ML4MOL

ML4Mol playlist

<https://www.youtube.com/playlist?list=PLmHiD62xzGu4FrJrlRrDEmRiEpdiDIQZ2>

Dataset Collection <https://moleculenet.org/datasets-1>

For env use base(python 3.11.7)

Gpt [ML4MOL](https://chatgpt.com/c/52473d46-bac8-4441-bd59-7cdcd21ea2ce) <https://chatgpt.com/c/52473d46-bac8-4441-bd59-7cdcd21ea2ce>

Large datasets of WDN

C:\Users\Dell Optiplex\Downloads\2404.15386v1.pdf

<https://zenodo.org/records/10974087>

<https://drive.google.com/drive/u/1/folders/1nPO7qfOBAoUSRLozyqfaf7hxrBnFV-7g>

## **Error:from** dgl.nn.pytorch import Set2Set

**FileNotFoundError**: Cannot find DGL C++ graphbolt library at c:\SPDP\Graph Neural Network\pppvenv\Lib\site-packages\dgl\graphbolt\graphbolt\_pytorch\_2.3.1.dll

<https://www.dgl.ai/pages/start.html>

# Since 2024.06.27, we have stopped providing packages for Windows and MacOS. The latest version of available package is 2.2.1. For newer versions, please install from source.

# If you have installed dgl-cuXX package, please uninstall it first.

pip install dgl -f https://data.dgl.ai/wheels/cu121/repo.html

gpt Uninstall the current version of PyTorch:

pip uninstall torch

<https://pytorch.org/get-started/previous-versions/>

# CUDA 12.1

pip install torch==2.2.1 torchvision==0.17.1 torchaudio==2.2.1 --index-url https://download.pytorch.org/whl/cu121

pip install dgl -f https://data.dgl.ai/wheels/cu121/repo.html

pip uninstall dgl

Successfully uninstalled dgl-2.2.1

pip install dgl -f https://data.dgl.ai/wheels/cu121/repo.html

**ModuleNotFoundError**: No module named 'pydantic'

pip uninstall torch

pip install torch==2.1.2 torchvision==0.16.2 torchaudio==2.1.2 --index-url https://download.pytorch.org/whl/cu121

pip uninstall dgl

pip install dgl -f <https://data.dgl.ai/wheels/cu121/repo.html>

I was not have success with pppvenv but base(python 3.11.7) is able to load necessary files

## **/Error:from** dgl.nn.pytorch import Set2Set