Title:-

Leveraging representation learning for drug discovery.

Abstract:-

Deciphering the secrets of cellular machinery and disease progression is critical for developing solutions in prognosis and in silico drug discovery. The ability to extract quantifiable information about cellular processes allows the profiling that is necessary to devise strategies for mitigating aberrations induced in a diseased state. Advances in high-throughput technologies have allowed characterisation of this information in the form of large-scale biological datasets at multiple levels of subcellular machinery. Traditional methods used to examine this data do not have sufficient sensitivity to identify correlations between molecular patterns and distinguishing characteristics of a disease. Moreover, such profiling methods do not allow for the stratification of high-risk malignancies at a molecular level. This is one of the primary drivers of research in personalized medicine. Over the years, machine learning algorithms have found their utility in analysing biological datasets due to their ability to model complex distributions and identify data patterns. However, there is a gap in methods to effectively represent biological datasets in a way that maximises the amount of information presented to the ML agent.

This talk has two parts. The first part is on the key notables that laid the foundation for AI in biomedical research. The second part of the talk will deal with how our group is developing frameworks capable of extracting relevant information from omics, sequence and structural datasets efficiently for downstream ML-based solutions in prognosis modelling and drug discovery.