# AAYUSH GROVER

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### PERSONAL PROFILE

I am a doctoral student at the Computational Cancer Genomics Lab (ETH Zürich). My research interest lies in deep learning and computational biology. Specifically, I am interested in understanding the mechanism of development and progression of cancer from an epigenetic viewpoint using deep learning.

#### **EDUCATION**

# **Doctoral Studies in Computer Science**

September 2021 - Present

ETH Zürich, Zürich, Switzerland

## Integrated Masters in Computer Science Engineering/Data Science

August 2016 - July 2021

International Institute of Information Technology, Bangalore, India

CGPA: 3.79/4.00

### **PUBLICATIONS**

Venkatesh G, Grover A, Srinivasaraghavan G, & Rao S (2020): "MHCAttnNet: predicting MHC-peptide bindings for MHC alleles classes I and II using an attention-based deep neural model" Bioinformatics, 36(Supplement\_1), i399-i406

· Built an end-to-end system to compute the binding affinity between a given peptide and a particular MHC allele. It not only predicted more accurately but also used an attention based scheme to analyze the subsequences of amino acids that are more important to make a particular prediction. This work was presented in ISMB-2020.

### RESEARCH EXPERIENCE

# Prediction of Enhancer-Promoter Interactions Computational Epi-Genetics of Cancer Lab, ETH Zürich

September 2021 - Present

Supervisor: Prof. Valentina Boeva

· While it is relatively straightforward to predict the effect of promoter deregulation on gene expression, one requires information about 3D enhancer-promoter interactions to assess the potential effect of enhancer activation/deactivation on the expression of neighboring genes. This 3D looping information is costly to obtain for each tumor of interest and it, therefore, should be substituted with in silico predictions. Prediction of enhancer-promoter interaction is a challenging task as enhancers can regulate promoters of distal target genes. We view this task analogous to the dependency parsing task of Natural Language Processing and therefore, are implementing a transformer-based approach to solve this task.

# Cancer Survival Prediction using Multi-omics Integration: A Few-Shot Learning Approach

Master Thesis, IIIT-Bangalore September 2020 - June 2021

Supervisors: Prof. G. Srinivasaraghavan & Prof. Laurent Gatto

· Built a few-shot learning model for predicting survival in cancer patients. Since the existing cancer patient data have very limited samples of each cancer type, training deep neural networks is not feasible. Therefore, we built the first few-shot learning model for this task that can be used to predict survival in patients suffering from any cancer type.

## Protein Subcellular Localization Prediction

Computational Biology and Bioinformatics Group, UCLouvain

Supervisor: Prof. Laurent Gatto

· Built a deep learning model for predicting protein subcellular localization using protein-protein interaction networks. Experimentally determining the localization of a protein can be challenging when a related antibody is unknown. Therefore, a multi-label predictive model that can annotate new proteins accurately is needed. This work has been made available on bioRxiv and was presented as a poster at the Applied Bioinformatics in Life Sciences conference.

# Novel Deep Learning Assisted Virtual Screening to Enhance Drug Discovery for COVID-19 IIIT-Bangalore & NCBS, Bangalore

May 2020 - March 2021

May 2020 - June 2021

Supervisors: Prof. G. Srinivasaraghayan, Prof. R. Sowdhamini & Prof. Neelam Sinha

· Built an attention-based graph neural model for ranking the molecules from SuperNatural and Drugbank databases on the basis of their docking with the NSP-1 protein of SARS-CoV-2. The experimental dataset consisted so of molecular fingerprints of drug molecules. The top ranked molecules were validated experimentally.

### **SKILLS**

Programming Languages Python, C++, Java, MySQL, C, Ocaml, Prolog

Tools Jupyter, LaTeX, Integrative Genomics Viewer (IGV), NetLogo

Python Libraries Pytorch, Pandas, Numpy, Scipy, Scikit-learn, OpenCV, Matplotlib,

Goatools, Seaborn, Torchtext, Torchvision, Biopython

### SERVICE TO FIELD

· Reviewer for top AI conferences like NeurIPS 2022 - Datasets and Benchmarks, ICML 2022 - AI for Science Workshop, ICLR 2022 - Deep Generative Models for Highly Structured Data Workshop, NeurIPS 2021 - AI for Science Workshop, AAMAS 2020

· Member of ISCB-Student Council

2020-Present

· Reviewer for journals like PLOS ONE & Springer's Sadhana Journal

### OTHER RESPONSIBILITIES

- · IT Coordinator at the Computational Cancer Genomics Lab (ETH Zürich).
- · Teaching Assistant: Computational Biomedicine (Fall 2021), Machine Learning for Genomics (Spring 2022), Probabilistic Artificial Intelligence (Fall 2022)
- · Supervision of Master and Bachelor Students: 4 (S. Gao, S. Häfliger, L. Kasak, P. Dominique)

### AWARDS

· Awarded the Swiss Government Excellence Scholarship for doctorate at ETH Zurich

2021

· Awarded the DAAD WISE scholarship for summer internship in Germany

2019

· Dean's Merit List, International Institute of Information Technology, Bangalore

2016-2021

## EXTRA-CURRICULAR INVOLVEMENTS

· Secretary of RSG-India

2020-Present

· Head of College Sports Committee

2018/19

· Captain of College Football Team

2018/19 & 2019/20

· Head Organizer of the RMIT Conference

2017-2019