New approach for structure reconstruction with machine learning methods in XFEL and Cryo-EM experiments.

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Structure reconstruction is one of important goals of modern science. Knowledge of atomic structure lead to significant achievements in various science fields. Rapid evolution in machine learning provide new instruments for data analysis in computer vision, classification, and other fields.

The rapid development of neural networks allowed to create new algorithms and data analysis schemes that are highly competitive with the best existing algorithms that have developed over the decades. In this work we present review of current state of art machine learning techniques for experimental data processing and 3d structure reconstruction of nanoscale particles and macromolecules. The methods are designed for X-ray Free Electron Lasers (XFEL) and Cryogenic Microscopy (CryoEM) experiments. We show our machine learning techniques to be effective for experimental data filtering and sorting and be promising for particle orientation determination. We examine various algorithms including Neural Networks, Decision Trees, Support Vector Machines and show their applicability and optimal sets of parameters for different stages of analysis. Our work is a joint effort of teams from Kurchatov Institute Supercomputer, CryoEM laboratory and DESY.