

國立中央大學統計研究所

學術演講

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講 題:CLEAPA: A Framework For Exploring The Conformational
Landscape of Cryo-EM Using Energy-Aware Pathfinding Algorithm

時 間:113年3月19日 (星期二) 上午11:00 ~ 12:00

地 點:鴻經館M429室

茶 會:上午 10:30 ~ 11:00 地 點:鴻經館M510室

ABSTRACT

Cryo-electron microscopy (cryo-EM) has emerged as a leading method for deciphering the functional landscapes of proteins by resolving their conformational dynamics. The identification of trajectories within these landscapes is a pivotal component of the cryo-EM methodology, dependent on the outcomes of 3D conformational analyses. However, the evaluation and validation of these critical trajectories remain underexplored in existing literature. Addressing this gap, our talk emphasizes the necessity of establishing benchmarks for trajectory analysis, thereby enhancing the reliability of computational tools in revealing protein functions and understand their limitations. We will unveil a new framework designed for trajectory validation, highlighting a synthetic dataset creation process that generates data embodying major conformational changes, and introducing metrics for trajectory benchmarking. The presentation further explores an innovative method that incorporates statistical measures of local density into the trajectory search process's objective function. We will also discuss ongoing research efforts, including the application of kernel methods to refine density estimations. Expected to propel the cryo-EM field forward, our findings promise significant implications for dynamic protein research, potentially accelerating drug and vaccine discovery. The presentation showcases collaborative efforts with Teng-Yu Lin, and the publicly accessible source code can be found at https://github.com/tengyulin/energy_aware_pathfinding.

Keywords: Cryogenic electron microscopy, minimum energy path, dimension reduction, manifold learning, graph traversal

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