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Job Title Postdoctoral researcher positions in Probabilistic

Machine Learning research group, Aalto University

**Department** T313 Dept. Computer Science

**Institution** Aalto University

, , Finland

Date Posted Aug. 15, 2024

Application Deadline Open until filled

Position Start Date Available immediately

Job Categories Post-Doc

Academic Field(s) Computer Science

Job Website https://aalto.wd3.myworkdayjobs.com/aalto/job/Otaniemi-

Espoo-Finland/Postdoctoral-researcher-positions-in-Probabilistic-Machine-Learning-research-group--Aalto-

University R40446-5

Apply By Email

**Job Description** 

Samuel Kaski's research group on Probabilistic Machine Learning ([url=https://research.cs.aalto.fi/pml/]https://research.cs.aalto.fi/pml/) is searching for postdocs to work on AI fundamentals in exciting projects. The work includes collaboration with the [url=https://fcai.fi]Finnish Center for Artificial Intelligence (FCAI), the [url=https://ai-fun.manchester.ac.uk]Centre for AI Fundamentals at the University of Manchester, the Alan Turing Institute, ELLIS, and researchers from other fields.

Prof Kaski is Professor of Computer Science in Aalto University and Professor of AI in the University of Manchester. He is Director of Finnish Center for Artificial Intelligence and ELLIS Unit Helsinki, and Research Director of the Pankhurst Institute for Healthcare Technology. His research group develops



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machine learning principles and methods focusing on a few key topics (see "Machine learning foundations" below), often working with researchers of other fields in new exciting applications (see the other topics below).

**Topics** 

### Machine learning foundations

Keywords: probabilistic modelling, Bayesian inference, simulation-based / likelihood-free inference, multi-agent RL and collaborative AI, sequential decision making and experimental design, privacy-preserving learning, Bayesian deep learning, generative models

We are looking for a new postdoc in the team which develops probabilistic modelling and Bayesian inference methods. The team has several exciting new machine learning formulations we work on, and opportunities for applying the methods with top-notch collaborators. The core is always development of new methods, and with this call we are looking for talented researchers with background in machine learning, stats or CS (or other directly relevant topics) who are keen on developing the new methods. In the cover letter, let us know what you are interested in - if we are already working on it, all the better, but we are willing to listen to new ideas too.

### Machine learning for drug design

Keywords: probabilistic modelling, generative models, drug design, molecular modelling, deep learning

Recent progress in machine learning for generative and predictive models of molecules brings us towards computational, automatised drug design. We develop statistical methods and models for molecular structures, energies and interactions with the help of deep learning. A number of open problems reside in developing neural network models with physics-based inductive biases, in generative models in 3D spaces, in modelling the property landscapes of molecules, and in generalizing outside the training distribution in molecular design.

We are looking for motivated candidates with background in computational sciences, machine learning, statistics. Stong interest in drug design is necessary, prior experience a big plus.

Team: this position is in the Probabilistic Machine Learning (PML) research group at Aalto, [url=https://research.cs.aalto.fi//pml]https://research.cs.aalto.fi//pml and will involve collaboration with Prof. Vikas Garg ([url=https://www.aalto.fi/en/people/vikas-kumar-garg]https://www.aalto.fi/en/people/vikas-kumar-garg) and Dr [url=https://users.aalto.fi/~heinom10/]Markus Heinonen.

Machine learning for synthetic biology and biodesign



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Keywords: AI-based design, human-in-the-loop machine learning, collaborative AI, molecular modeling, reinforcement learning, deep learning algorithms, generative models

We are searching for early career scientists to join our research team working towards next-generation machine learning methods for synthetic biology. The position is available in a new large multi-year project, the Virtual Laboratory for Biodesign (BIODESIGN), implemented in collaboration between FCAI and VTT Technical Research Centre of Finland.

Supported by a 2 million EUR grant from the Jane and Aatos Erkko Foundation, the BIODESIGN project aims for breakthroughs in AI techniques for protein design by combining the strength of novel deep learning models with AI-based design and human feedback in a Design-Build-Test-Learn cycle. The virtual laboratory is envisioned to have wide-range applications in industry (e.g., new biochemicals, biomaterials and drugs) and to help the transition to a carbon-neutral society.

We are looking for applicants with a strong academic record in computer science, mathematics, or statistics. Solid research experience in one or more of the following fields is beneficial: Al-based design, Deep learning algorithms, Generative models, Human-in-the-loop machine learning, Collaborative Al, Molecular modeling, Reinforcement learning, Structured prediction.

We invite applications from early-career scientists at levels of Postdoctoral researcher and Research fellow.

The successful applicants will join a world-class research team where top AI researchers in FCAI (led by Professors Samuel Kaski, Juho Rousu and Vikas Garg) join forces with synthetic biology experts of VTT (led by Prof. Merja Penttilä).

Team: this project will involve collaboration with Prof. Juho Rousu ([url=https://www.aalto.fi/en/people/juho-rousu]https://www.aalto.fi/en/people/juho-rousu) and Prof. Vikas Garg ([url=https://www.aalto.fi/en/people/vikas-kumar-garg]https://www.aalto.fi/en/people/vikas-kumar-garg).

Deep learning with differential privacy Keywords: Deep learning, hyperparameter learning, differential privacy

Differential privacy allows developing machine learning algorithms with strong privacy guarantees. Recent work shows it is possible to combine strong privacy and high accuracy by pre-training models on public data and only fine-tuning the model with the sensitive data. However, high accuracy still requires a few key problems to be solved. The aim of this project is to develop methods that make it



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easier to train high accuracy private models. The project will benefit from a very large grant of compute time on LUMI, 3rd fastest supercomputer in the world. The project requires a background in deep learning.

Team: this project will involve collaboration with Prof. Antti Honkela ([url=https://www.cs.helsinki.fi/u/ahonkela/]https://www.cs.helsinki.fi/u/ahonkela/).

Machine learning for personalized medicine Keywords: Causal inference, differential privacy, graph neural networks, user models

We are looking for postdocs to join our research team working towards new machine learning methods for personalized medicine. The fundamental machine learning challenges underlying modern data-based personalized medicine stem from the discrepancy that individual healthcare decisions need to be personalized to an individual, whereas any data-driven model needs to generalize over a larger set of individuals.

This project utilizes unique datasets such as the FinRegistry research project ([url=http://www.finregistry.fi]www.finregistry.fi), which combines data across 18 registries covering the Finnish population's healthcare visits, medications and socio-demographics for 7.2 million individuals. Patient data is characterized by limited data availability determined by how frequently a patient interacts with the healthcare system, and heterogeneity in the disease phenotypes being predicted. By developing new meta-learning methods for this data, we aim to address how risk assessments and treatments can be improved. This requires new approaches that learn from relational data (e.g., population-scale family networks and doctor-patient networks), while respecting data privacy and accounting for user models and distribution shift.

We are looking for applicants with a strong academic record in computer science, mathematics, or statistics. Solid research experience in one or more of the following fields is beneficial: meta-learning, causal inference, user models, distribution shift, differential privacy, graph neural networks.

Team: this project will be carried out with collaborators at the Institute for Molecular Medicine Finland (led by Associate Professor Andrea Ganna), Finnish Institute of Health and Welfare (led by Professor Markus Perola), and the Christabel Pankhurst Institute at the University of Manchester.

Real-time Al-assistance with computationally rational user models Keywords: collaborative Al, human-in-the-loop ML/RL, reinforcement learning, user modelling

Despite recent advances in AI and machine learning, there are few AI solutions that can be applied



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when we cannot precisely specify the objective or do not have suitable data to learn from. This is particularly salient and challenging in ad hoc assistance for human users in complex tasks such as scientific discovery.

This project aims to address this issue by learning these objectives, and to assist, directly from interaction with the users. To do so, we develop reinforcement learning techniques for Al-assistants and computationally rational user models that take into account factors such as cognitive biases to reason about human decision-making. We push state-of-the-art in Al that, through inference over - and planning with - such user models, is able to tackle problems that are otherwise out of reach of mainstream Al solutions.

Supported by a High-performance computing grant from the Research Council of Finland, we are looking to strengthen this team with postdocs with a strong academic record in computer science, mathematics, or statistics. Solid research experience in one or more of the fields listed under this topic is beneficial.

Team: this project will be carried out with a top expert on computational rationality, Prof. Andrew Howes of University of Exeter, and experts in application domains.

Next generation distribution shifts

Keywords: distribution shift, out-of-distribution generalization, robust deployment, deep learning, experimental design

Robust algorithms for machine learning models are vital as the deployed scenario can differ from the training scenario in unexpected ways. Placing assumptions on the kind of distribution shift we expect, such as covariate or label shift, and accounting for it during training is common practice. However, these assumptions are often too restrictive for real-world settings, as the shifts encountered are typically more complex. Moreover, it is difficult to know a priori which shifts we need to account for. This project focuses on developing novel machine learning methods that demonstrate robust performance by adapting to unforeseen shifts and diverse datasets during deployment.

We are looking for applicants with a strong academic record in computer science, mathematics, or statistics. Solid research experience in one or more of the following fields is beneficial: distribution shift, out-of-distribution generalization, out-of-domain generalization, sequential experimental design. Your experience and ambitions

We expect the candidates to hold or be close to getting a relevant doctoral degree and have a solid background in the mathematics/statistics/computer science needed in machine learning. Previous experience in the application fields is an advantage. Capability of both independent work and



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teamwork, and excellent written and spoken English are necessary. What we offer We provide

### 1) RESEARCH ENVIRONMENT

You will work in Professor Samuel Kaski's research group

([url=https://research.cs.aalto.fi/pml/]Probabilistic Machine Learning Group). We design the collaboration as we go, according to what the research needs. Collaborators include but are not restricted to the other groups in the Finnish Center for Artificial Intelligence ([url=https://fcai.fi/researchers]FCAI), other sites of the European Laboratory for Learning and Intelligent Systems ([url=https://fcai.fi/ellis-unit-helsinki]ELLIS), [url=https://aifun.manchester.ac.uk]Centre for AI Fundamentals of the University of Manchester, the Turing Institute, and a number of excellent researchers in other fields in our applications.

### 2) JOB DETAILS

Postdoc positions are typically made for up to two years. Starting dates are flexible. All positions are negotiated on an individual basis. We are strongly committed to offering everyone an inclusive and non-discriminating working environment. We warmly welcome qualified candidates from all backgrounds to apply and particularly encourage applications from women and other groups underrepresented in the field.

The salaries are based on the Finnish universities' pay scale. The contract includes occupational healthcare.

Ready to apply?

Submit your application through our recruitment system Workday by the link below. The deadline for applications is 15th September at 23:59 Finnish time (UTC +3) 2024.

Required attachments

Cover letter (1-2 pages).

CV

List of publications (please do not attach full copies of publications)

A transcript of doctoral study

The degree certificate of your latest degree. If you don't yet have a PhD degree, a plan of completion must be submitted.

Contact details of two senior academics who can provide references. We will contact your referees if we need recommendation letters.

All materials should be submitted in English in a PDF format. Note: You can upload max. five files to



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the recruitment system, each max. 5MB.

Please note: Aalto University's employees and visitors should apply for the position via our internal system Workday -> find jobs (not external aalto.fi webpage on open positions) by using their existing Workday user account.

Contacts: Coordinator Fang Wang (fang.wang@aalto.fi)

More Information

We are part of [url=https://fcai.fi/]Finnish Centre for Artificial Intelligence FCAI and [url=https://fcai.fi/ellis-unit-helsinki]ELLIS Unit Helsinki. More information on their pages, and the frequently asked questions on [url=https://fcai.fi/we-are-hiring]this page.

Aalto University is a community of bold thinkers where science and art meet technology and business. We are committed to identifying and solving grand societal challenges and building an innovative future. Aalto has six schools with nearly 12 000 students and a staff of more than 4000, of which 400 are professors. Our main campus is located in Espoo, Finland. Diversity is part of who we are, and we actively work to ensure our community's diversity and inclusiveness. This is why we warmly encourage qualified candidates from all backgrounds to join our community.

The Department of Computer Science is an internationally-oriented community and home to world-class research in modern computer science, combining research on foundations and innovative applications. With over 40 professors and more than 450 employees from 50 countries, it is the largest department at Aalto University and the largest computer science unit in Finland. Computer science research at Aalto University ranks high in several prominent surveys (47th worldwide and 9th in Europe in Shanghai subject ranking 2019; and 56th worldwide in Times Higher Education subject ranking 2020).

#### **About Finland**

Finland is a great place for living with or without family - it is a safe, politically stable and well-organized Nordic society. Finland is consistently ranked high in quality of life and was just listed again as the happiest country in the world: [url=https://worldhappiness.report/news/its-a-three-peat-finland-keeps-top-spot-as-happiest-country-in-world/]https://worldhappiness.report/news/its-a-three-peat-finland-keeps-top-spot-as-happiest-country-in-world/. For more information about living in Finland: [url=https://www.aalto.fi/services/about-finland]https://www.aalto.fi/services/about-finland

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Please reference Academickeys in your cover letter when applying for or inquiring about this job announcement.

Contact

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