Job Title: Machine Learning Engineer, Department of Computer Science

Reports to: Dr. Rintu Kutum, Department of Computer Science and Dr. Sourav Chatterjee, Department of Chemistry

Location: Ashoka University, Plot No. 2, Rajiv Gandhi Education City, Rai, Sonipat, Haryana 131029

Experience (in years): 0-1 years

Nature of work: On-site, full time 40 hr/week

Salary (consolidated): Up to 45,000/- (based on experience)

About Ashoka University:

Ashoka University is India's premier interdisciplinary teaching and research university, an institution that has become a beacon of academic excellence in the less than 10 years since its inception. At Ashoka, we encourage you to embrace change, learn and grow continuously, and strive for excellence in what you do.

As part of our thriving and committed workforce, you will:
Be Mission-Driven: Champion interdisciplinary learning, innovative pedagogy, and academic rigor to transform Indian higher education.
Think Strategically: Collaborate with other innovative colleagues to shape the future of higher education through strategic planning and a forward-thinking approach.
Act Authentically: Embrace authenticity and integrity, fostering an inclusive and supportive environment where every voice is valued.
Take Accountability: Own your work and drive positive change, as an individual seeking to make a meaningful contribution.
Build Collaboration: Experience the power of teamwork and diverse perspectives, working collectively towards our shared goals.
Deliver Excellence: Strive for high quality in all aspects, upholding the highest standards of academic excellence, student support, and professional development opportunities.

At Ashoka University, we are on a mission to redefine higher education and create a remarkable space where innovation and collaboration thrives. As a **pioneering force in interdisciplinary learning**, we **continually grow and adapt** to stay at the forefront of educational excellence with emphasis on inclusivity and equal opportunity. Our philosophy revolves around **care, well-being, and connection**, which are deeply embedded in everything we do.

When you join our community, you become part of an extraordinary journey in which you can enhance your potential and make a meaningful impact.

About the Department of Computer Science:

The unique positioning of our department in a liberal arts environment in India engenders opportunities to apply computational thinking to the sciences and the social sciences, as well as take advantage of the cross-pollination of ideas from other disciplines to generate and define problems in CS. We are actively doing impactful research towards disciplinary questions in CS as well as bringing CS methods into the natural and social sciences. In particular, the department is actively engaged in digitisation and data questions in health, education and welfare; cryptography, privacy and security; data science and AI for public good; epidemiology and modeling; molecular and systems biology; quantum computing; psychology; environment; elections and politics.

Role and Responsibilities:

The candidate will dedicatedly work in the screening of small molecule modulators for target proteins of interest using machine learning. The candidate will be responsible for literature review, drafting manuscript, experimental design and closely work with our collaborator (Dr. Sourav Chatterjee, Department of Chemistry, Ashoka University).

Briefly, the project focuses on developing geometric machine learning algorithms (such as predicting drug-target binding affinity with GNN) to predict active molecules against proteins of interest from a curated database (~4 million small molecules/compounds). The project also involves benchmarking state

of the art existing algorithms in this area and identifying potential inhibitors.

Qualifications and Skills Required:

- BS-MS in physics/chemistry with strong computational and machine learning experience (during dissertation).
- BTech in CSE (specialization in graph neural networks) + minimum 1 year of experience.
- MTech with specialization in machine learning.
- High proficiency in Python/C++/Julia.
- Contribution to open source libraries (highly preferred).
- Experience in graph representation learning and good track record of publications in reputed machine learning conferences (such as NeurIPS, ICLR, ICML, etc.) (highly preferred).
- Planning for pursuing Ph.D. in the intersection of graph machine learning, drug discovery and precision health (highly preferred).

  Individuals who are self driven, motivated and interested in working with interdisciplinary research groups are highly encouraged to apply.

Application Submission Process:

Submit your application to Dr. Rintu Kutum, Department of Computer Science to ensure your candidacy receives the attention it deserves, kindly follow the application submission process outlined below:

Prepare an Updated CV: Showcase your professional accomplishments, skills, and experiences in an updated curriculum vitae. Kindly also include publications (can be pre-print) and GitHub repository of your previous contributions in machine learning.

Submit Your Application: Email your CV to rintu.kutum@ashoka.edu.in, ensuring the subject line reads as follows: "ML Engineer – Drug Target Binding Affinity – <Applicant Name>". Candidates should also fill out the form below.
Link to form: https://forms.gle/h95XdB3F1YcvVVZa9

Include Essential Details: Along with your latest CV with publications (can be pre-print) and GitHub repository of your previous contributions in machine learning, kindly share the following documents:

- Statement of Purpose (1 page) - your motivation for the position and long term plan.
- One letter of recommendation from the previous guide (can be academic thesis mentor)

Only shortlisted candidates will be contacted as part of our rigorous selection process.

Adherence to Deadlines: To ensure fairness and efficiency, please submit your application by **10th Sept, 2024**. Applications received after the deadline will not be considered.