

Message Passing Simplicial Network on SRG

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Introduction

Problem and Approach

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Simplex, WL

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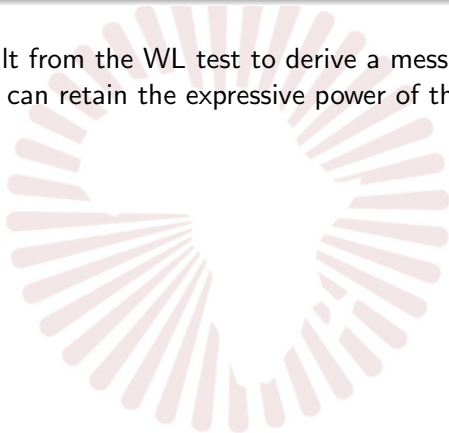
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- Formally, a simplicial complex is a collection of nonempty subsets of a vertex set V that contain all the singleton subsets of V and is closed under the operation of taking subsets.
- A simplex can have an orientation but not for SRG.

Simplicial WL Test

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This test is built from the WL test to derive a message-passing procedure that can retain the expressive power of the test[1].



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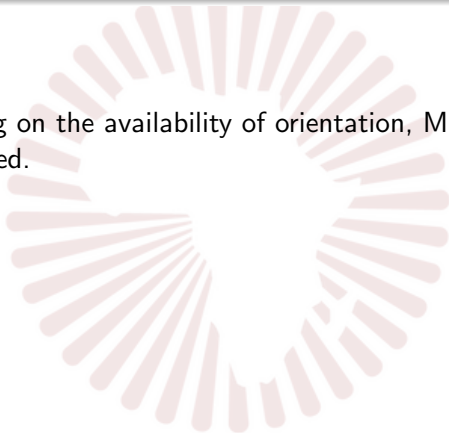
Simplicial WL Algorithm

- 1 Given a simplicial complex \mathbb{K} , all the simplices $\sigma \in \mathbb{K}$ are initialised with the same colour.
- 2 Given the colour c_σ^t of simplex σ at iteration t , compute c_σ^{t+1} by perfectly hashing the multi-set of colours belonging to the adjacent simplices of σ .
- 3 The algorithm stops once a stable colouring is reached. If the colour histogram is not the same, there's no isomorphism.

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- The model does message aggregation on the different boundary adjacency conditions of simplices in \mathbb{K} .
- Just as in k -WL tests, the update operation takes into account the different types of incoming messages and the previous colour of the simplex and then hash the multi-set of colours.

Data and Implementation

- Strongly regular graphs of at most 35 vertices were studied.
- The code is incomplete, for not many failure rates were registered.

References



Bodnar, Cristian and Frasca, Fabrizio and Wang, Yu Guang and Otter, Nina and Montúfar, Guido and Lio, Pietro and Bronstein, Michael

Weisfeiler and lehman go topological: Message passing simplicial networks.

arXiv preprint arXiv:2103.03212, 2021

Acknowledgements



Thanks for your attention!