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TorsionNet

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Abstract

We propose `TorsionNet`, an open-source deep reinforcement learning library designed for molecular conformer generation using Python. `TorsionNet` features several pre-built environments and baseline agents based on state-of-the-art algorithms in the field. The environments and agents are built on a modular interface, allowing users to easily build and test new implementations. Additionally, `TorsionNet` comes with extensive logging and visualization tools for evaluation of agents and generated conformers, as well as a toolkit for generating and modifying molecules. `TorsionNet` is well-tested and thoroughly documented, and is available through on PyPi and on Github: `https://github.com/ZimmermanGroup/conformer-ml`.

Keywords: reinforcement learning, deep learning, deep reinforcement learning, open source, conformer generation, computational chemistry

1. Introduction

In the past decade, deep reinforcement learning has been increasingly explored in the field of computational chemistry, including tasks such as protein folding [], improving chemical reactions [], and conformer generation [].

2. TorsionNet Architecture

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2.1 Environments

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2.2 Molecule Generation

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2.3 Agents

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2.4 Models

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2.5 Logging and Analysis

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3. Future Work

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4. Conclusions

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Acknowledgments

We would like to acknowledge ...

References

Appendix A.