Alessio **Gravina**

PhD Student in Computer Science

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Education

PhD in Computer Science, UNIVERSITY OF PISA, ITALY Nov. 2020 - PRESENT • Thesis title: Information propagation dynamics in Deep Graph Networks Main Theme: Representation learning for graphs inspired by dynamical systems and neural differential equations. • Supervisors: Prof. Davide Bacciu and Prof. Claudio Gallicchio. **Oxford Machine Learning Summer School**, VIRTUAL Aug. 2021 • 15-days specialized AI school that covers the topics of Rep. Learning & Statistical ML, ML in Healthcare, NLP, and AI for Good. • Acceptance rate 15%. MSc in Computer Science, University of Pisa, Italy • Curriculum: Artificial Intelligence. • Thesis: Machine Learning prediction of compounds impact on Schizophrenia treatment (110/110 Hons., equiv. GPA: 4/4). ERASMUS+ Student Programme, University College Dublin, Ireland Jan. 2019 - May 2019 • Student at the Computer Science Department in the framework of the EU Erasmus+ programme. • Main Theme: Artificial Intelligence and Cognitive Science. BSc in Computer Science, University of Pisa, Italy Sep. 2014 - Mar. 2018 • Thesis: Machine Learning for the prediction of Bronchopulmonary dysplasia risk (103/110, equiv. GPA: 3.75/4). Experience ____ Research scholarship, UNIVERSITY OF PISA, ITALY Nov. 2023 - PRESENT • Main Theme: Representation learning for dynamic graphs • Reference: decree of the Director n. 615/2023, 25/10/2023 Machine Learning Research Intern, Huawei Research Center, Munich, Germany Mar. 2023 - Aug. 2023 • Supervisors: Claas Grohnfeldt, Giulio Lovisotto and Michele Russo. · Joined the AI4Sec team to work on dynamical systems-based neural architectures for long-range propagation within Continuous-Time Dynamic Graphs, achieving state-of-the-art performance on various synthetic and real-world benchmarks. Visiting Phd Student, IDSIA USI-SUPSI, SWITZERLAND Apr. 2022 - Jul. 2022 • Supervisors: Prof. Cesare Alippi and Daniele Zambon • Designed a general modeling framework (by means of dynamical systems) for temporal graphs that can effectively operate with irregularly and sparsely sampled observations, achieving state-of-the-art performance on various synthetic and real-world benchmarks. Teaching Assistant, University of Pisa, Italy Feb. 2021 - May 2021 Course: Introduction to Programming and Algorithms • Reference: protocol n. 249/2021, protocol date: 11/02/2021 Weekly office hours for homework assistance and reinforcement of learned concepts. Research scholarship, UNIVERSITY OF PISA, ITALY Jul. 2020 - Nov. 2020 Main Theme: Deep learning per biomedical data • Reference: decree of the Director n. 797/2020, 20/05/2020 • Released a resource that collects all the clinical evidence on COVID-19 and the human genomic and proteomic information to foster COVID-19 research.

• Developed Deep Learning for graphs method in *Python* to repurpose drugs given sets of proteins. The model has been used to propose a list of 27 COVID-19 candidate drugs.

Machine Learning Engineer, Vydiant

• Developed an NLP model in Python to identify sentences containing relations between entities from a biomedical corpus, improving precision by 3%.

Visiting Student Researcher, Stanford University, USA

- Developed a Graph Deep Learning model in Python to automatize drug repurposing screenings in the field of Schizophrenia treatment, discovering 64 new candidate drugs.
- Research in collaboration with SPARK research group.

Jan. 2020 - Jun. 2020

Sep. 2019 - Dec. 2019

Sep. 2018 - Mar. 2020

Publications

- A. Gravina, D. Zambon, D. Bacciu, C. Alippi. Temporal Graph ODEs for Irregularly-Sampled Time Series. In IJCAI 2024.
- A. Gravina*, G. Lovisotto*, C. Gallicchio, D. Bacciu, C. Grohnfeldt. Long Range Propagation on Continuous-Time Dynamic Graphs. In ICML 2024. (* Equal Contrib.)

Also accepted in Temporal Graph Learning Workshop, NeurIPS 2023 under the title Effective Non-Dissipative Propagation for Continuous-Time Dynamic Graphs.

- A. Gravina and D. Bacciu. Deep learning for dynamic graphs: models and benchmarks. In IEEE TNNLS 2024.
- J. Reha, G. Lovisotto, M. Russo, A. Gravina, and C. Grohnfeldt. Continuous-Time Temporal Graph Learning on Provenance Graphs. In Temporal Graph Learning Workshop, NeurIPS 2023.
- A. Gravina, C. Gallicchio, and D. Bacciu. Non-Dissipative Propagation by Randomized Anti-Symmetric Deep Graph Networks. In Deep Learning meets Neuromorphic Hardware Workshop, ECML-PKDD 2023.
- F. Errica*, A. Gravina*, D. Bacciu., A. Micheli. Hidden Markov Models for Temporal Graph Representation Learning. In ESANN, 2023. (* Equal Contrib.)
- A. Gravina, D. Bacciu, and C. Gallicchio. Anti-Symmetric DGN: a stable architecture for Deep Graph Networks. In ICLR 2023. Also accepted in DGL-AAAI'23 workshop, AAAI 2023 under the title Non-Dissipative Propagation by Anti-Symmetric Deep Graph Networks and awarded with the Best Student Paper Award.
- D. Bacciu, F. Errica, A. Gravina*, L. Madeddu, M. Podda, and G. Stilo. Deep Graph Networks for Drug Repurposing with Multi-Protein Targets. In IEEE Transactions on Emerging Topics in Computing 2023. (* First Author - Alphabetical Order)
- A. Gravina, J.L. Wilson, D. Bacciu, K.J. Grimes, and C. Priami. Controlling astrocyte-mediated synaptic pruning signals for schizophrenia drug repurposing with Deep Graph Networks. In PLOS Computational Biology, 2022.
- A. Gravina*, F. Rossetto*, S. Severini*, and G. Attardi. A comparative study of models for answer sentence selection. In CLiC-it, 2019. (* Equal Contrib.)
- A. Gravina*, F. Rossetto*, S. Severini*, and G. Attardi. Cross attention for selection-based question answering. In NL4AI@AI*IA, 2018. (* Equal Contrib.)

Projects

Continuous-Time Graph Anti-Symmetric Network

- URL: https://github.com/gravins/non-dissipative-propagation-CTDGs
- Used Python and Pytorch to develop a deep graph network inspired on non-dissipative dynamical systems to achieve long-range information propagation between nodes within dynamic graphs.
- The model outperforms state-of-the-art deep graph networks on synthetic long-range tasks but as well as several real-world benchmark datasets.

Temporal Graph Ordinary Differential Equation

- URL: https://github.com/gravins/TG-ODE
- Used Python and Pytorch to develop a deep graph network inspired on dynamical systems for learning complex spatio-temporal patterns of dynamic graphs under the real-world assumption of irregularly and severely under-sampled data, thus overcoming the common assumption of dealing with regularly sampled temporal graph snapshots.
- The model outperforms modern deep graph networks on synthetic and real-world benchmarks.

Anti-SymmetricDGN

- URL: https://github.com/gravins/Anti-SymmetricDGN
- Used Python and Pytorch to develop a deep graph network inspired on non-dissipative dynamical systems to achieve long-range information propagation between nodes within static graphs.
- The model outperforms classical deep graph networks over several datasets even when dozens of layers are used.

NumGraph, GROUP PROJECT

- URL: https://github.com/gravins/NumGraph
- Num(py)Graph is a library for synthetic graph generation. The main principle of NumGraph is to be a lightweight library (i.e., Numpy is the only dependency) that generates graphs from a broad range of distributions in both the static and temporal domain.

Deep Graph Networks for Drug Repurposing with Multi-Protein Targets

- URL: https://github.com/gravins/covid19-drug-repurposing-with-DGNs
- Developed Deep Learning for graphs method in <u>Python</u> and <u>Pytorch</u> to repurpose drugs given sets of proteins instead of singleprotein/single-drug associations (as widespread in literature), increasing the AUROC by 9% with respect to the single-protein repurposing scenario.
- The model was used to discover 27 new potential COVID-19 candidate drugs.

2024

2024

2021

2021

2023

Graph learning for Schizophrenia treatment

- URL: https://github.com/gravins/DGNs-for-schizophrenia
- Used <u>Python</u> and <u>Pytorch</u> to develop a ML for graph framework to predict compounds that can reduce glial phagocytic activity in Schizophrenia patients.
- The framework was used by SPARK research group at Stanford to optimize drug phenotypic screens, discovering 64 new potential drug candidates.

Cross-Attentive CNN for QA, GROUP PROJECT

- 1st Place, Fujitsu AI-NLP Challenge, Prize \$20,000
- Implemented a Cross-Attentive Convolutional Neural Network (using *Python* and *Keras*) to tackle the task of Answer Sentence Selection. The model was assessed over SelQA and WikiQA datasets with different types of word embeddings: FastText, GloVe, and ELMo.

Awards_____

2023	Research Scholarhip , Research scholarhip funded by University of Pisa from November 2023 for 1 year	University of Pisa
2023	Best Student Paper Award, Non-Dissipative Propagation by Anti-Symmetric Deep Graph Net- works	DGL-AAAI'23 workshop, AAAI
2020	PhD Scholarhip , Full Scholarship for the Ph.D. programme in Computer Science, funded by Regione Toscana from November 2020 to November 2023	University of Pisa
2020	Research Scholarhip , Research scholarhip funded by University of Pisa from July 2020 for 5 months	University of Pisa
2018	1st Place, Fujitsu AI-NLP Challenge, <i>Prize \$20,000</i>	Contest
Intellige Presentati 9th Inte Applica Presenta	ropean Symposium on Artificial Neural Networks, Computational ence and Machine Learning (ESANN), BRUGES, BELGIUM ion of the paper "Hidden Markov Models for Temporal Graph Representation Learning" ernational Workshop on Deep Learning on Graphs: Method and tions (DLG-AAAI'23), WASHINGTON D.C., USA tion of the paper "Non-Dissipative Propagation by Anti-Symmetric Deep Graph Networks"	Oct 2023 Feb 2023
Revie	ewing activity	
2024 2024 2024 2023-202 2023-202	Neural Networks, ISSN: 0893-6080 International Joint Conference on Neural Networks (IJCNN), International Conference on Artificial Neural Networks (ICANN), 44 IEEE Transactions on Neural Networks and Learning Systems (TNNLS), ISSN: 2162-237X European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning (ESANN),	Journal Conference Conference Journal Conference

Skills_

ProgrammingPython, Java, C, C++Frameworks/LibrariesPytorch, Sklearn, Numpy, Pandas, KerasLanguagesItalian (Native), English (Fluent), Spanish (Elementary)

I hereby authorize the processing of my personal data in accordance with the current data protection regulations, specifically the European General Data Protection Regulation (GDPR) 2016/679, the Italian Legislative Decree No. 196 of 30 June 2003, and any subsequent amendments and additions.

2018