AKSHAY SUBRAMANIAN

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EDUCATION

Indian Institute of Technology Roorkee *August 2017 - August 2021*
In Progress
Bachelor in Technology (B.Tech.)
Metallurgical and Materials Engineering Cumulative GPA: 9.308/10

National Public School, Bangalore, India *June 2016 - May 2017*
Computer Science Stream
Central Board of Secondary Education (CBSE) Overall Percentage: 96.0

PUBLICATIONS

Inverse Design of Potential Singlet Fission Molecules using a Transfer Learning Based Approach
Implemented a deep generative model to predict novel Singlet Fission molecules for Solar Cell applications. A paper based on this work has been submitted for publication in a top journal and is under review.
[arxiv preprint]

WORK EXPERIENCE

Research Intern, AI and Text mining team *May 2020 - Present*
Prof. Gerbrand Ceder | Lawrence Berkeley National Laboratory (LBNL)

- Part of the team responsible for the development of [CovidScholar]. The aim of this effort is to curate and tag COVID-19 related research work to make them easily accessible to researchers and thereby accelerate research in this area. Relations between papers and tagging of papers into categories are achieved using Deep learning based approaches.
- Working on automated analysis of XRD and TEM diffraction pattern images using Computer Vision techniques.

Summer Research Intern, Department of Materials Engg. *May 2019 - August 2019*
Dr. Praveen Kumar | Indian Institute of Science, Bangalore
Worked on a project titled 'Investigation of effect of electric current loading on the morphology of the crack in thin sheets of metals'. Primarily worked on healing fatigue cracks in metal sheets by application of electric pulses.
[Certificate]

PROJECTS

Multitask Learning to predict crystal strains from EBSD diffraction patterns *July 2019 - Present*
Dr. K.S. Suresh | Indian Institute of Technology Roorkee
Implemented a Deep Convolutional Neural Network and employed Multitask learning to predict crystal strain components from Kikuchi Diffraction Patterns.

Repurposing Commercially available drugs for inhibition of the coronavirus using Machine Learning Techniques *April 2020*
Dr. Soumitra Satapathi | Indian Institute of Technology Roorkee
Experimented with a variety of Machine Learning techniques to predict potential inhibitors of the SARS coronavirus proteas molecule. Among others, made use of Graph Neural Networks, Random Forests and vanilla Deep Neural Networks.

PyTorch Implementation of 'Optimization of Molecules via Deep Reinforcement Learning' *April 2020*
Individual Work
Implemented and reproduced the results obtained in 'Optimization of Molecules via Deep Reinforcement Learning'. Made a couple of improvements to the original implementation to stabilize training:

- Utilized an additional target Q-Network to stabilize training as opposed to the single Q-Network used in the original TensorFlow implementation by the authors.
- Updated the target Q-Network periodically using Polyak averaging.

[`Code on GitHub`]

PyTorch Implementation of 'Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules' *May 2019 - July 2019*
Individual Work
Implemented and reproduced the results obtained in 'Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules'.
[`Code on GitHub`]

OPEN SOURCE CONTRIBUTIONS

Chainer *January 2019 - September 2019*
ChainerX is a versatile ndarray implementation with special support of deep learning-specific operations. I worked on supporting many fundamental operators usually available for ndarray libraries (e.g. those provided by NumPy and SciPy) as well as special operators focusing deep learning applications (e.g. convolution, pooling, activation functions, etc.).
`[Report] [Contributions]`

DeepChem April 2020
The DeepChem project is an open source framework that provides tools for drug discovery, materials science, quantum chemistry, and biology. I have implemented the approaches described in 'Optimization of Molecules via Deep Reinforcement Learning' and 'ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition' for TorchChem, which is a PyTorch version of the DeepChem framework.
`[GitHub link]`

TECHNICAL SKILLS

Programming Languages	Python, C++, C, Java, Javascript
Frameworks	PyTorch, Tensorflow, Keras, Chainer
Software & Tools	Git, CUDA, Docker, SLURM
Equipment and Instruments	Instron Fatigue test, SEM, Electrical Discharge Wire Cutting (EDSWC)

NOTABLE ACHIEVEMENTS

I am ranked 1st out of 80 students in my department at IIT Roorkee based on overall academic performance.

Selected for the prestigious MITACS Globalink Research Internship 2020 program that funds Summer research internships at Canadian Universities.

Was awarded the IIT Roorkee Heritage Excellence Award 2019 for outstanding academic, co-curricular and extra-curricular achievements.

Was among the top 0.1 percent in the country in the Chemistry Examination of the 12th Grade CBSE Board Examinations.(Scored 100/100)

Was ranked 17th in the state of Karnataka in the State Level National Talent Search Examination 2015 and was awarded a scholarship by the Department of State Educational Research and Training (DSERT) for being one out of 151 students from Karnataka to qualify the examination.

EXTRA-CURRICULARS

Member of Data Science Group, SDSLabs - a group in campus responsible for fostering a culture of Data Science by organizing Machine Learning and Deep Learning related competitions and Lectures.

Awarded the K.V. Mittal Memorial Award twice for securing the 1st position in the Institute Open tennis tournament held in 2017 and 2019.

Secretary of the IIT Roorkee tennis team for the session 2019-2020.

Captained the IIT Roorkee Tennis team at the prestigious Inter IIT Sports Meet held in IIT Madras in 2017, IIT Guwahati in 2018 and IIT Kharagpur in 2019.

Captain of Tennis and Table Tennis teams, National Public School Koramangala, Bangalore

REFERENCES

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