On Variants of Graph Neural Networks with Stronger Expressive Power

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Outline

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Introduction

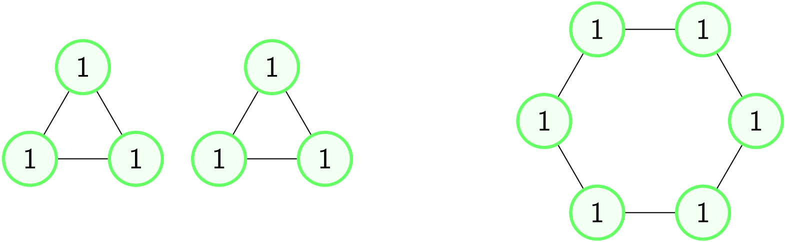
- Graph neural networks (GNNs) are a type of neural network
- GNNs have seen a lot of success representing graph data
  - Physics
  - Bioinformatics
  - Finance
  - Electronic engineering
  - Operations research

Classic GNNs

- Implemented on a graph
- Each node has an initial *node feature*
- In a message-passing step, the node features of each vertex are simultaneously updated based on
  - the previous node features of the vertex
  - the multiset of previous node features of its neighbors
- After some number of message passes, an output is determined based on the final node features.
  - Graph-level: output for the whole graph
  - Node-level: output for each node

Classic GNNs

- GNNs are not perfect; e.g. any classic GNN will produce the same output when run on the two graphs below



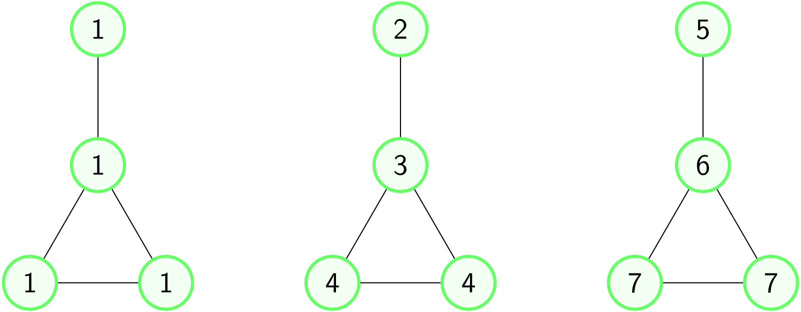
- Goal: modify GNNs to have stronger separation power

Outline

Weisfeiler-Lehman (WL) test

- Test for graph isomorphism
- Implemented on a graph with node features
- Label for each vertex initiated based on its node feature
- In a message-passing step, the label of each vertex is simultaneously updated based on
  - the previous label of the vertex
  - the multiset of previous labels of its neighbors
- After some number of message passes, the multiset of labels is output

WL test example



- The labels given by the WL test eventually stabilize

Separation power of GNNs and WL test

Theorem (Xu et al., 2018)

Given two graphs G and $\hat{G}$, the following are equivalent:

1. *There exists some GNN F such that $F(G) \neq F(\hat{G})$;*
2. *There exist hash functions such that, under the WL test, the multiset outputs for G and $\hat{G}$ are different.*

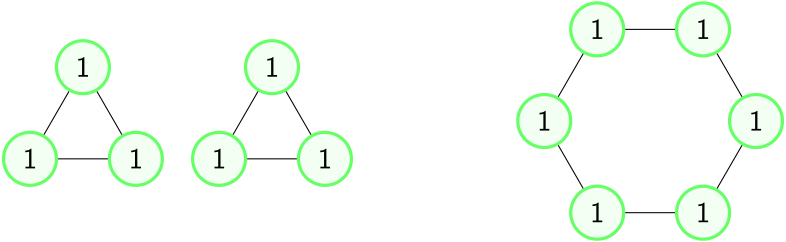
Outline

Variants of the WL test

- GNNs and the WL test have the same separation power, so it suffices to consider the WL test only
- Idea: the WL test can only use local information, so collect more local information
- Depth k subgraph: considers labels of vertices of at most distance k away and surrounding induced subgraph structure
- Depth k neighborhood: only considers labels of vertices of at most distance k away

Examples

- The classic WL test cannot distinguish between all pairs of non-isomorphic graphs



- But the depth 2 neighborhood WL test and the depth 1 subgraph WL test work for this example

Results

Conjecture

Let k be a positive integer, and let G_1 and G_2 be non-isomorphic connected graphs whose longest cycles contain at most $2k+1$ vertices. Then, G_1 and G_2 can be distinguished by the depth k subgraph WL test.

Results

Theorem

Let k be a positive integer, and let G_1 and G_2 be (possibly infinite) non-isomorphic connected graphs, with node features, whose longest cycles contain at most $2k+1$ vertices. Suppose that if the depth k subgraph WL test is run on G_1 and G_2, then any two vertices such that the distance between them is at most $2k$ are of different labels. Then, G_1 and G_2 can be distinguished by the WL test of depth k.

- Similar result for neighborhood WL test, except $2k+1$ is replaced by $2k-1$
- The condition can be replaced by simpler but stronger conditions

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