Dr Asif Khan

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Education

- **Harvard Medical School** — Boston, USA
  Postdoctoral Fellow — *Jan. 2024 - Present*
  Advisor: Prof. Chris Sander
  My research focuses on developing machine learning and AI algorithms to advance cancer therapy. The emphasis of my work lies on interpretable approaches that can guide clinical decision-making and ultimately improve patient outcomes. I am currently targeting two primary goals in this domain. Firstly, I am developing deep sequential models incorporating feature selection and uncertainty quantification techniques to predict cancer risk with greater precision and reliability over time. Secondly, I am utilising machine learning approaches to analyse spatial omics data of triple-negative breast cancer to predict the response of patients to chemotherapy.

- **The University of Edinburgh** — Edinburgh, United Kingdom
  Ph.D. in Machine Learning — *Oct. 2019 - Oct. 2023*
  Advisor: Prof. Amos Storkey
  PhD in machine learning. My thesis is on geometry for deep representation learning, focusing on applications related to disentanglement, robustness, and non-Euclidean data domains.

- **University of Bonn** — Bonn, Germany
  MSc., Computer Science; GPA: 1.1 (best: 1.0, worst: 5.0) — *Oct. 2017 - Sep. 2019*
  Advisor: Prof. Asja Fischer

Experience

- **Huawei Noah's Ark Lab** — London, United Kingdom
  Research Scientist Intern, Manager: Dr. Haitham Bou-Ammar — *Sept. 2021 - Dec. 2021*
  I led a project within a collaborative research environment implementing a combinatorial Bayesian optimisation framework for designing the CDRH3 region of antibody sequences. We demonstrated the effectiveness of the approach on several antigens of therapeutic interest. The project resulted in a research paper that got accepted for publication in Cell Reports Methods.

- **Sony** — Stuttgart, Germany
  Research Intern, Manager: Dr. Fabien Cardinaux — *March 2019 - August 2019*
  I developed a generative adversarial network (GAN) framework for unsupervised speech-to-speech conversion. I used the Librispeech corpus for training and validation. I was fortunate that my team fostered a collaborative research environment where I learned from and complemented the skills of other members.

- **Smart Data Analytics, University of Bonn** — Bonn, Germany
  Research Assistant, Supervisor: Prof. Jens Lehmann — *Oct 2017 - Feb 2019*
  I developed a representation learning method to incorporate attribute and relational triples for improving link prediction in knowledge graphs. The outcome of the project was published as a conference paper.

- **Bio-Ontology Research Group, KAUST** — Jeddah, Saudi Arabia
  Research Assistant, Supervisor: Prof. Robert Hoehndorf — *Jan. 2016 - May 2017*
  I provided machine learning expertise for solving life science problems. The key projects I worked on:
  - Ontology-aware hierarchical neural network for predicting Gene Ontology (GO) functions from protein sequences.
  - Representation learning of nodes and relations in a biological knowledge graph.
  - Representation learning of disease and gene entities from natural language text and a biological knowledge graph.

- **Rapid Rich Object Search Lab, Nanyang Technological University** Singapore
  Research Intern, Supervisor: Prof. Alex C. Kot *May 2015 - July 2015*
  I developed a deep convolutional neural network for fine-grained classification with an application to a dataset of visually similar handbags (developed by ROSE Lab). I integrated a new layer for feature selection in Caffe (a deep learning framework) implemented in C++. It was my first hands-on experience with deep learning, where I learned from various experts and delivered working software as an outcome.

Selected Publications

1. **A Khan**, A Storkey, Adversarial robustness of VAEs through the lens of local geometry. In International Conference on Artificial Intelligence and Statistics (AISTATS) 2023.
   Short Version: Workshop on New Frontiers in Adversarial Machine Learning, ICML 2022.
2. **A Khan***, A I Cowen-Rivers*, A Grosnit, P A Robert, V Greiff, E Smorodina, P Rawat, R Akbar, K Dreczkowski, R Tutunov, D Bou-Ammar, J Wang, A Storkey, H Bou-Ammar, Towards Real-World Automated Antibody Design with Combinatorial Bayesian Optimisation. Cell Reports Methods 2023,
   Short Version: In The 2022 ICML Workshop on Computational Biology. ***(* Equal Contribution)***
3. **A Khan**, A Storkey, HAmiltonian Latent Operator for content and motion disentanglement in image sequences. In Advances in Neural Information Processing Systems (NeurIPS) 2022.
4. Cowen-Rivers, A I, P J Gorinski, A Sootla, **A Khan**, L Furui, J Wang, J Peters, and H B Ammar, Structured Q-learning For Antibody Design. In Reinforcement Learning for Real Life Workshop, NeurIPS 2022. *(Spotlight)*
5. A Kristiadi*, **M Asif Khan***, Denis Lukovnikov, Jens Lehmann, Asja Fischer, LiteralE: Incorporating literals into knowledge graph embeddings. In Proceedings of the 18th International Semantic Web Conference (ISWC), Springer 2019. ***(* Equal Contribution)***
6. A Kukleva*, **M Asif Khan***, H Farazi, and S Behnke, Utilizing Temporal Information in Deep Convolutional Network for Efficient Soccer Ball Detection and Tracking. In the 23rd RoboCup International Symposium (RCS) 2019. *(Oral),* ***(* Equal Contribution)***
7. M Kulmanov, **M Asif Khan**, R. Hoehndorf, DeepGO: Predicting protein functions from sequence and interactions using a deep ontology-aware classifier. In Bioinformatics 2017, pp. 660-668.
8. M Alshahrani, **M Asif Khan**, OMaddouri, A R Kinjo, NQ Rosinach, R. Hoehndorf, Neuro-symbolic representation learning on biological knowledge graphs. In Bioinformatics 2017, pp. 2723-2730.

Skills

- **Programming**: Python, Bash, C, SQL, SPARQL.
- **ML topics**: Deep generative models, representation learning, self-supervised learning, Bayesian optimisation, transformers, geometric deep learning, physics prior in neural networks, topological data analysis.
- **ML tools**: Pytorch, Caffe, Keras, NumPy, Scipy, Scikit-learn, Matplotlib, wandb, huggingface, gensim.
- **Others**: Linux, GIT, LaTeX.

Academic Activities

- **Teaching**
  University of Edinburgh, United Kingdom *Oct 2019 – Oct 2023*
  - Tutor for Probabilistic Modeling and Reasoning. Delivered tutorial to a group of 15 students.
  - Marker for Probabilistic Modeling and Reasoning, Machine Learning Practical, Introductory Applied Machine Learning and Data Mining & Exploration. I was responsible for evaluating coursework, final exams and project reports.

  University of Bonn, Germany *Oct 2017 – Feb 2019*
  - Teaching Assistant for Knowledge Graph Analysis. I delivered tutorials to two groups of 30 students and marked exams. Also, I prepared theoretical and programming exercises for the course https://github.com/SmartDataAnalytics/Knowledge-Graph-Analysis-Programming-Exercises.
- **Reviewing**
  Journals

* JMLR.

Conferences

* NeurIPS 2022/2023, ICML 2023/2024, AISTATS 2022/2023, ICLR 2022.

Workshops

* SynS & ML Workshop ICML 2023, ML4PS Workshop NeurIPS 2021/2022/2023.

Awards

- **2023**: Top Reviewer NeurIPS.
- **2022**: Scholar Award NeurIPS.
- **2022**: Top Reviewer NeurIPS.
- **2022**: Highlighted Reviewer ICLR.
- **2022**: Top Reviewer AISTATS.
- **2019**: PhD Scholarship.