ReadMe

This is a light forum for the application of AI in molecule science.

For related review, see `./review` folder.

For models, see `./model` folder.

Here presents a short description.

Database

2020 ChemDataExtractor

Comment: Extract experimental data to construct a database.

2020 experiment-oriented

Comment: Extract experimental data to construct a database. Trained an AI to predict new electrolytes.

2022 RedDB

Comment: Construct a database with a specified core.

ML Review

2020 Descriptor

Physics-Inspired Structural Representations for Molecules and Materials

Cite This: https://doi.org/10.1021/acs.chemrev.1c00021

Comment:

A summary of cutting-edge descriptors.

A very detailed guide to building the description module with respect to Symmetry, Smoothness, Completeness, Locality, and Additivity.

2020 4generation

Four Generations of High-Dimensional Neural Network Potentials.

Cite This: https://doi.org/10.1021/acs.chemrev.0c00868

Comment:

A very much detailed description of the history of NNP.

1: without any symmetry considered.

2: with symmetry considered, yet limited to the local environment.

3: with long-range electrostatic interactions considered.

4: with non-local charge transfer considered.

Some description is hard to understand.

2020 MLFF

Machine Learning Force Fields

Cite This: https://dx.doi.org/10.1021/acs.chemrev.0c01111

Comment:

Focusing on FF(sGDML), which is a relatively cheap.

2020 October. not cutting-edge.

Focusing on the work of Klaus-Robert Müller.

2021 DIG

DIG: A Turnkey Library for Diving into Graph Deep Learning Research

Journal of Machine Learning Research 22 (2021) 1-9

Comment:

Focusing on the work of Shuiwang Ji, Texas A&M University.

A summary of GNN-related works, including graph generation, self-supervised learning, interpretability, and deep learning.

2022 road_map

Roadmap on Machine learning in electronic structure. Electron. Struct. 4 (2022) 023004

Comment:

Covered multiple applications:

- Predicting material properties
- Construction of accurate force fields and beyond
- Solving the many-body problem with machine learning, etc.

An overview of current research hotspots is brought out, yet the description is relatively short.

2023 SchNetPack 2.0

SchNetPack 2.0: A neural network toolbox for atomistic machine learning

J. Chem. Phys. 158, 144801 (2023)
https://doi.org/10.1063/5.0138367

Comment:

Focusing on the work of Klaus-Robert Müller.

A summary of cutting-edge models, including SchNet and multiple successors.

Model

A summary of recent models. (To do: add DeepMD community works)

They are divided into pro-DFT and pro-GNN models. Some tricks are summarized in the trick folder.

pro-DFT

2017 DTNN

Comment: The Quantum-chemical inspired model. Father of schnet.

2018 SchNet_JCP

Comment: Schnet.

Add a continuous-filter convolutional layer for better simulation of the basis set in DFT.

2019 SchNOrb

Comment: Extension to predict HOMO-LUMO

2021 FieldSchNet

Comment: Extension to predict solvent effects

2021 SpookyNet (3M parameters)

Comment:

Add support for non-local effects.

Add support for Charge input.

Add support for multiplicity input.

2022 Kernel-Based MLFF

Comment: Update on Kernel-Based MLFF (old-school)

2023 sGDML

Comment: MLFF for giant systems (200~400)

2023 SchNetPack 2.0

Comment: A summary of schnet techs.

pro-GNN

2020 DimeNet (key to add ang info)

Comment: Directional MPNN (add angular information for the first time)

2020 DimeNet++

Comment: update of some key modules to enhance performance.

2022 SMP

(preprint as spherenet in 2021)

Comment: Add torsion information (huge computational cost) (dis, ang, tor)

2021 PAINN

Comment: Add Angular information to schnet but non-directional MPNN (dis, ang)

2022 ComENet

Comment: update of spherenet but non-directional MPNN (dis, ang, tor)

2022 NequIP (key to point out E3)

Comment: Better integration of E3 (dis, ang)

2022 So3krates

Comment: update of PAINN with better integration of SO3 and attention modules. (**SODA** on MD17) (dis, ang)

unpublished left_net

Comment: update of ComENet, extend SO3 to 3D Isomorphism

trick

self-supervised learning

2022 GEM

Comment:
(1) the bond lengths prediction;
(2) the bond angles prediction;
(3) the atomic distance matrices prediction.
(GEM-2 is outperformed by uni-mol+ in recent months)
(outdated)

2022 MolCLR

Comment:
(1) Atom masking
(2) Bond deletion
(3) Subgraph removal

2023 uni_mol (47M parameters)

Comment: add noise on atom positions

2023 uni_mol +

Comment: very few steps to optimize (within the model, no need for optimizers) the geometry to an equrilibrim state.

Molecule generation

2019 G-Schnet

Comment: Extension of schnet to generate molecules.

2022 G-SphereNet

Comment: Extension of spherenet to generate molecules.

Moieties_ML

2023 ProNet

Comment: an extension of subgraph-level (moity) GNN for proteins. Better encode of Amino Acid.

unpublished_MoINN

Comment: Tool for moiety identification and Coarse-graining (CG) MD.