Shaurya Seth

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Overview

- Machine learning engineer with experience building and deploying models that outperform human experts in real-world drug discovery pipelines.
- Published researcher with co-authored work in *Nature Chemical Biology* and *Royal Society of Chemistry*, and foundational training under Richard Sutton and Martha White in reinforcement learning.
- Recipient of multiple competitive research awards, including the Alberta Innovates Studentship and GlycoNet Summer Award, recognizing innovation at the intersection of AI and biology.

Experience

48Hour Discovery Inc. *Apr 2023 – Present*
Machine Learning Engineer Edmonton, AB

- Founded and led the company's **machine learning team**, establishing a pipeline for weekly experimental validation of AI-designed molecules.
- Designed **molecular-binding models (XGBoost)** that consistently outperformed expert-designed compounds, validated by biochemical assays.
- Processed **5+ terabytes of paired-end Illumina data (FASTQ)** using custom barcodes for genomic analysis.
- Built and deployed **internal tools (AWS)** that became core infrastructure; widely adopted across lab staff.

Research

Reinforcement Learning & Artificial Intelligence (RLAI) *Apr 2021 – Aug 2021*
Undergraduate Researcher; Supervisor: Martha White & Adam White (DeepMind) Edmonton, AB

- Collaborated with leading RL researchers to **automate a real-world water treatment plant** using reinforcement learning.
- Benchmarked the first predictive agent for the plant by applying **Q-learning and SARSA with linear function approximation** on sensory data.
- Demonstrated that **classical methods outperformed deep RL (e.g., DQN with replay buffers)** on key benchmarks, supporting simpler, more interpretable deployment in industrial systems.

Derda Research Group *Apr 2019 – Jun 2021*
Undergraduate Researcher; Supervisor: Ratmir Derda & Russ Greiner (Amii) Edmonton, AB

- Pioneered the first ML project in the glycomics lab, developing a **deep learning model (GlyNet)** to predict protein–carbohydrate interactions from molecular structure.
- Developed a **novel fingerprint encoding for carbohydrates**, enabling accurate binding predictions across thousands of protein targets; the resulting multi-output neural network achieved an **R^2 of 0.78**.
- Published GlyNet in the Royal Society of Chemistry; the **model remains in active use today** and has enabled successful experimental validations of novel glycan–protein interactions.
- Presented research at **major scientific conferences (GlycoNet)**, communicating technical findings through posters and talks; awarded three competitive undergraduate research scholarships during this time.

Skills

Programming - Python, R, Swift, SQL
Frameworks - PyTorch, scikit-learn, XGBoost, NumPy, Polars, RDKit
Algorithms - Transformers, LLMs, MLPs, CNNs, SARSA, Q-Learning

Education

University of Alberta *Sep 2018 – May 2023*
B.Sc. in Physics; GPA: 3.2 Edmonton, AB

- Reinforcement Learning I (CMPUT 397) with Martha White; Grade: A
- Reinforcement Learning II (CMPUT 609) with Richard S. Sutton; Grade: A-

Awards

Alberta Innovates Summer Research Studentship 2021
GlycoNet Summer Award for Undergraduate Students 2021
Undergraduate Research Initiative Stipend 2020

Publications

[1] GlyNet: a multi-task neural network for predicting protein–glycan interactions. ***Royal Society of Chemistry***, 2022.
[2] Genetically encoded multivalent liquid glycan array displayed on M13 bacteriophage. ***Nature Chemical Biology***, 2021.