

CRYO-ELECTRON MICROSCOPY IMAGES ARE LOW-DIMENSIONAL

PILAR COSSIO

Simulation-based inference has been successful in the analysis of cryo-electron microscopy, particularly for estimating biomolecular conformations from individual images. However, the latent representations learned during training contain more information, which can support or complement the predictions learned in supervised mode. Here, with images of hemagglutinin, we demonstrate that the simulated and experimental data representations can be modeled as a low-dimensional smooth manifold. We identify the (non-linear) directions of variation of the main parameters of interest, and link physical parameter values to the experimental images. By using state-of-the-art manifold learning, we provide accurate visualizations of the data, quantitative supporting evidence to validate the neural predictions with insights into physical properties of the latent representation.