ALEXANDRE DUVAL

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

CentraleSupélec Paris Saclay
PhD – Graph ML – with Fragkiskos Malliaros 2021 - 2023
- 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 From Feb. 2022
- Designed scalable and expressive symmetry-preserving GNNs to predict the relaxed adsorption energy of a catalyst-adsorbate system. Used it within our flow-based generative method for catalyst discovery.

Teaching Assistant Paris Saclay
CentraleSupelec - master students - Course: "Machine Learning for Network Science" 2021-2023
- Taught 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: GraphSVX.

Student researcher 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

- Mistal[1], Yoshua Bengio (2023). *Crystal-GFlowNet: sampling materials with desirable properties and constraints.* Under submission at NeurIPS AI4MAt workshop.
- Alvaro Carbonero, Alexandre Duval, Victor Schmidt, Santiago Miret, Alex Hernandez-Garcia, Yoshua Bengio, David Rolnick (2023). *On the importance of relative 3D information in the prediction of catalyst-adsorbate relaxed energy with Disconnected GNN*. Under submission at NeurIPS AI4MAt workshop.
- Duval, A., Schmidt, V., Miret, S., Bengio, Y., Hernández-García, A., Rolnick, D. (2023). *FAENet: Frame Averaging Equivariant GNNs for Materials Modeling*. Accepted at ICML 2023.
- 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*. Accepted at JMLR.
- 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 and Knowledge Management (pp. 426-435).

[1]team name denoting the equal contribution of all authors

- 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., 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).

ONGOING WORK

- Uncertainty Prediction method for Graph Neural Networks (GNN).
- Generative AI for crystals and electro-catalysts, using GFlowNet.
- Active Learning for the Open Catalyst Project.
- A hitchhiker's guide to Geometric GNNs for 3D atomic systems.
- FAENet++: an improved GNN model for materials and molecules property prediction.

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"*.
- Paper presentation at Institut Polytechnique de Paris: *"FAENet"*.

ACADEMIC SERVICE

- Co-organizer of the International Learning-on-Graphs (LoG) Conference 2023.
- Organizer of local graph meetups in Paris ($\sim$ 100 attendees).
- Reviewer for ICML, the Web Conference, LoG and NeurIPS.
- Contributor of Pytorch Geometric.
- Lab representative.
- Supervisor of 1 MSc. intern at Mila.
- Research Project Advisor for 2 groups of final-year students at CentraleSupelec and MVA.

AWARDS

- *Mitacs Globalink Scholarship* in 2022 for my work on catalysis discovery.
- *SIGIR Student Travel Grant* to participate in CIKM 2022, Atlanta (US).
- *Runner-up* award in the 3 Minutes Thesis competition with Université Paris-Saclay.

SKILLS AND INTERESTS

Programming: Python, MATLAB, bash, Java, AWS, DL libraries (Pytorch, Tensorflow, PyG, networkx).
Tools: LaTeX, Git, ssh, Markdown, Liquid, Jekyll, HTML5, CSS, Draw.io, etc.
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: passionate, team worker, persistent, cheerful, leadership, efficient, autonomous, organized.
Interests: football, sustainable development, surf, cinema, new technologies, paintings.