ALEXANDRE DUVAL

PhD Student – Graph Representation Learning – CentraleSupélec & Inria & Mila
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EDUCATION

CentraleSupélec Paris Saclay
PhD – Graph ML – with Fragkiskos Malliaros 2021 - 2024
- Design expressive, explainable and scalable Graph Neural Networks spanning a broad range of applications.

MSc in Artificial Intelligence - Highest honours 2019 - 2020
- Modules: Deep Learning, NLP, RL, CV, Network Analytics, Big Data, Optimization, etc.

University of Warwick Coventry, UK
BsC and MASt in Mathematical Sciences - Highest honours 2015 - 2019
- Modules: ML, Graph Theory, Bayesian Stats, Stochastic Analysis, Functional Analysis, Algebra etc.
- Research Project on Explainable AI with the *Alan Turing Institute* - survey of most promising methods: mathematical definitions, improvements and application on a customer churn use case, survival analysis.

EXPERIENCE

Visiting researcher Montreal
Mila – Quebec AI Institute – with David Rolnick and Yoshua Bengio Feb. 2022 - 2023
- Designed scalable and expressive symmetry-preserving GNNs to predict the relaxed adsorption energy of a catalyst-adsorbate system. Combine it with a generative method (e.g. GFlowNet) for catalyst discovery.

Teaching Assistant Paris Saclay
CentraleSupelec - master students - Course: "Machine Learning for Network Science" From 2021
- Teach this module covering basic graph theory, GNNs, community detection and information propagation.

Research intern Paris Saclay
Inria - Opis team June - Dec. 2020
- Proposed a unified view of existing GNN explainability methods along with a new explainer.

Research intern Grenoble
Naver Labs, with Matthias Gallé March - June. 2020
- Worked on controlled and contextualised text generation for novel authors. Open-source writing assistant.

SCIENTIFIC PUBLICATIONS

- Duval, A., Lamson, T., de Kérouara, G. D. L., Gallé, M. (2020). *Breaking Writer's Block: Low-cost Fine-tuning of Natural Language Generation Models*. In Proceedings of the 15th Conference of the European Chapter of the Association for Computational Linguistics (EACL 2021).
- Duval, A., Malliaros, F. D. (2021). *Graphsvx: Shapley value explanations for graph neural networks*. In Machine Learning and Knowledge Discovery in Databases. Research Track: European Conference, ECML PKDD 2021, Bilbao, Spain, September 13–17, 2021, Proceedings, Part II 21 (pp. 302-318). Springer International Publishing.
- Duval, A., Malliaros, F. (2022, October). *Higher-order clustering and pooling for graph neural networks*. In Proceedings of the 31st ACM International Conference on Information Knowledge Management (pp. 426-435).
- Duval, A., Schmidt, V., Miret, S., Bengio, Y., Hernández-García, A., Rolnick, D. (2022). *PhAST: Physics-Aware, Scalable, and Task-specific GNNs for Accelerated Catalyst Design*. NeurIPS AI4Mat workshop. Under review at JMLR.
- Duval, A., Schmidt, V., Miret, S., Bengio, Y., Hernández-García, A., Rolnick, D. (2023). *FAENet: Frame Averaging Equivariant GNNs for Materials Modeling*. Under review at ICML.

TALKS

- Keynote speaker at CIKM 2022 in the AIMLAI workshop: *"Explainability for Graph Neural Networks"*.
- Seminar Talk for the CRUNCH group of Brown University: *"Accelerated catalysis discovery"*.

ACADEMIC SERVICE

- Co-organizer of the Learning-on-Graphs (LoG) conference 2023.
- Organizer of local graph meetups in Paris.
- Reviewer for ICML 2021, the Web Conference 2021, LoG 2022 and NeurIPS 2022.
- Contributor of Pytorch Geometric.

AWARDS

- *Mitacs Globalink Scholarship* in 2022 for my work on catalysis discovery.
- *SIGIR Student Travel Grant* to participate in CIKM 2022, Atlanta (US).

SKILLS AND INTERESTS

Tools: Python, R, Java, Matlab, LaTeX, git, AWS, Spark, DL libraries (Pytorch, PyG, DGL, networkx).
AI for Tomorrow: write articles about AI, discuss challenges and promote beneficial usage.
Languages: French (Native), English (Fluent), Spanish and Chinese (Conversational ability)
Personality traits: efficient, passionate, team worker, persistent, cheerful, leadership, autonomous, organized.
Interests: football, sustainable development, cinema, new technologies, art.