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Time Frequency Like Representation and Forward Design in Molecular Design Using Signal Processing and Machine Learning

Sergey Han*

Managing Editor, Journal of Space Exploration, China

***Corresponding author:** Sergey Han, Managing Editor, Journal of Space Exploration, China, E-mail: spaceexploration@scholarres.org

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Abstract

The accumulation of molecular data from Quantum Mechanics (QM) theories such as Density Functional Theory (DFTQM) allows Machine Learning (ML) to speed up the discovery of new molecules, drugs, and materials. Models that combine QM and ML (QMML) have proven to be very effective in delivering QM precision at ML speed. In this paper, we show that by incorporating well-known Signal Processing (SP) techniques (such as short time Fourier transform, continuous wavelet analysis, and Wigner-Ville distribution) into the QMML pipeline, we can obtain a Powerful Machinery (QMSPML) that can be used for molecule representation, visualization, and forward design.

Keywords: Machine learning, Molecular design, Molecular visualization, Quantum mechanics, Signal processing

Introduction

The ultimate goal of many chemical, agrochemical, and pharmaceutical industries is to design drugs and materials with the properties we desire. Throughout history, researchers have devised various approaches to this problem. That is, creating molecules with specific properties. Among these techniques, the most time-consuming and expensive process is trial and error, which is still used today. Breakthroughs in Quantum Mechanics (QM) and Molecular Design (MD) at the turn of the century attempted to solve this problem more scientifically by solving the Schrodinger Equations (SE), which govern the system dynamics at the atomic scale. For large systems, this equation is extremely difficult to solve, prompting the development of a number of approaches for approximately solving the SEs. This question has already been thoroughly addressed in the literature on cheminformatics and Quantitative Structure Property Relationships (QSPRs), and numerous molecular descriptors have been proposed. Unfortunately, they frequently necessitate a significant amount of domain knowledge and are not always transferable across the entire CCS. The advances in precision achieved for QM9's energetic properties are truly remarkable. However, much work remains to be done in areas such as molecular representation that captures all of the molecule's features, or the development of new approaches for predicting a broader range of molecular properties below acceptable chemical accuracy. The goal of this research is to look at the MD problem from a different angle, using techniques inspired by and deeply rooted in SP. The challenge is to do it within the SP

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framework, in a way that performs similarly or better than current state-of-the-art techniques, while also demonstrating the benefits of using SP within the MD pipeline. The success of TFL representations of molecules in predicting their properties with MAEs lower than chemical accuracy indicates that these representations encode highly relevant information about the molecules. The TFL representations are inferred from the CM, which are computed using the atomic coordinates, so the connection between the TFL representations and the molecule structure is obvious.

Conclusion

We demonstrated in this study that time-frequency-like representations of molecules are a powerful tool for molecular representation and visualisation. We showed that these representations encode molecules' structural, geometric, energetic, electronic, and thermodynamic properties. We demonstrated a clear relationship between time-frequency-like representations and the structure, energetic, electronic, and thermodynamic properties of molecules using a deep convolutional neural networks approach in a regression framework and the benchmark QM9 dataset. As supporting documents, all of the codes and data generated and used in this study are available.