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Deep Learning for Energetic Material Detonation Performance
BRIAN BARNES, US Army Research Laboratory — We present advances in accurate, extremely rapid prediction of detonation performance for energetic molecules. These models may be integrated into larger efforts for high-throughput virtual screening, molecular optimization, or an experimentalists selection of molecules before attempting a hazardous synthesis. Our machine learning workflow utilizes (a) a reference dataset generated from quantum mechanical calculations and the Cheetah thermochemical code, and (b) a message-passing neural network (MPNN) for nonlinear regression. The MPNN is a graph convolutional deep learning model best used with large datasets such as the one in this study. We create models to predict detonation velocity, detonation pressure, heat of formation, and density. Critically, prediction of the detonation properties requires absolutely no information other than the skeletal formula for a molecule. Molecules evaluated are CHNO-containing molecules from public datasets and known explosives. Neural net architecture and training are discussed. The MPNN is also evaluated against baseline models such as a feed-forward network, LASSO, random forest regression, and kernel ridge regression. The Python workflow for parallel, automated dataset generation and analysis is also discussed.

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