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Generating Efficient Neural Networks for Protein Diffraction Data

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Proteins and other biological molecules are responsible for many vital cellular functions, such as transport, signaling, or catalysis, and dysfunction can result in diseases. Information on the 3-dimensional (3D) structures of biological molecules and their dynamics is essential to understand mechanisms of their functions, leading to medicinal applications such as drug design. Different proteins have different structures; proteins in the same family share similar substructures and thus may share similar functions. Additionally, one protein may exhibit several structural states, also named conformations. X-ray Free Electron Laser (XFEL) beams are used to create diffraction patterns (images) that can reveal protein structure and function. The translation from diffraction patterns in the XFEL images to protein structures and functionalities is nontrivial.
We present A4NN (analytics for neural networks) applied to protein structure identification. In our previous talk, we reviewed our framework XPSI (XFEL-based Protein Structure Identifier). XPSI combines DL (autoencoder) and ML (kNN) to capture key information that allows the identification of structural properties, such as spatial orientation, protein conformation, and protein type from the diffraction patterns. In this talk, we will discuss improvements to protein structure identification with neural networks and neural architecture search. We will show improvements in accuracy, efficiency, and accessibility. In particular, we will demonstrate how the NSGA-Net workflow increases access to machine learning for domain scientists. We will also deliver a Jupyter Notebook.
As next steps, we are working on 1) testing the framework with additional neural architecture search workflows; and 2) understanding the qualities of successful neural architectures for classification and regression problems.
This project is collaborative research between RIKEN, GCLab, and ICL.

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