A Theory of Link Prediction via Relational Weisfeiler-Leman on Knowledge Graphs

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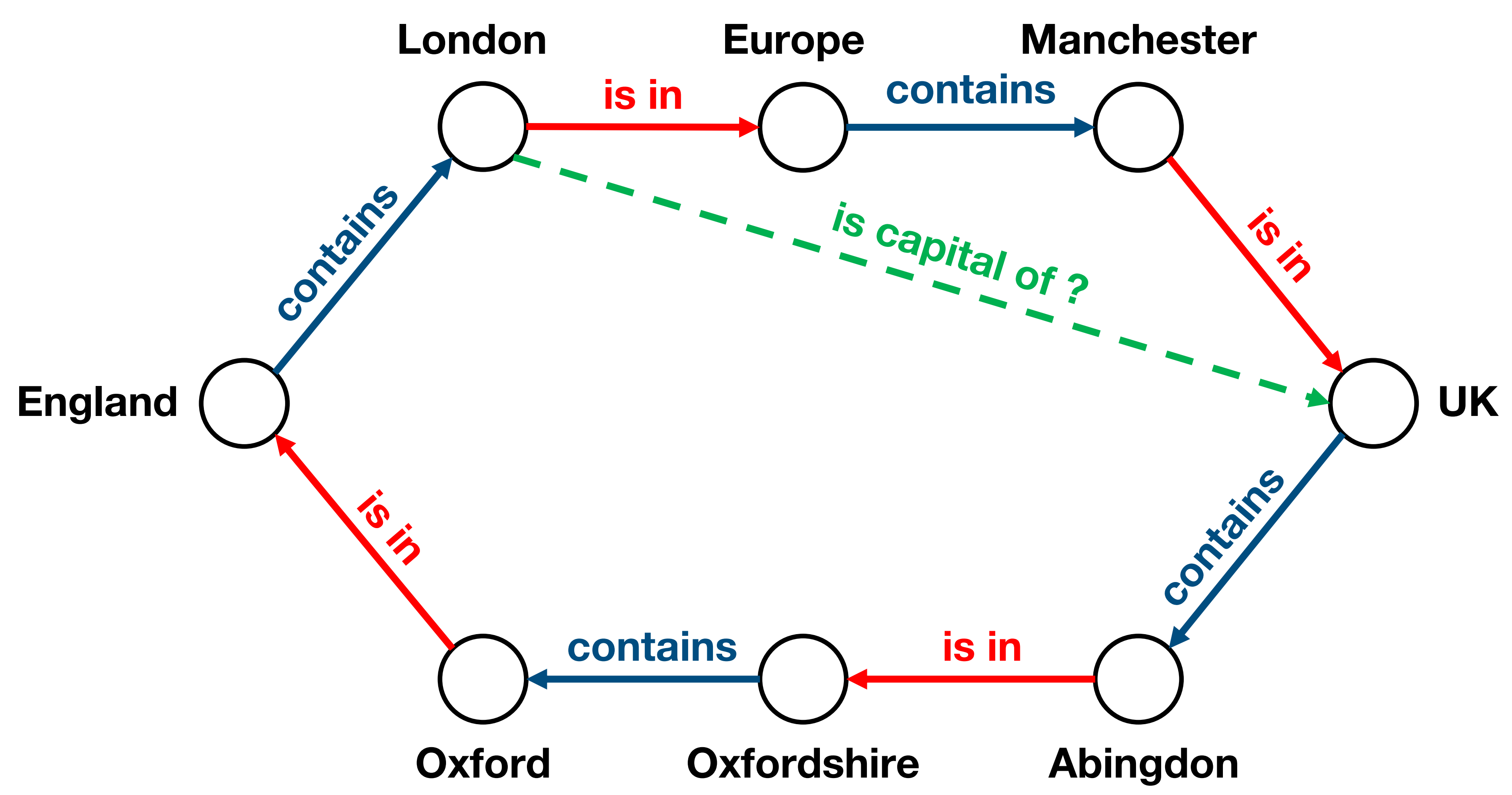
UNIVERSITY OF OXFORD

CENTRO NACIONAL DE INTELIGENCIA ARTIFICIAL

NEURAL INFORMATION PROCESSING SYSTEMS

Link Prediction on Knowledge Graphs



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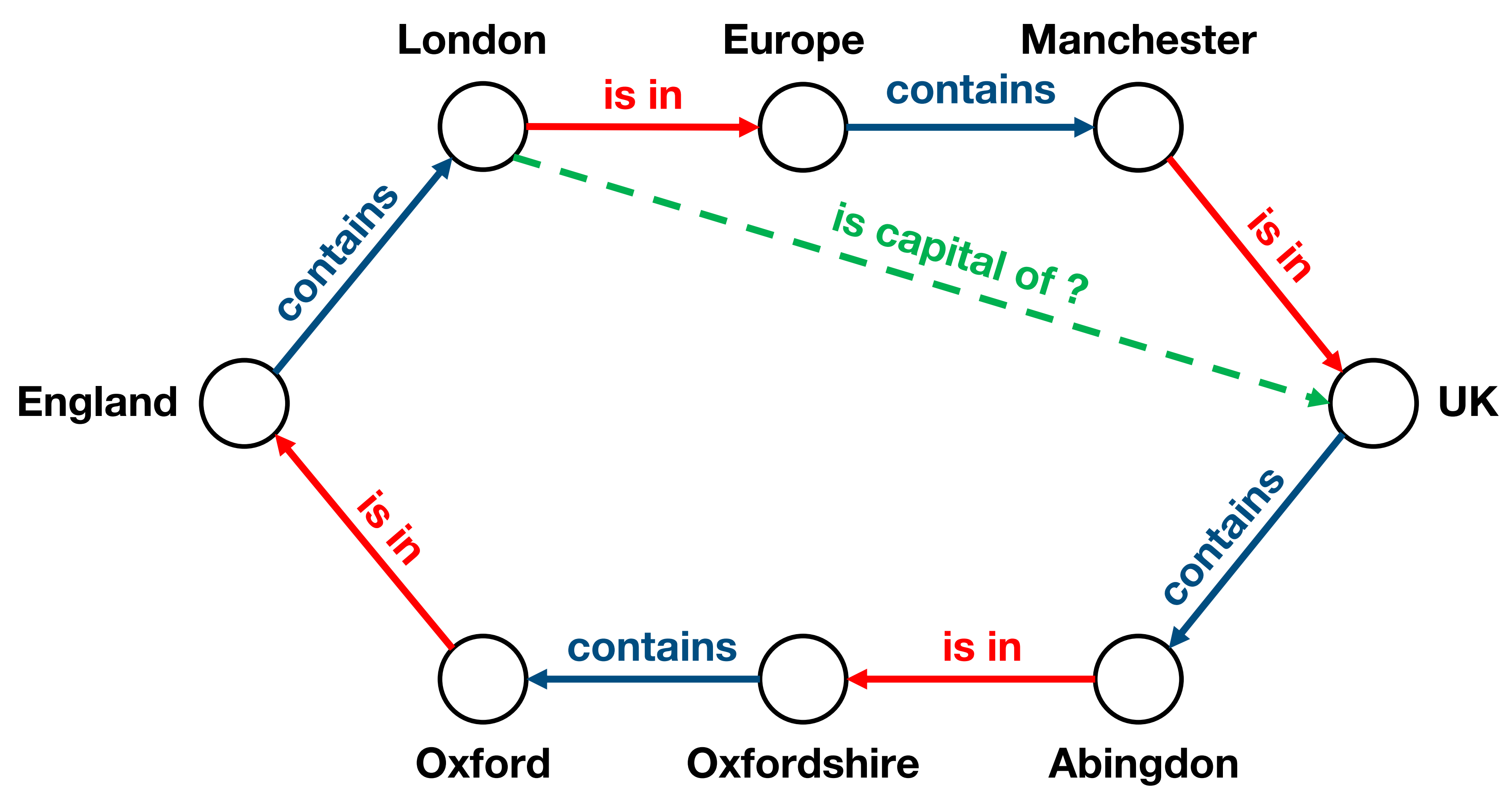

Knowledge graph is a graph with edges labelled with relation types.

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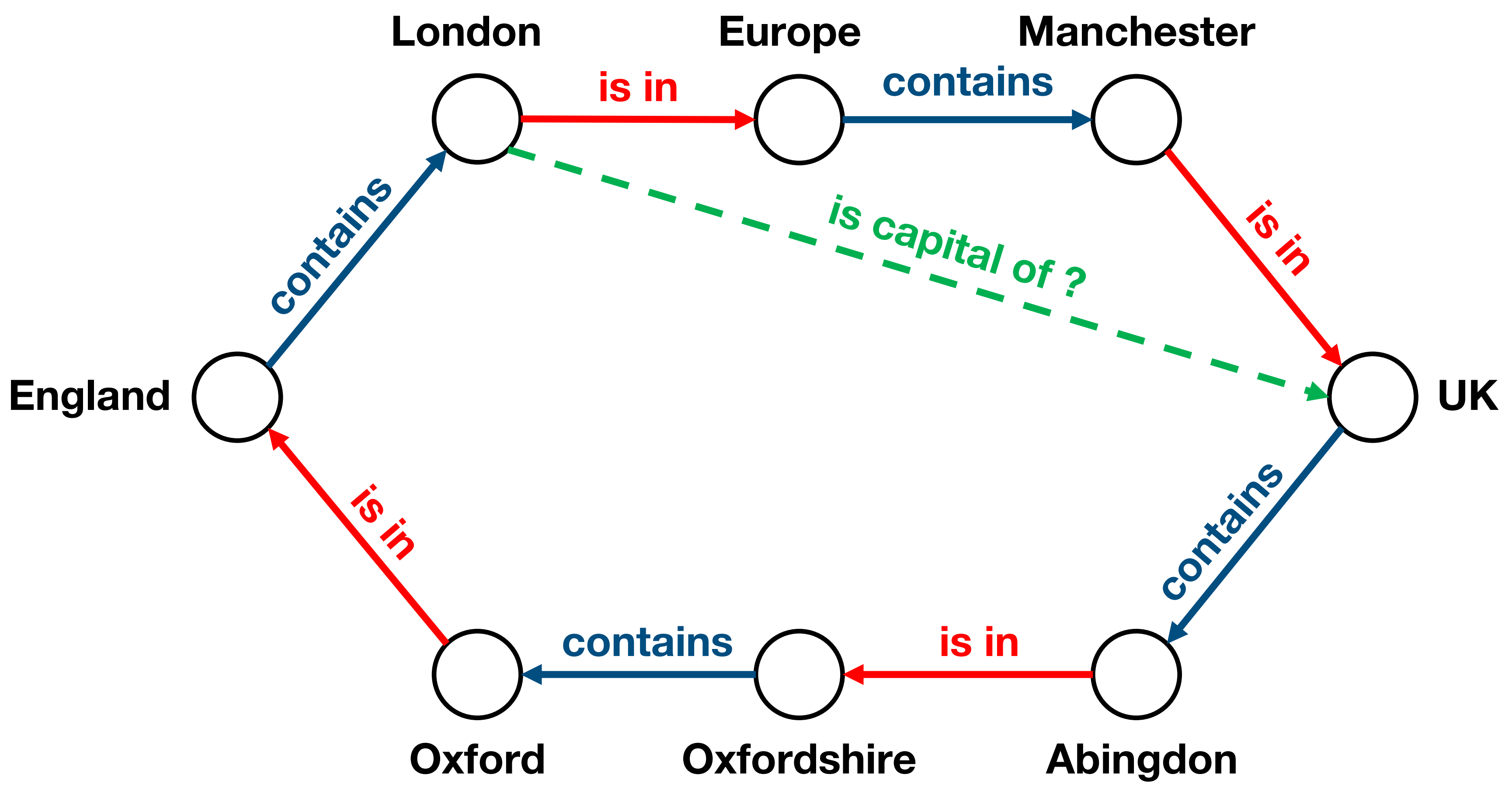
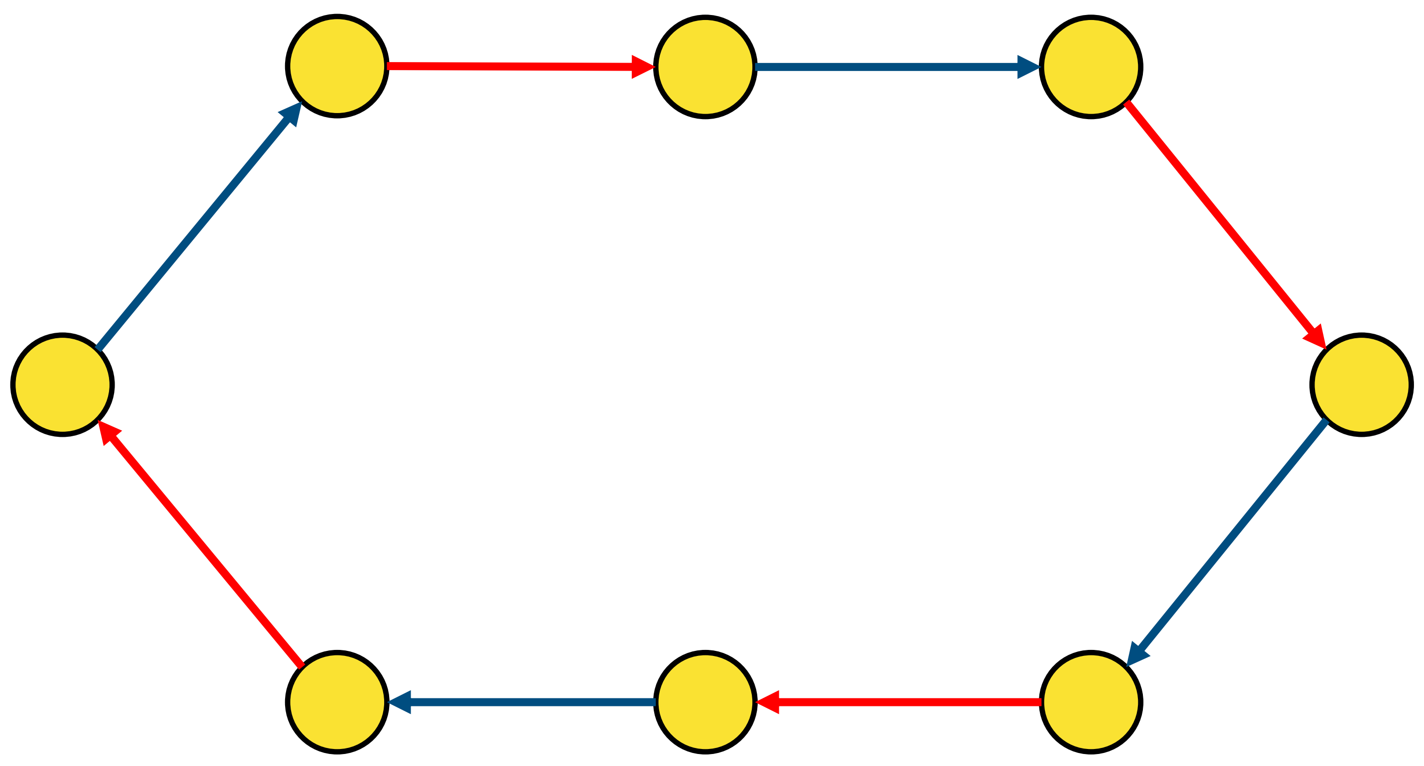


Knowledge graph is a graph with edges labelled with relation types.

Link prediction is to predict missing link or relation on pairs of nodes.

Relational Message Passing Neural Networks



$$\boxed{\boldsymbol{h}_v^{(0)} = \boldsymbol{x}_v}$$

$$\boldsymbol{h}_v^{(t+1)} = \textsc{Upd}\left(\boldsymbol{h}_v^{(f(t))}, \textsc{Agg}(\{\!\!\{\textsc{Msg}_r(\boldsymbol{h}_w^{(t)}) |\, w \in \mathcal{N}_r(v), r \in R\}\!\!\}), \textsc{Read}(\{\!\!\{\boldsymbol{h}_w^{(t)} \mid w \in V\}\!\!\})\right),$$

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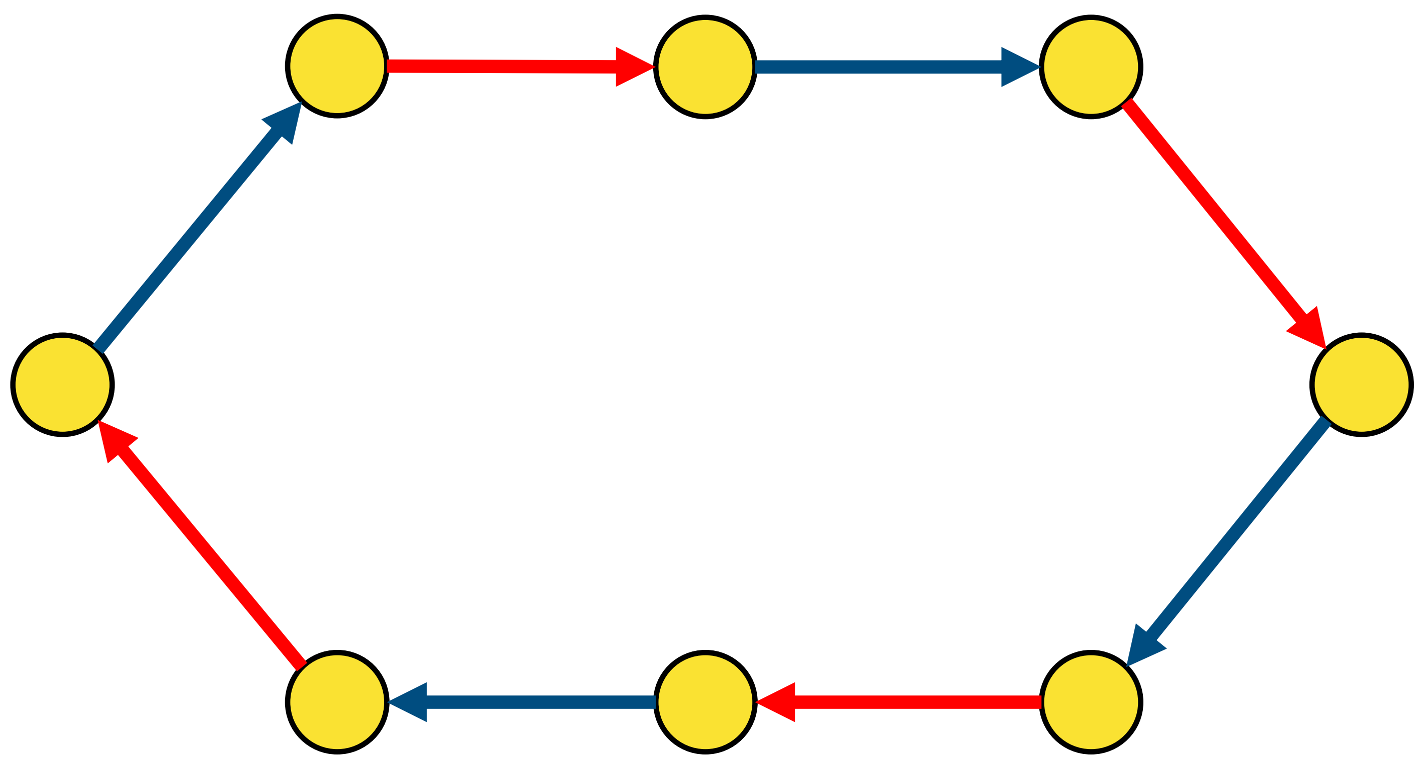

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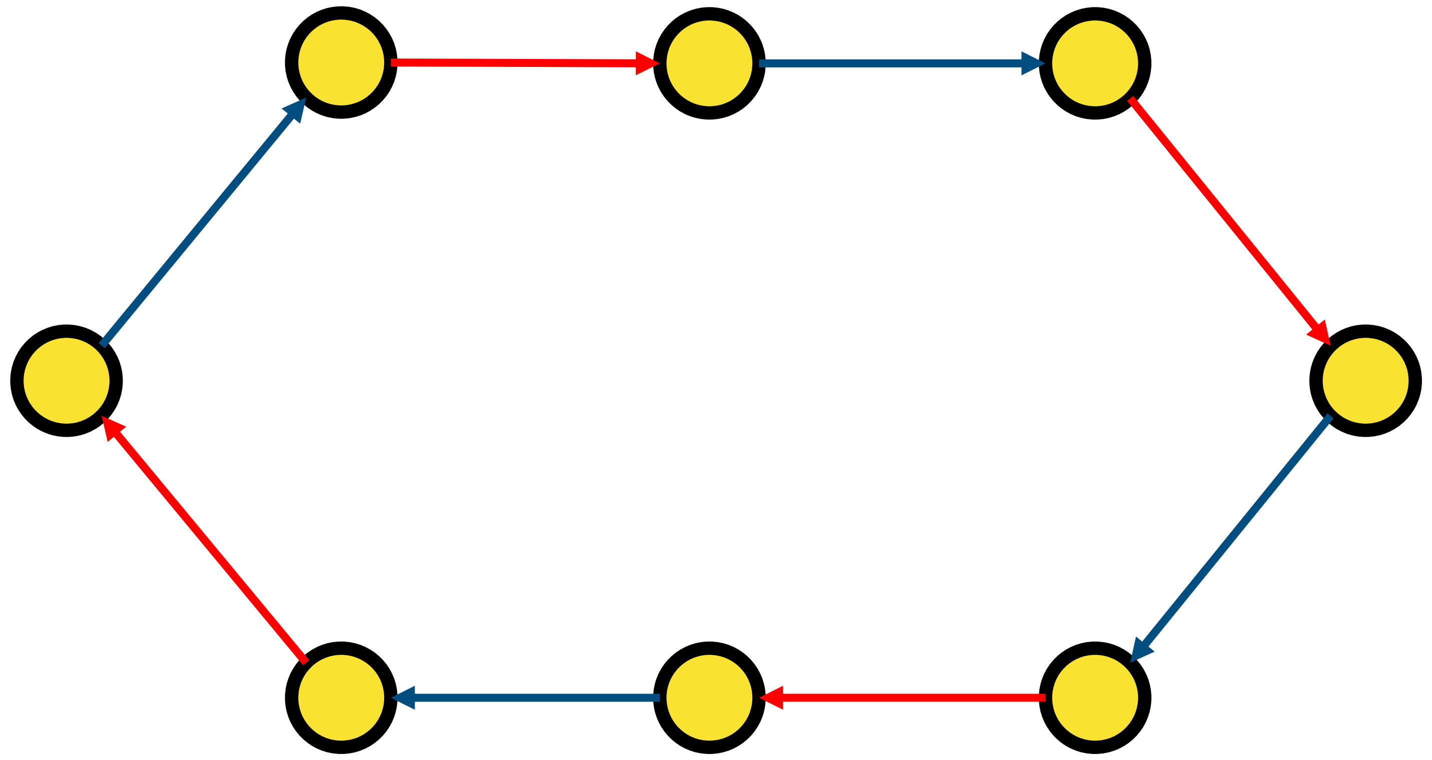

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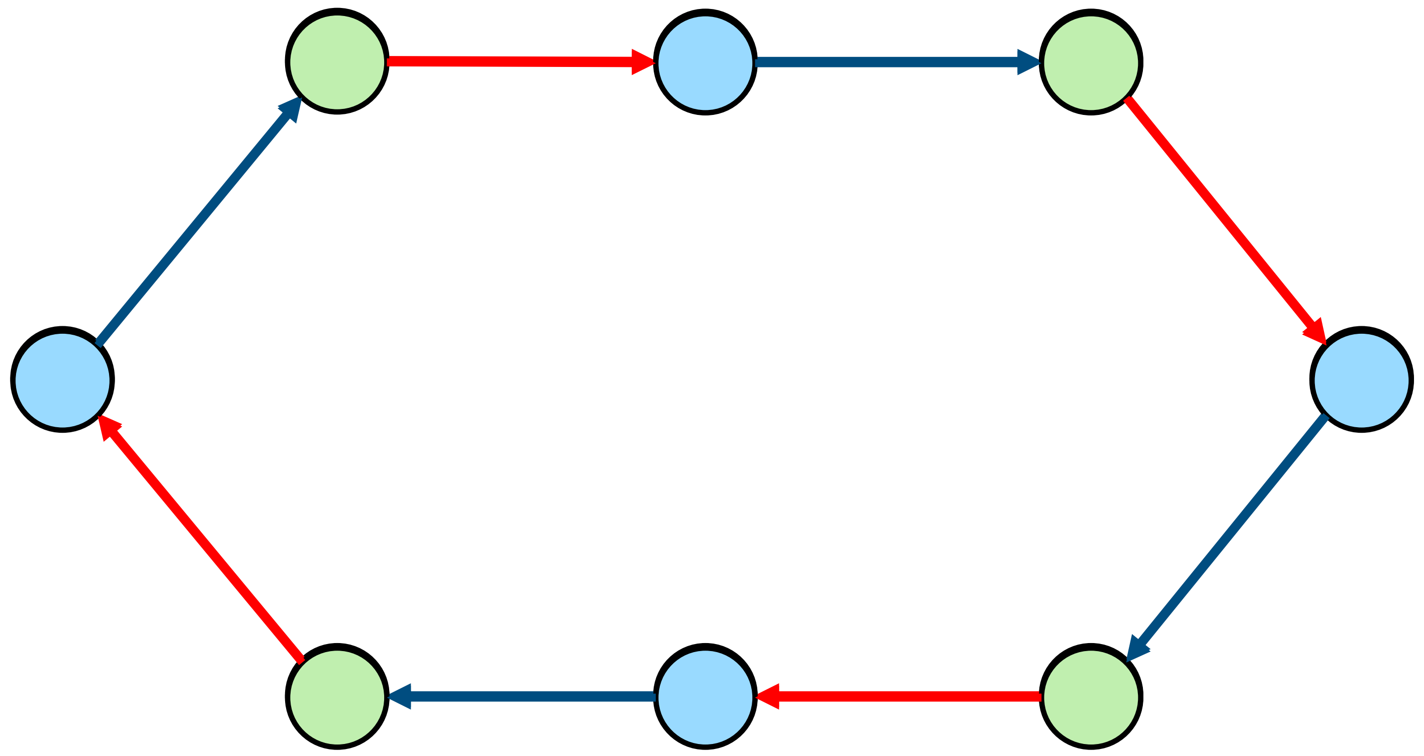

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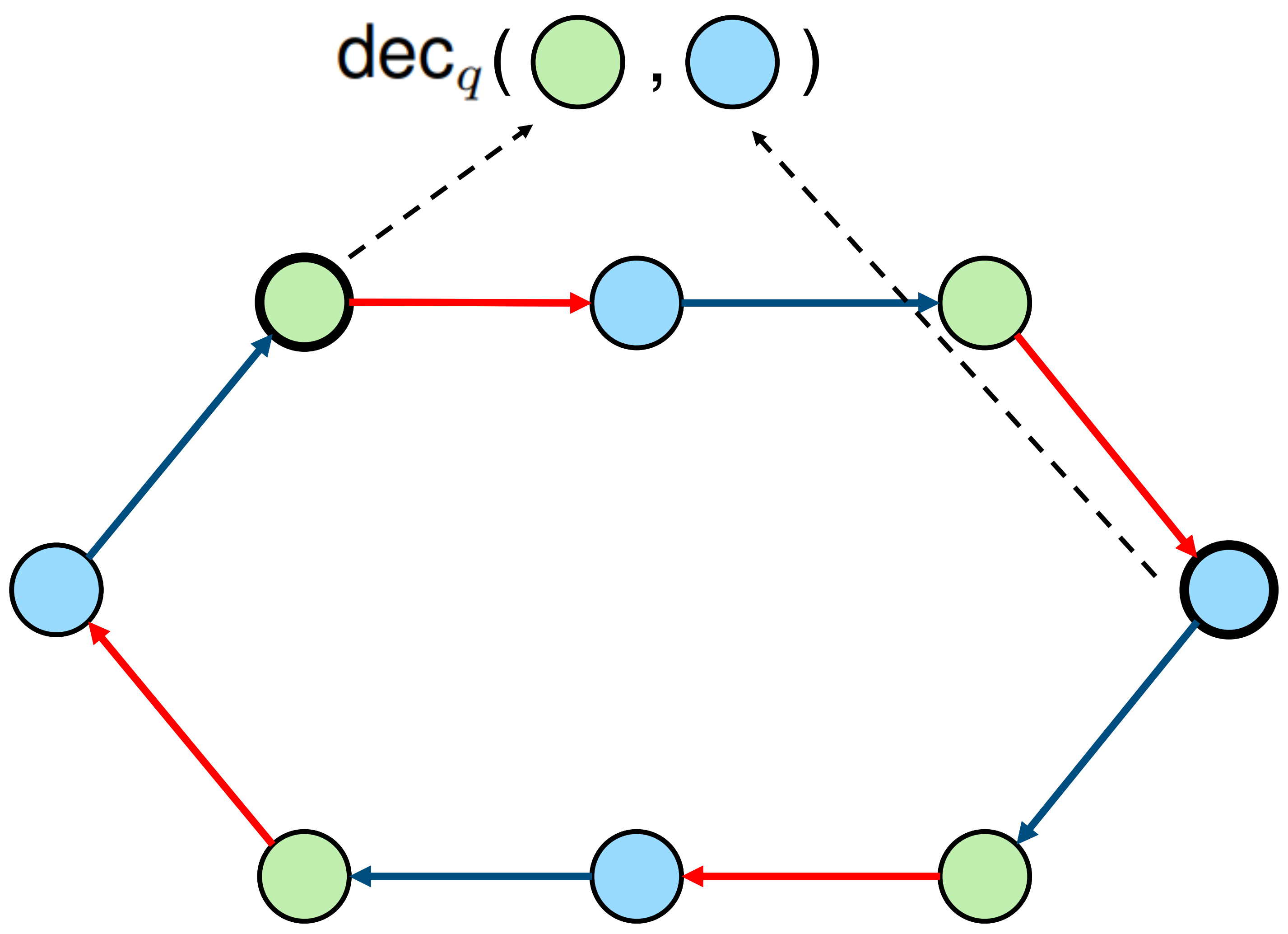

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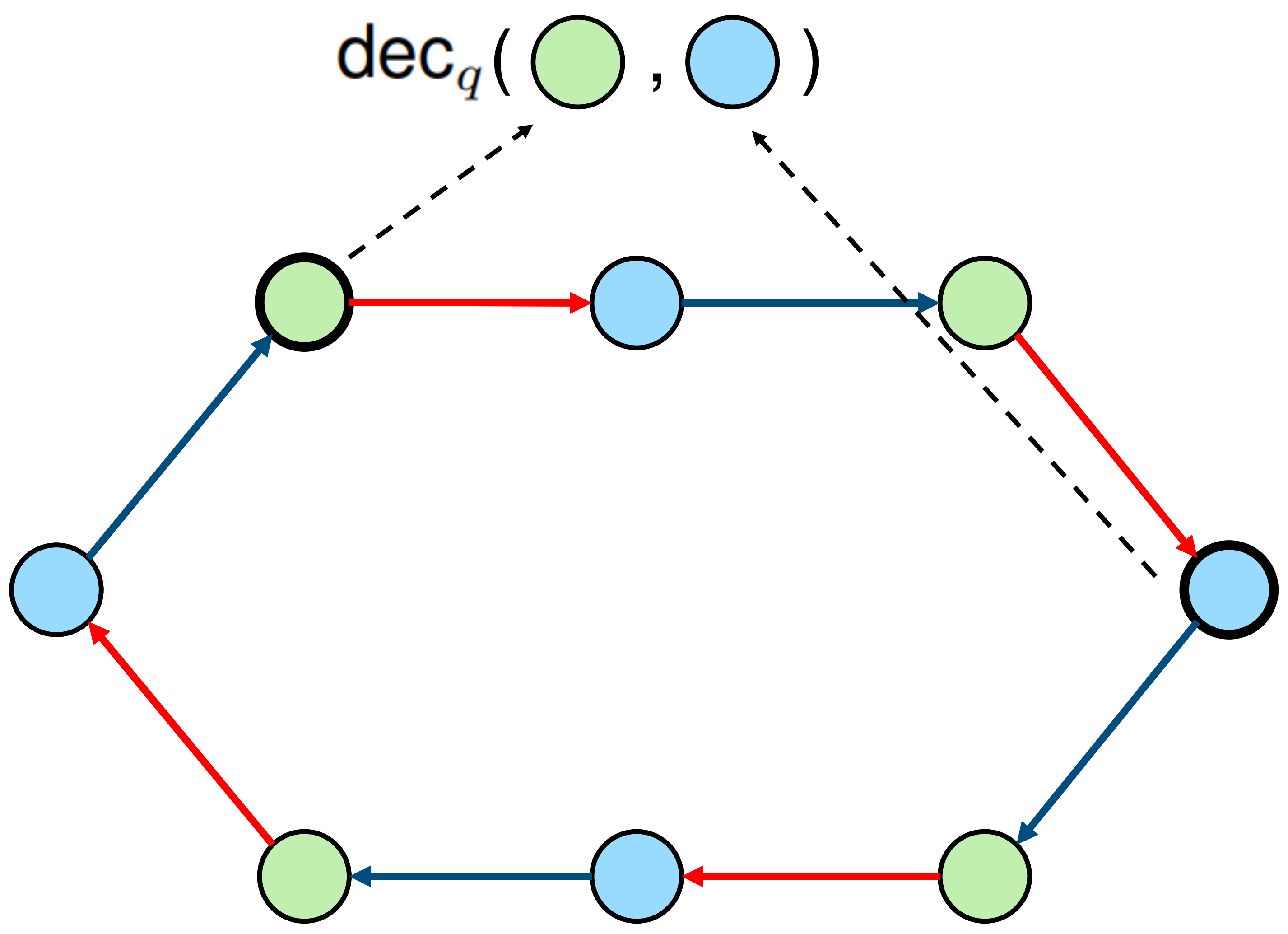
Relational Message Passing Neural Networks

R-MPNNs relies on binary decoder for link prediction.



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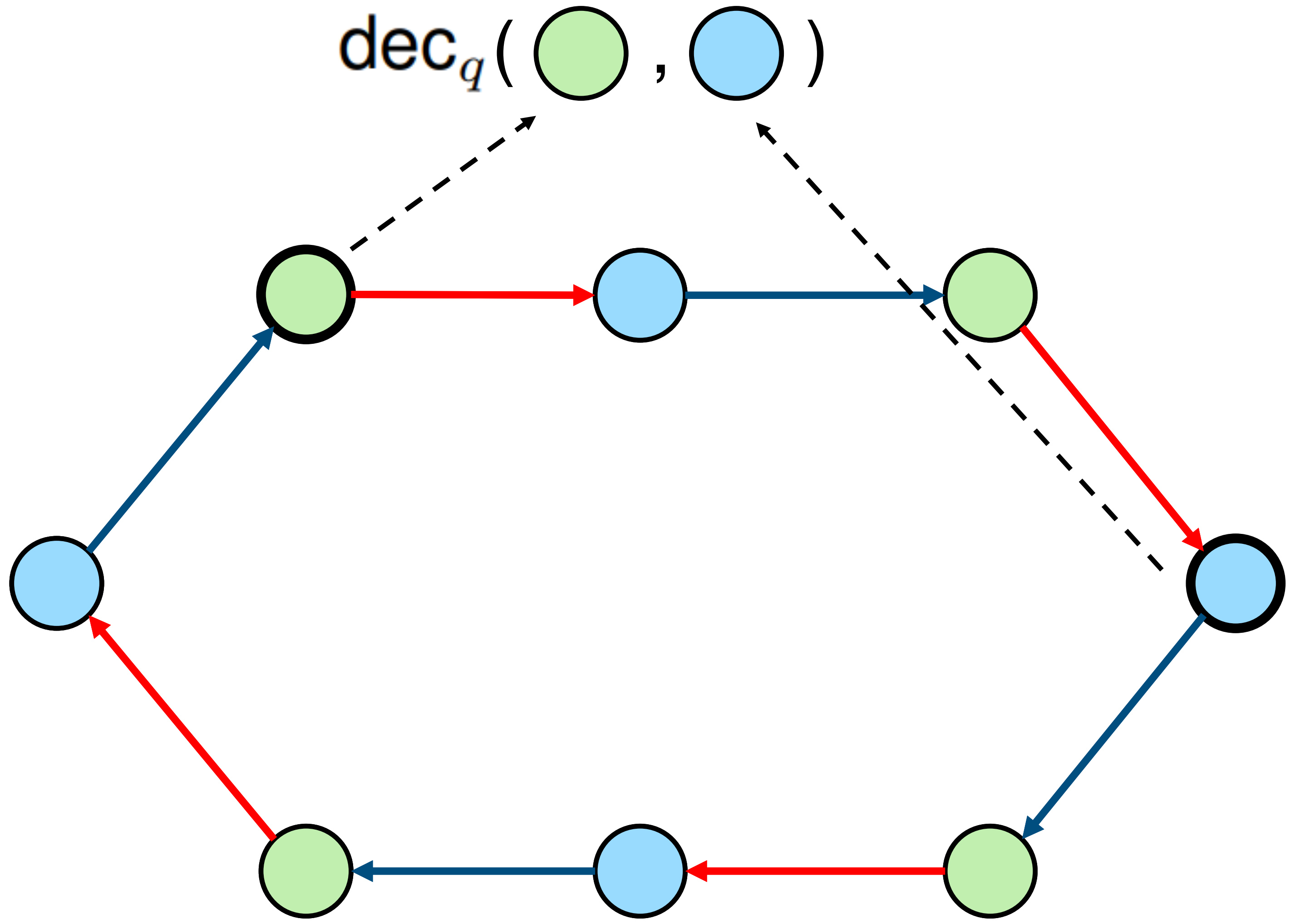

Prominent examples are RGCN [1] and CompGCN [2].

$$
\begin{aligned}
\boldsymbol{h}_v^{(0)} &= \boldsymbol{x}_v \\
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\end{aligned}
$$

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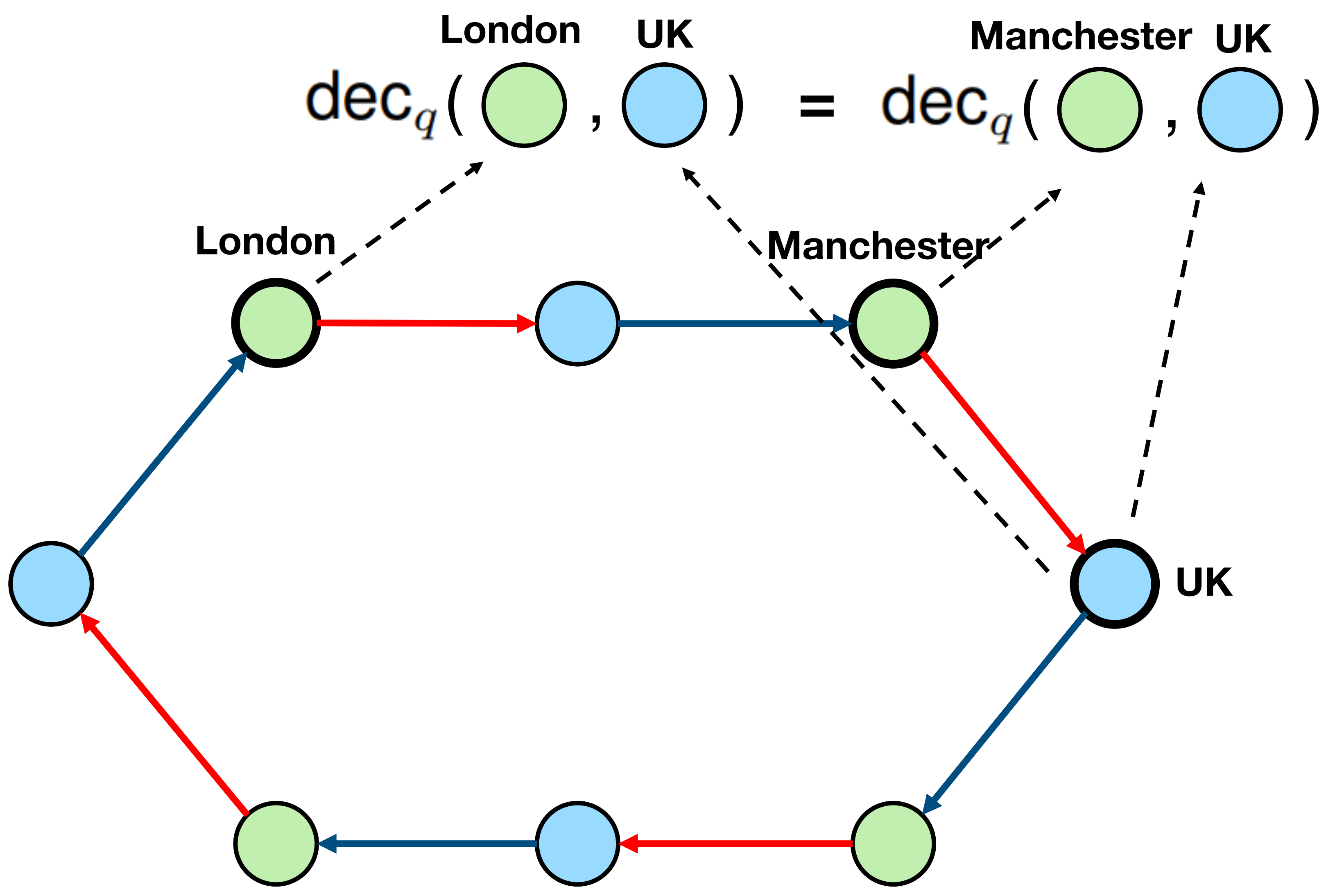

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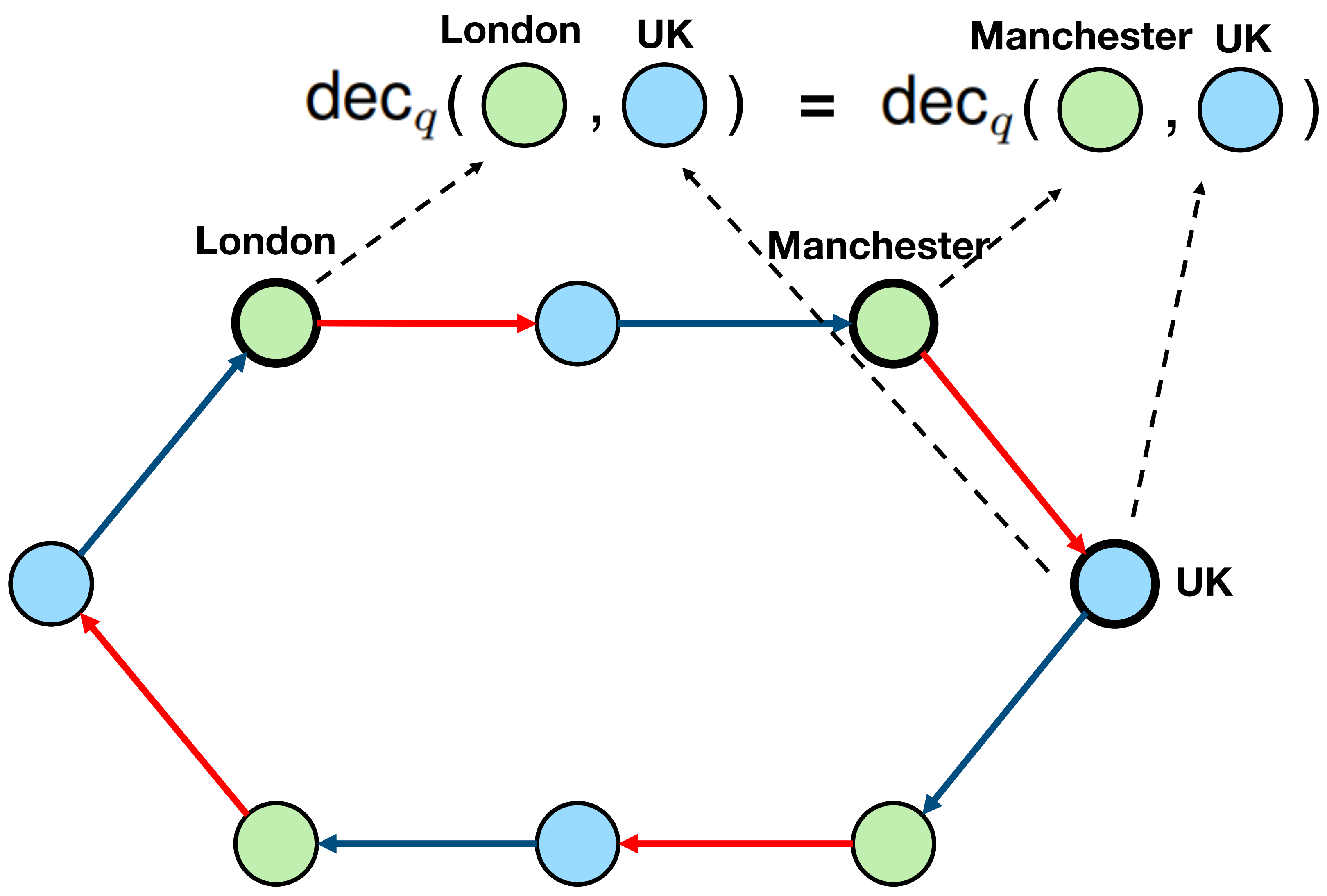
Relational Message Passing Neural Networks

R-MPNNs are at most as powerful as *relational local 1-WL test* [3].



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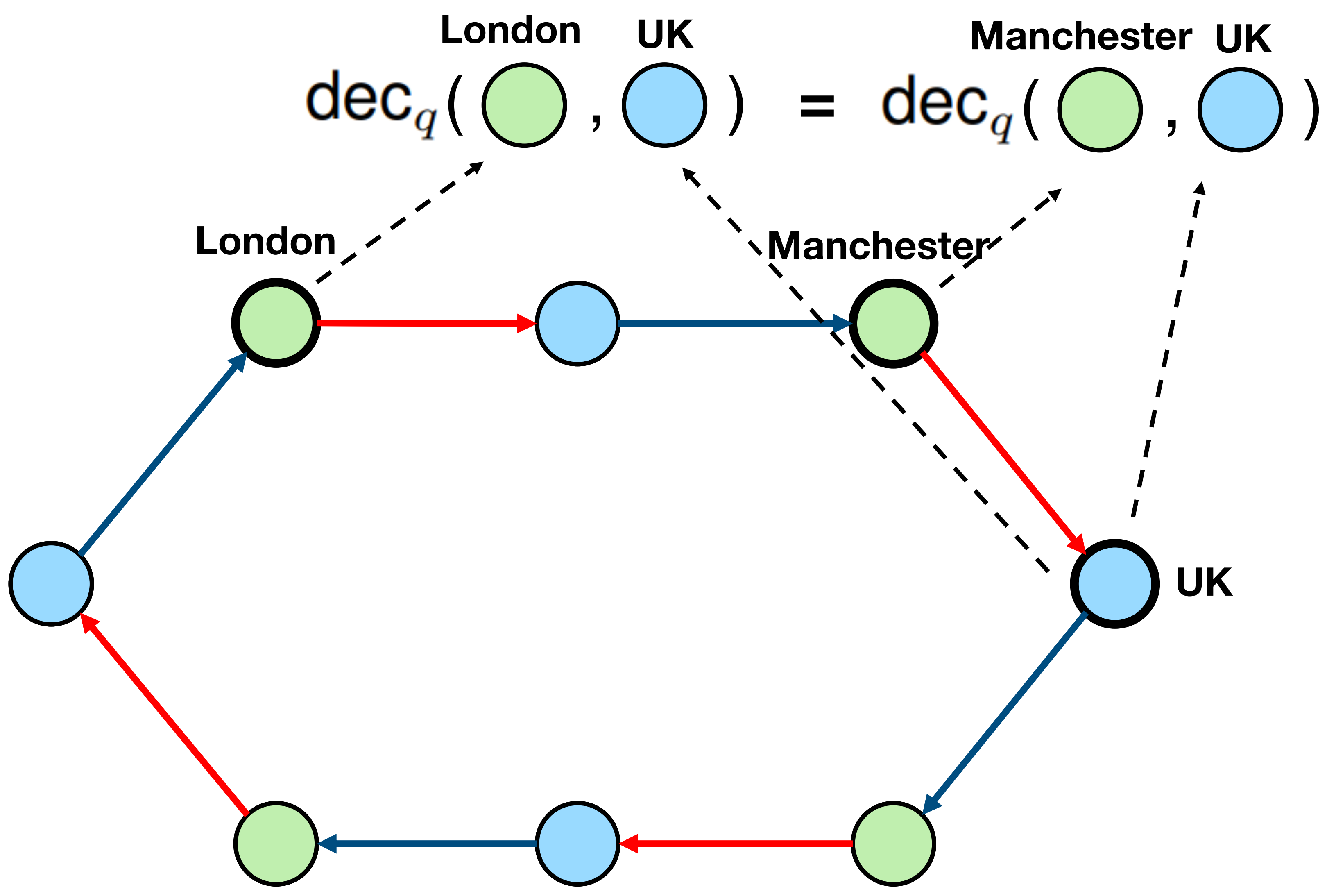

Higher order method is computationally prohibitive.

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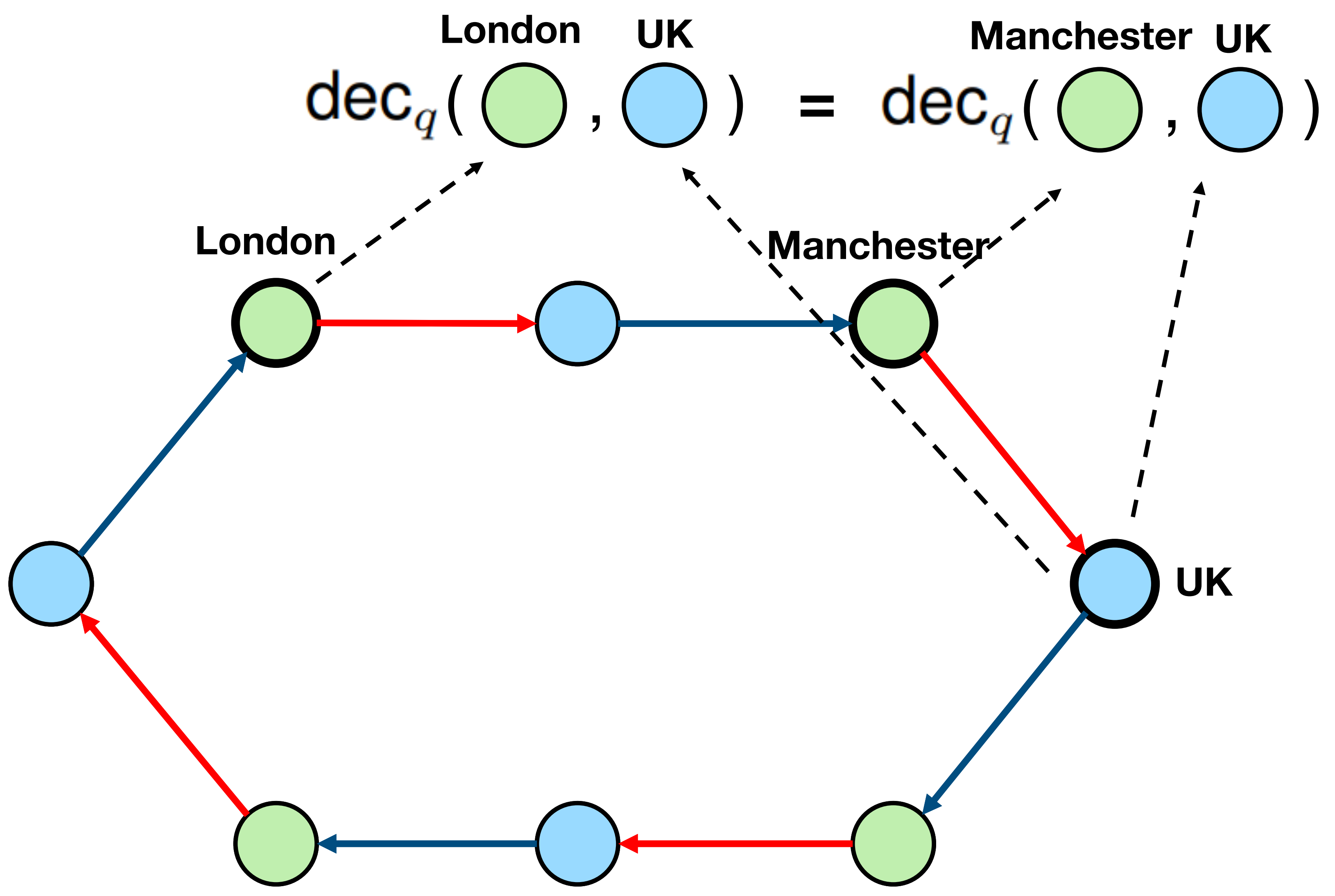

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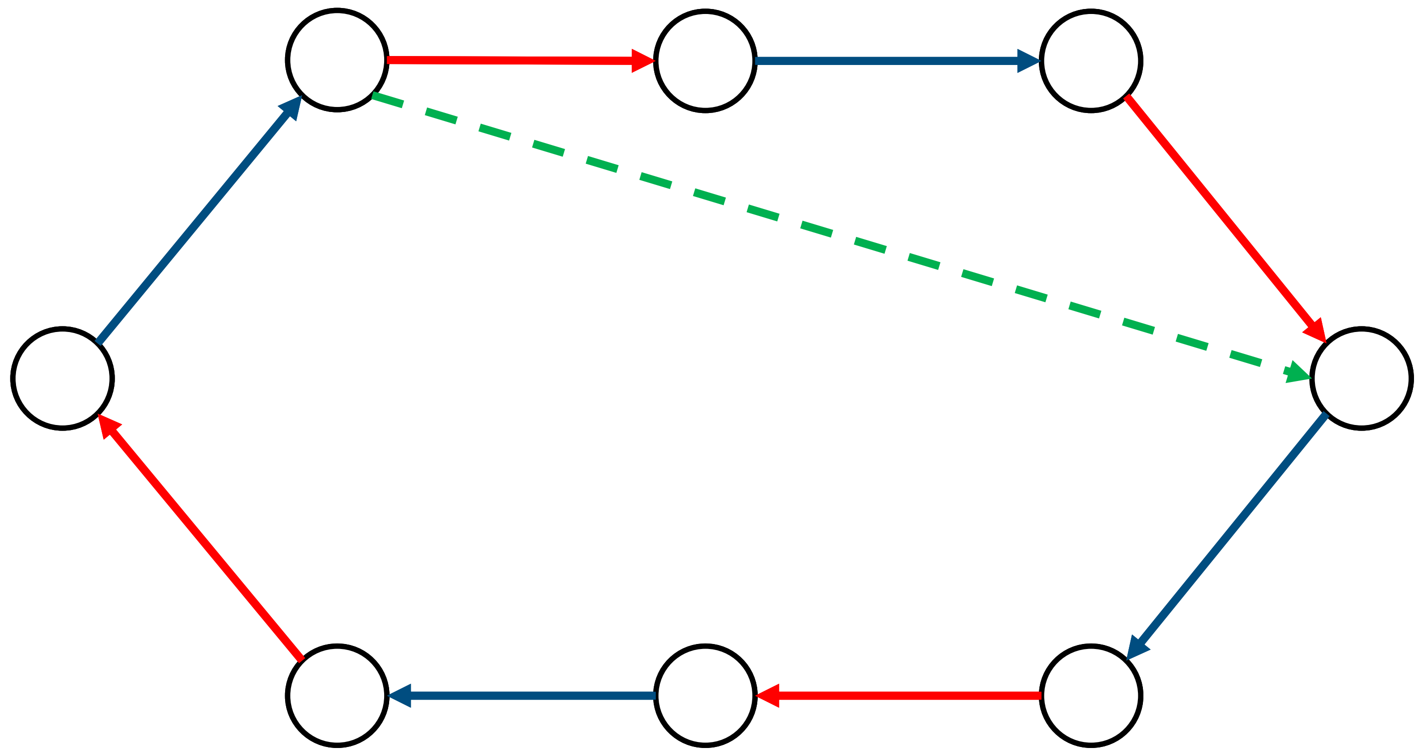
What is a good trade off between expressivity and scalability?

Conditional Message Passing Neural Networks (C-MPNNs)

Conditional Message Passing Neural Networks

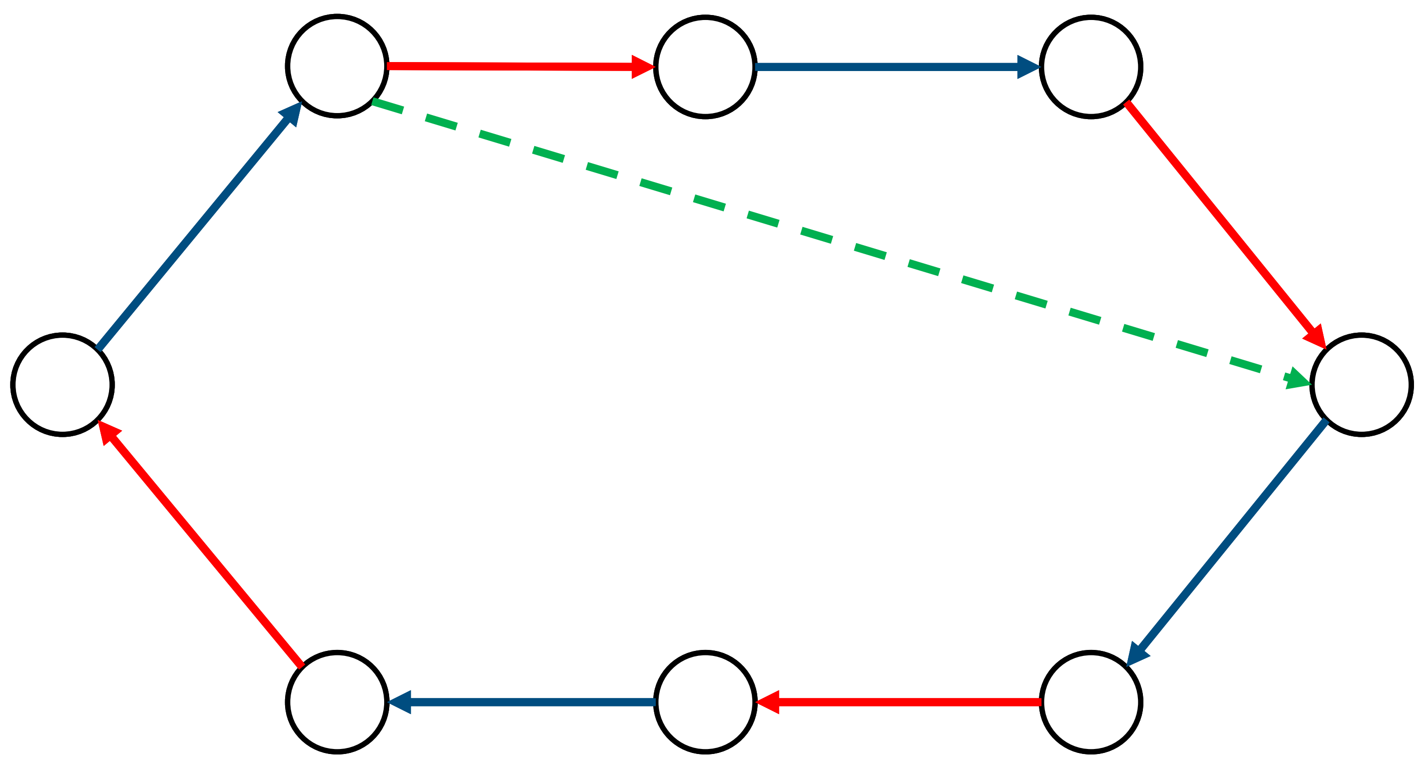


$$\boldsymbol{h}_{v|u,q}^{(0)} = \textsc{Init}(u, v, q)$$

$$\boldsymbol{h}_{v|u,q}^{(t+1)} = \textsc{Upd}(\boldsymbol{h}_{v|u,q}^{f(t)}, \textsc{Agg}(\{\!\{\textsc{Msg}_r(\boldsymbol{h}_{w|u,q}^{(t)}, \boldsymbol{z}_q) | \; w \in \mathcal{N}_r(v), r \in R\}\!\}), \textsc{Read}(\{\!\{\boldsymbol{h}_{w|u,q}^{(t)} \mid w \in V\}\!\})),$$

Conditional Message Passing Neural Networks

NBFNet [4] locally computes pairwise representations by conditioning.



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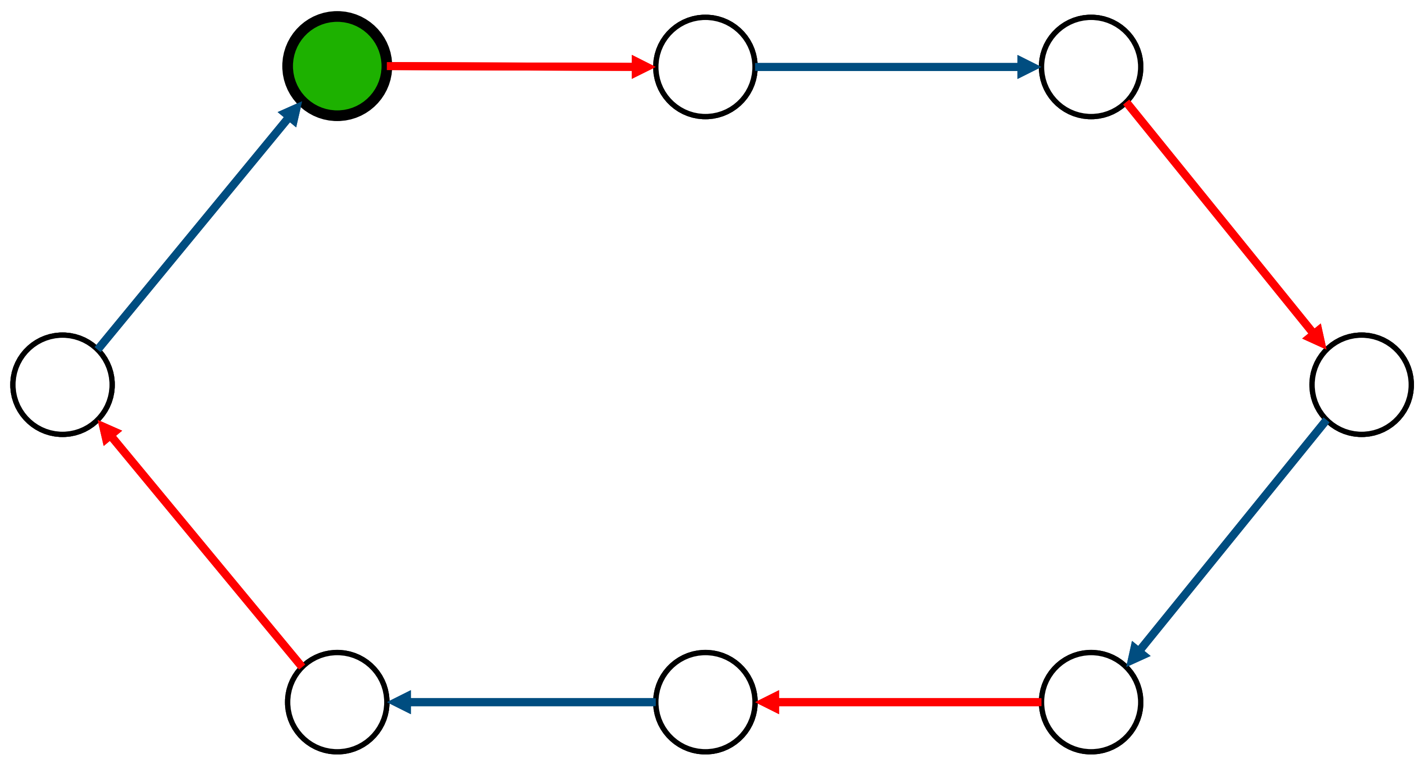

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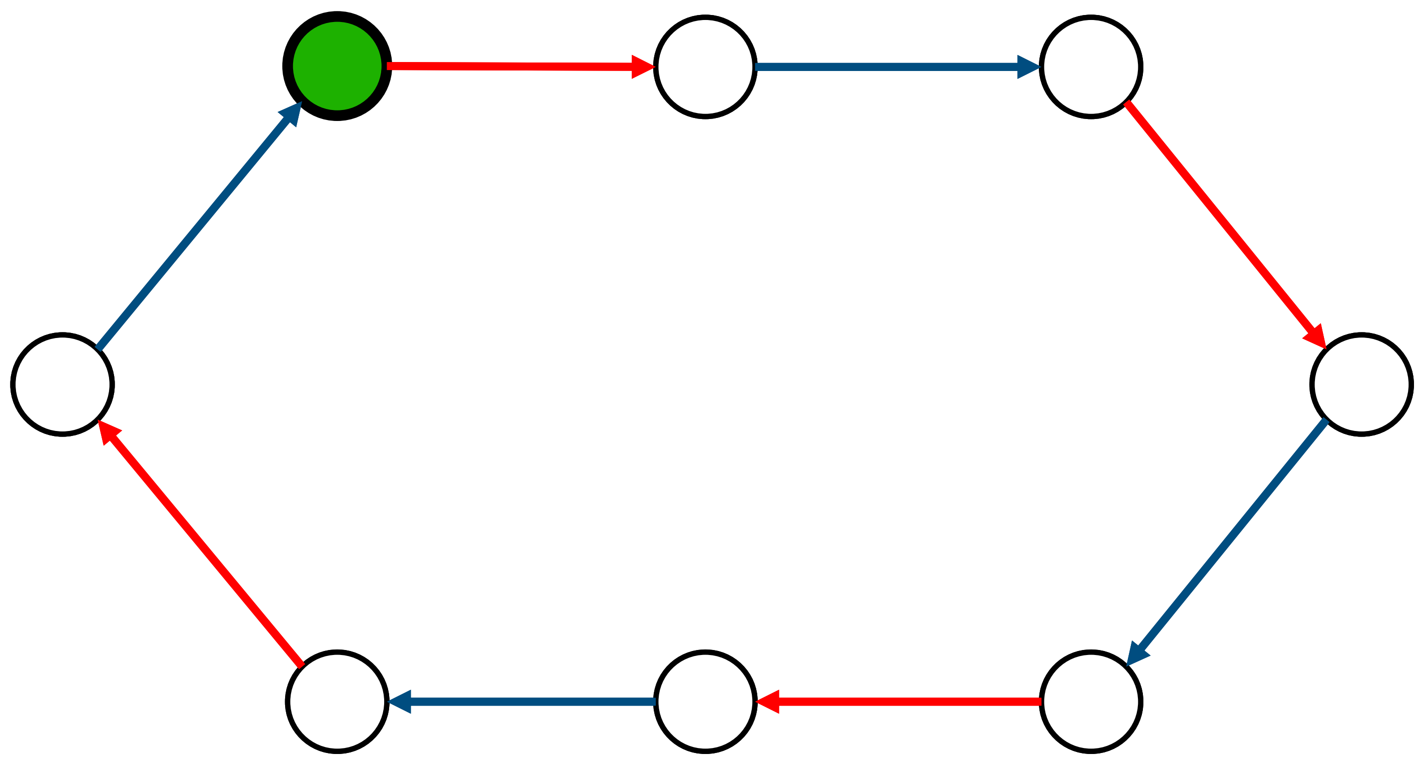

The initialization function must satisfy target node distinguishability.

$$\boxed{\boldsymbol{h}_{v|u,q}^{(0)} = \textsc{Init}(u, v, q)}$$

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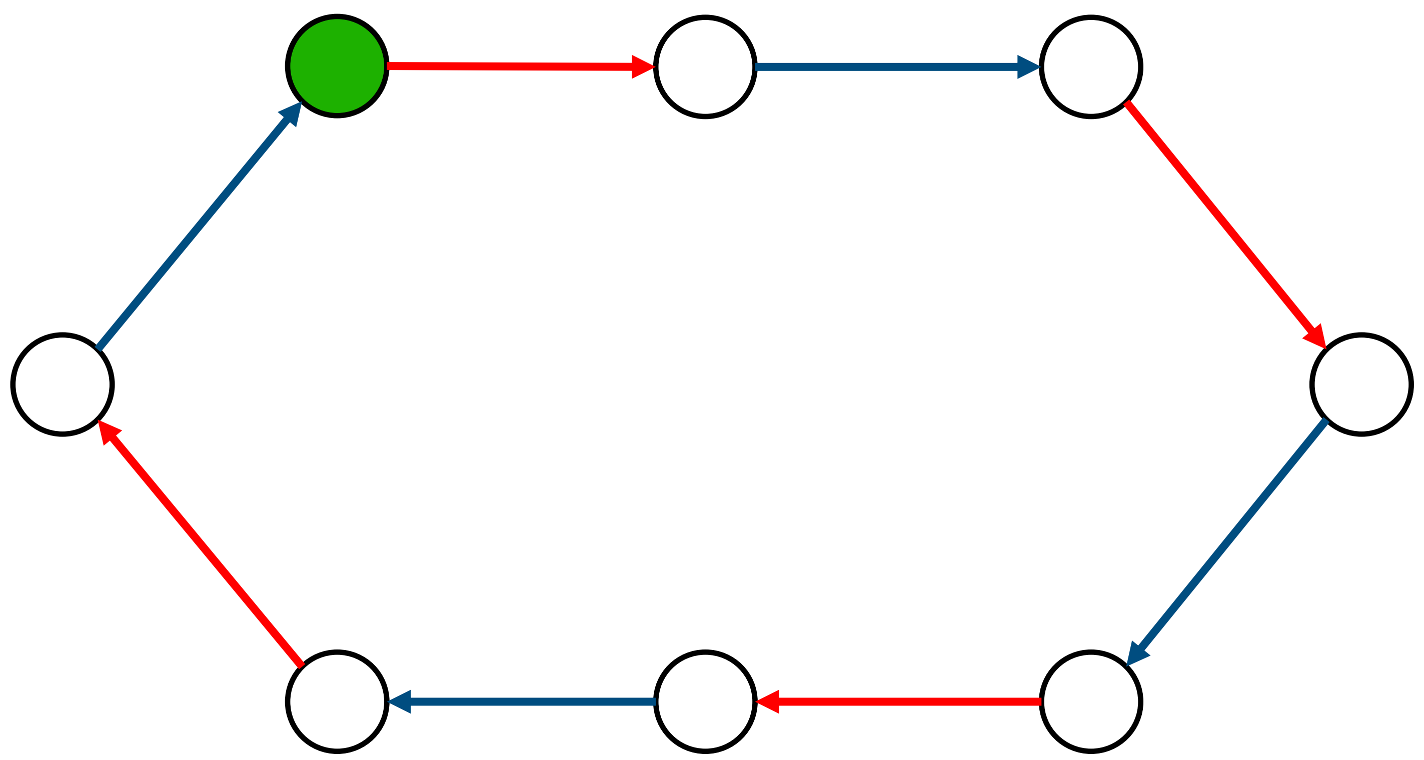

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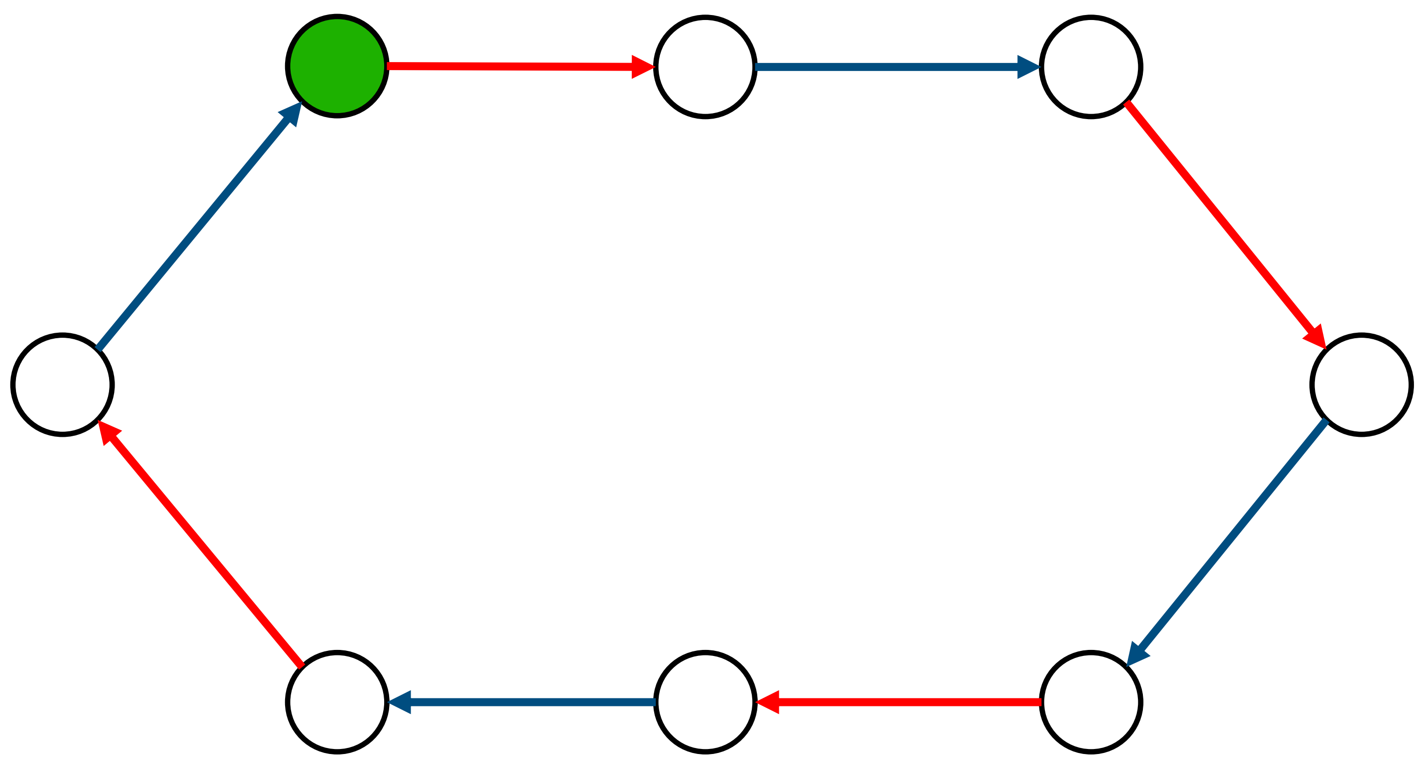
Conditional Message Passing Neural Networks

The history function shows which historical self-representation we choose to update.



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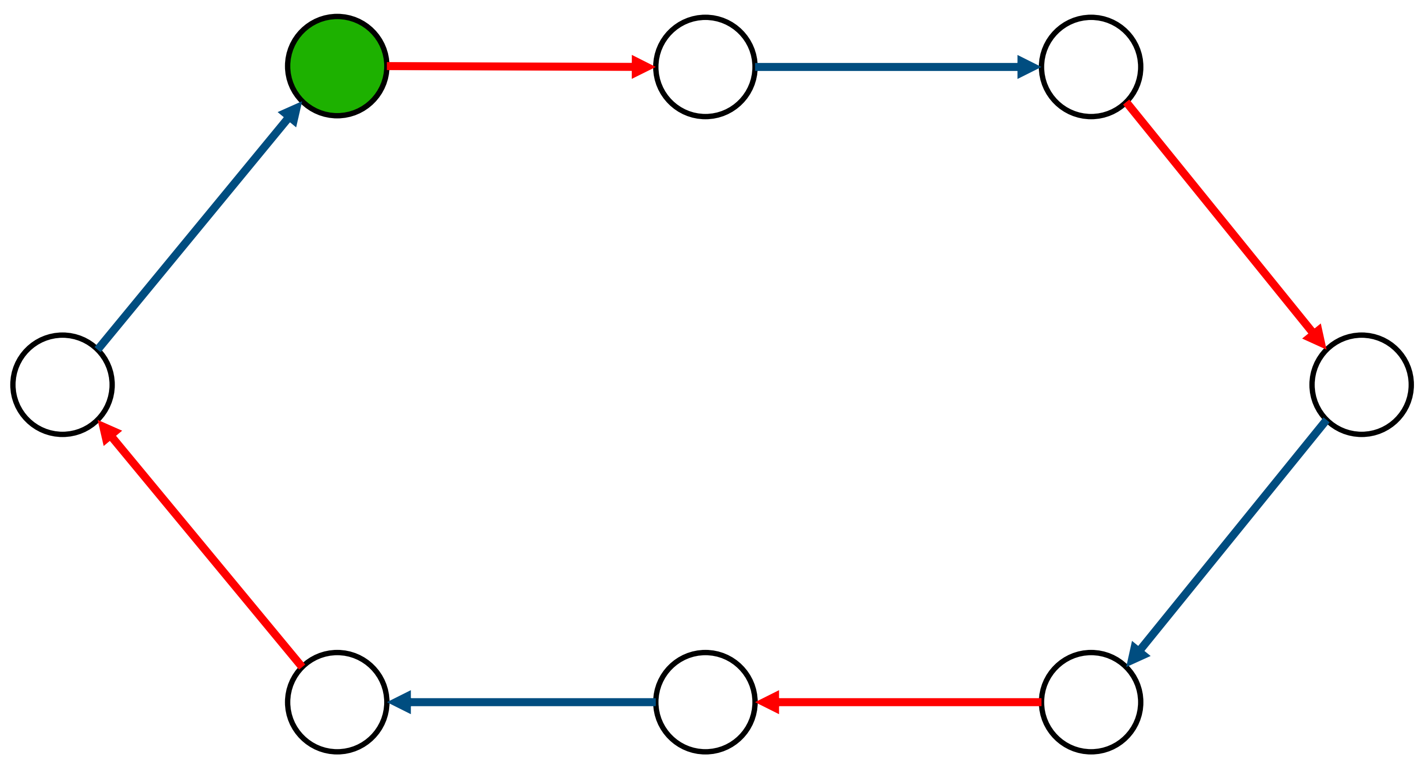

We prove that the choice of the historic function is irrelevant in theoretical expressiveness.

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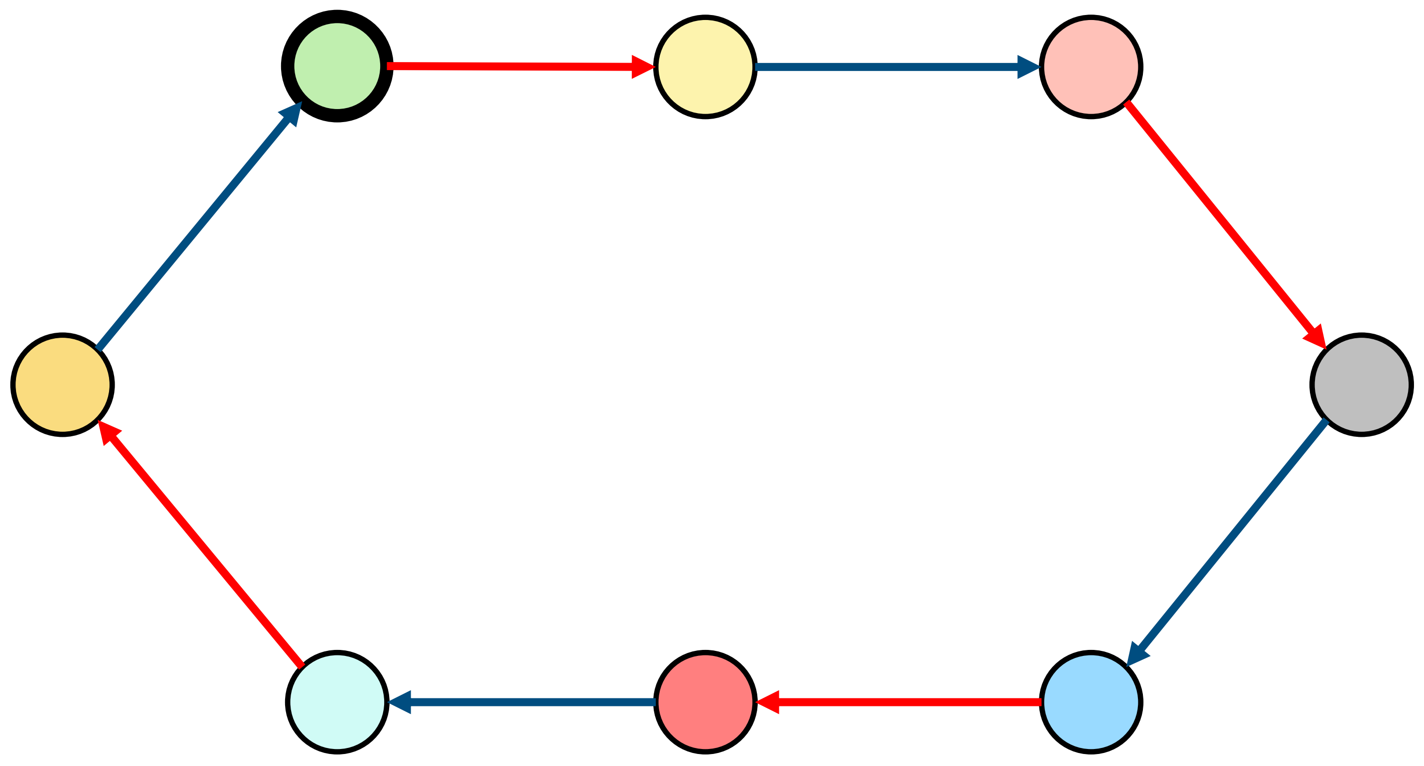

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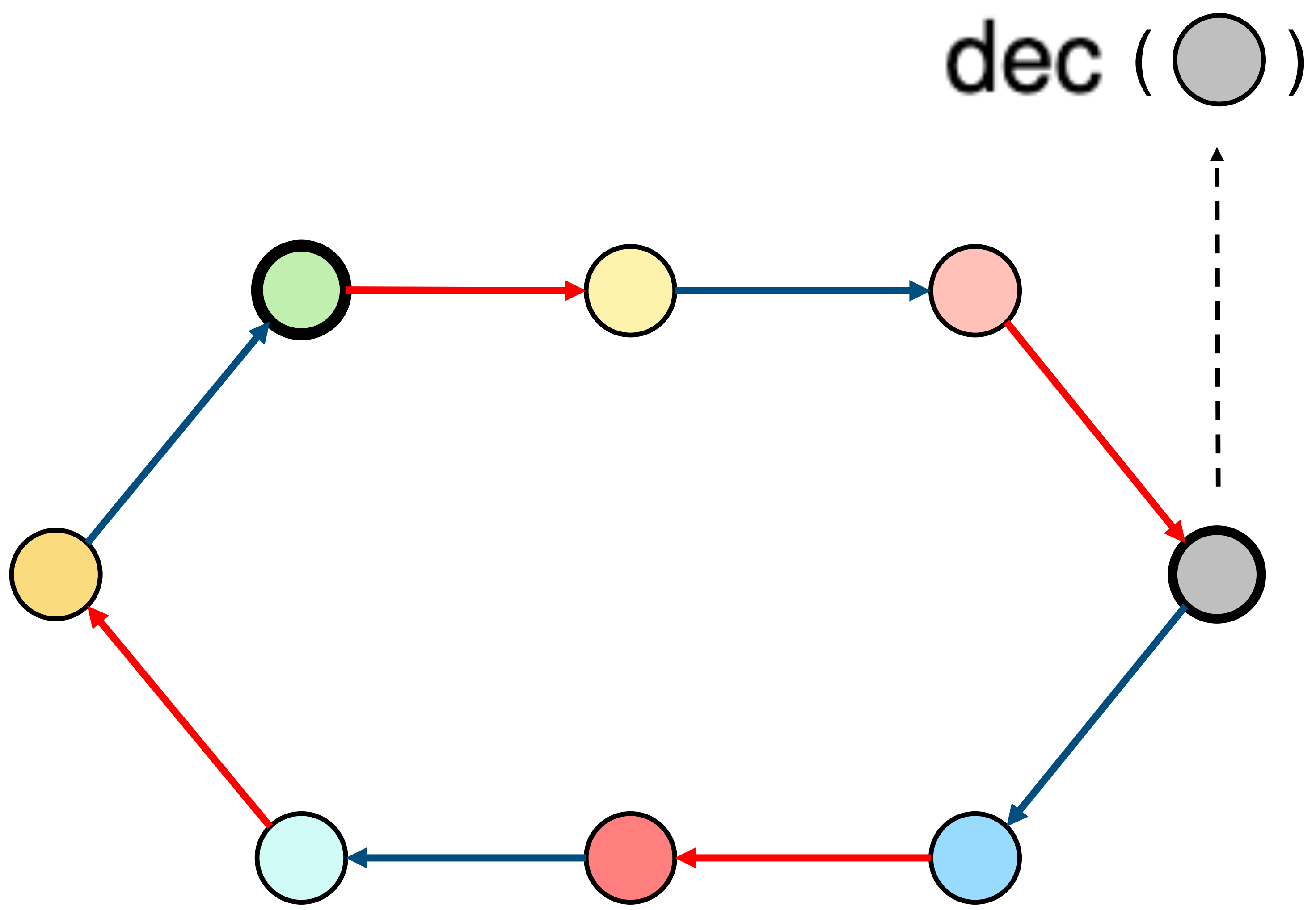

$$\boldsymbol{h}^{(0)}_{v|u,q} = \textsc{Init}(u, v, q)$$

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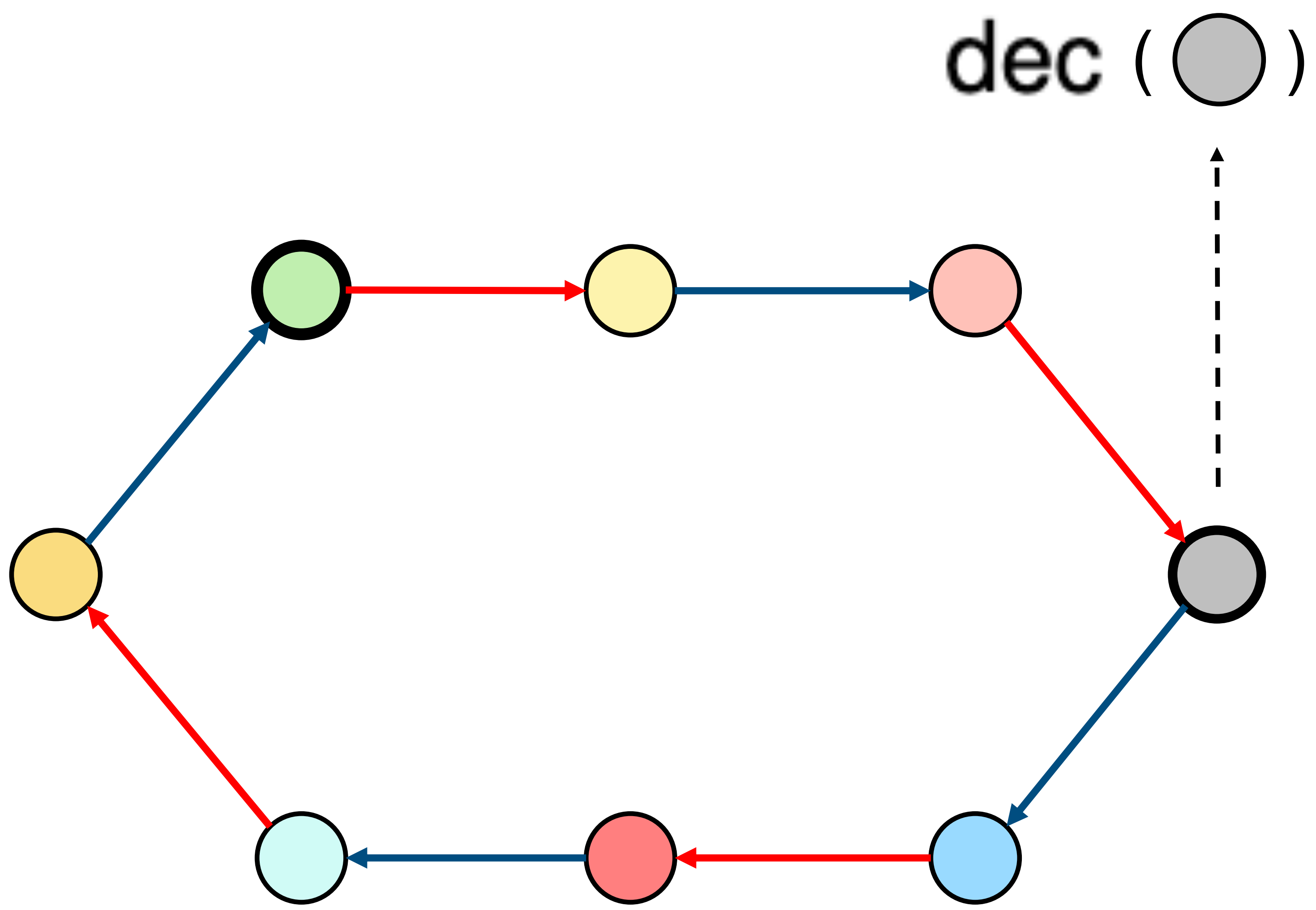

C-MPNNs relies on unary decoder for link prediction.

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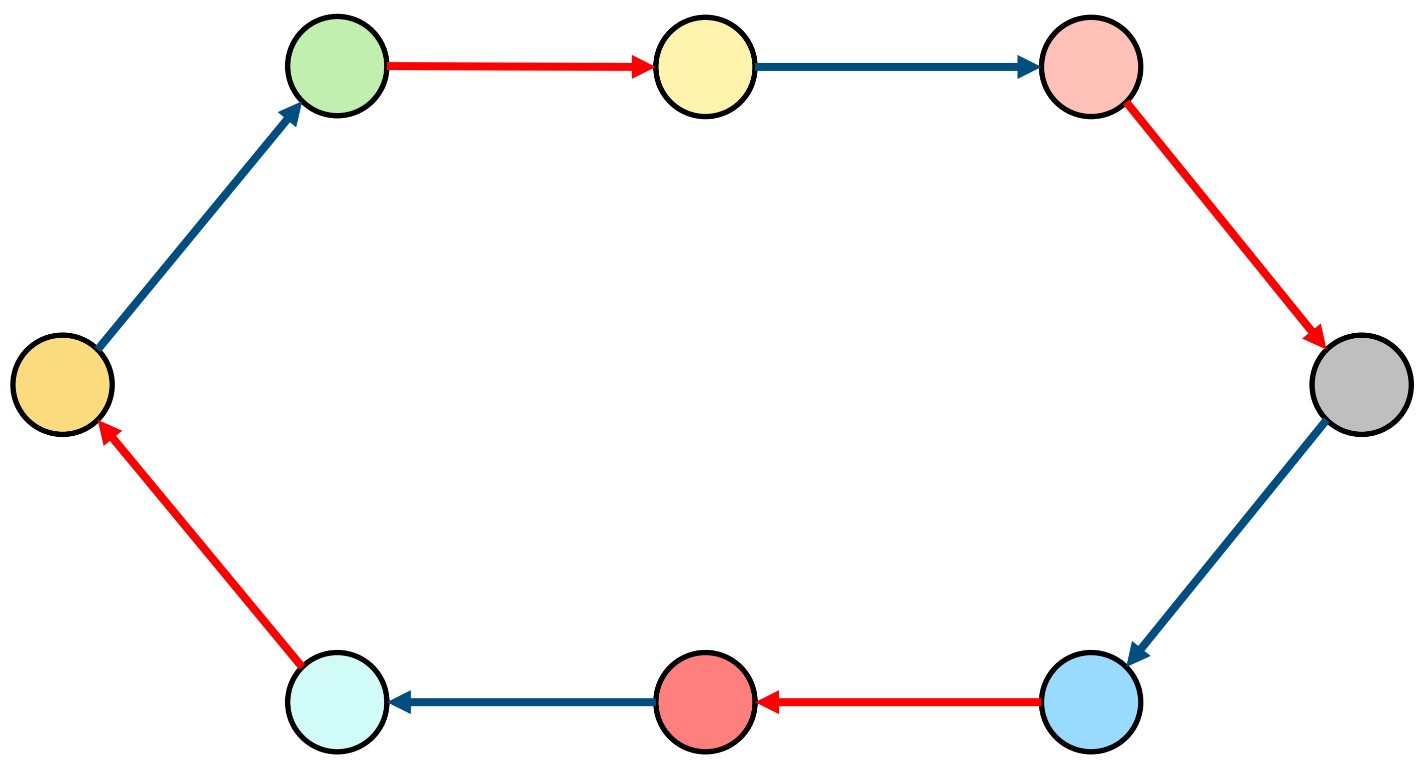
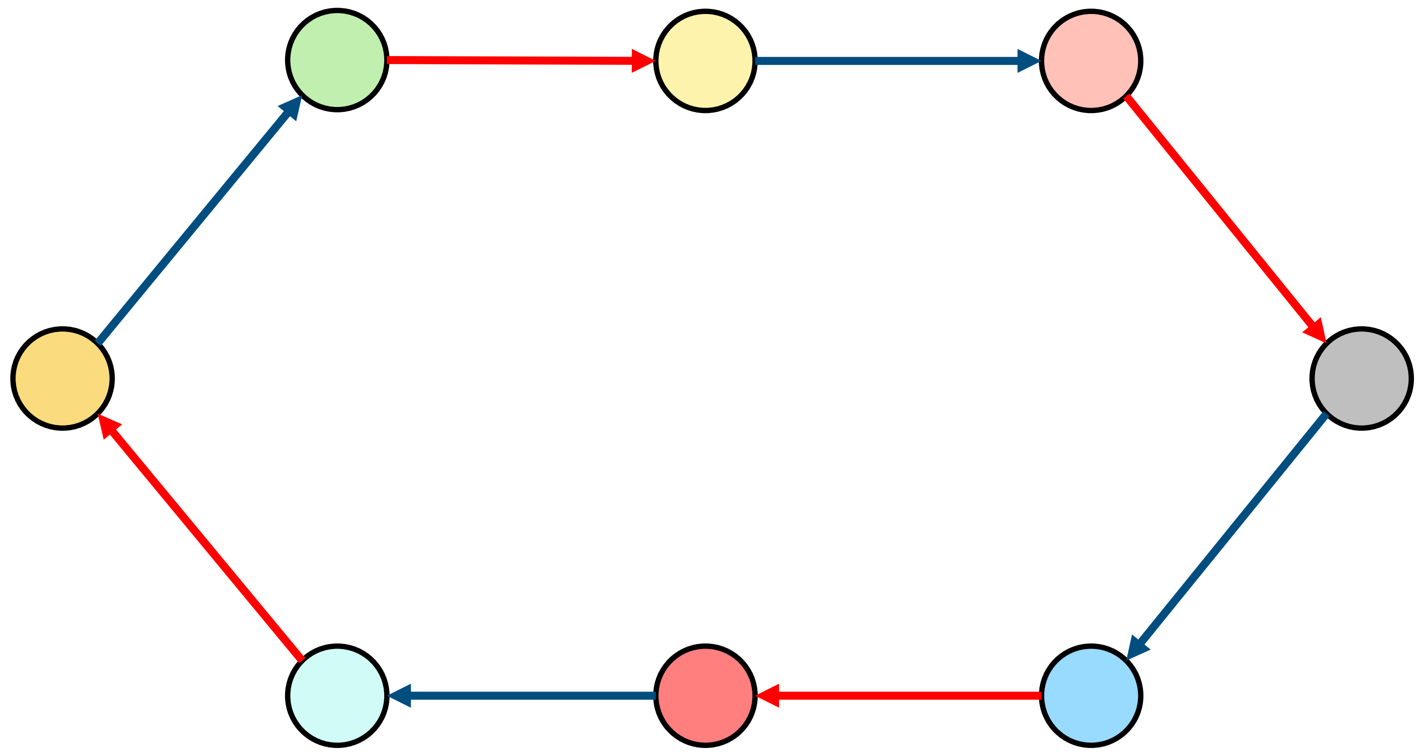
Expressiveness of C-MPNNs



$$\mathsf{rawl}_2^{(0)}(u,v) = \eta(u,v),$$
$$\mathsf{rawl}_2^{(t+1)}(u,v) = \tau\big(\mathsf{rawl}_2^{(t)}(u,v), \{\!\{(\mathsf{rawl}_2^{(t)}(u,w), r) \mid w \in \mathcal{N}_r(v), r \in R)\}\!\}\big),$$

Expressiveness of C-MPNNs

C-MPNNs are at most as expressive as relational asymmetric local 2-WL (rawl_2).



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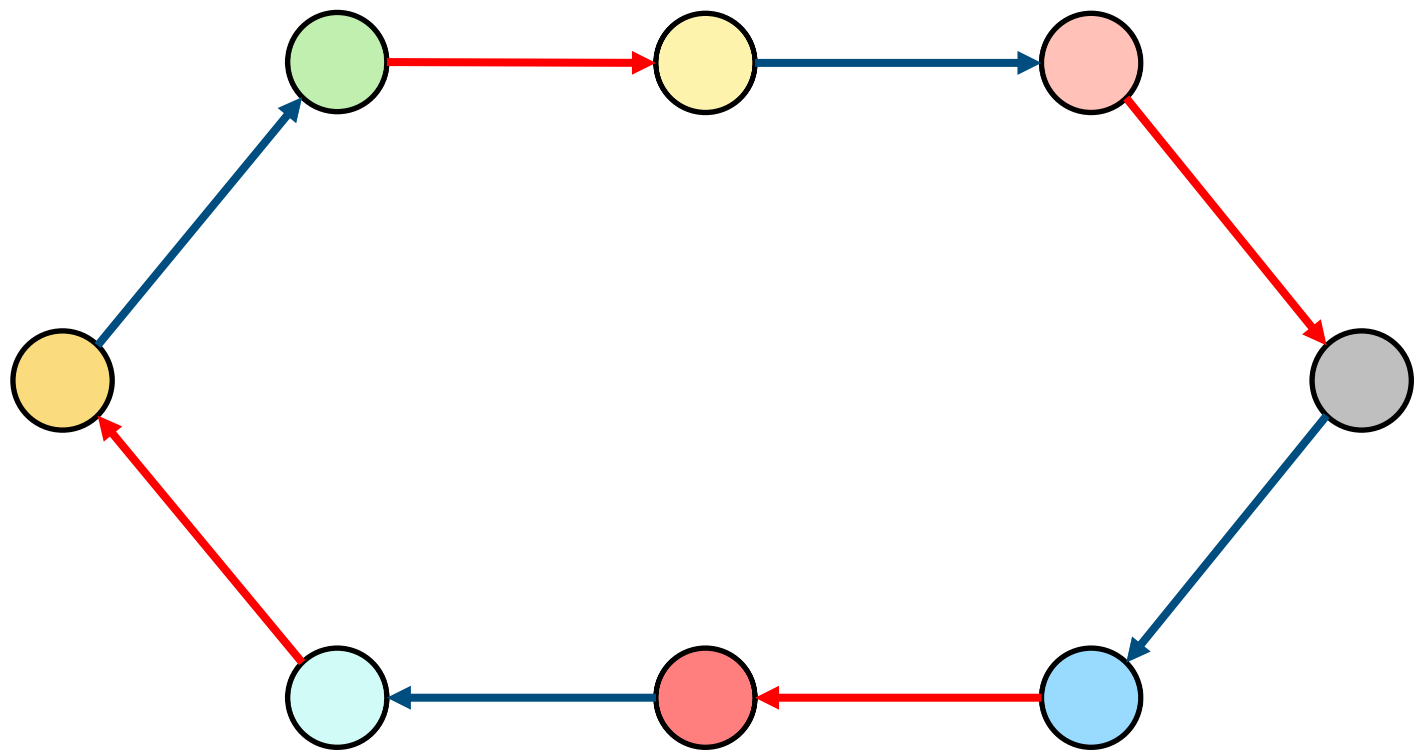

There exists a C-MPNN (even without readout) that achieves the same express power of rawl_2.

$$\text{rawl}_2^{(0)}(u,v) = \eta(u,v),$$
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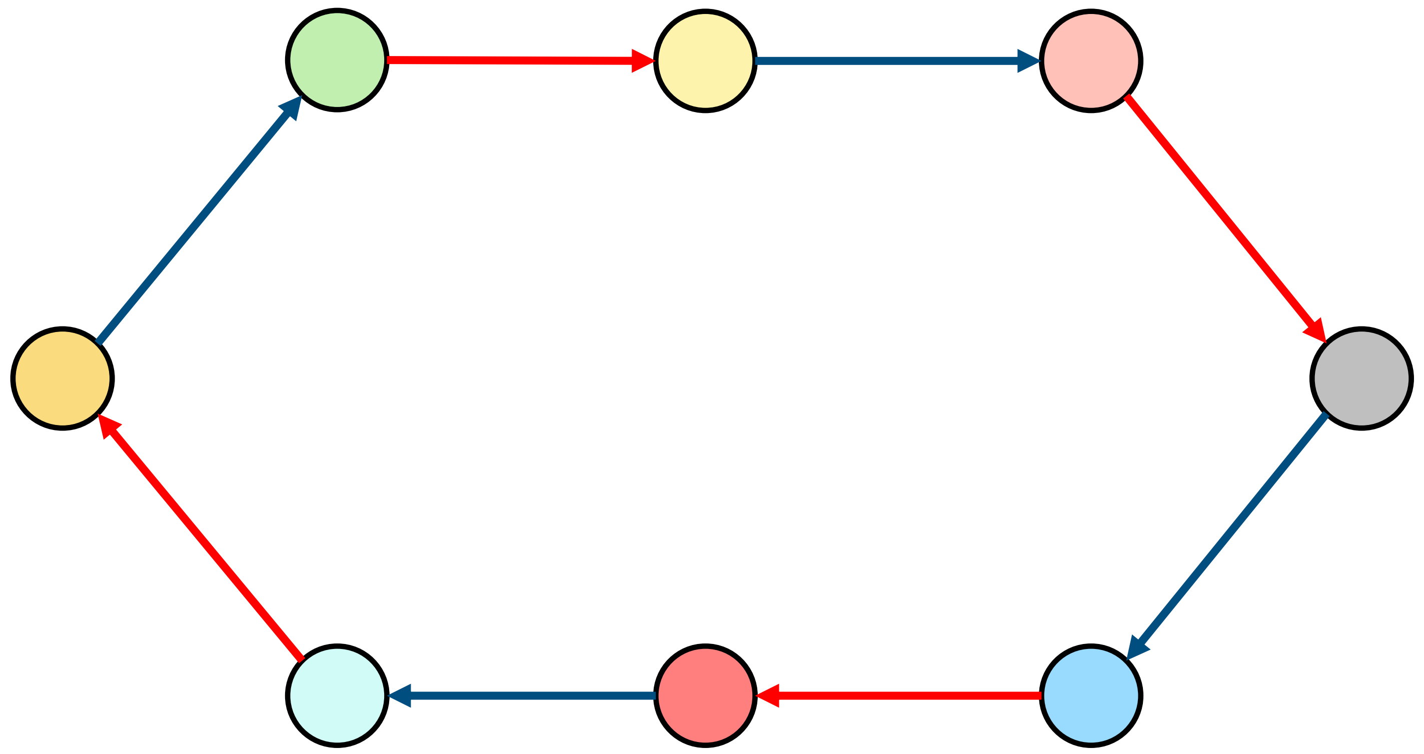
Logical Characterization of C-MPNNs

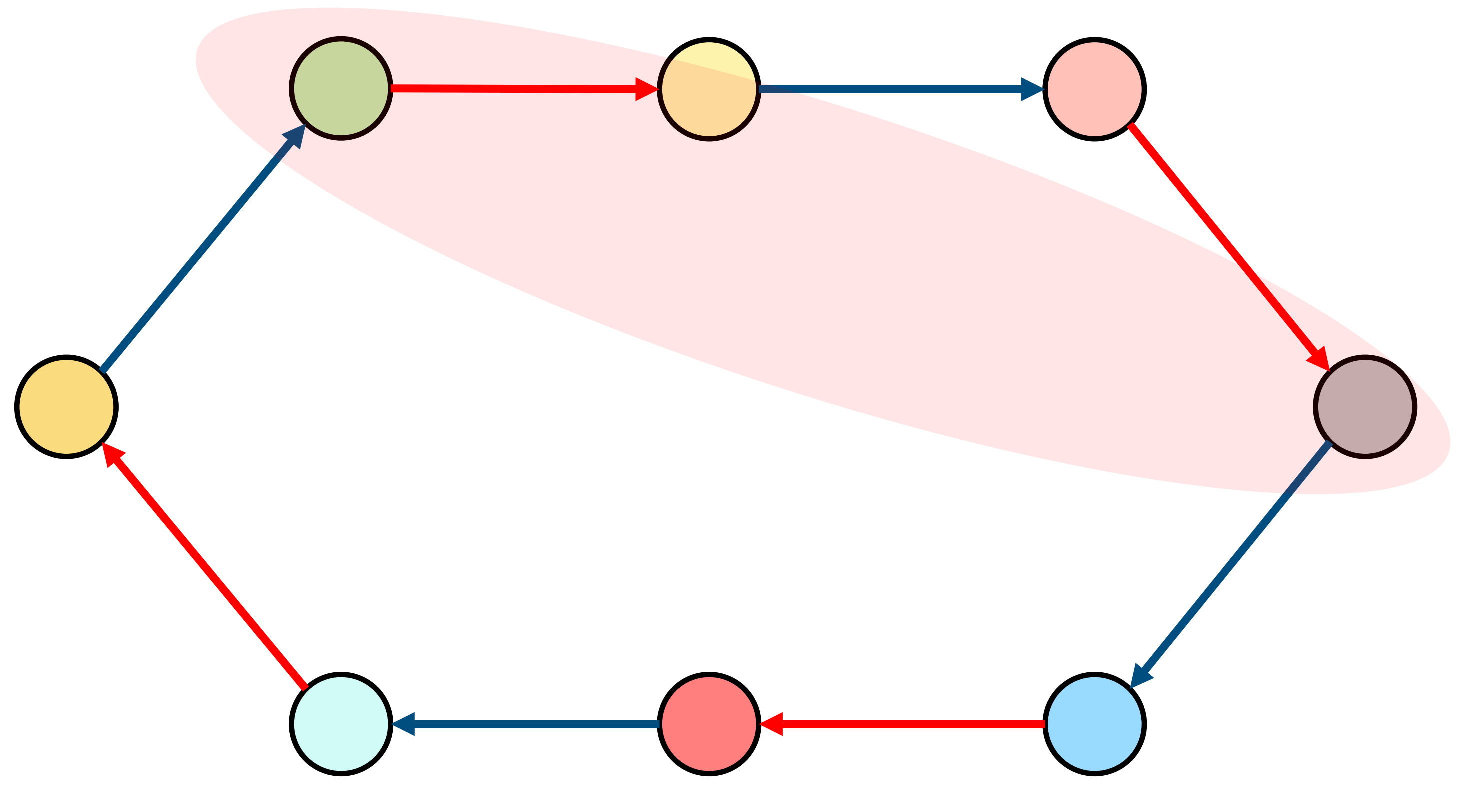


C-MPNNs (without readout) can uniformly express precisely functions in $\mathsf{rFO}^3_{\mathrm{cnt}}$.

C-MPNNs (with readout) can uniformly express all functions in $\mathsf{erFO}^3_{\mathrm{cnt}}$.

Summary and Outlook

Pairwise representation: C-MPNNs encodes pairwise node representations conditioned on source node.



Expressiveness results: C-MPNNs can match the expressive power of relational asymmetric local 2-WL, and logical characterizations.

Experimental validation: Experimental analysis is carried out to verify the impact of model choices to validate our theoretical findings.

Thank you!

Selected References

[1] Michael Sejr Schlichtkrull, Thomas N. Kipf, Peter Bloem, Rianne van den Berg, Ivan Titov, and Max Welling. Modeling relational data with graph convolutional networks. In ESWC, 2018.

[2] Shikhar Vashishth, Soumya Sanyal, Vikram Nitin, and Partha Talukdar. Composition-based multi-relational graph convolutional networks. In ICLR, 2020.

[3] Pablo Barceló, Mikhail Galkin, Christopher Morris, and Miguel Romero. Weisfeiler and leman go relational. In LoG, 2022.

[4] Zhaocheng Zhu, Zuobai Zhang, Louis-Pascal Xhonneux, and Jian Tang. Neural bellman-ford networks: A general graph neural network framework for link prediction. In NeurIPS, 2021.