Aleksandra Kalisz

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Education

THE UNIVERSITY OF OXFORD | PhD Programme
Sustainable Approaches to Biomedical Sciences, Centre for Doctoral Training
October 2022 - Present | Oxford, UK
➔ Researching **Modern Machine Learning Technologies for Drug Discovery** under supervision of Jakob Foerster and Francesca Vianello from Exscientia.

THE UNIVERSITY OF EDINBURGH | Bachelor of Science with Honours
Artificial Intelligence and Computer Science
September 2015 - July 2019 | Edinburgh, UK
➔ First Class Degree with an **85% grade average**.
➔ Dissertation topic: '**Encoding Cooperation in Multi-Agent Reinforcement Learning**' under prof. Stefano Albrecht's supervision.

CALIFORNIA INSTITUTE OF TECHNOLOGY | Undergraduate Exchange Programme
Computer Science Major
September 2017 - June 2018 | Pasadena, California, USA
➔ Cumulative **GPA of 4.1/4.0**.
➔ Exchange year focused on Machine Learning and Theoretical Computer Science.
➔ Worked on research projects involving **Reinforcement Learning and Imitation Learning** like path planning for NASA Mars rovers, NIPS Learning to Run competition or Two Sigma Halite AI challange.

Work Experience

EXSCIENTIA | Senior AI Research Scientist
January 2020 – April 2024 | Oxford, UK
➔ Currently collaborating with Exscientia on my PhD project.
➔ Lead an **AI Technology: Generative Molecule Design** group. Recruited the team with support from the larger AI Technology group. Developed a roadmap for the team, proposed research projects to focus on. Provided research supervision for the team members.
➔ Co-developed a **de-novo generative design algorithm** that uses Reinforcement Learning to fine-tune a Language Model which generates string representations of molecules. It has successfully supported multiple in-house drug design projects.

A*STAR Agency for Science, Technology and Research | Research Intern
August 2019 – November 2019 | Singapore
➔ Received a Singapore International Pre-Graduate Award (SIPGA).
➔ Worked on a project where we applied Reinforcement Learning to find an **optimal pruning of large neural network architectures** like ResNet50. We submitted our work on neural network pruning to the **MicroNet Challange at NeurIPS 2019**.

CALIFORNIA INSTITUTE OF TECHNOLOGY DOLCIT Group | Research Intern
June 2018 – August 2018 | Pasadena, California, USA
➔ Received a Summer Undergraduate Research Fellowship (SURF).
➔ Worked with prof. Yisong Yue on a project in Multi-Agent Reinforcement Learning which involved **encoding cooperation between agents** in order to optimise the exploration process.

JPMORGAN CHASE & CO. CIB Treasury Tech team | Technology Analyst Intern
June 2017 – August 2017 | Glasgow, UK
➔ Improved the database and code release process
➔ Designed and implemented elements of the continuous deployment pipeline

Publications & Talks

Towers, S.*, Kalisz, A.*, Robert, P. A., Higueruelo, A., Vianello, F., Tsai, M. C., Steel, H., Foerster, J. N. (2024)
Opponent Shaping for Antibody Development | Preprint
(Paper Link🔗)

Mokaya, M., Imrie, F., van Hoorn, W. P., Kalisz, A., Bradley, A. R., Deane, C. M. (2023)
Testing the limits of SMILES-based de novo molecular generation with curriculum and deep reinforcement learning | Nature Machine Intelligence
(Paper Link 🔗)

Gupta, M., Aravindan, S., Kalisz, A., Chandrasekhar, V., Jie, L. (2020)
Learning to Prune Deep Neural Networks via Reinforcement Learning. | 7th ICML Workshop on Automated Machine Learning
(Paper Link 🔗)

Kalisz, A., (2020)
Can AI Design Drugs? | FUTURE Conference, Edinburgh
(Talk Recording 🔗)

Volunteering

OXWEST MENTORING SCHEME | Mentor
Nov 2021 - Feb 2022 | Oxford, UK
Mentored a STEM student from the University of Oxford. Helped her with creating a strong job application, adviced her on choosing a career path in tech.

INFPALS University of Edinburgh | Student Leader
September 2016 - January 2017 | Edinburgh, UK
Planned and organised weekly sessions for students. Monitored the students' progress and adjusted the sessions as needed.

Techincal skills

Reinforcement Learning • Machine Learning • Python • Pytorch • Pandas • Numpy • Git and Github • AWS • Weights and Biases