Dr Asif Khan

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EDUCATION

### Harvard Medical School

Postdoctoral Fellow

Boston, USA

Jan. 2024 - Present

Advisor: Prof. Chris Sander

Research Interests: 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

Oct. 2019 - Oct. 2023

Ph.D. in Machine Learning Advisor: Prof. Amos Storkey

Research Interests: I hold a 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

# LNM Institute of Information Technology

Jaipur, India

Bachelor of Technology in Electronics and Communication; GPA: 8.94/10.0

July. 2012 - July. 2016

#### 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)
- 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

 $* \ \mathrm{JMLR}.$ 

#### Conferences

 $\ast\,$  NeurIPS 2022/2023, ICML 2023, AISTATS 2022/2023, ICLR 2022.

## Workshops

 $\ast\,$  Syn<br/>S & 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.