國立中山大學應用數學系 學術演講

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講 題:Einstein from noise and statistical de-noising

for cryo-EM Image Analysis

時 間:2018/10/18(星期四)14:10~15:00

地 點:理學院四樓理 SC 4009-1 室

茶 會:15:00 於理 SC 4010 室 (系辦公室)

摘 要

Single particle cryogenic electron microscopy (cryo-EM) has become a mainstream method for structural determination of biological molecules to near atomic resolution that the major developers were awarded 2017 Nobel Prize in Chemistry. Single particle cryo-EM images are extremely noisy due to low exposure to reduce radiation-damage. Besides, these images do not contain orientation information required for 3D structure reconstruction. Often times, reference is used to initiate the search of orientation, which has incurred the risk of coalescing images with low or no signal to the reference, known as the 'Einstein from noise' problem. Because nowadays a high-resolution image is composed of more than tens of thousands of pixels and sub-millions of images of molecule are routinely collected to realize near-atomic resolution, modern cryo-EM data is thereby characterized by high dimensionality as number of pixels (p) and large sample size as number of images (n), in addition to intrinsic low signal-to-noise-ratio (SNR). Here, we set out to investigate the phenomenon from model- bias viewpoint in terms of image dimensionality and sample size. By using mathematical modeling, we derive a surprisingly simple form of asymptotic distribution that shows the correlation between Einstein face and the spurious images from averaging the sorted m copies of images of pure identically independent Gaussian noise increases with n and m but decreased with p. To avoid 'Einstein from noise' pitfall, we propose a dimension reduction method as a data pre-processing tool to increase the SNR. We observe that this tool makes significant improvement in either computation time or clustering average quality in 2D clustering of various cryo-EM analysis packages.

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