



PPD Seminar

Decision-making for workflows in computational biology, using AI and classical statistical approaches

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Modern computational science increasingly relies on complex workflows in which many decisions must be made: which data to process, which algorithms to apply, how their parameters should be chosen, and when a result is good enough to proceed. While similar challenges arise across many areas of computational science, they are important problems in computational biology, where workflows often involve many interdependent processing, modelling and analysis steps. In this seminar, we will discuss early-stage ALC-funded projects at STFC exploring how we are addressing these problems within computational biology, using complementary approaches ranging from classical statistical methods to machine learning and AI. Information from previous computations can be used to understand the behaviour of scientific workflows, predict outcomes, and guide future decisions. Doing this reliably raises fundamental questions about how success should be defined and measured, how uncertainty and heterogeneous data should be handled, and how optimisation objectives can be aligned with the scientific outcomes we actually care about. Using examples from computational structural biology, we will introduce the problems we are tackling, the approaches we are developing, and some of the challenges involved in making better-informed decisions within complex computational workflows.

