Bioinformatics Seminar Series

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14:00-15:00 at CB207

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Building and Validating Biomolecular Structure Models for cryo-EM Maps Using Deep Learning

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Cryo-electron microscopy (cryo-EM) has become one of the main experimental methods for determining biomolecular structures including proteins and nucleic acids. Molecular structure modeling from cryo-EM is in general more difficult than conventional methods such as X-ray crystallography since the resolution of maps is often not high enough to specify atom positions. We have been developing a series of computational methods for modeling protein and nucleic acid structures from cryo-EM maps. For maps at medium resolution, deep learning can detect characteristic local density features of amino acids and secondary structures, which can be used to guide structure modeling. Local density features are also used for validating existing protein structure models in PDB. The protein model quality assessment score, DAQ, we developed recently, compares local density patterns captured by deep learning with amino acid positions in a model and detects potential errors in the model. In a large-scale analysis of protein models from cryo-EM, we found that a substantial small number of models may have some errors. All the tools we developed are available at https://kiharalab.org/emsuites/.