

Lecture "Science in the Age of Machine Learning"

Monday, 13 September 2021 15:15 (1 hour)

Traditionally the “best” observations are those with the largest signal from the most tightly controlled systems. In a wide range of phenomena –the dance of proteins in function, femtosecond breaking of molecular bonds, the gestation of fetuses –tight control is neither feasible, nor desirable. Modern machine-learning techniques extract far more information from sparse random sightings than usually obtained from set-piece experiments. I will describe on-going efforts to extract structural and dynamical information from noisy, random snapshots recorded with very poor, or non-existent timing information. Examples will include functional motions of molecular machines, and ultrafast dynamics of photo-induced reactions.

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Session Classification: Machine Learning - Theory