統計科學研
INSTITUTE (

統計所學術演 中研院統計

學 術 演 講

講　題：Tukey計畫報告

講　者：Dr. Tso-Jung Yen and Dr. Frederick Kin Hing Phoa
顏佐榕博士與潘建興博士
(中央研究院統計科學研究所)

時　間：2023年12月4日(星期一)，10:30-11:00

地　點：統計所B1演講廳

Abstract

Dr. Frederick Kin Hing Phoa

In the second part of this talk, we introduce a brand new approach to molecular optimization via swarm intelligence. It involves a new MIX operation that accomodates the constrained chemical reactions for molecular formation. We compare the results of our methods with those of the existing methods, showing superior performance in terms of traditional criteria like QED. We further decompose QED into its original eight important molecule-like chemical properties and propose a new multi-objective optimization method to handle this 8-dimensional MOO problem. A Pareto front is formed associated to the results and we indicate where the best-known QED-optimal particles from existing methods are located in our solution domain. This work is a joint work with my doctoral student Ms. Hsin-Ping Liu of National Taiwan University, and my postdoctoral researcher Dr. Saykat Dutta of Academia Sinica.

Dr. Tso-Jung Yen

2nd Year Progress Report on the Fisher and Tukey Project

In this talk we report our progress in the Fisher and Tukey Project that focuses on using a data-driven approach to the property estimation and structural generation of molecules via deep learning. We first describe an on-going effort on building prediction intervals for molecular property prediction. We then discuss challenges we face when tackling the molecule generation problem and tools we may adopt for solving the generation problem. We also report our study on point cloud reconstruction using generative models trained under the denoising diffusion probabilistic model (DDPM) framework. This study shows that generative models trained under DDPM are capable for high-dimensional point simulation, and DDPM may serve as a benchmark framework for model training for solving the molecule generation problem.

※ 茶　會：10：10開始。

※ 實體演講，不開放線上視訊。