

Lista de papers 2024-2

Poder expresivo de GNNs: comparación con WL, lógica, otros

1. Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks.
Christopher Morris, Martin Ritzert, Matthias Fey, William L. Hamilton, Jan Eric Lenssen, Gaurav Rattan, Martin Grohe.
2. Weisfeiler and Leman Go Relational.
Pablo Barceló, Mikhail Galkin, Christopher Morris, Miguel Romero.
3. Expressiveness and Approximation Properties of Graph Neural Networks.
Floris Geerts, Juan L. Reutter.
4. The Logical Expressiveness of Graph Neural Networks.
Pablo Barceló, Egor V. Kostylev, Mikael Monet, Jorge Pérez, Juan L. Reutter, Juan Pablo Silva.
5. On dimensionality of feature vectors in MPNNs.
César Bravo, Alexander Kozachinskiy, Cristóbal Rojas.
6. Let's Agree to Degree: Comparing Graph Convolutional Networks in the Message-Passing Framework.
Floris Geerts, Filip Mazowiecki, Guillermo A. Pérez.
7. Weisfeiler and Leman go sparse: Towards scalable higher-order graph embeddings.
Christopher Morris, Gaurav Rattan, Petra Mutzel.
8. Fine-grained Expressivity of Graph Neural Networks.
Jan Böker, Ron Levie, Ningyuan Huang, Soledad Villar, Christopher Morris.
9. Are Targeted Messages More Effective?.
Martin Grohe, Eran Rosenbluth.

Otras propiedades sobre GNNs

1. Three iterations of $(d - 1)$ -WL test distinguish non isometric clouds of d -dimensional points.
Valentino Delle Rose, Alexander Kozachinskiy, Cristóbal Rojas, Mircea Petrache, Pablo Barceló.
2. Some Might Say All You Need Is Sum.
Rosenbluth, Eran, Jan Toenshoff, and Martin Grohe.
3. The Descriptive Complexity of Graph Neural Networks.
Martin Grohe.

4. WL meet VC.
Christopher Morris, Floris Geerts, Jan Tönshoff, Martin Grohe.
5. Generalization and Representational Limits of Graph Neural Networks.
Vikas K. Garg, Stefanie Jegelka, and Tommi S. Jaakkola.
6. Weisfeiler-Leman at the margin: When more expressivity matters.
Billy J. Franks, Christopher Morris, Ameya Velingker, Floris Geerts.
7. On the Power of the Weisfeiler-Leman Test for Graph Motif Parameters.
Matthias Lanzinger, Pablo Barceló.
8. Almost Surely Asymptotically Constant Graph Neural Networks.
Sam Adam-Day, Michael Benedikt, Ismail Ilkan Ceylan, Ben Finkelshtein.
9. Homomorphism Counts for Graph Neural Networks: All About That Basis.
Emily Jin, Michael Bronstein, Ismail Ilkan Ceylan, Matthias Lanzinger.
10. Decidability of Graph Neural Networks via Logical Characterizations.
Michael Benedikt, Chia-Hsuan Lu, Boris Motik, Tony Tan.
11. How does over-squashing affect the power of GNNs?
Francesco Di Giovanni, T. Konstantin Rusch, Michael M. Bronstein, Andreea Deac, Marc Lackenby, Siddhartha Mishra, Petar Velickovic.
12. Zero-One Laws of Graph Neural Networks.
Sam Adam-Day, Theodor Mihai Iliant, Ismail Ilkan Ceylan.

Variantes y extensiones de GNNs

1. The Surprising Power of Graph Neural Networks with Random Node Initialization.
Ralph Abboud, Ismail Ilkan Ceylan, Martin Grohe, Thomas Lukasiewicz.
2. Probabilistically Rewired Message-Passing Neural Networks.
Chendi Qian, Andrei Manolache, Kareem Ahmed, Zhe Zeng, Guy Van den Broeck, Mathias Niepert, Christopher Morris.
3. Graph Neural Networks with Local Graph Parameters.
Pablo Barceló, Floris Geerts, Juan L. Reutter, Maksimilian Ryschkov.
4. Ordered Subgraph Aggregation Networks.
Chendi Qian, Gaurav Rattan, Floris Geerts, Mathias Niepert, Christopher Morris.
5. Neural Bellman-Ford Networks: A General Graph Neural Network Framework for Link Prediction.
Zhaocheng Zhu, Zuobai Zhang, Louis-Pascal Xhonneux, Jian Tang.
6. A*Net: A Scalable Path-based Reasoning Approach for Knowledge Graphs.
Zhaocheng Zhu, Xinyu Yuan, Mikhail Galkin, Sophie Xhonneux, Ming Zhang, Maxime Gazeau, Jian Tang.
7. A Theory of Link Prediction via Relational Weisfeiler-Leman on Knowledge Graphs.
Xingyue Huang, Miguel Romero, Ismail Ilkan Ceylan, Pablo Barceló.

8. Link Prediction with Relational Hypergraphs.
Xingyue Huang, Miguel Romero, Pablo Barceló, Michael M. Bronstein, Ismail Ilkan Ceylan.
9. GraphAny: A Foundation Model for Node Classification on Any Graph.
Jianan Zhao, Hesham Mostafa, Mikhail Galkin, Michael Bronstein, Zhaocheng Zhu, Jian Tang.
10. Towards Foundation Models for Knowledge Graph Reasoning.
Mikhail Galkin, Xinyu Yuan, Hesham Mostafa, Jian Tang, Zhaocheng Zhu.
11. Walking Out of the Weisfeiler Leman Hierarchy: Graph Learning Beyond Message Passing.
Jan Tönshoff, Martin Ritzert, Hinrikus Wolf, Martin Grohe.
12. Cooperative Graph Neural Networks.
Ben Finkelshtein, Xingyue Huang, Michael Bronstein, Ismail Ilkan Ceylan.

Graph Transformers

1. Attending to Graph Transformers.
Luis Müller, Mikhail Galkin, Christopher Morris, Ladislav Rampásek.
2. Towards Principled Graph Transformers.
Luis Müller, Daniel Kusuma, Blai Bonet, Christopher Morris.
3. Recipe for a General, Powerful, Scalable Graph Transformer.
Ladislav Rampásek, Michael Galkin, Vijay Prakash Dwivedi, Anh Tuan Luu, Guy Wolf, Dominique Beaini. https://proceedings.neurips.cc/paper_files/paper/2022/hash/5d4834a159f1547b267a05a4e2b7cf5e-.html
4. Expormer: Sparse Transformers for Graphs.
Hamed Shirzad, Ameeya Velingker, Balaji Venkatachalam, Danica J. Sutherland, Ali Kemal Sinop-
5. Distinguished In Uniform: Self Attention Vs. Virtual Nodes.
Eran Rosenbluth, Jan Tönshoff, Martin Ritzert, Berke Kisin, Martin Grohe.
6. Aligning Transformers with Weisfeiler-Leman.
Luis Müller, Christopher Morris.

GNNs y Graph Query Answering

1. Message passing query embedding.
Daza, Daniel, and Michael Cochez.
2. Neural-Symbolic Models for Logical Queries on Knowledge Graphs.
Zhaocheng Zhu, Mikhail Galkin, Zuobai Zhang, Jian Tang.
3. A Neuro-Symbolic Framework for Answering Graph Pattern Queries in Knowledge Graphs.
Tamara Cucumides, Daniel Daza, Pablo Barceló, Michael Cochez, Floris Geerts, Juan L Reutter, Miguel Romero.
4. Zero-shot Logical Query Reasoning on any Knowledge Graph.
Mikhail Galkin, Jincheng Zhou, Bruno Ribeiro, Jian Tang, Zhaocheng Zhu.

GNNs y problemas de Optimización

1. Combinatorial optimization and reasoning with graph neural networks.
Quentin Cappart, Didier Chételat, Elias Khalil, Andrea Lodi, Christopher Morris, Petar Velickovic.
2. MIP-GNN: A Data-Driven Framework for Guiding Combinatorial Solvers.
Elias B. Khalil, Christopher Morris, Andrea Lodi.
3. Exploring the Power of Graph Neural Networks in Solving Linear Optimization Problems.
Chendi Qian, Didier Chételat, Christopher Morris.
4. One Model, Any CSP: Graph Neural Networks as Fast Global Search Heuristics for Constraint Satisfaction.
Jan Tönshoff, Berke Kisin, Jakob Lindner, Martin Grohe.

GNNs y aplicaciones

1. Solving AC Power Flow with Graph Neural Networks under Realistic Constraints.
Luis Böttcher, Hinrikus Wolf, Bastian Jung, Philipp Lutat, Marc Trageser, Oliver Pohl, Andreas Ulbig, Martin Grohe.
2. Physical Pooling Functions in Graph Neural Networks for Molecular Property Prediction.
Artur M. Schweidtmann, Jan G. Rittig, Jana M. Weber, Martin Grohe, Manuel Dahmen, Kai Leonhard, Alexander Mitsos.
3. RelBench: A Benchmark for Deep Learning on Relational Databases.
Joshua Robinson, Rishabh Ranjan, Weihua Hu, Kexin Huang, Jiaqi Han, Alejandro Dobles, Matthias Fey, Jan E. Lenssen, Yiwen Yuan, Zecheng Zhang, Xinwei He, Jure Leskovec.
4. Learning production functions for supply chains with graph neural networks.
Serina Chang, Zhiyin Lin, Benjamin Yan, Swapnil Bembde, Qi Xiu, Chi Heem Wong, Yu Qin, Frank Kloster, Alex Luo, Raj Palleti, Jure Leskovec.
5. VQA-GNN: Reasoning with Multimodal Knowledge via Graph Neural Networks for Visual Question Answering.
Yanan Wang, Michihiro Yasunaga, Hongyu Ren, Shinya Wada, Jure Leskovec.
6. QA-GNN: Reasoning with language models and knowledge graphs for question answering.
Michihiro Yasunaga, Hongyu Ren, Antoine Bosselut, Percy Liang, Jure Leskovec.