Learning with Graphs

Roger Wattenhofer
Machine Learning Deals with ...
High-res 3D simulations

up to 19k particles

2 different simulators (MPM & SPH)
Refik Anadol, Unsupervised, MOMA
Graph Classification

Node Classification
Graph Neural Networks
Graph Neural Networks
Graph Neural Networks

\[ a_v = \text{AGGREGATE} \left( \{ \{ h_u \} \mid u \in N(v) \} \right) \quad (\text{Min, Max, Mean, Sum}) \]
Graph Neural Networks

\[ a_v = \text{AGGREGATE} \left( \{ h_u \mid u \in N(v) \} \right) \quad \text{(Min, Max, Mean, Sum)} \]

\[ h_v^{(t+1)} = \text{UPDATE} \left( h_v, a_v \right) \]
Graph Neural Networks

\[ a_v = \text{AGGREGATE} \left( \left\{ h_u \mid u \in N(v) \right\} \right) \]  

\[ h_v^{(t+1)} = \text{UPDATE} \left( h_v, a_v \right) \]  

(Min, Max, Mean, Sum)  

(Little Neural Network)
Graph Neural Networks
GNN Limitations?
Limits of GNNs
Limits of GNNs
More Expressive GNNs?
DropGNN: Random Dropouts Increase the Expressiveness of Graph Neural Networks
GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability $p$ independently
GNNs with Dropouts

Multiple runs of the GNN
Each node removed with probability $p$ independently

Run #1
GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability $p$ independently

Run #1
GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability $p$ independently

Run #2
GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability $p$ independently

Run #2
GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability $p$ independently

Run #3
GNNs with Dropouts
Port Numbers
Angle Features
Random Features
Easier Learning                    More Expressivity

Base GNN                          DropGNN                      Ports                          Rand IDs
Efficiently
Learn
Compute
Extrapolation
Without Aggregation?
GwAC: GNNs with Asynchronous Communication

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I am an H

An H? Not interesting to me

I am an H

OH! I have an H neighbor

Then this is an alcohol
AGENT-BASED GRAPH NEURAL NETWORKS

Karolis Martinkus¹, Pál András Papp², Benedikt Schesch¹, Roger Wattenhofer¹
¹ETH Zurich ²Computing Systems Lab, Huawei Zurich Research Center

I've been there 3 steps ago!
Agent-based Graph Neural Networks

Karolis Martinkus\textsuperscript{1}, Pál András Papp\textsuperscript{2}, Benedikt Schesch\textsuperscript{1}, Roger Wattenhofer\textsuperscript{1}

The Graph has triangles!

I see a triangle!

I didn't see a triangle.

Me neither.

1. Node Update
2. Neighborhood Aggregation
3. Agent Update
4. Agent Transition

I've been there 3 steps ago!

I keep seeing these nodes!
<table>
<thead>
<tr>
<th>Model</th>
<th>4-CYCLES [59]</th>
<th>CIRCULAR SKIP LINKS [15]</th>
<th>2-WL</th>
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<td>GIN [75]</td>
<td>50.0 ±0.0</td>
<td>10.0 ±0.0</td>
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<td>GIN with random features [64; 1]</td>
<td>99.7 ±0.4</td>
<td>95.8 ±2.1</td>
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<td>SMP [71]</td>
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<td><strong>RANDOM WALK AGENTNET</strong></td>
<td><strong>100.0 ±0.0</strong></td>
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SPECTRE: Spectral Conditioning Helps to Overcome the Expressivity Limits of One-shot Graph Generators

Karolis Martinkus\textsuperscript{1} Andreas Loukas\textsuperscript{2,3} Nathanaël Perraudin\textsuperscript{3} Roger Wattenhofer\textsuperscript{1}
def outer_loop():
    for i in range(N):
        inner_loop()

def inner_loop():
    for j in range(i):
        float00 = random(0, 1)
        bool00 = float00 < 0.4
        if bool00:
            add_edge(i, j)

outer_loop()
Automating Rigid Origami Design
Jeremia Geiger, Karolis Martinkus, Oliver Richter, Roger Wattenhofer
Graph Explanation
GraphChef: Learning the Recipe of Your Dataset
The Bigger Picture
User: what is 5 times 7?

Assistant: 5 times 7 equals 35.

User: what is 384903720 times 538982734?

Assistant: 384,903,720 times 538,982,734 equals 207,559,081,508,668,480.
what is 384903720 times 538982734?

384,903,720 times 538,982,734 equals 207,559,081,508,668,480.
Thinking Slow Benchmark?
FACT: Learning Governing Abstractions Behind Integer Sequences

Peter Belcák, Ard Kastrati, Flavio Schenker, Roger Wattenhofer
Simon Tatham's Portable Puzzle Collection
Loopy (Takegaki, Slitherlink, Ouroboros, Suriza, ...
RLP: A Reinforcement Learning Benchmark for Neural Algorithmic Reasoning
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<th>Puzzle</th>
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<tr>
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<td>3x3b1</td>
<td>4742.1 ± 2960.1</td>
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<td>Same Game</td>
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<td>11.5 ± 0.1</td>
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<td></td>
<td>5x5c3s2</td>
<td>1009.3 ± 1089.4</td>
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<td>2294.7 ± 2121.2</td>
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100% 2k fail
Sudoku
Sudoku
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Kakuro GNN Step: 0
Tents
Atari Games

Puzzle Games

Intuition

Involuntary control

Speed

Reason

Patience

Concentration

Constructed thoughts

Effort

Effortlessness

Analytics

Innate skills

Reflex
Deep Neural Networks

BRAIN SYSTEMS

1. Effortlessness
   - Reflex
   - Innate skills
   - Speed

2. Constructed thoughts
   - Reason
   - Analytics
   - Effort
   - Concentration
   - Patience
   - Intuition
   - Involuntary control

Signal layer
Hidden layer 1
Hidden layer 2
Hidden layer 3
Output layer

THOMAS H. CORMEN
CHARLES E. LEISERSON
RONALD L. RIVEST
CLIFFORD STEIN

INTRODUCTION TO ALGORITHMS
FOURTH EDITION
Over 1 MILLION copies sold worldwide
Summary
Thank You!

Any questions or comments?

Thanks to co-authors: Peter Belcak, Benjamin Estermann, Lukas Faber, Florian Grötschla, Luca Lanzendörfer, Karolis Martinkus, Joël Mathys, Pal Andras Papp, etc.

Roger Wattenhofer