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Researches on Molecular Geometry and Related Applications

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Biomolecules such as proteins are the basic functional units of life activities. Geometric modeling on biomolecules is widely used in molecular visualization, geometric calculation, computer-aided drug design, biophysics and cheminformatics. Due to the irregularity and complexity of the geometric shape of biomolecules, it is an open challenge to effectively represent the molecular shape of biomolecules in high quality. This talk focuses on some related researches of molecular geometry and its application in molecular biology, image representation and numerical solution of partial differential equations.

The structures and shapes of biomolecules provide essential information about their interactions and functions. The computational cost of biomolecular shape representation increases rapidly as the number of atoms increase. We have developed an ellipsoid radial basis function neural network (ERBFNN) and an algorithm for sparsely representing molecular shape. The machine learning model were trained by optimizing a nonlinear loss function with L1 regularization. Experimental results reveal that our algorithm can represent the original molecular shape with a relatively higher accuracy and fewer scale of ERBFNN.

Furthermore, the sparse representation method is applied to the image field. For complicated image data, the anisotropic elliptic Gaussian radial basis function neural network with sparse optimization technique is used to represent the image sparsely. The experimental results show that our method can represent the input image with fewer elliptic Gaussian functions, and the accuracy is high.

The Poisson-Boltzmann (PB) equation and Poisson-Nernst-Planck (PNP) equations are two most commonly used continuum models describe the electrostatic interaction and diffusion process in electrolyte solution system. Conventional numerical methods such as the finite element method often led to divergence or abnormal numerical results while dealing with the continuum models. In recent years, machine learning has inspired a large number of new ideas in the field of numerical computing. Therefore, we solve the continuum models by using physics-informed neural networks (PINNs). The results show that the method can approximate the solution of the models well and is not sensitive to the convection dominated problem in the PNP model.