Towards a graph neural network solver for granular dynamics

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ABSTRACT

The discrete element method (DEM) is a versatile but computationally intensive method for granular dynamics simulation. We investigate the possibility of accelerating DEM simulations using graph neural networks (GNN), which automatically support variable connectivity between particles. This approach was recently found promising for particle-based simulation of complex fluids [1]. We start from a time-implicit, or nonsmooth, DEM [2], where the computational bottleneck is the process of solving a mixed linear complementarity problem (MLCP) to obtain the contact forces and particle velocity update. This solve step is substituted by a GNN, trained to predict the MLCP solution. Following [1], we employ an encoder-process-decoder structure for the GNN. The particle and connectivity data is encoded in an input graph with particle mass, external force, and previous velocity as node attributes, and contact overlap, normal, and tangent vectors as edge attributes. The sought solution is represented in the output graph with the updated particle velocities as node attributes and the contact forces as edge attributes. In the intermediate processing step, the input graph is converted to a latent graph, which is then advanced with a fixed number of message passing steps involving a multilayer perceptron neural network for updating the edge and node values. The output graph, with the approximate solution to the MLCP, is finally computed by decoding the last processed latent graph.

Both a supervised and unsupervised method are tested for training the network on granular simulation of particles in a rotating or static drum. AGX Dynamics [3] is used for running the simulations, and Pytorch [4] in combination with the Deep Graph Library [5] for the learning. The supervised model learns from ground truth MLCP solutions, computed using a projected Gauss-Seidel (PGS) solver, sampled from 1200 simulations involving 50-150 particles. The unsupervised model learns to minimize a loss function derived from the MLCP residual function using particle configurations extracted from the same simulations but ignoring the approximate solution from the PGS solver. The simulation samples are split into training data (80%), validation data (10%), and test data (10%). Network hyperparameter optimization is performed. The supervised GNN solver reaches an error level of 1% for the contact forces and 0.01% on the particle velocities for a static drum. For a rotating drum, the respective errors are 10% and 1%. The unsupervised GNN solver reaches 1% velocity errors, 5% normal forces errors, but it has significant problems with predicting the friction forces. The latter is presumably because of the discontinuous loss function that follows from the Coulomb friction law and therefore we explore regularization of it. Finally, we discuss the potential scalability and performance for large particle systems.

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