

Yashaswi Pathak

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EDUCATION

IIIT HYDERABAD

B.TECH IN COMPUTER SCIENCE AND
M.S. BY RESEARCH IN
COMPUTATIONAL NATURAL SCIENCE

Aug 2016 - April 2021

Cum. GPA : 9.18 / 10

Branch Rank: 1

Deans Academic Merit List (top 5%)
for all semesters

DPS, PATNA

Graduated May 2016 | Patna, India

Senior Secondary, CBSE - 93%

LINKS

Homepage: [Link](#)

Github: [yp201](#)

LinkedIn: [yashaswipathak](#)

Google Scholar: [Yashaswi Pathak](#)

COURSEWORK

Machine Learning

Information Retrieval and Extraction

NLP Applications

Machine Learning for Science

Distributed Systems

Database Systems

Compilers

Computer Graphics

(Teaching Asst 1x)

Software Architecture

(Teaching Asst 1x)

Data Structures and Algorithms

Operating Systems

Discrete Mathematics

(Teaching Asst 1x)

Technology Product Entrepreneurship

(Teaching Asst 1x)

SKILLS

Programming Languages:

Python • C • C++ • Bash • Javascript

Machine Learning:

PyTorch • Keras • SciKit Learn • Pandas

Web Dev:

HTML • CSS • React JS • Django

Miscellaneous:

Git • AWS • MySQL • OpenGL • WebGL

AWARDS & POSITIONS

- AAI and IIIT travel grant to attend AAI 2020.
- Captain of Institute's Football Team, IIIT Hyderabad (Sept 2018-Present)

EXPERIENCE

99ANDBEYOND | MACHINE LEARNING RESEARCHER

Jan 2020 – Aug 2020 | Montreal, Canada

- Part of the team that developed PGFS: Reinforcement Learning based agent that can search for readily-producible small molecules in a very large discrete action space
- Designed a Max Reward formulation in reinforcement learning with direct applications in drug discovery and gold mining.

CCNSB, IIIT HYDERABAD | RESEARCH ASSISTANT

May 2018 – Present | Hyderabad, India

- Working with **Dr. U Deva Priyakumar**
- Developed autonomous methods for molecular/material property prediction for drug/material design and discovery based on deep graph neural networks, attention mechanism and conditional variational autoencoders
- From NMR spectra to Molecule: Alpha zero (Deep learning + MCTS) like algorithm to find molecule directly from NMR spectrum.

MATSCI AI | RESEARCH ANALYST INTERN

June 2019 – Aug 2019 | Hyderabad, India

- Developed Pipeline for various NLP Tasks.
- Worked on Database design and efficient Data extraction design for a huge data set of Industry materials.

PROJECTS

- **Compiler Frontend:** Developed a compiler frontend that included lexical and syntax analysis, AST generation, interpreter and LLVM code generator.
- **OpenGL Game Development:** Built a 2D game similar to Pacman Killer and a 3D game similar to the Legend of Zelda using OpenGL and C++
- **Linux Shell:** Custom shell in C++ with support for features like foreground and background processes, input-output piping and redirection etc.
- **Search Engine:** Created a search engine using inverted index on wikipedia data (70GB) that was able to retrieve top K articles for a query via relevance ranking, implemented using tf-idf scoring.
- **Hate Speech Detection** Structured based Tree-LSTM model implemented on twitter dataset to detect hatefulness.

PUBLICATIONS

- [1] S. K. Gottipati, B. Sattarov, S. Niu, **Pathak, Yashaswi**, et al. Learning to navigate the synthetically accessible chemical space using reinforcement learning. *ICML*, 2020.
- [2] S. K. Gottipati, **Pathak, Yashaswi**, and others. Maximum reward formulation in reinforcement learning. *Under review at ICLR*, 2020.
- [3] S. Laghuvarapu, **Pathak, Yashaswi**, and U. D. Priyakumar. Band nn: A deep learning framework for energy prediction and geometry optimization of organic small molecules. *J. Comp. Chem*, 2020.
- [4] **Pathak, Yashaswi**, K. S. Juneja, et al. Deep learning enabled inorganic material generator. 2020.
- [5] **Pathak, Yashaswi**, S. Laghuvarapu, et al. Chemically interpretable graph interaction network for prediction of pharmacokinetic properties of drug-like molecules. *AAAI*, 2020.