

Opportunities and challenges of graph learning in biomedicine

Pietro Lio (University of Cambridge)

In this talk I will focus on Graph representation learning in bioinformatics and medicine. The aim is to characterise what AI scientists think doctors want and what is expected to be delivered, in other words solving the conundrum at the heart of AI and Medicine. I will introduce the molecular scale and the challenges of diffusion models in protein design. Then the cell scale and the role of cancer graph signature. The cell and tissue scales allow for hypergraph neural networks methodologies. The patient scale provides the opportunities to discuss temporal graph networks. I will then focus on how to build a digital patient twin using graph representation and considering physiological (cardiovascular), clinical (inflammation) and molecular variables (multi omics and genetics). I will consider different pathologies such as inflammaging and immune senescence through the use of neural graph ODEs. I will discuss how this approach could also keep the clinician in the loop to avoid excessive automatisisation using logic and explainer frameworks. In particular inputting logic to recover interpretability and explainability would also enable Doctors in the loop.

I will conclude with some brief intro to Beyond Graph neural networks: the sheaves.