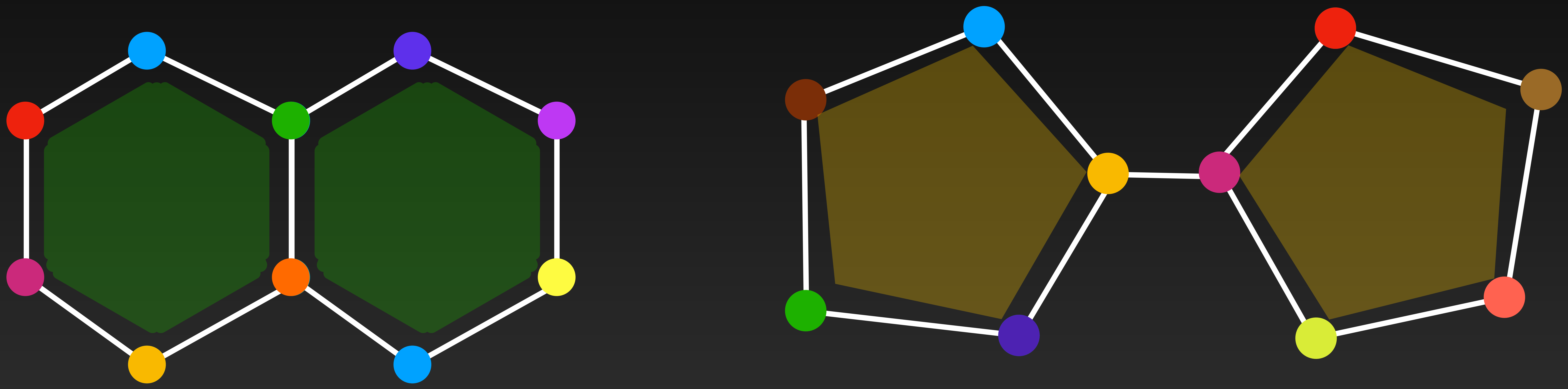


Extension of GNNs

GSN - Back to the WL-Test

Problem 2: GNNs are at most powerful as the WL-test



2-WL would fail here, while GSNs can distinguish

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Discussion

Some Inspirations

1. What is the problem with **invariance in expectation**?
2. Which approach do you think is superior? Why?
3. What is the advantage of increasing mean expressiveness?