Machine Learning for Developing Understanding in Soft Matter Systems

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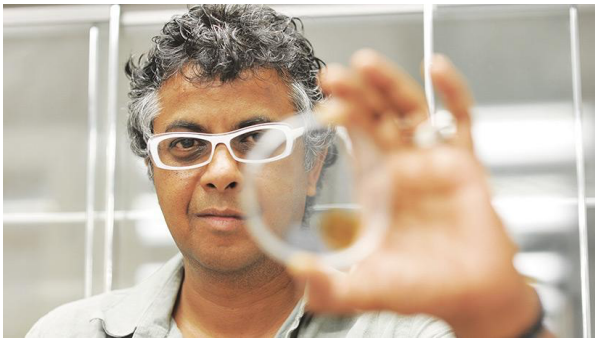

While much focus has been placed on the use of AI tools in the context of large data sets, their applicability to soft matter systems, where data sets are small ("precious data"), is significantly less explored. This will be the topic of this talk. We focus first of all on the applicability of machine learning as a tool for optimized materials design. While the forward problem, taking experimental inputs and predicting properties, is relatively straightforward to implement and obtain reliable predictions, the reverse problem, of designing a material with desired properties, is fraught with difficulties. The primary barriers here are the availability of sufficient high-quality data, while a second issue is data representation. These difficulties also apply to the more difficult, but important, problem of interpretable AI – namely understanding the key variables that underpin a physical situation. While we show that the tools of AI could have tremendous valuable, they should be used with considerable care in the context of experimental systems where data sets are typically small. We illustrate our approaches through two canonical problems – one in the design of membranes for gas separation, and the second towards controlling the properties of polymer-nanoparticle composites.