DR. ALEXANDRE DUVAL

Co-Founder and Chief Science Officer of Entalpic

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EDUCATION

CentraleSupélec Paris Saclay

PhD in Graph Machine Learning - with Fragkiskos Malliaros and Hugues Talbot

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

Co-Founder & CS(cience)O

Paris, France

Entalpic

May 2024 - Present

- AI-guided materials discovery to promote a fair ecological transition

Applied Scientist

Cambridge, UK

Amazon - AGI Foundation Team

Dec. 2023 – May 2024

- Enriched LLMs with API tools

Visiting researcher

Montreal

Mila - Quebec AI Institute - with David Rolnick and Yoshua Bengio

Feb. 2022 - Nov 2023

- Built several Geometric GNNs for property prediction of 3D atomic systems.
- Designed flow-based generative methods for materials 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

- Ramlaoui, A., Saulus, T., Terver, B., Schmidt, V., Rolnick, D., Malliaros, F. D., Duval, A. (2024). Improving Molecular Modeling with Geometric GNNs: an Empirical Study. Accepted at ICML ML4LMS workshop.
- Mila AI4Science¹, Bengio Y. (2023). Crystal-GFlowNet: sampling materials with desirable properties and constraints. Accepted at NeurIPS AI4Mat workshop.

¹team name denoting the equal contribution of all authors

- Duval A., Mathis S., Joshi C., Schmidt V., Miret S., Malliaros F., Cohen T., Lio P., Bengio Y., Bronstein M. (2023) A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems.
- Carbonero A., Duval A., Schmidt V., Miret S., Hernández-García, A., Bengio Y., Rolnick, D. (2023). On the importance of catalyst-adsorbate 3D interactions for relaxed energy prediction.. Accepted 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). Higher-order clustering and pooling for graph neural networks. Accepted at CIKM.
- Duval, A., Malliaros, F. D. (2021). Graphsvx: Shapley value explanations for graph neural networks. Accepted at ECML PKDD.
- 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. Accepted at EACL.

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.

TALKS

- Talk and panel session at ICML 2024 in Vienna: "AI for materials discovery"
- Paper presentation at the Molecular ML Conference (MoML) in Montreal, Canada.
- Paper presentation at Institut Polytechnique de Paris.
- Seminar Talk for the CRUNCH group of Brown University: "Accelerated catalysis discovery".
- Keynote speaker at CIKM 2022 in the AIMLAI workshop: "Explainability for Graph Neural Networks".

ACADEMIC SERVICE

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

AWARDS

- Reviewer award in Learning-on-Graphs international conference 2023.
- Runner-up award in the 3 Minutes Thesis competition 2023 with Université Paris-Saclay.
- 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

Programming: Python, bash, AWS, DL libraries (Pytorch, PyG, PymatGen, networkx, transformers).

Tools: LaTeX, Git, ssh, Markdown, Liquid, Jekyll, HTML5, CSS, Draw.io, Wandb, 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.