Title: Random walk-based molecule encoding for drug property prediction

Abstract: In this paper, we propose a method for molecular property prediction, with applications to drug discovery. Density Functional Theory has been used in the past to calculate molecular properties, however its computational complexity prevents it from being used on the modern large-scale sets of molecules that are necessary for effective drug discovery. Machine learning methods have been introduced to more efficiently approximate molecular features, with graph-based neural networks currently being used most commonly. We present a random walk-based image encoding of molecules, which preserves the structural information of the molecules while enabling the use of standard convolutional neural networks for property prediction. In order to validate our method, we present experimental results on the widely used QM8 and QM9 datasets, which require the prediction of quantum mechanical properties of molecules. We reach the state of the art on certain features, while out-performing most conventional models on nearly all others.