Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

Structure Recognition with Graph Neural Networks

A project for the lab-course
Advanced Projects in Computational Physics 2

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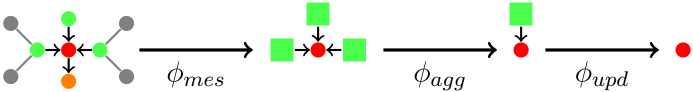
Theoretical Background - Message Passing

Overview:

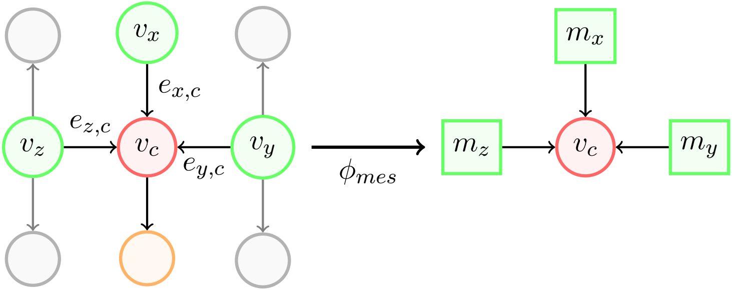


Message passing consists of three steps:

1. Computing messages (ϕ_{mes})
2. Aggregating messages (ϕ_{agg})
3. Updating node values (ϕ_{upd})

Theoretical Background - Message Passing

Step 1: Compute Messages

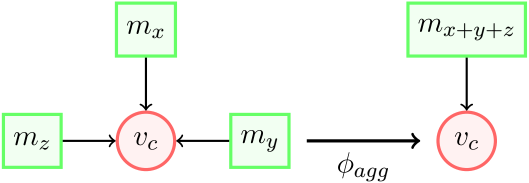


For $i \in \{x, y, z\}$ calculate:

$$m_i \coloneqq \phi_{mes}(v_c, v_i, e_{i,c})$$

Theoretical Background - Message Passing

Step 2: Aggregate Messages

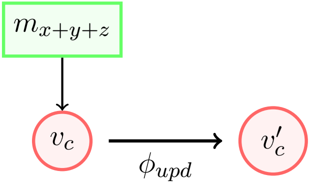


Calculate total message:

$$m_{x+y+z} \coloneqq \phi_{agg}(m_x, m_y, m_z)$$

Theoretical Background - Message Passing

Step 3: Update node value



Calculate new node value:

$$v'_c := \phi_{upd}(v_c, m_{x+y+z})$$

Question: What exactly are $\phi_{mes}, \phi_{agg}, \phi_{upd}$?

Theoretical Background - Message Passing

Common example for $\phi_{mes}, \phi_{agg}, \phi_{upd}$:
GIN-Layer [4] given by:

$$\phi_{mes}(v_c, v_i, e_{i,c}) = v_i$$

$$\phi_{agg}(m_1, ..., m_n) = \sum_{i=1}^{n} m_i$$

$$\phi_{upd}(v_c, m_{agg}) = h_\theta\left((1+\epsilon)v_c + m_{agg}\right)$$

Theoretical Background - Message Passing

Common example for $\phi_{mes}, \phi_{agg}, \phi_{upd}$:
GIN-Layer [4] given by:

$$\phi_{mes}(v_c, v_i, e_{i,c}) = v_i \rightarrow \text{ReLU}(v_i + e_{i,c}) \quad \text{GINE [3]}$$

$$\phi_{agg}(m_1, ..., m_n) = \sum_{i=1}^{n} m_i$$

$$\phi_{upd}(v_c, m_{agg}) = h_\theta\left((1+\epsilon)v_c + m_{agg}\right)$$

In general, $\phi_{mes}, \phi_{agg}, \phi_{upd}$ can be (almost) anything
$\implies$ in particular: arbitrary feed forward neural networks

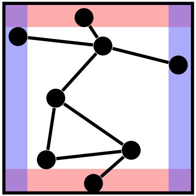
Theoretical Background - Percolation

Given are

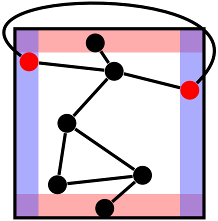
- graph $G = (V, E)$
- one position (n_x, n_y) inside unit square for each node $n \in V$
- small stripes at the edges of the unit square

G is called percolating, if there are nodes $n, m \in V$ such that

1. there is a cycle containing n and m
2. n and m are connected by an edge
3. n and m lie in opposite stripes



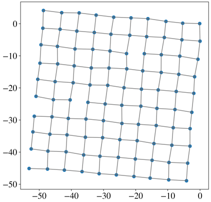
(a) non-percolating



(b) percolating

Goals

Experiment 1
Input: Bravais lattice (in 2D, 3D), e.g.:

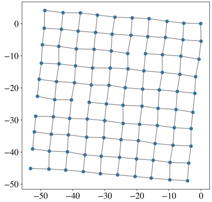


Expected output: Bravais class, e.g. square
Question: What are suitable choices for ϕ's?

Experiment 2

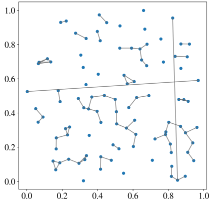
Goals

Experiment 1
Input: Bravais lattice (in 2D, 3D), e.g.:



Expected output: Bravais class, e.g. square
Question: What are suitable choices for ϕ's?

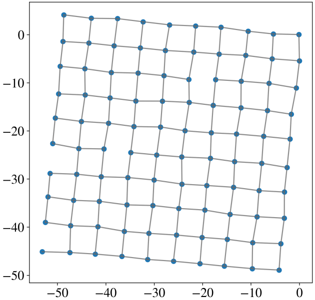
Experiment 2
Input: Graph inside unit-square, e.g.:



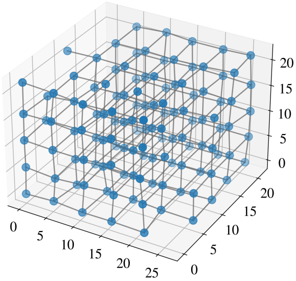
Expected output: percolating or not
Question: Can this problem be solved by a GNN?

Results - Bravais Lattices 2D (Experiment 1)

Input data:



(a) 2d (square)



(b) 3d (cubic)

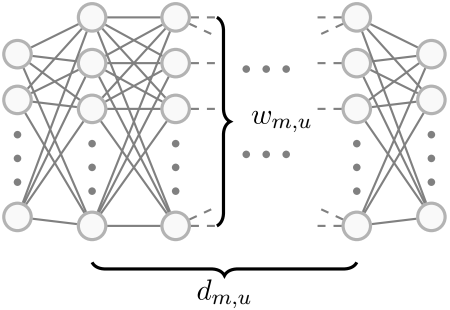
with node features = 1, edge features = direction

Expected output: Bravais class

Results - Bravais Lattices 2D (Experiment 1)

parameters varied: w_u, w_m, d_u, d_m

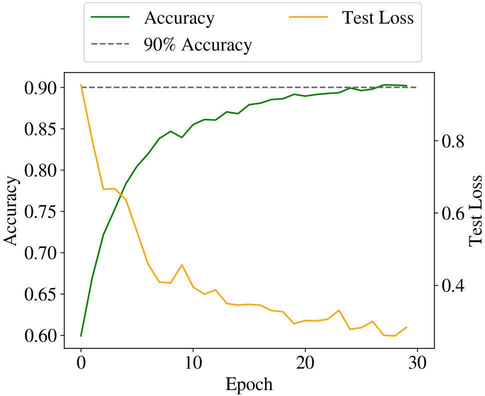
$\phi_{mes}, \phi_{upd} =$ general feed forward neural network with certain width $w_{m,u}$, depth $d_{m,u}$



$$d_m \in \{1, 2, 3\}, \quad w_m \in \{10, 20, 30\},$$
$$d_u \in \{1, 2\}, \quad w_u \in \{5, 10\}$$

Results - Bravais Lattices 2D (Experiment 1)

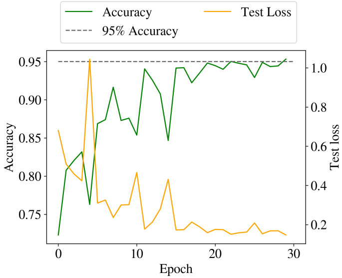
Averaged performance (over all 36 models):



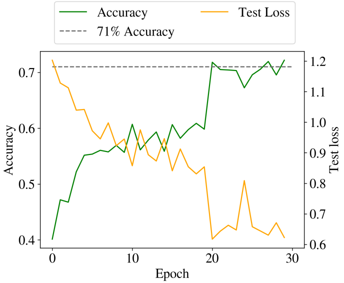
Question: Do different models lead to different accuracies?

Results - Bravais Lattices 2D (Experiment 1)

Best and worst performing models:



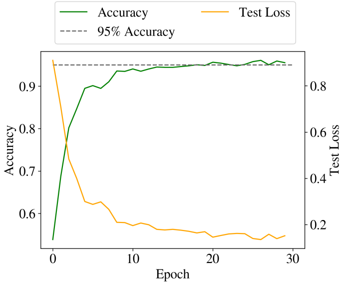
(a) Best performing model ($(d_m, w_m, d_u, w_u) = (2, 30, 1, 10)$).



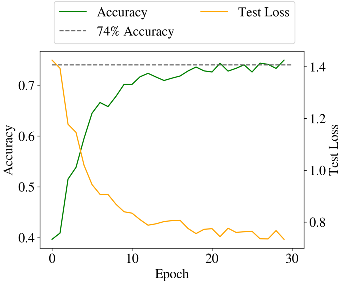
(b) Worst performing model ($(d_m, w_m, d_u, w_u) = (3, 30, 2, 5)$)

Results - Bravais Lattices 3D (Experiment 1)

Training of best and worst performing models on 3D dataset:



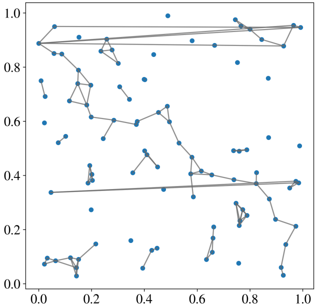
(a) Best performing model $((d_m, w_m, d_u, w_u) = (2, 30, 1, 10))$.



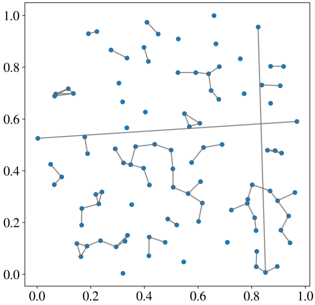
(b) Worst performing model $((d_m, w_m, d_u, w_u) = (3, 30, 2, 5))$

Results - Percolation (Experiment 2)

Input data:



(a) Percolating



(b) Non-Percolating

with node features = position, edge features = 1
Expected output: percolating or not

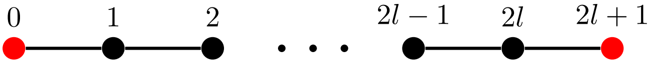
Results - Percolation (Experiment 2)

Observation: GNN can solve percolation problem $\implies$ GNN can solve connection problem
Question: Can a GNN solve the connection problem?
Assumption: there is a GNN with **1** layer capable of solving the connection problem

After one message passing step:

Results - Percolation (Experiment 2)

Observation: GNN can solve percolation problem $\implies$ GNN can solve connection problem
Question: Can a GNN solve the connection problem?
Assumption: there is a GNN with l layers capable of solving the connection problem



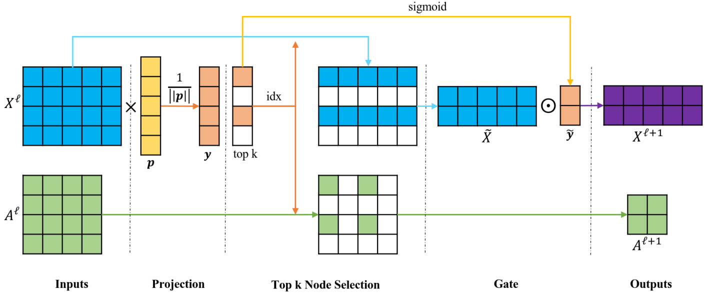
Answer: No!

Results - Percolation (Experiment 2)

Problem: size of graph, too many nodes

$\implies$ pooling might help ([2])

Example: Top K Pooling ([1])



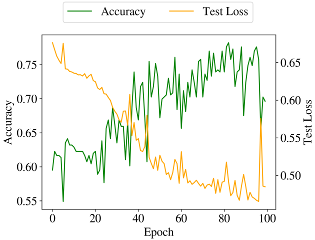
X^l = node features, A^l = adjacency matrix

Results - Percolation (Experiment 2)

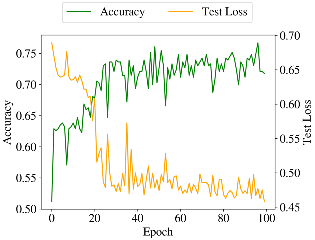
Why Top K Pooling might not help:

- deletion of nodes/edges
- connected components not preserved

Training results:



(a) Without Pooling



(b) With Pooling

Conclusion and Outlook

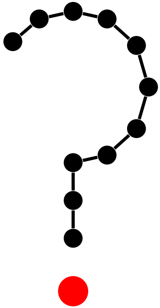
What we have learned:

- GNN capable of classifying Bravais lattices
- Correlation between width, depth and accuracies rather complicated
- Connection problem can not be solved
  $\Longrightarrow$ percolation problem can not be solved

What can be done next:

- Bravais lattices: vary node, edge features
- Percolation Problem: experiment with layers that preserve topological properties

Time for Discussion and Questions



References

[1] Hongyang Gao and Shuiwang Ji. "Graph U-Nets". In: *CoRR* abs/1905.05178 (2019). arXiv: 1905.05178. URL: http://arxiv.org/abs/1905.05178.

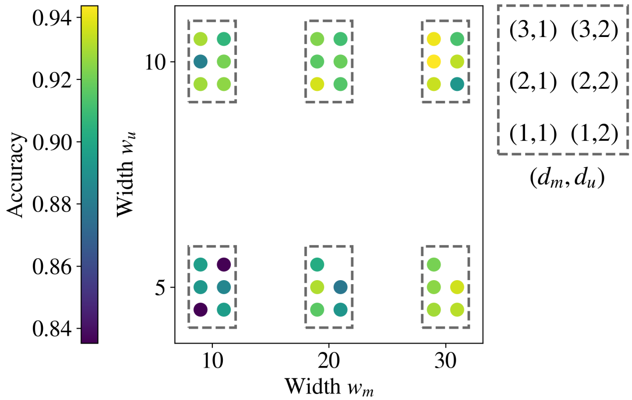
[2] Daniele Grattarola et al. "Understanding Pooling in Graph Neural Networks". In: *CoRR* abs/2110.05292 (2021). arXiv: 2110.05292. URL: https://arxiv.org/abs/2110.05292.

[3] Weihua Hu et al. *Strategies for Pre-training Graph Neural Networks*. 2020. arXiv: 1905.12265 [cs.LG]. URL: https://arxiv.org/abs/1905.12265.

[4] Keyulu Xu et al. "How Powerful are Graph Neural Networks?" In: *CoRR* abs/1810.00826 (2018). arXiv: 1810.00826. URL: http://arxiv.org/abs/1810.00826.

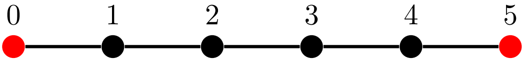
Results - Bravais Lattices 2D (Experiment 1)

Correlation between w_m and w_u:



Results - Percolation (Experiment 2)

Observation: GNN can solve percolation problem $\implies$ GNN can solve connection problem
Question: Can a GNN solve the connection problem?
Answer: No!
Assumption: there is a GNN with **2** layers capable of solving the connection problem



After one message passing steps:

After two message passing step:

Results - Percolation (Experiment 2)

Claim: GNN can solve percolation problem $\Longrightarrow$ GNN can solve connection problem

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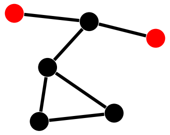
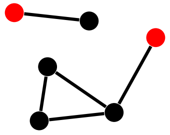
Procedure:

1. Start with arbitrary Graph G, select two nodes n, m



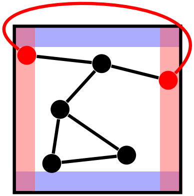


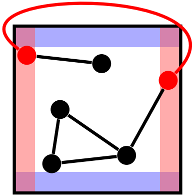
Results - Percolation (Experiment 2)

Claim: GNN can solve percolation problem $\implies$ GNN can solve connection problem

Procedure:

1. Start with arbitrary Graph G, select two nodes n, m
2. Place G inside unit square, move n, m to edges, add edge (n, m) $\implies$ new graph $\tilde{G}$



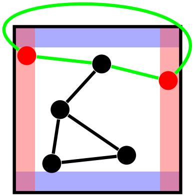


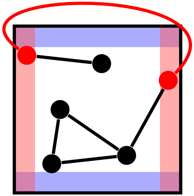
Results - Percolation (Experiment 2)

Claim: GNN can solve percolation problem $\implies$ GNN can solve connection problem

Procedure:

1. Start with arbitrary Graph G, select two nodes n, m
2. Place G inside unit square, move n, m to edges, add edge (n, m) $\implies$ new graph $\tilde{G}$
3. Run GNN on $\tilde{G}$ $\implies$ either $\tilde{G}$ is percolating (i.e. there is a cycle containing n, m and the new edge) or not





Results - Percolation (Experiment 2)

Claim: GNN can solve percolation problem $\implies$ GNN can solve connection problem

Procedure:

1. Start with arbitrary Graph G, select two nodes n, m
2. Place G inside unit square, move n, m to edges, add edge (n, m) $\implies$ new graph $\tilde{G}$
3. Run GNN on $\tilde{G}$
4. $\tilde{G}$ percolating $\iff$ n, m connected in G