

### The Seminars on “Information Technology Outlook” - PhD Program in Computer Science and Mathematics



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## Mechanism-aware deep learning for biomedicine

In recent biomedical research, deep learning has been widely used for the exploitation of omics data when predicting the cell phenotype, suffering however from a lack of biological interpretability. In parallel, constraint-based mathematical modelling of metabolism has gained popularity due to its scope and flexibility, enabling mechanistic insights into the genotype-phenotype-environment relationship within cells. These two computational frameworks have mostly been used in isolation, having distinct research communities associated with them. However, their complementary characteristics and common mathematical bases make them particularly suitable to be combined. I will describe how machine learning can be combined with constraint-based modelling, discuss the mathematical and practical aspects involved, and show several applications in biotechnology and biomedicine. Instead of applying machine learning to omics data directly, we propose a multi-view approach merging experimental omics data and model-generated predictions, based on known biochemistry. This architecture can contribute with disjoint information towards biologically-informed and interpretable machine learning, including key mechanistic information in an otherwise biology-agnostic learning process.

*Claudio Angione is a Professor of Artificial Intelligence at Teesside University (TU), and a Turing Academic Liaison between TU and The Alan Turing Institute. He joined TU after a PostDoc at the University of Cambridge, and a research intern position at Microsoft Research UK. He holds a PhD in Computer Science from the University of Cambridge. His research group develops multi-modal AI tools that include mechanistic information, with recent projects being published in eLife, Cell Reports Methods, and PNAS. CA received a research award from the Italian Embassy in 2016, and a Turing Network Development Award from The Alan Turing Institute in 2022. He is currently the PI of a £550k BBSRC grant (BB/Y01278X/1), and a WP Lead of a £4.5m Horizon Europe grant (101182278).*