DATA SCIENCE COLLOQUIUM (SUMMER TERM 2022)



April 21st, 2022 at 2 PM DESY Auditorium & Online (Zoom)

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Statistical Challenges in Protein Dynamics Modelling

Collective atomic motions dominate the molecular dynamics of biological macromolecules such as proteins. Likewise, the functional dynamics of these molecules is accomplished by fine-tuned collective modes of atomic motion. Identification of the small set of collective degrees of freedom from a high-dimensional atomic space, that drive a certain protein function is of critical importance.

In this talk we consider several examples of protein dynamics modelling and discuss statistical challenges that arise due to complex and/or hierarchical protein structures, low variability of relevant atoms and temporal dependence in the data.

Chair: Prof. Nina Rohringer

MEET THE SPEAKER: All on-site attendees are invited to stay for a cup of coffee and a snack for further discussions and exchange after the official talk.

Please write a short email to <u>dashh-office@desy.de</u> or subscribe here (<u>https://lists.desy.de/sympa/subscribe/datasciencecolloquium</u>) to our mailing list for the Zoom link of the online event and registration to the on-site event.



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