

# Asif Khan

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Personal: <https://mdasifkhan.github.io/>

GitHub: <https://github.com/MdAsifKhan>

## EDUCATION

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- **The University of Edinburgh** Edinburgh, United Kingdom  
*Ph.D. in Machine Learning* *Oct. 2019 - Aug. 2023 (Expected)*  
*Advisor:* Prof. Amos Storkey  
*Research Interests:* My PhD focuses on deep generative modelling and structured representation learning. My work has particular applications to disentanglement, robustness and non-Euclidean data domains.  
  
I am also passionate about using machine learning to develop efficient solutions to complex life science problems, especially protein engineering and drug discovery. In recent work, I proposed a combinatorial BO framework that offers a sample-efficient solution for designing the CDRH3 region of antibody sequences using the biophysical properties of sequences as a trust region.
- **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  
*Key Courses:* Computational Topology, Randomised Algorithms & Probabilistic Analysis, Cluster Analysis, Machine Learning, Deep Learning for Visual Recognition, Game AI, Knowledge Graph Analysis, Audio Signal Processing.
- **LNM Institute of Information Technology** Jaipur, India  
*Bachelor of Technology in Electronics and Communication; GPA: 8.94/10.0* *July. 2012 - July. 2016*

## EXPERIENCE

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- **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

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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.

## ACADEMIC ACTIVITIES

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### • **Teaching**

*University of Edinburgh*

*Oct 2019 – Present*

- 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 and Exploration. I was responsible for evaluating coursework, final exams and project reports.

*University of Bonn*

*Oct 2017 – Feb 2019*

- Teaching Assistant for Knowledge Graph Analysis. I was responsible for delivering tutorials to two groups of 30 students each and marking exams. I prepared theoretical and programming exercises for the course <https://github.com/SmartDataAnalytics/Knowledge-Graph-Analysis-Programming-Exercises>.

### • **Reviewing**

NeurIPS 2023, ICML 2023, AISTATS 2023, NeurIPS 2022, ICLR 2022, AISTATS 2022, ML4PS Workshop NeurIPS 2021/2022.

## AWARDS

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- **2022**: Scholar Award NeurIPS.
- **2022**: Top Reviewer NeurIPS.
- **2022**: Highlighted Reviewer ICLR.

- **2022:** Top Reviewer AISTATS.
- **2019:** PhD Scholarship.

## SKILLS

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- **Programming:** Python, C, SQL, SPARQL.
- **ML topics:** Deep generative models, representation learning, self-supervised learning, Physics prior in neural networks, large transformer networks, topological data analysis, graph neural networks.
- **ML tools:** Pytorch, Caffe, Keras, Numpy, Scipy, Matplotlib.
- **Others:** Linux, GIT,  $\text{\LaTeX}$ .