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Explore Heterogeneous Data Structures using Persistent Homology

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To explore the structural information of a heterogeneous dataset projected into lower dimensional representations, e.g. high-resolution microscopy where three dimensions (3D) marked histone position are projected into two dimensions (2D) focal plane, powerful tools to solve the following questions are highly wanted. 1) What kinds of robust measurements can make structures visible from structureless datasets? 2) Do projections conceal important structural information from the original data? 3) How can we characterize these structures?

To address this questions, we propose a topological method based on persistent diagrams (PDs). This method aims to capture multiscale shapes from model data. A well-known heterogeneous system, Lennard-Jones (LJ) is introduced as a physical model. Using molecular dynamics simulations, we generated a 3D LJ fluid as input. Several 2D projections are obtained from slices of different thickness of its linear system size. The resulting persistent homology calculations render up to two-dimensional PDs. Specific distributions in the PDs identify essential shape characteristics (cavities, tunnels) in the model atomic configuration. Physical properties like compressibility can be interpreted from the number and size of cavities in 3D and rings in 2D. Additional analysis is provided using three parameters from conventional methods in statistical mechanic: radial distribution function(RDF), the reduced fourth-order cumulant, isothermal compressibility. By comparing our approach with these conventional methods, we elucidate how we provide a unified approach that can not only classify topological features in all scale but also extract geometrical information in greater depth.