Paul Scherer

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Education

University of Cambridge PhD Computer Science

My current research interests lie within graph representation learning and its applications in biomedical informatics. However, I carry a general interest in the design of inductive biases for learning algorithms, and machine learning applications in scientific research.

In addition to publishing research on biomedical informatics, I have authored several open source Python libraries for learning with graph structured data and active learning. I am supervised by Profs. Pietro Liò and Mateja Jamnik.

University of Cambridge MPhil. Advanced Computer Science (Graduated with Distinction)

Undertook modules in machine learning and algorithms for data mining, biomedical information processing, affective computing, and natural language processing. A substantial focus of the degree was on critically assessing and replicating research papers as well as proposing original research.

Completed self-proposed dissertation on graph kernels supervised by Professor Pietro Liò

University of Edinburgh

BSc. Artificial Intelligence and Computer Science (Graduated with 1st Class Honours)

Dissertation in developing clustering algorithms applicable to protein-protein interaction networks which incorporate biological knowledge encoded in ontologies.

Selected Publications

Ramon Viñas Torné*, **Paul Scherer***, Nikola Simidjievski, Mateja Jamnik, Pietro Liò "Spatio-relational inductive biases in spatial cell-type deconvolution". (ICML2023 CompBio Workshop) 2023.

Paul Scherer, Pietro Liò, Mateja Jamnik "Distributed representations of graphs for drug pair scoring" (LoG2022). 2022. **Best reviewer award**.

Paul Scherer, Thomas Gaudelet, Alison Pouplin, Suraj M.S., Jyothish Soman, Lindsay Edwards, Jake Taylor-King. "PyRelationAL: A Library for Active Learning Research and Development." arXiv preprint 2022 (Under review).

Benedek Rozemberczki, **Paul Scherer**, Yixuan He, George Panagopoulos, Alexander Riedel, Maria Astefanoaei, Oliver Kiss, Ferenc Beres, Guzmán López, Nicolas Collignon, and Rik Sarkar. 2021. "PyTorch Geometric Temporal: Spatiotemporal Signal Processing with Neural Machine Learning Models." (CIKM 2021), **Best resource paper award**

Paul Scherer, Pietro Liò "Learning distributed representations of graphs with Geo2DR" (ICML 2020 Workshop in Graph Representation Learning and Beyond), 2020

Nikola Simidjievski, Cristian Bodnar, Ifrah Tariq, **Paul Scherer**, Helena Andres-Terre, Zohreh Shams, Mateja Jamnik, Pietro Liò "Variational Autoencoders for Cancer Data Integration: Design Principles and Computational Practice" (Frontiers Genetics), 2019

Select Open Source Projects

PyRelationAL (2021-Present) - Author/maintainer of modular open source active learning library for research and development.

Pytorch Geometric Temporal (2020-Present) - Part of the developing team for a dynamic extension of the Pytorch Geometric library for graph representation learning.

(Oct 2017 - Nov 2018)

(Sep 2012- Jun 2016)

(Jan 2019 - Present)

Research Intern / Research Consultant - Relation Therapeutics

Proposed and started the development of PyRelationAL a modular open source Python library for active learning. The package is now publicly available for research purposes.

Part-time Research Assistant / Consultant - University of Cambridge

Developed an interactive ABM-CA platform for the Department of Land Economy. It is now used as a research and teaching tool for postgraduate students within the University. (2019-2022)

Investigated role privacy of multi-robot formations using generative adversarial networks (2018).

Data Scientist - MRC Epidemiology Unit

Developed data harmonisation and analysis methods for an EU-FP7 funded epidemiological study using federated analysis techniques. This included onboarding 8 international institutions to participate under strict data governance rules. The pilot study has lead to a publication in the international journal for obstetrics and gynaecology BJOG.

Informatics Supervisor - University of Edinburgh

Prepared and gave seminar like classes on topics covered in Computation and Logic and Object Oriented *Programming*. Wrote supplementary materials and enjoyed high attendance (>90%) in classes.

Software Engineering Intern - Metasystems Asia Hong Kong Office

Implemented scrape and import tools for phpBB forums, e-mails, and SVN logs in PHP, Shell, and Python to transfer their entire internal knowledge-base off deprecated tools to Atlassian Confluence.

Resident Assistant - University of Edinburgh

As a live-in RA the role focused on building relationships with residents and empathising with their needs, aspirations, and interests so that they can make the most out of University life.

Awarded the Edinburgh and Edinburgh Leadership Award for services to improve student well-being.

Student Software Developer - Lightfields GmbH

Developed an in-house continuous integration suite and analysed different server/application monitoring tools to increase rate of development and maintenance.

ADHS Voice Study Assistant - Charité Universitätsmedizin

Processed, analysed, and organized voice samples gathered from research subjects for the computational analysis and biometric diagnosis of ADHS (ADHD).

Technical skills

Python (Proficient): Regularly use NumPy, SciPy, Pandas, Scikit-Learn, NetworkX, PyTorch, and comfortable using the Python ecosystem across operating systems.

R (Proficient): For data exploration, wrangling, visualisations, and quick observations.

NetLogo (Familiar): For agent based modelling and GIS simulation research.

General: Comfortable developing on Linux and Windows and modern coding practices.

Always happy to learn more! I have learned and used other languages (e.g. PHP, Java) on the job.

Personal details

German national with full settled status in the UK.

Fluent in: English and German. Intermediate level: Japanese and Spanish.

Professional

(Sep 2015 - Jun 2016)

(Jun 2012 - Aug 2014)

(Jul 2016 - Sep 2017)

(Aug 2014 - Jun 2016)

(Jun 2015 - Aug 2015)

(Nov 2010 - Apr 2011)

(Jul 2018 - Present)

(Jan 2021 - Oct 2021)