DeePMD-kit

Deep Modeling

Oct 15, 2021

GETTING STARTED

DeePMD-kit is a package written in Python/C++, designed to minimize the effort required to build deep learning based model of interatomic potential energy and force field and to perform molecular dynamics (MD). This brings new hopes to addressing the accuracy-versus-efficiency dilemma in molecular simulations. Applications of DeePMD-kit span from finite molecules to extended systems and from metallic systems to chemically bonded systems.

Important: The project DeePMD-kit is licensed under GNU LGPLv3.0. If you use this code in any future publications, please cite this using *Han Wang, Linfeng Zhang, Jiequn Han, and Weinan E. "DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics." Computer Physics Communications 228 (2018): 178-184.*

CHAPTER

ONE

GETTING STARTED

In this text, we will call the deep neural network that is used to represent the interatomic interactions (Deep Potential) the model. The typical procedure of using DeePMD-kit is

1.1 Easy install

There various easy methods to install DeePMD-kit. Choose one that you prefer. If you want to build by yourself, jump to the next two sections.

After your easy installation, DeePMD-kit (`dp`) and LAMMPS (`lmp`) will be available to execute. You can try `dp -h` and `lmp -h` to see the help. `mpirun` is also available considering you may want to train models or run LAMMPS in parallel.

- *Install off-line packages*
- *Install with conda*
- *Install with docker*

1.1.1 Install off-line packages

Both CPU and GPU version offline packages are available in the Releases page.

Some packages are splited into two files due to size limit of GitHub. One may merge them into one after downloading:

```
cat deepmd-kit-2.0.0-cuda11.3_gpu-Linux-x86_64.sh.0 deepmd-kit-2.0.0-cuda11.3_gpu-Linux-
↪x86_64.sh.1 > deepmd-kit-2.0.0-cuda11.3_gpu-Linux-x86_64.sh
```

1.1.2 Install with conda

DeePMD-kit is avaiable with conda. Install Anaconda or Miniconda first.

One may create an environment that contains the CPU version of DeePMD-kit and LAMMPS:

```
conda create -n deepmd deepmd-kit=*=*cpu libdeepmd=*=*cpu lammps-dp -c https://conda.
↪deepmodeling.org
```

Or one may want to create a GPU environment containing CUDA Toolkit:

```
conda create -n deepmd deepmd-kit=*=*gpu libdeepmd=*=*gpu lammps-dp cudatoolkit=11.3␣
↪horovod -c https://conda.deepmodeling.org
```

One could change the CUDA Toolkit version from `10.1` or `11.3`.

One may speficy the DeePMD-kit version such as `2.0.0` using

```
conda create -n deepmd deepmd-kit=2.0.0=*cpu libdeepmd=2.0.0=*cpu lammps-dp=2.0.0␣
↪horovod -c https://conda.deepmodeling.org
```

One may enable the environment using

```
conda activate deepmd
```

1.1.3 Install with docker

A docker for installing the DeePMD-kit is available here.

To pull the CPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.0.0_cpu
```

To pull the GPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.0.0_cuda10.1_gpu
```

1.2 Prepare data with dpdata

One can use the a convenient tool `dpdata` to convert data directly from the output of first priciple packages to the DeePMD-kit format.

To install one can execute

```
pip install dpdata
```

An example of converting data VASP data in `OUTCAR` format to DeePMD-kit data can be found at

```
$deepmd_source_dir/examples/data_conv
```

Switch to that directory, then one can convert data by using the following python script

```
import dpdata
dsys = dpdata.LabeledSystem('OUTCAR')
dsys.to('deepmd/npy', 'deepmd_data', set_size = dsys.get_nframes())
```

`get_nframes()` method gets the number of frames in the `OUTCAR`, and the argument `set_size` enforces that the set size is equal to the number of frames in the system, viz. only one `set` is created in the `system`.

The data in DeePMD-kit format is stored in the folder `deepmd_data`.

A list of all supported data format and more nice features of `dpdata` can be found at the official website.

1.3 Training a model

Several examples of training can be found at the `examples` directory:

```
$ cd $deepmd_source_dir/examples/water/se_e2_a/
```

After switching to that directory, the training can be invoked by

```
$ dp train input.json
```

where `input.json` is the name of the input script.

By default, the verbosity level of the DeePMD-kit is `INFO`, one may see a lot of important information on the code and environment showing on the screen. Among them two pieces of information regarding data systems worth special notice.

```
DEEPMD INFO    ---Summary of DataSystem: training     -----------------------------------
↪------------
DEEPMD INFO    found 3 system(s):
DEEPMD INFO                                        system  natoms  bch_sz   n_bch   prob␣
↪ pbc
DEEPMD INFO                          ../data_water/data_0/     192       1      80  0.250␣
↪   T
DEEPMD INFO                          ../data_water/data_1/     192       1     160  0.500␣
↪   T
DEEPMD INFO                          ../data_water/data_2/     192       1      80  0.250␣
↪   T
DEEPMD INFO    ---------------------------------------------------------------------------
↪------------
DEEPMD INFO    ---Summary of DataSystem: validation   -----------------------------------
↪------------
DEEPMD INFO    found 1 system(s):
DEEPMD INFO                                        system  natoms  bch_sz   n_bch   prob␣
↪ pbc
DEEPMD INFO                           ../data_water/data_3     192       1      80  1.000␣
↪   T
DEEPMD INFO    ---------------------------------------------------------------------------
↪------------
```

The DeePMD-kit prints detailed informaiton on the training and validation data sets. The data sets are defined by `"training_data"` and `"validation_data"` defined in the `"training"` section of the input script. The training data set is composed by three data systems, while the validation data set is composed by one data system. The number of atoms, batch size, number of batches in the system and the probability of using the system are all shown on the screen. The last column presents if the periodic boundary condition is assumed for the system.

During the training, the error of the model is tested every `disp_freq` training steps with the batch used to train the model and with `numb_btch` batches from the validating data. The training error and validation error are printed correspondingly in the file `disp_file` (default is `lcurve.out`). The batch size can be set in the input script by the key `batch_size` in the corresponding sections for training and validation data set. An example of the output

```
#  step      rmse_val    rmse_trn    rmse_e_val  rmse_e_trn    rmse_f_val  rmse_f_trn    ␣
↪     lr
      0      3.33e+01    3.41e+01      1.03e+01    1.03e+01      8.39e-01    8.72e-01    ␣
↪1.0e-03
```

(continues on next page)

(continued from previous page)

```
    100      2.57e+01    2.56e+01      1.87e+00    1.88e+00      8.03e-01    8.02e-01   ␣
↪1.0e-03
    200      2.45e+01    2.56e+01      2.26e-01    2.21e-01      7.73e-01    8.10e-01   ␣
↪1.0e-03
    300      1.62e+01    1.66e+01      5.01e-02    4.46e-02      5.11e-01    5.26e-01   ␣
↪1.0e-03
    400      1.36e+01    1.32e+01      1.07e-02    2.07e-03      4.29e-01    4.19e-01   ␣
↪1.0e-03
    500      1.07e+01    1.05e+01      2.45e-03    4.11e-03      3.38e-01    3.31e-01   ␣
↪1.0e-03
```

The file contains 8 columns, form right to left, are the training step, the validation loss, training loss, root mean square (RMS) validation error of energy, RMS training error of energy, RMS validation error of force, RMS training error of force and the learning rate. The RMS error (RMSE) of the energy is normalized by number of atoms in the system. One can visualize this file by a simple Python script:

```
import numpy as np
import matplotlib.pyplot as plt

data = np.genfromtxt("lcurve.out", names=True)
for name in data.dtype.names[1:-1]:
    plt.plot(data['step'], data[name], label=name)
plt.legend()
plt.xlabel('Step')
plt.ylabel('Loss')
plt.xscale('symlog')
plt.yscale('symlog')
plt.grid()
plt.show()
```

Checkpoints will be written to files with prefix `save_ckpt` every `save_freq` training steps.

1.3.1 Warning

It is warned that the example water data (in folder `examples/water/data`) is of very limited amount, is provided only for testing purpose, and should not be used to train a productive model.

1.4 Freeze a model

The trained neural network is extracted from a checkpoint and dumped into a database. This process is called "freezing" a model. The idea and part of our code are from Morgan. To freeze a model, typically one does

```
$ dp freeze -o graph.pb
```

in the folder where the model is trained. The output database is called `graph.pb`.

1.5 Test a model

The frozen model can be used in many ways. The most straightforward test can be performed using `dp test`. A typical usage of `dp test` is

```
dp test -m graph.pb -s /path/to/system -n 30
```

where `-m` gives the tested model, `-s` the path to the tested system and `-n` the number of tested frames. Several other command line options can be passed to `dp test`, which can be checked with

```
$ dp test --help
```

An explanation will be provided

```
usage: dp test [-h] [-m MODEL] [-s SYSTEM] [-S SET_PREFIX] [-n NUMB_TEST]
               [-r RAND_SEED] [--shuffle-test] [-d DETAIL_FILE]

optional arguments:
  -h, --help            show this help message and exit
  -m MODEL, --model MODEL
                        Frozen model file to import
  -s SYSTEM, --system SYSTEM
                        The system dir
  -S SET_PREFIX, --set-prefix SET_PREFIX
                        The set prefix
  -n NUMB_TEST, --numb-test NUMB_TEST
                        The number of data for test
  -r RAND_SEED, --rand-seed RAND_SEED
                        The random seed
  --shuffle-test        Shuffle test data
  -d DETAIL_FILE, --detail-file DETAIL_FILE
                        The file containing details of energy force and virial
                        accuracy
```

1.6 Run MD with LAMMPS

Running an MD simulation with LAMMPS is simpler. In the LAMMPS input file, one needs to specify the pair style as follows

```
pair_style      deepmd graph.pb
pair_coeff      * *
```

where `graph.pb` is the file name of the frozen model. It should be noted that LAMMPS counts atom types starting from 1, therefore, all LAMMPS atom type will be firstly subtracted by 1, and then passed into the DeePMD-kit engine to compute the interactions.

CHAPTER

TWO

INSTALLATION

2.1 Easy install

There various easy methods to install DeePMD-kit. Choose one that you prefer. If you want to build by yourself, jump to the next two sections.

After your easy installation, DeePMD-kit (`dp`) and LAMMPS (`lmp`) will be available to execute. You can try `dp -h` and `lmp -h` to see the help. `mpirun` is also available considering you may want to train models or run LAMMPS in parallel.

- *Install off-line packages*
- *Install with conda*
- *Install with docker*

2.1.1 Install off-line packages

Both CPU and GPU version offline packages are available in the Releases page.

Some packages are splited into two files due to size limit of GitHub. One may merge them into one after downloading:

```
cat deepmd-kit-2.0.0-cuda11.3_gpu-Linux-x86_64.sh.0 deepmd-kit-2.0.0-cuda11.3_gpu-Linux-
↪x86_64.sh.1 > deepmd-kit-2.0.0-cuda11.3_gpu-Linux-x86_64.sh
```

2.1.2 Install with conda

DeePMD-kit is avaiable with conda. Install Anaconda or Miniconda first.

One may create an environment that contains the CPU version of DeePMD-kit and LAMMPS:

```
conda create -n deepmd deepmd-kit=*=*cpu libdeepmd=*=*cpu lammps-dp -c https://conda.
↪deepmodeling.org
```

Or one may want to create a GPU environment containing CUDA Toolkit:

```
conda create -n deepmd deepmd-kit=*=*gpu libdeepmd=*=*gpu lammps-dp cudatoolkit=11.3␣
↪horovod -c https://conda.deepmodeling.org
```

One could change the CUDA Toolkit version from `10.1` or `11.3`.

One may speficy the DeePMD-kit version such as `2.0.0` using

```
conda create -n deepmd deepmd-kit=2.0.0=*cpu libdeepmd=2.0.0=*cpu lammps-dp=2.0.0␣
↪horovod -c https://conda.deepmodeling.org
```

One may enable the environment using

```
conda activate deepmd
```

2.1.3 Install with docker

A docker for installing the DeePMD-kit is available here.

To pull the CPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.0.0_cpu
```

To pull the GPU version:

```
docker pull ghcr.io/deepmodeling/deepmd-kit:2.0.0_cuda10.1_gpu
```

2.2 Install from source code

Please follow our github webpage to download the latest released version and development version.

Or get the DeePMD-kit source code by `git clone`

```
cd /some/workspace
git clone --recursive https://github.com/deepmodeling/deepmd-kit.git deepmd-kit
```

The `--recursive` option clones all submodules needed by DeePMD-kit.

For convenience, you may want to record the location of source to a variable, saying `deepmd_source_dir` by

```
cd deepmd-kit
deepmd_source_dir=`pwd`
```

2.2.1 Install the python interface

Install the Tensorflow's python interface

First, check the python version on your machine

```
python --version
```

We follow the virtual environment approach to install the tensorflow's Python interface. The full instruction can be found on the tensorflow's official website. Now we assume that the Python interface will be installed to virtual environment directory `$tensorflow_venv`

```
virtualenv -p python3 $tensorflow_venv
source $tensorflow_venv/bin/activate
pip install --upgrade pip
pip install --upgrade tensorflow
```

It is notice that everytime a new shell is started and one wants to use `DeePMD-kit`, the virtual environment should be activated by

```
source $tensorflow_venv/bin/activate
```

if one wants to skip out of the virtual environment, he/she can do

```
deactivate
```

If one has multiple python interpreters named like python3.x, it can be specified by, for example

```
virtualenv -p python3.7 $tensorflow_venv
```

If one does not need the GPU support of deepmd-kit and is concerned about package size, the CPU-only version of tensorflow should be installed by

```
pip install --upgrade tensorflow-cpu
```

To verify the installation, run

```
python -c "import tensorflow as tf;print(tf.reduce_sum(tf.random.normal([1000, 1000])))"
```

One should remember to activate the virtual environment every time he/she uses deepmd-kit.

Install the DeePMD-kit's python interface

Execute

```
cd $deepmd_source_dir
pip install .
```

One may set the following environment variables before executing `pip`:

Environment variables	Allowed value	Default value	Usage
DP_VARIANT	`cpu`, `cuda`, `rocm`	`cpu`	Build CPU variant or GPU variant with CUDA or ROCM support.
CUDA_TOOLKIT_ROOT_DIR	Path	Detected automatically	The path to the CUDA toolkit directory.
ROCM_ROOT	Path	Detected automatically	The path to the ROCM toolkit directory.

To test the installation, one should firstly jump out of the source directory

```
cd /some/other/workspace
```

then execute

```
dp -h
```

It will print the help information like

```
usage: dp [-h] {train,freeze,test} ...

DeePMD-kit: A deep learning package for many-body potential energy
representation and molecular dynamics

optional arguments:
  -h, --help            show this help message and exit

Valid subcommands:
  {train,freeze,test}
    train               train a model
    freeze              freeze the model
    test                test the model
```

Install horovod and mpi4py

Horovod and mpi4py is used for parallel training. For better performance on GPU, please follow tuning steps in Horovod on GPU.

```
# With GPU, prefer NCCL as communicator.
HOROVOD_WITHOUT_GLOO=1 HOROVOD_WITH_TENSORFLOW=1 HOROVOD_GPU_OPERATIONS=NCCL HOROVOD_
↪NCCL_HOME=/path/to/nccl pip install horovod mpi4py
```

If your work in CPU environment, please prepare runtime as below:

```
# By default, MPI is used as communicator.
HOROVOD_WITHOUT_GLOO=1 HOROVOD_WITH_TENSORFLOW=1 pip install horovod mpi4py
```

To ensure Horovod has been built with proper framework support enabled, one can invoke the `horovodrun --check-build` command, e.g.,

```
$ horovodrun --check-build

Horovod v0.22.1:

Available Frameworks:
    [X] TensorFlow
    [X] PyTorch
    [ ] MXNet

Available Controllers:
    [X] MPI
    [X] Gloo

Available Tensor Operations:
    [X] NCCL
    [ ] DDL
    [ ] CCL
    [X] MPI
    [X] Gloo
```

From version 2.0.1, Horovod and mpi4py with MPICH support is shipped with the installer.

If you don't install horovod, DeePMD-kit will fallback to serial mode.

2.2.2 Install the C++ interface

If one does not need to use DeePMD-kit with Lammps or I-Pi, then the python interface installed in the previous section does everything and he/she can safely skip this section.

Install the Tensorflow's C++ interface

Check the compiler version on your machine

```
gcc --version
```

The C++ interface of DeePMD-kit was tested with compiler gcc >= 4.8. It is noticed that the I-Pi support is only compiled with gcc >= 4.8.

First the C++ interface of Tensorflow should be installed. It is noted that the version of Tensorflow should be in consistent with the python interface. You may follow the instruction to install the corresponding C++ interface.

Install the DeePMD-kit's C++ interface

Now goto the source code directory of DeePMD-kit and make a build place.

```
cd $deepmd_source_dir/source
mkdir build
cd build
```

I assume you want to install DeePMD-kit into path `$deepmd_root`, then execute cmake

```
cmake -DTENSORFLOW_ROOT=$tensorflow_root -DCMAKE_INSTALL_PREFIX=$deepmd_root ..
```

where the variable `tensorflow_root` stores the location where the TensorFlow's C++ interface is installed.

One may add the following arguments to `cmake`:

CMake Aurgements	Allowed value	Default value	Usage
-DTENSORFLOW_ROOT=<value>	Path	-	The Path to TensorFlow's C++ interface.
-DCMAKE_INSTALL_PREFIX=<value>	Path	-	The Path where DeePMD-kit will be installed.
-DUSE_CUDA_TOOLKIT=<value>	`TRUE` or `FALSE`	`FALSE`	If `TRUE`, Build GPU support with CUDA toolkit.
-DCUDA_TOOLKIT_ROOT_DIR=<value>	Path	Detected automatically	The path to the CUDA toolkit directory.
-DUSE_ROCM_TOOLKIT=<value>	`TRUE` or `FALSE`	`FALSE`	If `TRUE`, Build GPU support with ROCM toolkit.
-DROCM_ROOT=<value>	Path	Detected automatically	The path to the ROCM toolkit directory.
-DLAMMPS_VERSION_NUMBER=<value>	Number	`20210929`	Only neccessary for LAMMPS built-in mode. The version number of LAMMPS (yyyymmdd).
-DLAMMPS_SOURCE_ROOT=<value>	Path	-	Only neccessary for LAMMPS plugin mode. The path to the LAMMPS source code (later than 8Apr2021). If not assigned, the plugin mode will not be enabled.

If the cmake has executed successfully, then

```
make -j4
make install
```

The option `-j4` means using 4 processes in parallel. You may want to use a different number according to your hardware.

If everything works fine, you will have the following executable and libraries installed in `$deepmd_root/bin` and `$deepmd_root/lib`

```
$ ls $deepmd_root/bin
dp_ipi      dp_ipi_low
$ ls $deepmd_root/lib
libdeepmd_cc_low.so  libdeepmd_ipi_low.so  libdeepmd_lmp_low.so  libdeepmd_low.so       ␣
↪  libdeepmd_op_cuda.so  libdeepmd_op.so
libdeepmd_cc.so      libdeepmd_ipi.so      libdeepmd_lmp.so      libdeepmd_op_cuda_low.
↪so  libdeepmd_op_low.so   libdeepmd.so
```

2.3 Install LAMMPS

There are two ways to install LAMMPS: the built-in mode and the plugin mode. The built-in mode builds LAMMPS along with the DeePMD-kit and DeePMD-kit will be loaded automatically when running LAMMPS. The plugin mode builds LAMMPS and a plugin separately, so one need to use `plugin load` command to load the DeePMD-kit's LAMMPS plugin library.

2.3.1 Install LAMMPS's DeePMD-kit module (built-in mode)

DeePMD-kit provide module for running MD simulation with LAMMPS. Now make the DeePMD-kit module for LAMMPS.

```
cd $deepmd_source_dir/source/build
make lammps
```

DeePMD-kit will generate a module called `USER-DEEPMD` in the `build` directory. If you need low precision version, move `env_low.sh` to `env.sh` in the directory. Now download the LAMMPS code (`29Oct2020` or later), and uncompress it:

```
cd /some/workspace
wget https://github.com/lammps/lammps/archive/stable_29Sep2021.tar.gz
tar xf stable_29Sep2021.tar.gz
```

The source code of LAMMPS is stored in directory `lammps-stable_29Sep2021`. Now go into the LAMMPS code and copy the DeePMD-kit module like this

```
cd lammps-stable_29Sep2021/src/
cp -r $deepmd_source_dir/source/build/USER-DEEPMD .
```

Now build LAMMPS

```
make yes-kspace
make yes-user-deepmd
make mpi -j4
```

If everything works fine, you will end up with an executable `lmp_mpi`.

```
./lmp_mpi -h
```

The DeePMD-kit module can be removed from LAMMPS source code by

```
make no-user-deepmd
```

2.3.2 Install LAMMPS (plugin mode)

Starting from `8Apr2021`, LAMMPS also provides a plugin mode, allowing one build LAMMPS and a plugin separately.

Now download the LAMMPS code (`8Apr2021` or later), and uncompress it:

```
cd /some/workspace
wget https://github.com/lammps/lammps/archive/stable_29Sep2021.tar.gz
tar xf stable_29Sep2021.tar.gz
```

The source code of LAMMPS is stored in directory `lammps-stable_29Sep2021`. Now go into the LAMMPS code and create a directory called `build`

```
mkdir -p lammps-stable_29Sep2021/build/
cd lammps-stable_29Sep2021/build/
```

Now build LAMMPS. Note that `PLUGIN` and `KSPACE` package must be enabled, and `BUILD_SHARED_LIBS` must be set to `yes`. You can install any other package you want.

```
cmake -D PKG_PLUGIN=ON -D PKG_KSPACE=ON -D LAMMPS_INSTALL_RPATH=ON -D BUILD_SHARED_
↪LIBS=yes -D CMAKE_INSTALL_PREFIX=${deepmd_root} -D CMAKE_INSTALL_LIBDIR=lib -D CMAKE_
↪INSTALL_FULL_LIBDIR=${deepmd_root}/lib ../cmake
make -j4
make install
```

If everything works fine, you will end up with an executable `${deepmd_root}/lmp`.

```
${deepmd_root}/lmp -h
```

2.4 Install i-PI

The i-PI works in a client-server model. The i-PI provides the server for integrating the replica positions of atoms, while the DeePMD-kit provides a client named `dp_ipi` that computes the interactions (including energy, force and virial). The server and client communicates via the Unix domain socket or the Internet socket. A full instruction of i-PI can be found here. The source code and a complete installation instructions of i-PI can be found here. To use i-PI with already existing drivers, install and update using Pip:

```
pip install -U i-PI
```

Test with Pytest:

```
pip install pytest
pytest --pyargs ipi.tests
```

2.5 Install GROMACS with DeepMD

2.5.1 Patch source code of GROMACS

Download source code of a supported gromacs version (2020.2) from https://manual.gromacs.org/2020.2/download.html. Run the following command:

```
export PATH=$PATH:$deepmd_kit_root/bin
dp_gmx_patch -d $gromacs_root -v $version -p
```

where `deepmd_kit_root` is the directory where the latest version of deepmd-kit is installed, and `gromacs_root` refers to source code directory of gromacs. And `version` represents the version of gromacs, **only support 2020.2 now**. You may patch another version of gromacs but still setting `version` to `2020.2`. However, we cannot ensure that it works.

2.5.2 Compile GROMACS with deepmd-kit

The C++ interface of `deepmd-kit 2.x` and `tensorflow 2.x` are required. And be aware that only deepmd-kit with **high precision** is supported now, since we cannot ensure single precision is enough for a GROMACS simulation. Here is a sample compile scipt:

```
#!/bin/bash
export CC=/usr/bin/gcc
export CXX=/usr/bin/g++
export CMAKE_PREFIX_PATH="/path/to/fftw-3.3.9" # fftw libraries
mkdir build
cd build

cmake3 .. -DCMAKE_CXX_STANDARD=14 \ # not required, but c++14 seems to be more␣
↪compatible with higher version of tensorflow
          -DGMX_MPI=ON \
          -DGMX_GPU=CUDA \ # Gromacs on ROCm has not been fully developed yet
          -DCUDA_TOOLKIT_ROOT_DIR=/path/to/cuda \
          -DCMAKE_INSTALL_PREFIX=/path/to/gromacs-2020.2-deepmd
make -j
make install
```

2.6 Building conda packages

One may want to keep both convenience and personalization of the DeePMD-kit. To achieve this goal, one can consider builing conda packages. We provide building scripts in deepmd-kit-recipes organization. These building tools are driven by conda-build and conda-smithy.

For example, if one wants to turn on `MPIIO` package in LAMMPS, go to `lammps-dp-feedstock` repository and modify `recipe/build.sh`. `-D PKG_MPIIO=OFF` should be changed to `-D PKG_MPIIO=ON`. Then go to the main directory and executing

```
./build-locally.py
```

This requires the Docker has been installed. After the building, the packages will be generated in `build_artifacts/linux-64` and `build_artifacts/noarch`, and then one can install then executing

```
conda create -n deepmd lammps-dp -c file:///path/to/build_artifacts -c https://conda.
↪deepmodeling.org -c nvidia
```

One may also upload packages to one's Anaconda channel, so they can be installed on other machines:

```
anaconda upload /path/to/build_artifacts/linux-64/*.tar.bz2 /path/to/build_artifacts/
↪noarch/*.tar.bz2
```

CHAPTER

THREE

DATA

In this section, we will introduce how to convert the DFT labeled data into the data format used by DeePMD-kit.

The DeePMD-kit organize data in `systems`. Each `system` is composed by a number of `frames`. One may roughly view a `frame` as a snap short on an MD trajectory, but it does not necessary come from an MD simulation. A `frame` records the coordinates and types of atoms, cell vectors if the periodic boundary condition is assumed, energy, atomic forces and virial. It is noted that the `frames` in one `system` share the same number of atoms with the same type.

3.1 Data conversion

One needs to provide the following information to train a model: the atom type, the simulation box, the atom coordinate, the atom force, system energy and virial. A snapshot of a system that contains these information is called a **frame**. We use the following convention of units:

Property	Unit
Time	ps
Length	Å
Energy	eV
Force	eV/Å
Virial	eV
Pressure	Bar

The frames of the system are stored in two formats. A raw file is a plain text file with each information item written in one file and one frame written on one line. The default files that provide box, coordinate, force, energy and virial are `box.raw`, `coord.raw`, `force.raw`, `energy.raw` and `virial.raw`, respectively. *We recommend you use these file names*. Here is an example of force.raw:

```
$ cat force.raw
-0.724  2.039 -0.951  0.841 -0.464  0.363
 6.737  1.554 -5.587 -2.803  0.062  2.222
-1.968 -0.163  1.020 -0.225 -0.789  0.343
```

This `force.raw` contains 3 frames with each frame having the forces of 2 atoms, thus it has 3 lines and 6 columns. Each line provides all the 3 force components of 2 atoms in 1 frame. The first three numbers are the 3 force components of the first atom, while the second three numbers are the 3 force components of the second atom. The coordinate file `coord.raw` is organized similarly. In `box.raw`, the 9 components of the box vectors should be provided on each line. In `virial.raw`, the 9 components of the virial tensor should be provided on each line in the order `XX XY XZ YX YY YZ ZX ZY ZZ`. The number of lines of all raw files should be identical.

We assume that the atom types do not change in all frames. It is provided by `type.raw`, which has one line with the types of atoms written one by one. The atom types should be integers. For example the `type.raw` of a system that has 2 atoms with 0 and 1:

```
$ cat type.raw
0 1
```

Sometimes one needs to map the integer types to atom name. The mapping can be given by the file `type_map.raw`. For example

```
$ cat type_map.raw
O H
```

The type `0` is named by "`O`" and the type `1` is named by "`H`".

The second format is the data sets of `numpy` binary data that are directly used by the training program. User can use the script `$deepmd_source_dir/data/raw/raw_to_set.sh` to convert the prepared raw files to data sets. For example, if we have a raw file that contains 6000 frames,

```
$ ls
box.raw  coord.raw  energy.raw  force.raw  type.raw  virial.raw
$ $deepmd_source_dir/data/raw/raw_to_set.sh 2000
nframe is 6000
nline per set is 2000
will make 3 sets
making set 0 ...
making set 1 ...
making set 2 ...
$ ls
box.raw  coord.raw  energy.raw  force.raw  set.000  set.001  set.002  type.raw  virial.
↪raw
```

It generates three sets `set.000`, `set.001` and `set.002`, with each set contains 2000 frames. One do not need to take care of the binary data files in each of the `set.*` directories. The path containing `set.*` and `type.raw` is called a *system*.

If one needs to train a non-periodic system, an empty `nopbc` file should be put under the system directory. `box.raw` is not necessary is a non-periodic system.

3.2 Prepare data with dpdata

One can use the a convenient tool `dpdata` to convert data directly from the output of first priciple packages to the DeePMD-kit format.

To install one can execute

```
pip install dpdata
```

An example of converting data VASP data in `OUTCAR` format to DeePMD-kit data can be found at

```
$deepmd_source_dir/examples/data_conv
```

Switch to that directory, then one can convert data by using the following python script

```
import dpdata
dsys = dpdata.LabeledSystem('OUTCAR')
dsys.to('deepmd/npy', 'deepmd_data', set_size = dsys.get_nframes())
```

`get_nframes()` method gets the number of frames in the `OUTCAR`, and the argument `set_size` enforces that the set size is equal to the number of frames in the system, viz. only one `set` is created in the `system`.

The data in DeePMD-kit format is stored in the folder `deepmd_data`.

A list of all supported data format and more nice features of `dpdata` can be found at the official website.

CHAPTER

FOUR

MODEL

4.1 Overall

A model has two parts, a descriptor that maps atomic configuration to a set of symmetry invariant features, and a fitting net that takes descriptor as input and predicts the atomic contribution to the target physical property. It's defined in the `model` section of the `input.json`, for example

```
"model": {
    "type_map":        ["O", "H"],
    "descriptor" :{
        "...": "..."
    },
    "fitting_net" : {
        "...": "..."
    }
}
```

Assume that we are looking for a model for water, we will have two types of atoms. The atom types are recorded as integers. In this example, we denote `0` for oxygen and `1` for hydrogen. A mapping from the atom type to their names is provided by `type_map`.

The model has two subsections `descritpor` and `fitting_net`, which defines the descriptor and the fitting net, respectively. The `type_map` is optional, which provides the element names (but not necessarily to be the element name) of the corresponding atom types.

DeePMD-kit implements the following descriptors:

1. *`se_e2_a`*: DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.
2. *`se_e2_r`*: DeepPot-SE constructed from radial information of atomic configurations. The embedding takes the distance between atoms as input.
3. *`se_e3`*: DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes angles between two neighboring atoms as input.
4. `loc_frame`: Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.
5. *`hybrid`*: Concate a list of descriptors to form a new descriptor.

The fitting of the following physical properties are supported

1. *`ener`*: Fitting the energy of the system. The force (derivative with atom positions) and the virial (derivative with the box tensor) can also be trained. See the example.

2. *dipole*: The dipole moment.
3. *polar*: The polarizability.

4.2 Descriptor "se_e2_a"

The notation of `se_e2_a` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from all information (both angular and radial) of atomic configurations. The `e2` stands for the embedding with two-atoms information. This descriptor was described in detail in the DeepPot-SE paper.

In this example we will train a DeepPot-SE model for a water system. A complete training input script of this example can be find in the directory.

```
$deepmd_source_dir/examples/water/se_e2_a/input.json
```

With the training input script, data are also provided in the example directory. One may train the model with the DeePMD-kit from the directory.

The construction of the descriptor is given by section `descriptor`. An example of the descriptor is provided as follows

```
    "descriptor" :{
        "type":             "se_e2_a",
        "rcut_smth":      0.50,
        "rcut":             6.00,
        "sel":            [46, 92],
        "neuron":             [25, 50, 100],
        "type_one_side":     true,
        "axis_neuron":     16,
        "resnet_dt":      false,
        "seed":             1
    }
```

- The `type` of the descriptor is set to `"se_e2_a"`.
- `rcut` is the cut-off radius for neighbor searching, and the `rcut_smth` gives where the smoothing starts.
- `sel` gives the maximum possible number of neighbors in the cut-off radius. It is a list, the length of which is the same as the number of atom types in the system, and `sel[i]` denote the maximum possible number of neighbors with type `i`.
- The `neuron` specifies the size of the embedding net. From left to right the members denote the sizes of each hidden layer from input end to the output end, respectively. If the outer layer is of twice size as the inner layer, then the inner layer is copied and concatenated, then a ResNet architecture is built between them.
- If the option `type_one_side` is set to `true`, then descriptor will consider the types of neighbor atoms. Otherwise, both the types of centric and neighbor atoms are considered.
- The `axis_neuron` specifies the size of submatrix of the embedding matrix, the axis matrix as explained in the DeepPot-SE paper
- If the option `resnet_dt` is set `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

4.3 Descriptor "se_e2_r"

The notation of `se_e2_r` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from the radial information of atomic configurations. The `e2` stands for the embedding with two-atom information.

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/se_e2_r/input.json
```

The training input script is very similar to that of `se_e2_a`. The only difference lies in the `descriptor` section

```
        "descriptor": {
            "type":                "se_e2_r",
            "sel":                 [46, 92],
            "rcut_smth":           0.50,
            "rcut":                6.00,
            "neuron":                [5, 10, 20],
            "resnet_dt":           false,
            "seed":                1,
            "_comment": " that's all"
        },
```

The type of the descriptor is set by the key "`type`".

4.4 Descriptor "se_e3"

The notation of `se_e3` is short for the Deep Potential Smooth Edition (DeepPot-SE) constructed from all information (both angular and radial) of atomic configurations. The embedding takes angles between two neighboring atoms as input (denoted by `e3`).

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/se_e3/input.json
```

The training input script is very similar to that of `se_e2_a`. The only difference lies in the `descriptor` section

```
        "descriptor": {
            "type":                "se_e3",
            "sel":                 [40, 80],
            "rcut_smth":           0.50,
            "rcut":                6.00,
            "neuron":                [2, 4, 8],
            "resnet_dt":           false,
            "seed":                1,
            "_comment":                " that's all"
        },
```

The type of the descriptor is set by the key "`type`".

4.5 Descriptor "hybrid"

This descriptor hybridize multiple descriptors to form a new descriptor. For example we have a list of descriptor denoted by D_1, D_2, ..., D_N, the hybrid descriptor this the concatenation of the list, i.e. D = (D_1, D_2, ..., D_N).

To use the descriptor in DeePMD-kit, one firstly set the `type` to `"hybrid"`, then provide the definitions of the descriptors by the items in the `list`,

```
        "descriptor" :{
            "type": "hybrid",
            "list" : [
                {
                    "type" : "se_e2_a",
                    ...
                },
                {
                    "type" : "se_e2_r",
                    ...
                }
            ]
        },
```

A complete training input script of this example can be found in the directory

```
$deepmd_source_dir/examples/water/hybrid/input.json
```

4.6 Fit energy

In this section, we will take `$deepmd_source_dir/examples/water/se_e2_a/input.json` as an example of the input file.

4.6.1 Fitting network

The construction of the fitting net is give by section `fitting_net`

```
        "fitting_net" : {
            "neuron":               [240, 240, 240],
            "resnet_dt":        true,
            "seed":                 1
        },
```

- `neuron` specifies the size of the fitting net. If two neighboring layers are of the same size, then a ResNet architecture is built between them.
- If the option `resnet_dt` is set `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

4.6.2 Loss

The loss function for training energy is given by

```
loss = pref_e * loss_e + pref_f * loss_f + pref_v * loss_v
```

where `loss_e`, `loss_f` and `loss_v` denote the loss in energy, force and virial, respectively. `pref_e`, `pref_f` and `pref_v` give the prefactors of the energy, force and virial losses. The prefectors may not be a constant, rather it changes linearly with the learning rate. Taking the force prefactor for example, at training step `t`, it is given by

```
pref_f(t) = start_pref_f * ( lr(t) / start_lr ) + limit_pref_f * ( 1 - lr(t) / start_lr )
```

where `lr(t)` denotes the learning rate at step `t`. `start_pref_f` and `limit_pref_f` specifies the `pref_f` at the start of the training and at the limit of `t -> inf`.

The `loss` section in the `input.json` is

```
    "loss" : {
        "start_pref_e":         0.02,
        "limit_pref_e":         1,
        "start_pref_f":         1000,
        "limit_pref_f":         1,
        "start_pref_v":         0,
        "limit_pref_v":         0
    }
```

The options `start_pref_e`, `limit_pref_e`, `start_pref_f`, `limit_pref_f`, `start_pref_v` and `limit_pref_v` determine the start and limit prefactors of energy, force and virial, respectively.

If one does not want to train with virial, then he/she may set the virial prefactors `start_pref_v` and `limit_pref_v` to 0.

4.7 Fit `tensor` like `Dipole` and `Polarizability`

Unlike `energy` which is a scalar, one may want to fit some high dimensional physical quantity, like `dipole` (vector) and `polarizability` (matrix, shorted as `polar`). Deep Potential has provided different API to allow this. In this example we will show you how to train a model to fit them for a water system. A complete training input script of the examples can be found in

```
$deepmd_source_dir/examples/water_tensor/dipole/dipole_input.json
$deepmd_source_dir/examples/water_tensor/polar/polar_input.json
```

The training and validation data are also provided our examples. But note that **the data provided along with the examples are of limited amount, and should not be used to train a productive model.**

Similar to the `input.json` used in `ener` mode, training json is also divided into `model`, `learning_rate`, `loss` and `training`. Most keywords remains the same as `ener` mode, and their meaning can be found *here*. To fit a tensor, one need to modify `model.fitting_net` and `loss`.

4.7.1 Fitting Network

The `fitting_net` section tells DP which fitting net to use.

The json of `dipole` type should be provided like

```
        "fitting_net" : {
                "type": "dipole",
                "sel_type": [0],
                "neuron": [100,100,100],
                "resnet_dt": true,
                "seed": 1,
        },
```

The json of `polar` type should be provided like

```
        "fitting_net" : {
                   "type": "polar",
                "sel_type": [0],
                "neuron": [100,100,100],
                "resnet_dt": true,
                "seed": 1,
        },
```

- `type` specifies which type of fitting net should be used. It should be either `dipole` or `polar`. Note that `global_polar` mode in version 1.x is already **deprecated** and is merged into `polar`. To specify whether a system is global or atomic, please see *here*.
- `sel_type` is a list specifying which type of atoms have the quantity you want to fit. For example, in water system, `sel_type` is `[0]` since `0` represents for atom `O`. If left unset, all type of atoms will be fitted.
- The rest `args` has the same meaning as they do in `ener` mode.

4.7.2 Loss

DP supports a combinational training of global system (only a global `tensor` label, i.e. dipole or polar, is provided in a frame) and atomic system (labels for **each** atom included in `sel_type` are provided). In a global system, each frame has just **one** `tensor` label. For example, when fitting `polar`, each frame will just provide a `1 x 9` vector which gives the elements of the polarizability tensor of that frame in order XX, XY, XZ, YX, YY, YZ, XZ, ZY, ZZ. By contrast, in a atomic system, each atom in `sel_type` has a `tensor` label. For example, when fitting dipole, each frame will provide a `#sel_atom x 3` matrix, where `#sel_atom` is the number of atoms whose type are in `sel_type`.

The `loss` section tells DP the weight of this two kind of loss, i.e.

```
loss = pref * global_loss + pref_atomic * atomic_loss
```

The loss section should be provided like

```
        "loss" : {
                "type":                 "tensor",
                "pref":                 1.0,
                "pref_atomic":          1.0
        },
```

- `type` should be written as `tensor` as a distinction from `ener` mode.

- `pref` and `pref_atomic` respectively specify the weight of global loss and atomic loss. It can not be left unset. If set to 0, system with corresponding label will NOT be included in the training process.

4.7.3 Training Data Preparation

In tensor mode, the identification of label's type (global or atomic) is derived from the file name. The global label should be named as `dipole.npy/raw` or `polarizability.npy/raw`, while the atomic label should be named as `atomic_dipole.npy/raw` or `atomic_polarizability.npy/raw`. If wrongly named, DP will report an error

```
ValueError: cannot reshape array of size xxx into shape (xx,xx). This error may occur␣
↪when your label mismatch it's name, i.e. you might store global tensor in `atomic_
↪tensor.npy` or atomic tensor in `tensor.npy`.
```

In this case, please check the file name of label.

4.7.4 Train the Model

The training command is the same as `ener` mode, i.e.

```
dp train input.json
```

The detailed loss can be found in `lcurve.out`:

```
#  step      rmse_val    rmse_trn    rmse_lc_val rmse_lc_trn rmse_gl_val rmse_gl_trn  lr
       0      8.34e+00    8.26e+00    8.34e+00    8.26e+00    0.00e+00    0.00e+00    1.0e-02
     100      3.51e-02    8.55e-02    0.00e+00    8.55e-02    4.38e-03    0.00e+00    5.0e-03
     200      4.77e-02    5.61e-02    0.00e+00    5.61e-02    5.96e-03    0.00e+00    2.5e-03
     300      5.68e-02    1.47e-02    0.00e+00    0.00e+00    7.10e-03    1.84e-03    1.3e-03
     400      3.73e-02    3.48e-02    1.99e-02    0.00e+00    2.18e-03    4.35e-03    6.3e-04
     500      2.77e-02    5.82e-02    1.08e-02    5.82e-02    2.11e-03    0.00e+00    3.2e-04
     600      2.81e-02    5.43e-02    2.01e-02    0.00e+00    1.01e-03    6.79e-03    1.6e-04
     700      2.97e-02    3.28e-02    2.03e-02    0.00e+00    1.17e-03    4.10e-03    7.9e-05
     800      2.25e-02    6.19e-02    9.05e-03    0.00e+00    1.68e-03    7.74e-03    4.0e-05
     900      3.18e-02    5.54e-02    9.93e-03    5.54e-02    2.74e-03    0.00e+00    2.0e-05
    1000      2.63e-02    5.02e-02    1.02e-02    5.02e-02    2.01e-03    0.00e+00    1.0e-05
    1100      3.27e-02    5.89e-02    2.13e-02    5.89e-02    1.43e-03    0.00e+00    5.0e-06
    1200      2.85e-02    2.42e-02    2.85e-02    0.00e+00    0.00e+00    3.02e-03    2.5e-06
    1300      3.47e-02    5.71e-02    1.07e-02    5.71e-02    3.00e-03    0.00e+00    1.3e-06
    1400      3.13e-02    5.76e-02    3.13e-02    5.76e-02    0.00e+00    0.00e+00    6.3e-07
    1500      3.34e-02    1.11e-02    2.09e-02    0.00e+00    1.57e-03    1.39e-03    3.2e-07
    1600      3.11e-02    5.64e-02    3.11e-02    5.64e-02    0.00e+00    0.00e+00    1.6e-07
    1700      2.97e-02    5.05e-02    2.97e-02    5.05e-02    0.00e+00    0.00e+00    7.9e-08
    1800      2.64e-02    7.70e-02    1.09e-02    0.00e+00    1.94e-03    9.62e-03    4.0e-08
    1900      3.28e-02    2.56e-02    3.28e-02    0.00e+00    0.00e+00    3.20e-03    2.0e-08
    2000      2.59e-02    5.71e-02    1.03e-02    5.71e-02    1.94e-03    0.00e+00    1.0e-08
```

One may notice that in each step, some of local loss and global loss will be `0.0`. This is because our training data and validation data consist of global system and atomic system, i.e.

```
        --training_data
                >atomic_system
                >global_system
```

(continues on next page)

(continued from previous page)

```
        --validation_data
                >atomic_system
                >global_system
```

During training, at each step when the lcurve.out is printed, the system used for evaluating the training (validation) error may be either with only global or only atomic labels, thus the corresponding atomic or global errors are missing and are printed as zeros.

4.8 Type embedding approach

We generate specific type embedding vector for each atom type, so that we can share one descriptor embedding net and one fitting net in total, which decline training complexity largely.

The training input script is similar to that of `se_e2_a`, but different by adding the `type_embedding` section.

4.8.1 Type embedding net

The `model` defines how the model is constructed, adding a section of type embedding net:

```
    "model": {
        "type_map":        ["O", "H"],
        "type_embedding":{
                        ...
        },
        "descriptor" :{
            ...
        },
        "fitting_net" : {
            ...
        }
    }
```

Model will automatically apply type embedding approach and generate type embedding vectors. If type embedding vector is detected, descriptor and fitting net would take it as a part of input.

The construction of type embedding net is given by `type_embedding`. An example of `type_embedding` is provided as follows

```
        "type_embedding":{
            "neuron":               [2, 4, 8],
            "resnet_dt":        false,
            "seed":                 1
        }
```

- The `neuron` specifies the size of the type embedding net. From left to right the members denote the sizes of each hidden layer from input end to the output end, respectively. It takes one-hot vector as input and output dimension equals to the last dimension of the `neuron` list. If the outer layer is of twice size as the inner layer, then the inner layer is copied and concatenated, then a ResNet architecture is built between them.
- If the option `resnet_dt` is set `true`, then a timestep is used in the ResNet.
- `seed` gives the random seed that is used to generate random numbers when initializing the model parameters.

A complete training input script of this example can be find in the directory.

```
$deepmd_source_dir/examples/water/se_e2_a_tebd/input.json
```

See *here* for further explanation of `type embedding`.

P.S.: You can't apply compression method while using atom type embedding

CHAPTER

FIVE

TRAINING

5.1 Training a model

Several examples of training can be found at the `examples` directory:

```
$ cd $deepmd_source_dir/examples/water/se_e2_a/
```

After switching to that directory, the training can be invoked by

```
$ dp train input.json
```

where `input.json` is the name of the input script.

By default, the verbosity level of the DeePMD-kit is `INFO`, one may see a lot of important information on the code and environment showing on the screen. Among them two pieces of information regarding data systems worth special notice.

```
DEEPMD INFO    ---Summary of DataSystem: training     -----------------------------------
↪------------
DEEPMD INFO    found 3 system(s):
DEEPMD INFO                                        system  natoms  bch_sz   n_bch   prob␣
↪ pbc
DEEPMD INFO                          ../data_water/data_0/     192       1      80  0.250␣
↪   T
DEEPMD INFO                          ../data_water/data_1/     192       1     160  0.500␣
↪   T
DEEPMD INFO                          ../data_water/data_2/     192       1      80  0.250␣
↪   T
DEEPMD INFO    -------------------------------------------------------------------------
↪------------
DEEPMD INFO    ---Summary of DataSystem: validation   -----------------------------------
↪------------
DEEPMD INFO    found 1 system(s):
DEEPMD INFO                                        system  natoms  bch_sz   n_bch   prob␣
↪ pbc
DEEPMD INFO                           ../data_water/data_3     192       1      80  1.000␣
↪   T
DEEPMD INFO    -------------------------------------------------------------------------
↪------------
```

The DeePMD-kit prints detailed informaiton on the training and validation data sets. The data sets are defined by `"training_data"` and `"validation_data"` defined in the `"training"` section of the input script. The training

data set is composed by three data systems, while the validation data set is composed by one data system. The number of atoms, batch size, number of batches in the system and the probability of using the system are all shown on the screen. The last column presents if the periodic boundary condition is assumed for the system.

During the training, the error of the model is tested every `disp_freq` training steps with the batch used to train the model and with `numb_btch` batches from the validating data. The training error and validation error are printed correspondingly in the file `disp_file` (default is `lcurve.out`). The batch size can be set in the input script by the key `batch_size` in the corresponding sections for training and validation data set. An example of the output

```
#  step      rmse_val    rmse_trn    rmse_e_val  rmse_e_trn    rmse_f_val  rmse_f_trn    ␣
↪     lr
      0      3.33e+01    3.41e+01      1.03e+01    1.03e+01      8.39e-01    8.72e-01    ␣
↪1.0e-03
    100      2.57e+01    2.56e+01      1.87e+00    1.88e+00      8.03e-01    8.02e-01    ␣
↪1.0e-03
    200      2.45e+01    2.56e+01      2.26e-01    2.21e-01      7.73e-01    8.10e-01    ␣
↪1.0e-03
    300      1.62e+01    1.66e+01      5.01e-02    4.46e-02      5.11e-01    5.26e-01    ␣
↪1.0e-03
    400      1.36e+01    1.32e+01      1.07e-02    2.07e-03      4.29e-01    4.19e-01    ␣
↪1.0e-03
    500      1.07e+01    1.05e+01      2.45e-03    4.11e-03      3.38e-01    3.31e-01    ␣
↪1.0e-03
```

The file contains 8 columns, form right to left, are the training step, the validation loss, training loss, root mean square (RMS) validation error of energy, RMS training error of energy, RMS validation error of force, RMS training error of force and the learning rate. The RMS error (RMSE) of the energy is normalized by number of atoms in the system. One can visualize this file by a simple Python script:

```
import numpy as np
import matplotlib.pyplot as plt

data = np.genfromtxt("lcurve.out", names=True)
for name in data.dtype.names[1:-1]:
    plt.plot(data['step'], data[name], label=name)
plt.legend()
plt.xlabel('Step')
plt.ylabel('Loss')
plt.xscale('symlog')
plt.yscale('symlog')
plt.grid()
plt.show()
```

Checkpoints will be written to files with prefix `save_ckpt` every `save_freq` training steps.

5.1.1 Warning

It is warned that the example water data (in folder `examples/water/data`) is of very limited amount, is provided only for testing purpose, and should not be used to train a productive model.

5.2 Advanced options

In this section, we will take `$deepmd_source_dir/examples/water/se_e2_a/input.json` as an example of the input file.

5.2.1 Learning rate

The `learning_rate` section in `input.json` is given as follows

```
    "learning_rate" :{
        "type":                "exp",
        "start_lr":         0.001,
        "stop_lr":         3.51e-8,
        "decay_steps":         5000,
        "_comment":         "that's all"
    }
```

- `start_lr` gives the learning rate at the beginning of the training.
- `stop_lr` gives the learning rate at the end of the training. It should be small enough to ensure that the network parameters satisfactorily converge.
- During the training, the learning rate decays exponentially from `start_lr` to `stop_lr` following the formula.

  ```
  lr(t) = start_lr * decay_rate ^ ( t / decay_steps )
  ```

  where `t` is the training step.

5.2.2 Training parameters

Other training parameters are given in the `training` section.

```
    "training": {
        "training_data": {
            "systems":                ["../data_water/data_0/", "../data_water/data_1/",
↪"../data_water/data_2/"],
            "batch_size":         "auto"
        },
        "validation_data":{
            "systems":                ["../data_water/data_3"],
            "batch_size":         1,
            "numb_btch":         3
        },

        "numb_step":         1000000,
        "seed":                1,
```

(continues on next page)

(continued from previous page)

```
        "disp_file":     "lcurve.out",
        "disp_freq":     100,
        "save_freq":     1000
    }
```

The sections "training_data" and "validation_data" give the training dataset and validation dataset, respectively. Taking the training dataset for example, the keys are explained below:

- systems provide paths of the training data systems. DeePMD-kit allows you to provide multiple systems with different numbers of atoms. This key can be a list or a str.
  - list: systems gives the training data systems.
  - str: systems should be a valid path. DeePMD-kit will recursively search all data systems in this path.
- At each training step, DeePMD-kit randomly pick batch_size frame(s) from one of the systems. The probability of using a system is by default in proportion to the number of batches in the system. More optional are available for automatically determining the probability of using systems. One can set the key auto_prob to
  - "prob_uniform" all systems are used with the same probability.
  - "prob_sys_size" the probability of using a system is in proportional to its size (number of frames).
  - "prob_sys_size; sidx_0:eidx_0:w_0; sidx_1:eidx_1:w_1;..." the list of systems are divided into blocks. The block i has systems ranging from sidx_i to eidx_i. The probability of using a system from block i is in proportional to w_i. Within one block, the probability of using a system is in proportional to its size.
- An example of using "auto_prob" is given as below. The probability of using systems[2] is 0.4, and the sum of the probabilities of using systems[0] and systems[1] is 0.6. If the number of frames in systems[1] is twice as system[0], then the probability of using system[1] is 0.4 and that of system[0] is 0.2.

```
        "training_data": {
            "systems":                ["../data_water/data_0/", "../data_water/data_1/",
↪"../data_water/data_2/"],
            "auto_prob":        "prob_sys_size; 0:2:0.6; 2:3:0.4",
            "batch_size":        "auto"
        }
```

- The probability of using systems can also be specified explicitly with key "sys_prob" that is a list having the length of the number of systems. For example

```
        "training_data": {
            "systems":                ["../data_water/data_0/", "../data_water/data_1/",
↪"../data_water/data_2/"],
            "sys_prob":        [0.5, 0.3, 0.2],
            "batch_size":        "auto:32"
        }
```

- The key batch_size specifies the number of frames used to train or validate the model in a training step. It can be set to
  - list: the length of which is the same as the systems. The batch size of each system is given by the elements of the list.
  - int: all systems use the same batch size.
  - "auto": the same as "auto:32", see "auto:N"

  - "auto:N": automatically determines the batch size so that the batch_size times the number of atoms in the system is no less than N.

- The key numb_batch in validate_data gives the number of batches of model validation. Note that the batches may not be from the same system

Other keys in the training section are explained below:

- numb_step The number of training steps.
- seed The random seed for getting frames from the training data set.
- disp_file The file for printing learning curve.
- disp_freq The frequency of printing learning curve. Set in the unit of training steps
- save_freq The frequency of saving check point.

5.2.3 Options and environment variables

Several command line options can be passed to dp train, which can be checked with

```
$ dp train --help
```

An explanation will be provided

```
positional arguments:
  INPUT                 the input json database

optional arguments:
  -h, --help            show this help message and exit

  --init-model INIT_MODEL
                        Initialize a model by the provided checkpoint

  --restart RESTART     Restart the training from the provided checkpoint

  --init-frz-model INIT_FRZ_MODEL
                        Initialize the training from the frozen model.
```

--init-model model.ckpt, initializes the model training with an existing model that is stored in the checkpoint model.ckpt, the network architectures should match.

--restart model.ckpt, continues the training from the checkpoint model.ckpt.

--init-frz-model frozen_model.pb, initializes the training with an existing model that is stored in frozen_model.pb.

On some resources limited machines, one may want to control the number of threads used by DeePMD-kit. This is achieved by three environmental variables: OMP_NUM_THREADS, TF_INTRA_OP_PARALLELISM_THREADS and TF_INTER_OP_PARALLELISM_THREADS. OMP_NUM_THREADS controls the multithreading of DeePMD-kit implemented operations. TF_INTRA_OP_PARALLELISM_THREADS and TF_INTER_OP_PARALLELISM_THREADS controls intra_op_parallelism_threads and inter_op_parallelism_threads, which are Tensorflow configurations for multithreading. An explanation is found here.

For example if you wish to use 3 cores of 2 CPUs on one node, you may set the environmental variables and run DeePMD-kit as follows:

```
export OMP_NUM_THREADS=6
export TF_INTRA_OP_PARALLELISM_THREADS=3
export TF_INTER_OP_PARALLELISM_THREADS=2
dp train input.json
```

One can set other environmental variables:

Environment variables	Allowed value	Default value	Usage
DP_INTERFACE_PREC	`high`, `low`	`high`	Control high (double) or low (float) precision of training.

5.3 Training Parameters

Note: One can load, modify, and export the input file by using our effective web-based tool DP-GUI. All training parameters below can be set in DP-GUI. By clicking "SAVE JSON", one can download the input file for furthur training.

model:

type: `dict`
argument path: `model`

type_map:

type: `list`, optional
argument path: `model/type_map`

A list of strings. Give the name to each type of atoms. It is noted that the number of atom type of training system must be less than 128 in a GPU environment.

data_stat_nbatch:

type: `int`, optional, default: `10`
argument path: `model/data_stat_nbatch`

The model determines the normalization from the statistics of the data. This key specifies the number of *frames* in each *system* used for statistics.

data_stat_protect:

type: `float`, optional, default: `0.01`
argument path: `model/data_stat_protect`

Protect parameter for atomic energy regression.

use_srtab:

type: `str`, optional
argument path: `model/use_srtab`

The table for the short-range pairwise interaction added on top of DP. The table is a text data file with (N_t + 1) * N_t / 2 + 1 columes. The first colume is the distance between atoms. The second to the last columes are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columes from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

smin_alpha:

type: `float`, optional
argument path: `model/smin_alpha`

The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by softmin. This parameter is the decaying parameter in the softmin. It is only required when *use_srtab* is provided.

sw_rmin:

type: `float`, optional
argument path: `model/sw_rmin`

The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when *use_srtab* is provided.

sw_rmax:

type: `float`, optional
argument path: `model/sw_rmax`

The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when *use_srtab* is provided.

type_embedding:

type: `dict`, optional
argument path: `model/type_embedding`

The type embedding.

neuron:

type: `list`, optional, default: `[2, 4, 8]`
argument path: `model/type_embedding/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`
argument path: `model/type_embedding/activation_function`

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”.

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model/type_embedding/resnet_dt`

Whether to use a “Timestep” in the skip connection

precision:

type: `str`, optional, default: `float64`
argument path: `model/type_embedding/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”.

trainable:

type: `bool`, optional, default: `True`
argument path: `model/type_embedding/trainable`

If the parameters in the embedding net are trainable

seed:

type: `int | NoneType`, optional
argument path: `model/type_embedding/seed`

Random seed for parameter initialization

descriptor:

type: `dict`
argument path: `model/descriptor`

The descriptor of atomic environment.

Depending on the value of *type*, different sub args are accepted.

type:

type: `str` (flag key)
argument path: `model/descriptor/type`
possible choices: *loc_frame*, *se_e2_a*, *se_e3*, *se_a_tpe*, *se_e2_r*, *hybrid*

The type of the descritpor. See explanation below.

- *loc_frame*: Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.
- *se_e2_a*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor.
- *se_e2_r*: Used by the smooth edition of Deep Potential. Only the distance between atoms is used to construct the descriptor.
- *se_e3*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Three-body embedding will be used by this descriptor.
- *se_a_tpe*: Used by the smooth edition of Deep Potential. The full relative coordinates are used to construct the descriptor. Type embedding will be used by this descriptor.
- *hybrid*: Concatenate of a list of descriptors as a new descriptor.

When type is set to `loc_frame`:

sel_a:

type: `list`
argument path: `model/descriptor[loc_frame]/sel_a`

A list of integers. The length of the list should be the same as the number of atom types in the system. *sel_a[i]* gives the selected number of type-i neighbors. The full relative coordinates of the neighbors are used by the descriptor.

sel_r:

type: `list`
argument path: `model/descriptor[loc_frame]/sel_r`

A list of integers. The length of the list should be the same as the number of atom types in the system. *sel_r[i]* gives the selected number of type-i neighbors. Only relative distance of the neighbors are used by the descriptor. sel_a[i] + sel_r[i] is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius.

rcut:

type: `float`, optional, default: `6.0`
argument path: `model/descriptor[loc_frame]/rcut`

The cut-off radius. The default value is 6.0

axis_rule:

type: `list`
argument path: `model/descriptor[loc_frame]/axis_rule`

A list of integers. The length should be 6 times of the number of types.

- axis_rule[i*6+0]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.
- axis_rule[i*6+1]: type of the atom defining the first axis of type-i atom.
- axis_rule[i*6+2]: index of the axis atom defining the first axis. Note that the neighbors with the same class and type are sorted according to their relative distance.
- axis_rule[i*6+3]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.
- axis_rule[i*6+4]: type of the atom defining the second axis of type-i atom.
- axis_rule[i*6+5]: class of the atom defining the second axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.

When type is set to `se_e2_a` (or its alias `se_a`):

sel:

type: `list | str`, optional, default: `auto`
argument path: `model/descriptor[se_e2_a]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- *List[int]*. The length of the list should be the same as the number of atom types in the system. *sel[i]* gives the selected number of type-i neighbors. *sel[i]* is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius. It is noted that the total sel value must be less than 4096 in a GPU environment.
- *str*. Can be "auto:factor" or "auto". "factor" is a float number larger than 1. This option will automatically determine the *sel*. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the "factor". Finally the number is wraped up to 4 divisible. The option "auto" is equivalent to "auto:1.1".

rcut:

type: `float`, optional, default: `6.0`
argument path: `model/descriptor[se_e2_a]/rcut`

The cut-off radius.

rcut_smth:

type: `float`, optional, default: `0.5`
argument path: `model/descriptor[se_e2_a]/rcut_smth`

Where to start smoothing. For example the 1/r term is smoothed from *rcut* to *rcut_smth*

neuron:

type: `list`, optional, default: `[10, 20, 40]`
argument path: `model/descriptor[se_e2_a]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: `int`, optional, default: `4`, alias: *n_axis_neuron*
argument path: `model/descriptor[se_e2_a]/axis_neuron`

Size of the submatrix of G (embedding matrix).

activation_function:

type: `str`, optional, default: `tanh`
argument path: `model/descriptor[se_e2_a]/activation_function`

The activation function in the embedding net. Supported activation functions are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu".

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_e2_a]/resnet_dt`

Whether to use a "Timestep" in the skip connection

type_one_side:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_e2_a]/type_one_side`

Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

precision:

type: `str`, optional, default: `float64`
argument path: `model/descriptor[se_e2_a]/precision`

The precision of the embedding net parameters, supported options are "default", "float16", "float32", "float64".

trainable:

type: `bool`, optional, default: `True`
argument path: `model/descriptor[se_e2_a]/trainable`

If the parameters in the embedding net is trainable

seed:

type: `int` | `NoneType`, optional
argument path: `model/descriptor[se_e2_a]/seed`

Random seed for parameter initialization

exclude_types:

type: `list`, optional, default: `[]`
argument path: `model/descriptor[se_e2_a]/exclude_types`

The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

set_davg_zero:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_e2_a]/set_davg_zero`

Set the normalization average to zero. This option should be set when *atom_ener* in the energy fitting is used

When type is set to `se_e3` (or its aliases `se_at`, `se_a_3be`, `se_t`):

sel:

type: `list | str`, optional, default: `auto`
argument path: `model/descriptor[se_e3]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- *List[int]*. The length of the list should be the same as the number of atom types in the system. *sel[i]* gives the selected number of type-i neighbors. *sel[i]* is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius. It is noted that the total sel value must be less than 4096 in a GPU environment.
- *str*. Can be "auto:factor" or "auto". "factor" is a float number larger than 1. This option will automatically determine the *sel*. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the "factor". Finally the number is wraped up to 4 divisible. The option "auto" is equivalent to "auto:1.1".

rcut:

type: `float`, optional, default: `6.0`
argument path: `model/descriptor[se_e3]/rcut`

The cut-off radius.

rcut_smth:

type: `float`, optional, default: `0.5`
argument path: `model/descriptor[se_e3]/rcut_smth`

Where to start smoothing. For example the 1/r term is smoothed from *rcut* to *rcut_smth*

neuron:

type: `list`, optional, default: `[10, 20, 40]`
argument path: `model/descriptor[se_e3]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`
argument path: `model/descriptor[se_e3]/activation_function`

The activation function in the embedding net. Supported activation functions are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu".

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_e3]/resnet_dt`

Whether to use a "Timestep" in the skip connection

precision:

type: `str`, optional, default: `float64`
argument path: `model/descriptor[se_e3]/precision`

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”.

trainable:

type: `bool`, optional, default: `True`
argument path: `model/descriptor[se_e3]/trainable`

If the parameters in the embedding net are trainable

seed:

type: `int | NoneType`, optional
argument path: `model/descriptor[se_e3]/seed`

Random seed for parameter initialization

set_davg_zero:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_e3]/set_davg_zero`

Set the normalization average to zero. This option should be set when *atom_ener* in the energy fitting is used

When type is set to `se_a_tpe` (or its alias `se_a_ebd`):

sel:

type: `list | str`, optional, default: `auto`
argument path: `model/descriptor[se_a_tpe]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- *List[int]*. The length of the list should be the same as the number of atom types in the system. *sel[i]* gives the selected number of type-i neighbors. *sel[i]* is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius. It is noted that the total sel value must be less than 4096 in a GPU environment.
- *str*. Can be “auto:factor” or “auto”. “factor” is a float number larger than 1. This option will automatically determine the *sel*. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the “factor”. Finally the number is wraped up to 4 divisible. The option “auto” is equivalent to “auto:1.1”.

rcut:

type: `float`, optional, default: `6.0`
argument path: `model/descriptor[se_a_tpe]/rcut`

The cut-off radius.

rcut_smth:

type: `float`, optional, default: `0.5`
argument path: `model/descriptor[se_a_tpe]/rcut_smth`

Where to start smoothing. For example the 1/r term is smoothed from *rcut* to *rcut_smth*

neuron:

type: `list`, optional, default: `[10, 20, 40]`
argument path: `model/descriptor[se_a_tpe]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

axis_neuron:

type: `int`, optional, default: `4`, alias: *n_axis_neuron*
argument path: `model/descriptor[se_a_tpe]/axis_neuron`

Size of the submatrix of G (embedding matrix).

activation_function:

type: `str`, optional, default: `tanh`
argument path: `model/descriptor[se_a_tpe]/activation_function`

The activation function in the embedding net. Supported activation functions are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu".

resnet_dt:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_a_tpe]/resnet_dt`

Whether to use a "Timestep" in the skip connection

type_one_side:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_a_tpe]/type_one_side`

Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

precision:

type: `str`, optional, default: `float64`
argument path: `model/descriptor[se_a_tpe]/precision`

The precision of the embedding net parameters, supported options are "default", "float16", "float32", "float64".

trainable:

type: `bool`, optional, default: `True`
argument path: `model/descriptor[se_a_tpe]/trainable`

If the parameters in the embedding net is trainable

seed:

type: `int` | `NoneType`, optional
argument path: `model/descriptor[se_a_tpe]/seed`

Random seed for parameter initialization

exclude_types:

type: `list`, optional, default: `[]`
argument path: `model/descriptor[se_a_tpe]/exclude_types`

The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

set_davg_zero:

type: `bool`, optional, default: `False`
argument path: `model/descriptor[se_a_tpe]/set_davg_zero`

Set the normalization average to zero. This option should be set when *atom_ener* in the energy fitting is used

type_nchanl:

type: `int`, optional, default: `4`
argument path: `model/descriptor[se_a_tpe]/type_nchanl`

number of channels for type embedding

type_nlayer:

type: `int`, optional, default: `2`
argument path: `model/descriptor[se_a_tpe]/type_nlayer`

number of hidden layers of type embedding net

numb_aparam:

type: `int`, optional, default: `0`
argument path: `model/descriptor[se_a_tpe]/numb_aparam`

dimension of atomic parameter. if set to a value > 0, the atomic parameters are embedded.

When type is set to `se_e2_r` (or its alias `se_r`):

sel:

type: `list | str`, optional, default: `auto`
argument path: `model/descriptor[se_e2_r]/sel`

This parameter set the number of selected neighbors for each type of atom. It can be:

- *List[int]*. The length of the list should be the same as the number of atom types in the system. *sel[i]* gives the selected number of type-i neighbors. *sel[i]* is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius. It is noted that the total sel value must be less than 4096 in a GPU environment.
- *str*. Can be "auto:factor" or "auto". "factor" is a float number larger than 1. This option will automatically determine the *sel*. In detail it counts the maximal number of neighbors with in the cutoff radius for each type of neighbor, then multiply the maximum by the "factor". Finally the number is wraped up to 4 divisible. The option "auto" is equivalent to "auto:1.1".

rcut:

type: `float`, optional, default: `6.0`
argument path: `model/descriptor[se_e2_r]/rcut`

The cut-off radius.

rcut_smth:

type: `float`, optional, default: `0.5`
argument path: `model/descriptor[se_e2_r]/rcut_smth`

Where to start smoothing. For example the 1/r term is smoothed from *rcut* to *rcut_smth*

neuron:

type: `list`, optional, default: `[10, 20, 40]`
argument path: `model/descriptor[se_e2_r]/neuron`

Number of neurons in each hidden layers of the embedding net. When two layers are of the same size or one layer is twice as large as the previous layer, a skip connection is built.

activation_function:

type: `str`, optional, default: `tanh`

argument path: model/descriptor[se_e2_r]/activation_function

The activation function in the embedding net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”.

resnet_dt:

type: bool, optional, default: False
argument path: model/descriptor[se_e2_r]/resnet_dt

Whether to use a “Timestep” in the skip connection

type_one_side:

type: bool, optional, default: False
argument path: model/descriptor[se_e2_r]/type_one_side

Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

precision:

type: str, optional, default: float64
argument path: model/descriptor[se_e2_r]/precision

The precision of the embedding net parameters, supported options are “default”, “float16”, “float32”, “float64”.

trainable:

type: bool, optional, default: True
argument path: model/descriptor[se_e2_r]/trainable

If the parameters in the embedding net are trainable

seed:

type: int | NoneType, optional
argument path: model/descriptor[se_e2_r]/seed

Random seed for parameter initialization

exclude_types:

type: list, optional, default: []
argument path: model/descriptor[se_e2_r]/exclude_types

The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

set_davg_zero:

type: bool, optional, default: False
argument path: model/descriptor[se_e2_r]/set_davg_zero

Set the normalization average to zero. This option should be set when *atom_ener* in the energy fitting is used

When type is set to hybrid:

list:

type: list
argument path: model/descriptor[hybrid]/list

A list of descriptor definitions

fitting_net:

type: dict
argument path: model/fitting_net

The fitting of physical properties.

Depending on the value of *type*, different sub args are accepted.

type:

type: str (flag key), default: ener
argument path: model/fitting_net/type
possible choices: *ener*, *dipole*, *polar*

The type of the fitting. See explanation below.

- *ener*: Fit an energy model (potential energy surface).
- *dipole*: Fit an atomic dipole model. Global dipole labels or atomic dipole labels for all the selected atoms (see *sel_type*) should be provided by *dipole.npy* in each data system. The file either has number of frames lines and 3 times of number of selected atoms columns, or has number of frames lines and 3 columns. See *loss* parameter.
- *polar*: Fit an atomic polarizability model. Global polarizazbility labels or atomic polarizability labels for all the selected atoms (see *sel_type*) should be provided by *polarizability.npy* in each data system. The file eith has number of frames lines and 9 times of number of selected atoms columns, or has number of frames lines and 9 columns. See *loss* parameter.

When type is set to ener:

numb_fparam:

type: int, optional, default: 0
argument path: model/fitting_net[ener]/numb_fparam

The dimension of the frame parameter. If set to >0, file *fparam.npy* should be included to provided the input fparams.

numb_aparam:

type: int, optional, default: 0
argument path: model/fitting_net[ener]/numb_aparam

The dimension of the atomic parameter. If set to >0, file *aparam.npy* should be included to provided the input aparams.

neuron:

type: list, optional, default: [120, 120, 120], alias: *n_neuron*
argument path: model/fitting_net[ener]/neuron

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: str, optional, default: tanh
argument path: model/fitting_net[ener]/activation_function

The activation function in the fitting net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”.

precision:

type: str, optional, default: float64
argument path: model/fitting_net[ener]/precision

The precision of the fitting net parameters, supported options are “default”, “float16”, “float32”, “float64”.

resnet_dt:

type: bool, optional, default: True
argument path: model/fitting_net[ener]/resnet_dt

Whether to use a “Timestep” in the skip connection

trainable:

type: list | bool, optional, default: True
argument path: model/fitting_net[ener]/trainable

Whether the parameters in the fitting net are trainable. This option can be

- bool: True if all parameters of the fitting net are trainable, False otherwise.
- list of bool: Specifies if each layer is trainable. Since the fitting net is composed by hidden layers followed by a output layer, the length of tihs list should be equal to len(*neuron*)+1.

rcond:

type: float, optional, default: 0.001
argument path: model/fitting_net[ener]/rcond

The condition number used to determine the inital energy shift for each type of atoms.

seed:

type: int | NoneType, optional
argument path: model/fitting_net[ener]/seed

Random seed for parameter initialization of the fitting net

atom_ener:

type: list, optional, default: []
argument path: model/fitting_net[ener]/atom_ener

Specify the atomic energy in vacuum for each type

When type is set to dipole:

neuron:

type: list, optional, default: [120, 120, 120], alias: *n_neuron*
argument path: model/fitting_net[dipole]/neuron

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: str, optional, default: tanh
argument path: model/fitting_net[dipole]/activation_function

The activation function in the fitting net. Supported activation functions are “relu”, “relu6”, “softplus”, “sigmoid”, “tanh”, “gelu”.

resnet_dt:

type: bool, optional, default: True
argument path: model/fitting_net[dipole]/resnet_dt

Whether to use a "Timestep" in the skip connection

precision:

type: str, optional, default: float64
argument path: model/fitting_net[dipole]/precision

The precision of the fitting net parameters, supported options are "default", "float16", "float32", "float64".

sel_type:

type: list | int | NoneType, optional, alias: *dipole_type*
argument path: model/fitting_net[dipole]/sel_type

The atom types for which the atomic dipole will be provided. If not set, all types will be selected.

seed:

type: int | NoneType, optional
argument path: model/fitting_net[dipole]/seed

Random seed for parameter initialization of the fitting net

When type is set to polar:

neuron:

type: list, optional, default: [120, 120, 120], alias: *n_neuron*
argument path: model/fitting_net[polar]/neuron

The number of neurons in each hidden layers of the fitting net. When two hidden layers are of the same size, a skip connection is built.

activation_function:

type: str, optional, default: tanh
argument path: model/fitting_net[polar]/activation_function

The activation function in the fitting net. Supported activation functions are "relu", "relu6", "softplus", "sigmoid", "tanh", "gelu".

resnet_dt:

type: bool, optional, default: True
argument path: model/fitting_net[polar]/resnet_dt

Whether to use a "Timestep" in the skip connection

precision:

type: str, optional, default: float64
argument path: model/fitting_net[polar]/precision

The precision of the fitting net parameters, supported options are "default", "float16", "float32", "float64".

fit_diag:

type: bool, optional, default: True
argument path: model/fitting_net[polar]/fit_diag

Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale:

type: `list | float`, optional, default: `1.0`
argument path: `model/fitting_net[polar]/scale`

The output of the fitting net (polarizability matrix) will be scaled by `scale`

shift_diag:

type: `bool`, optional, default: `True`
argument path: `model/fitting_net[polar]/shift_diag`

Whether to shift the diagonal of polar, which is beneficial to training. Default is true.

sel_type:

type: `list | int | NoneType`, optional, alias: *pol_type*
argument path: `model/fitting_net[polar]/sel_type`

The atom types for which the atomic polarizability will be provided. If not set, all types will be selected.

seed:

type: `int | NoneType`, optional
argument path: `model/fitting_net[polar]/seed`

Random seed for parameter initialization of the fitting net

modifier:

type: `dict`, optional
argument path: `model/modifier`

The modifier of model output.

Depending on the value of *type*, different sub args are accepted.

type:

type: `str` (flag key)
argument path: `model/modifier/type`
possible choices: *dipole_charge*

The type of modifier. See explanation below.

-*dipole_charge*: Use WFCC to model the electronic structure of the system. Correct the long-range interaction

When type is set to `dipole_charge`:

model_name:

type: `str`
argument path: `model/modifier[dipole_charge]/model_name`

The name of the frozen dipole model file.

model_charge_map:

type: `list`
argument path: `model/modifier[dipole_charge]/model_charge_map`

The charge of the WFCC. The list length should be the same as the *sel_type*.

sys_charge_map:

type: `list`
argument path: `model/modifier[dipole_charge]/sys_charge_map`

The charge of real atoms. The list length should be the same as the *type_map*

ewald_beta:

type: `float`, optional, default: `0.4`
argument path: `model/modifier[dipole_charge]/ewald_beta`

The splitting parameter of Ewald sum. Unit is A^-1

ewald_h:

type: `float`, optional, default: `1.0`
argument path: `model/modifier[dipole_charge]/ewald_h`

The grid spacing of the FFT grid. Unit is A

compress:

type: `dict`, optional
argument path: `model/compress`

Model compression configurations

Depending on the value of *type*, different sub args are accepted.

type:

type: `str` (flag key), default: `se_e2_a`
argument path: `model/compress/type`
possible choices: *`se_e2_a`*

The type of model compression, which should be consistent with the descriptor type.

When type is set to `se_e2_a` (or its alias `se_a`):

compress:

type: `bool`
argument path: `model/compress[se_e2_a]/compress`

The name of the frozen model file.

model_file:

type: `str`
argument path: `model/compress[se_e2_a]/model_file`

The input model file, which will be compressed by the DeePMD-kit.

table_config:

type: `list`
argument path: `model/compress[se_e2_a]/table_config`

The arguments of model compression, including extrapolate(scale of model extrapolation), stride(uniform stride of tabulation's first and second table), and frequency(frequency of tabulation overflow check).

min_nbor_dist:

type: `float`

argument path: `model/compress[se_e2_a]/min_nbor_dist`

The nearest distance between neighbor atoms saved in the frozen model.

loss:

type: `dict`, optional
argument path: `loss`

The definition of loss function. The loss type should be set to *tensor*, *ener* or left unset. .

Depending on the value of *type*, different sub args are accepted.

type:

type: `str` (flag key), default: `ener`
argument path: `loss/type`
possible choices: *ener*, *tensor*

The type of the loss. When the fitting type is *ener*, the loss type should be set to *ener* or left unset. When the fitting type is *dipole* or *polar*, the loss type should be set to *tensor*. .

When type is set to `ener`:

start_pref_e:

type: `float | int`, optional, default: `0.02`
argument path: `loss[ener]/start_pref_e`

The prefactor of energy loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the energy label should be provided by file energy.npy in each data system. If both start_pref_energy and limit_pref_energy are set to 0, then the energy will be ignored.

limit_pref_e:

type: `float | int`, optional, default: `1.0`
argument path: `loss[ener]/limit_pref_e`

The prefactor of energy loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_f:

type: `float | int`, optional, default: `1000`
argument path: `loss[ener]/start_pref_f`

The prefactor of force loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the force label should be provided by file force.npy in each data system. If both start_pref_force and limit_pref_force are set to 0, then the force will be ignored.

limit_pref_f:

type: `float | int`, optional, default: `1.0`
argument path: `loss[ener]/limit_pref_f`

The prefactor of force loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_v:

type: `float | int`, optional, default: `0.0`
argument path: `loss[ener]/start_pref_v`

The prefactor of virial loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the virial label should be provided by file virial.npy in each data system. If both start_pref_virial and limit_pref_virial are set to 0, then the virial will be ignored.

limit_pref_v:

type: `float` | `int`, optional, default: `0.0`

argument path: `loss[ener]/limit_pref_v`

The prefactor of virial loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_ae:

type: `float` | `int`, optional, default: `0.0`

argument path: `loss[ener]/start_pref_ae`

The prefactor of atom_ener loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the atom_ener label should be provided by file atom_ener.npy in each data system. If both start_pref_atom_ener and limit_pref_atom_ener are set to 0, then the atom_ener will be ignored.

limit_pref_ae:

type: `float` | `int`, optional, default: `0.0`

argument path: `loss[ener]/limit_pref_ae`

The prefactor of atom_ener loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

start_pref_pf:

type: `float` | `int`, optional, default: `0.0`

argument path: `loss[ener]/start_pref_pf`

The prefactor of atom_pref loss at the start of the training. Should be larger than or equal to 0. If set to none-zero value, the atom_pref label should be provided by file atom_pref.npy in each data system. If both start_pref_atom_pref and limit_pref_atom_pref are set to 0, then the atom_pref will be ignored.

limit_pref_pf:

type: `float` | `int`, optional, default: `0.0`

argument path: `loss[ener]/limit_pref_pf`

The prefactor of atom_pref loss at the limit of the training, Should be larger than or equal to 0. i.e. the training step goes to infinity.

relative_f:

type: `float` | `NoneType`, optional

argument path: `loss[ener]/relative_f`

If provided, relative force error will be used in the loss. The difference of force will be normalized by the magnitude of the force in the label with a shift given by *relative_f*, i.e. DF_i / (|| F || + relative_f) with DF denoting the difference between prediction and label and || F || denoting the L2 norm of the label.

When type is set to `tensor`:

pref:

type: `float` | `int`

argument path: `loss[tensor]/pref`

The prefactor of the weight of global loss. It should be larger than or equal to 0. If controls the weight of loss corresponding to global label, i.e. ‘polarizability.npy` or *dipole.npy*, whose shape should be #frames x [9 or 3]. If it’s larger than 0.0, this npy should be included.

pref_atomic:

type: `float | int`
argument path: `loss[tensor]/pref_atomic`

The prefactor of the weight of atomic loss. It should be larger than or equal to 0. If controls the weight of loss corresponding to atomic label, i.e. *atomic_polarizability.npy* or *atomic_dipole.npy*, whose shape should be #frames x ([9 or 3] x #selected atoms). If it’s larger than 0.0, this npy should be included. Both *pref* and *pref_atomic* should be provided, and either can be set to 0.0.

learning_rate:

type: `dict`
argument path: `learning_rate`

The definitio of learning rate

scale_by_worker:

type: `str`, optional, default: `linear`
argument path: `learning_rate/scale_by_worker`

When parallel training or batch size scaled, how to alter learning rate. Valid values are *linear`(default), `sqrt* or *none*.

Depending on the value of *type*, different sub args are accepted.

type:

type: `str` (flag key), default: `exp`
argument path: `learning_rate/type`
possible choices: *exp*

The type of the learning rate.

When type is set to `exp`:

start_lr:

type: `float`, optional, default: `0.001`
argument path: `learning_rate[exp]/start_lr`

The learning rate the start of the training.

stop_lr:

type: `float`, optional, default: `1e-08`
argument path: `learning_rate[exp]/stop_lr`

The desired learning rate at the end of the training.

decay_steps:

type: `int`, optional, default: `5000`
argument path: `learning_rate[exp]/decay_steps`

The learning rate is decaying every this number of training steps.

training:

type: `dict`

argument path: `training`

The training options.

training_data:

type: `dict`
argument path: `training/training_data`

Configurations of training data.

systems:

type: `list | str`
argument path: `training/training_data/systems`

The data systems for training. This key can be provided with a list that specifies the systems, or be provided with a string by which the prefix of all systems are given and the list of the systems is automatically generated.

set_prefix:

type: `str`, optional, default: `set`
argument path: `training/training_data/set_prefix`

The prefix of the sets in the *systems*.

batch_size:

type: `list | str | int`, optional, default: `auto`
argument path: `training/training_data/batch_size`

This key can be

- list: the length of which is the same as the *systems*. The batch size of each system is given by the elements of the list.
- int: all *systems* use the same batch size.
- string "auto": automatically determines the batch size so that the batch_size times the number of atoms in the system is no less than 32.
- string "auto:N": automatically determines the batch size so that the batch_size times the number of atoms in the system is no less than N.

auto_prob:

type: `str`, optional, default: `prob_sys_size`, alias: *auto_prob_style*
argument path: `training/training_data/auto_prob`

Determine the probability of systems automatically. The method is assigned by this key and can be

- "prob_uniform" : the probability all the systems are equal, namely 1.0/self.get_nsystems()
- "prob_sys_size" : the probability of a system is proportional to the number of batches in the system
- "prob_sys_size;stt_idx:end_idx:weight;stt_idx:end_idx:weight;..." : the list of systems is devided into blocks. A block is specified by *stt_idx:end_idx:weight*, where *stt_idx* is the starting index of the system, *end_idx* is then ending (not including) index of the system, the probabilities of the systems in this block sums up to *weight*, and the relatively probabilities within this block is proportional to the number of batches in the system.

sys_probs:

type: `list | NoneType`, optional, default: `None`, alias: *sys_weights*

argument path: `training/training_data/sys_probs`

A list of float if specified. Should be of the same length as *systems*, specifying the probability of each system.

validation_data:

type: `dict` | `NoneType`, optional, default: `None`
argument path: `training/validation_data`

Configurations of validation data. Similar to that of training data, except that a *numb_btch* argument may be configured

systems:

type: `list` | `str`
argument path: `training/validation_data/systems`

The data systems for validation. This key can be provided with a list that specifies the systems, or be provided with a string by which the prefix of all systems are given and the list of the systems is automatically generated.

set_prefix:

type: `str`, optional, default: `set`
argument path: `training/validation_data/set_prefix`

The prefix of the sets in the *systems*.

batch_size:

type: `list` | `str` | `int`, optional, default: `auto`
argument path: `training/validation_data/batch_size`

This key can be

- list: the length of which is the same as the *systems*. The batch size of each system is given by the elements of the list.
- int: all *systems* use the same batch size.
- string "auto": automatically determines the batch size so that the batch_size times the number of atoms in the system is no less than 32.
- string "auto:N": automatically determines the batch size so that the batch_size times the number of atoms in the system is no less than N.

auto_prob:

type: `str`, optional, default: `prob_sys_size`, alias: *auto_prob_style*
argument path: `training/validation_data/auto_prob`

Determine the probability of systems automatically. The method is assigned by this key and can be

- "prob_uniform" : the probability all the systems are equal, namely 1.0/self.get_nsystems()
- "prob_sys_size" : the probability of a system is proportional to the number of batches in the system
- "prob_sys_size;stt_idx:end_idx:weight;stt_idx:end_idx:weight;..." : the list of systems is devided into blocks. A block is specified by *stt_idx:end_idx:weight*, where *stt_idx* is the starting index of the system, *end_idx* is then ending (not including) index of the system, the probabilities of the systems in this block sums up to *weight*, and the relatively probabilities within this block is proportional to the number of batches in the system.

sys_probs:

type: list | NoneType, optional, default: None, alias: *sys_weights*
argument path: training/validation_data/sys_probs

A list of float if specified. Should be of the same length as *systems*, specifying the probability of each system.

numb_btch:

type: int, optional, default: 1, alias: *numb_batch*
argument path: training/validation_data/numb_btch

An integer that specifies the number of systems to be sampled for each validation period.

numb_steps:

type: int, alias: *stop_batch*
argument path: training/numb_steps

Number of training batch. Each training uses one batch of data.

seed:

type: int | NoneType, optional
argument path: training/seed

The random seed for getting frames from the training data set.

disp_file:

type: str, optional, default: lcurve.out
argument path: training/disp_file

The file for printing learning curve.

disp_freq:

type: int, optional, default: 1000
argument path: training/disp_freq

The frequency of printing learning curve.

numb_test:

type: list | str | int, optional, default: 1
argument path: training/numb_test

Number of frames used for the test during training.

save_freq:

type: int, optional, default: 1000
argument path: training/save_freq

The frequency of saving check point.

save_ckpt:

type: str, optional, default: model.ckpt
argument path: training/save_ckpt

The file name of saving check point.

disp_training:

type: bool, optional, default: True
argument path: training/disp_training

Displaying verbose information during training.

time_training:

type: `bool`, optional, default: `True`
argument path: `training/time_training`

Timing durining training.

profiling:

type: `bool`, optional, default: `False`
argument path: `training/profiling`

Profiling during training.

profiling_file:

type: `str`, optional, default: `timeline.json`
argument path: `training/profiling_file`

Output file for profiling.

tensorboard:

type: `bool`, optional, default: `False`
argument path: `training/tensorboard`

Enable tensorboard

tensorboard_log_dir:

type: `str`, optional, default: `log`
argument path: `training/tensorboard_log_dir`

The log directory of tensorboard outputs

tensorboard_freq:

type: `int`, optional, default: `1`
argument path: `training/tensorboard_freq`

The frequency of writing tensorboard events.

5.4 Parallel training

Currently, parallel training is enabled in a sychoronized way with help of Horovod. Depend on the number of training processes (according to MPI context) and number of GPU cards avaliable, DeePMD-kit will decide whether to launch the training in parallel (distributed) mode or in serial mode. Therefore, no additional options is specified in your JSON/YAML input file.

5.4.1 Tuning learning rate

Horovod works in the data-parallel mode, resulting in a larger global batch size. For example, the real batch size is 8 when `batch_size` is set to 2 in the input file and you launch 4 workers. Thus, `learning_rate` is automatically scaled by the number of workers for better convergence. Technical details of such heuristic rule are discussed at Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour.

The number of decay steps required to achieve same accuracy can decrease by the number of cards (e.g., 1/2 of steps in the above case), but needs to be scaled manually in the input file.

In some cases, it won't work well when scale learning rate by worker count in a `linear` way. Then you can try `sqrt` or `none` by setting argument `scale_by_worker` like below.

```
    "learning_rate" :{
        "scale_by_worker": "none",
        "type": "exp"
    }
```

5.4.2 Scaling test

Testing `examples/water/se_e2_a` on a 8-GPU host, linear acceleration can be observed with increasing number of cards.

Num of GPU cards	Seconds every 100 samples	Samples per second	Speed up
1	1.4515	68.89	1.00
2	1.5962	62.65*2	1.82
4	1.7635	56.71*4	3.29
8	1.7267	57.91*8	6.72

5.4.3 How to use

Training workers can be launched with `horovodrun`. The following command launches 4 processes on the same host:

```
CUDA_VISIBLE_DEVICES=4,5,6,7 horovodrun -np 4 \
    dp train --mpi-log=workers input.json
```

Need to mention, environment variable `CUDA_VISIBLE_DEVICES` must be set to control parallelism on the occupied host where one process is bound to one GPU card.

When using MPI with Horovod, `horovodrun` is a simple wrapper around `mpirun`. In the case where fine-grained control over options passed to `mpirun`, `mpirun` can be invoked directly, and it will be detected automatically by Horovod, e.g.,

```
CUDA_VISIBLE_DEVICES=4,5,6,7 mpirun -l -launcher=fork -hosts=localhost -np 4 \
    dp train --mpi-log=workers input.json
```

this is sometimes neccessary on HPC environment.

Whether distributed workers are initiated can be observed at the "Summary of the training" section in the log (`world size` > 1, and `distributed`).

```
[0] DEEPMD INFO    ---Summary of the training---------------------------------------
[0] DEEPMD INFO    distributed
[0] DEEPMD INFO    world size:          4
[0] DEEPMD INFO    my rank:             0
[0] DEEPMD INFO    node list:           ['exp-13-57']
[0] DEEPMD INFO    running on:          exp-13-57
[0] DEEPMD INFO    computing device:    gpu:0
[0] DEEPMD INFO    CUDA_VISIBLE_DEVICES: 0,1,2,3
[0] DEEPMD INFO    Count of visible GPU: 4
[0] DEEPMD INFO    num_intra_threads:   0
[0] DEEPMD INFO    num_inter_threads:   0
[0] DEEPMD INFO    -----------------------------------------------------------------
```

5.4.4 Logging

What's more, 2 command-line arguments are defined to control the logging behvaior when performing parallel training with MPI.

```
optional arguments:
  -l LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to disk, if not
                        specified, the logs will only be output to console
                        (default: None)
  -m {master,collect,workers}, --mpi-log {master,collect,workers}
                        Set the manner of logging when running with MPI.
                        'master' logs only on main process, 'collect'
                        broadcasts logs from workers to master and 'workers'
                        means each process will output its own log (default:
                        master)
```

5.5 TensorBoard Usage

TensorBoard provides the visualization and tooling needed for machine learning experimentation. A full instruction of tensorboard can be found here.

5.5.1 Highlighted features

DeePMD-kit can now use most of the interesting features enabled by tensorboard!

- **Tracking and visualizing metrics,** such as l2_loss, l2_energy_loss and l2_force_loss
- **Visualizing the model graph** (ops and layers)
- **Viewing histograms of weights, biases, or other tensors as they change over time.**
- **Viewing summaries of trainable viriables**

5.5.2 How to use Tensorboard with DeePMD-kit

Before running TensorBoard, make sure you have generated summary data in a log directory by modifying the the input script, set "tensorboard" true in training subsection will enable the tensorboard data analysis. eg. **water_se_a.json**.

```
    "training" : {
        "systems":        ["../data/"],
        "set_prefix":       "set",
        "stop_batch":       1000000,
        "batch_size":       1,

        "seed":               1,

        "_comment": " display and restart",
        "_comment": " frequencies counted in batch",
        "disp_file":       "lcurve.out",
        "disp_freq":       100,
        "numb_test":       10,
        "save_freq":       1000,
        "save_ckpt":       "model.ckpt",

        "disp_training":true,
        "time_training":true,
        "tensorboard":       true,
        "tensorboard_log_dir":"log",
        "tensorboard_freq": 1000,
        "profiling":       false,
        "profiling_file":"timeline.json",
        "_comment":       "that's all"
    }
```

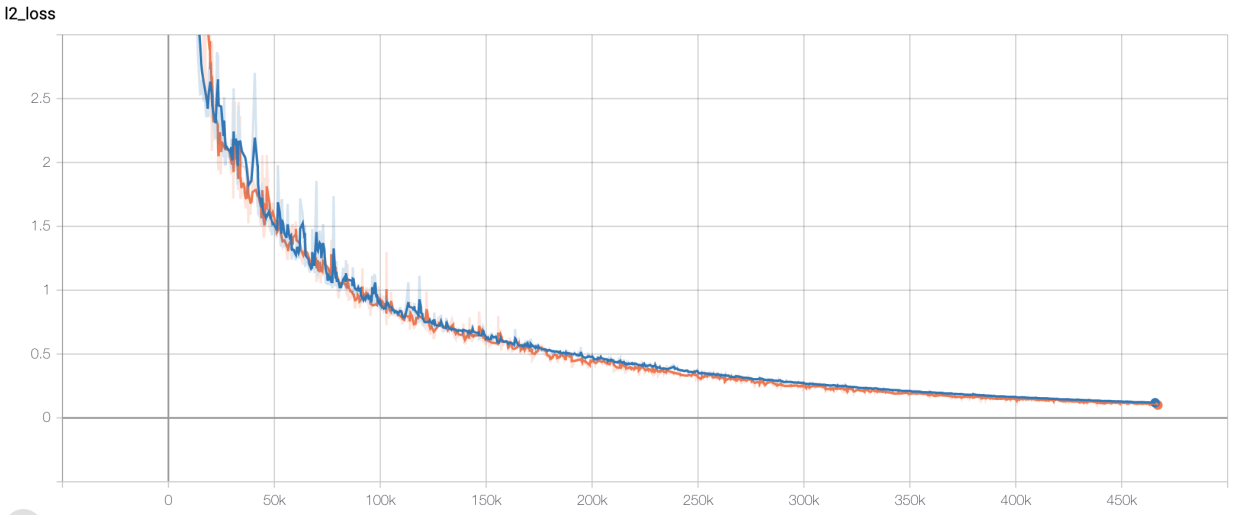
Once you have event files, run TensorBoard and provide the log directory. This should print that TensorBoard has started. Next, connect to http://tensorboard_server_ip:6006.

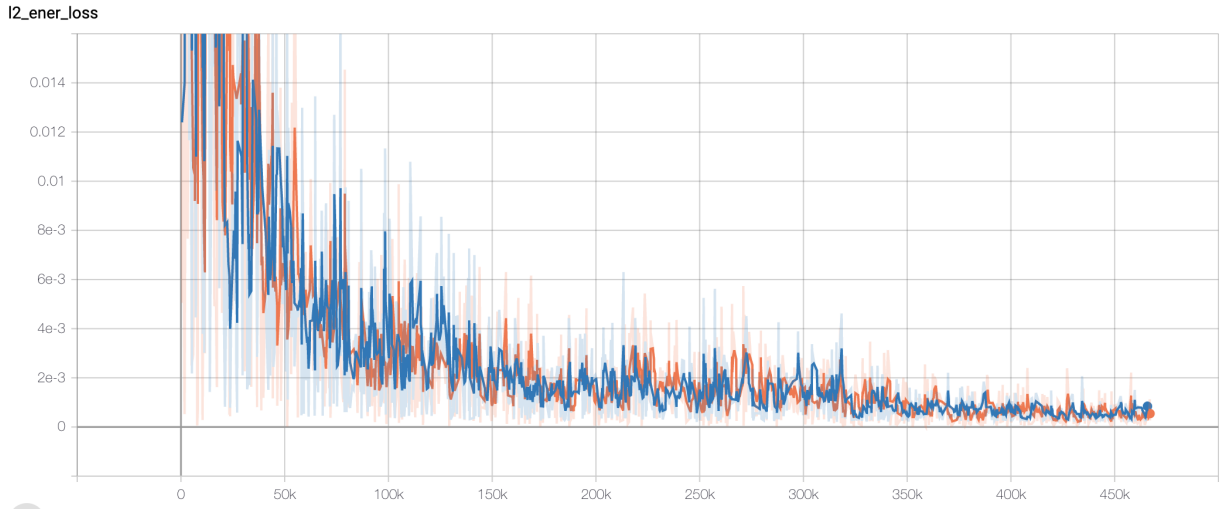
TensorBoard requires a logdir to read logs from. For info on configuring TensorBoard, run tensorboard –help. One can easily change the log name with "tensorboard_log_dir" and the sampling frequency with "tensorboard_freq".

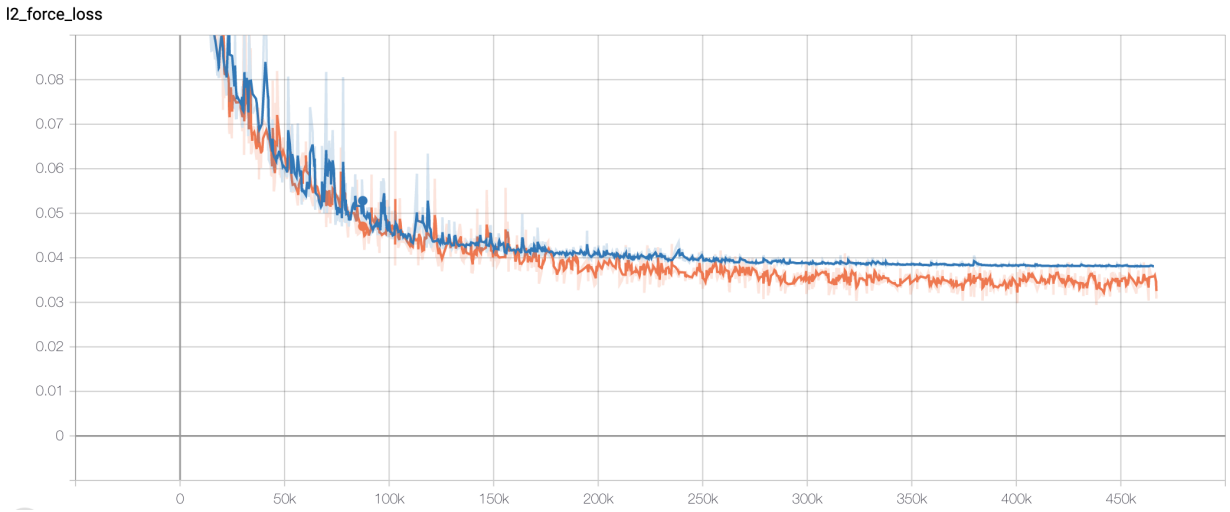
```
tensorboard --logdir path/to/logs
```

5.5.3 Examples

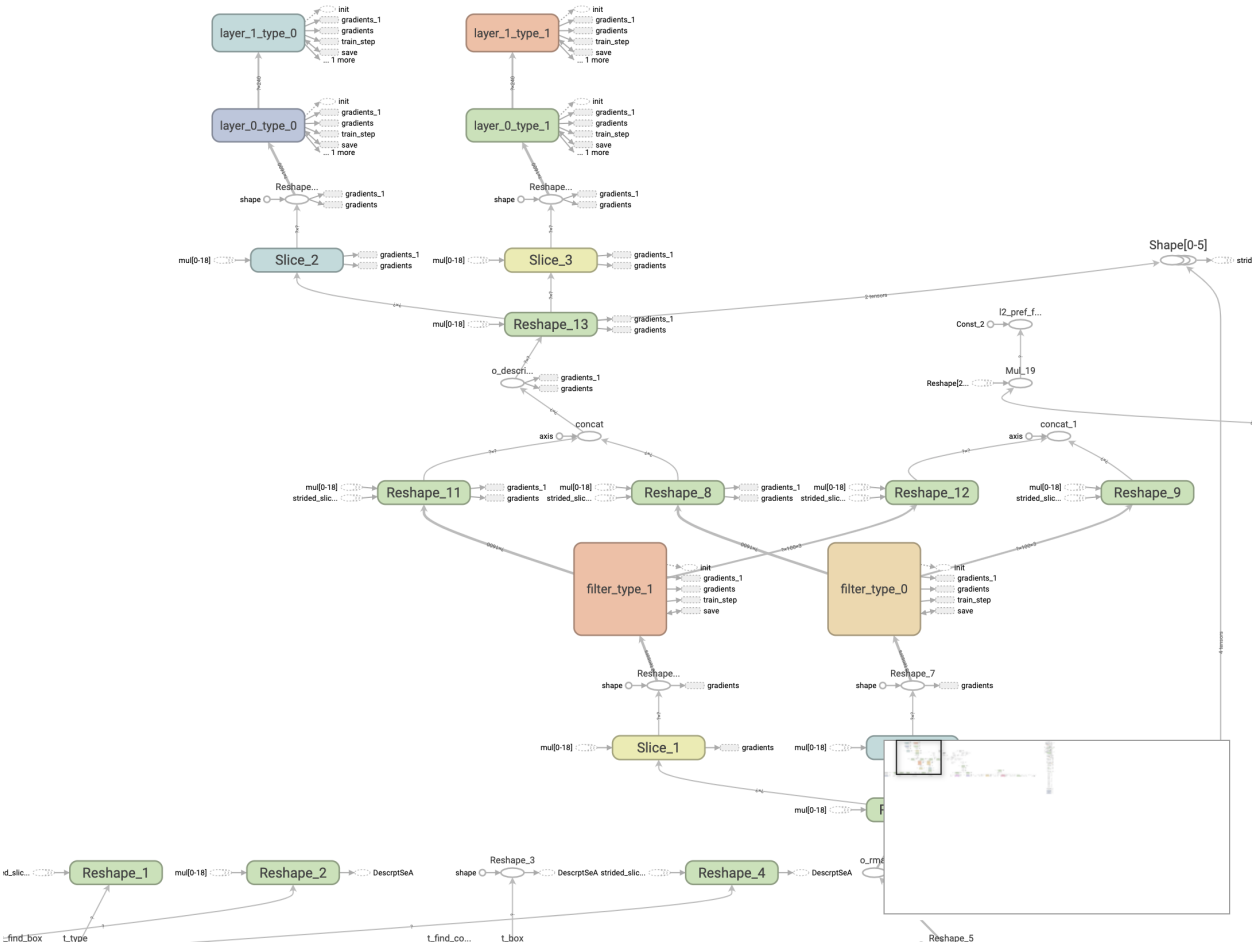
Tracking and visualizing loss metrics(red:train, blue:test)



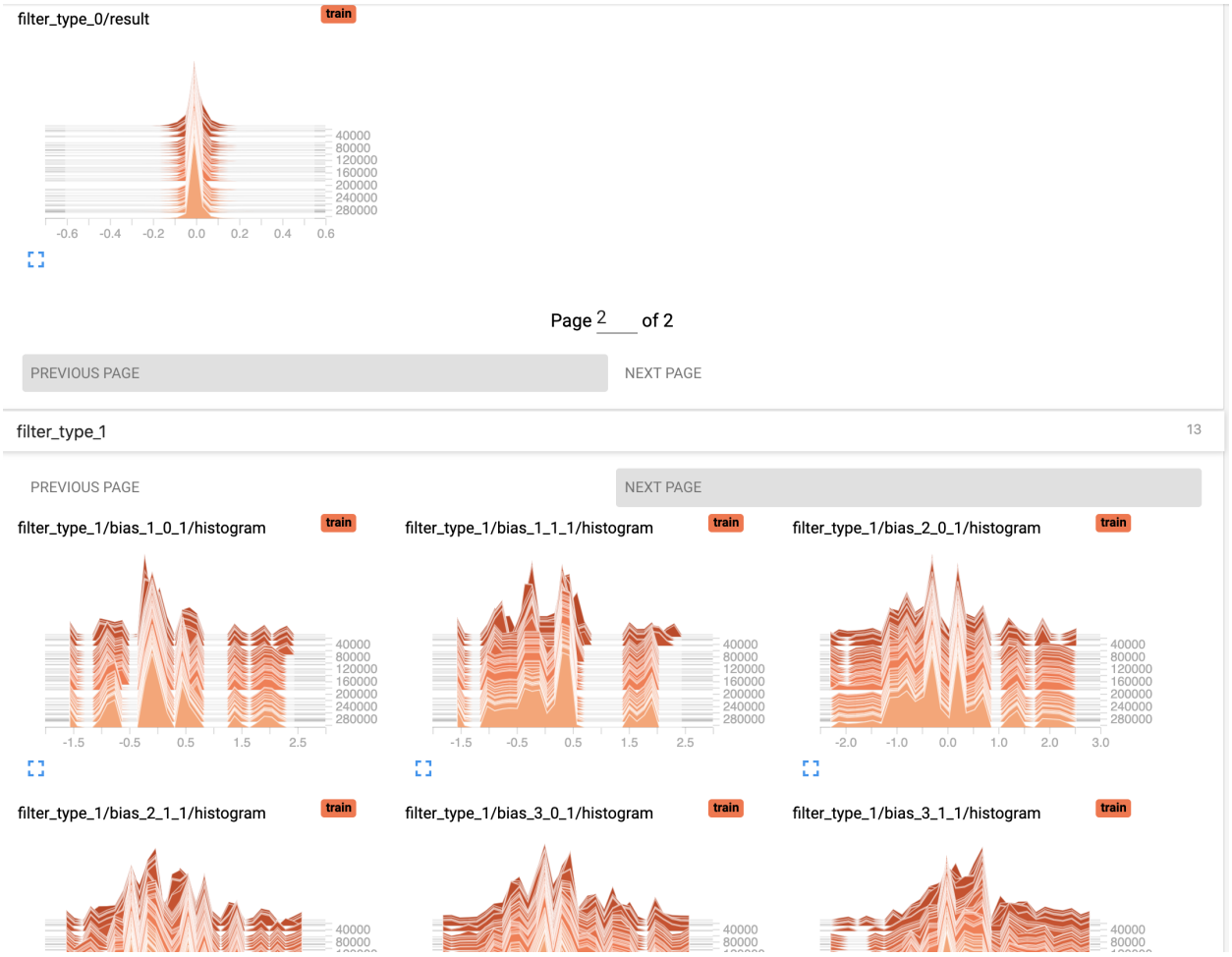




Visualizing deepmd-kit model graph



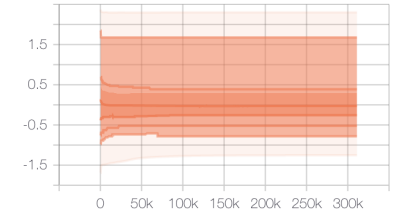
Viewing histograms of weights, biases, or other tensors as they change over time



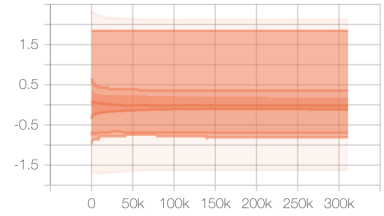
filter_type_0 13

PREVIOUS PAGE NEXT PAGE

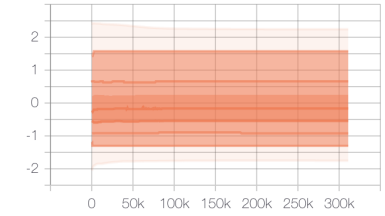
filter_type_0/bias_1_0_1/histogram train



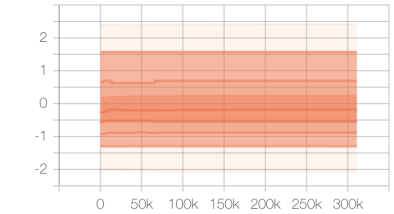
filter_type_0/bias_1_1_1/histogram train



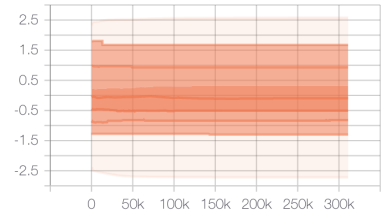
filter_type_0/bias_2_0_1/histogram train



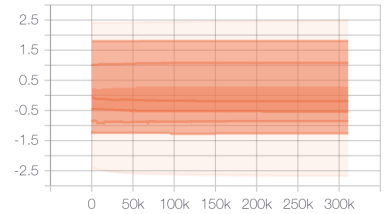
filter_type_0/bias_2_1_1/histogram train



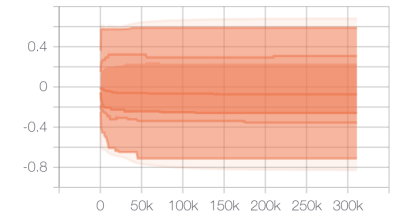
filter_type_0/bias_3_0_1/histogram train



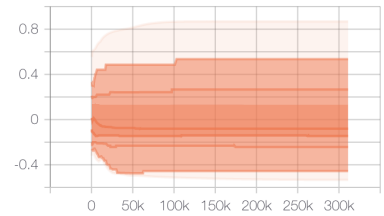
filter_type_0/bias_3_1_1/histogram train



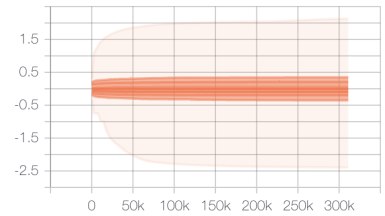
filter_type_0/matrix_1_0_1/histogram train



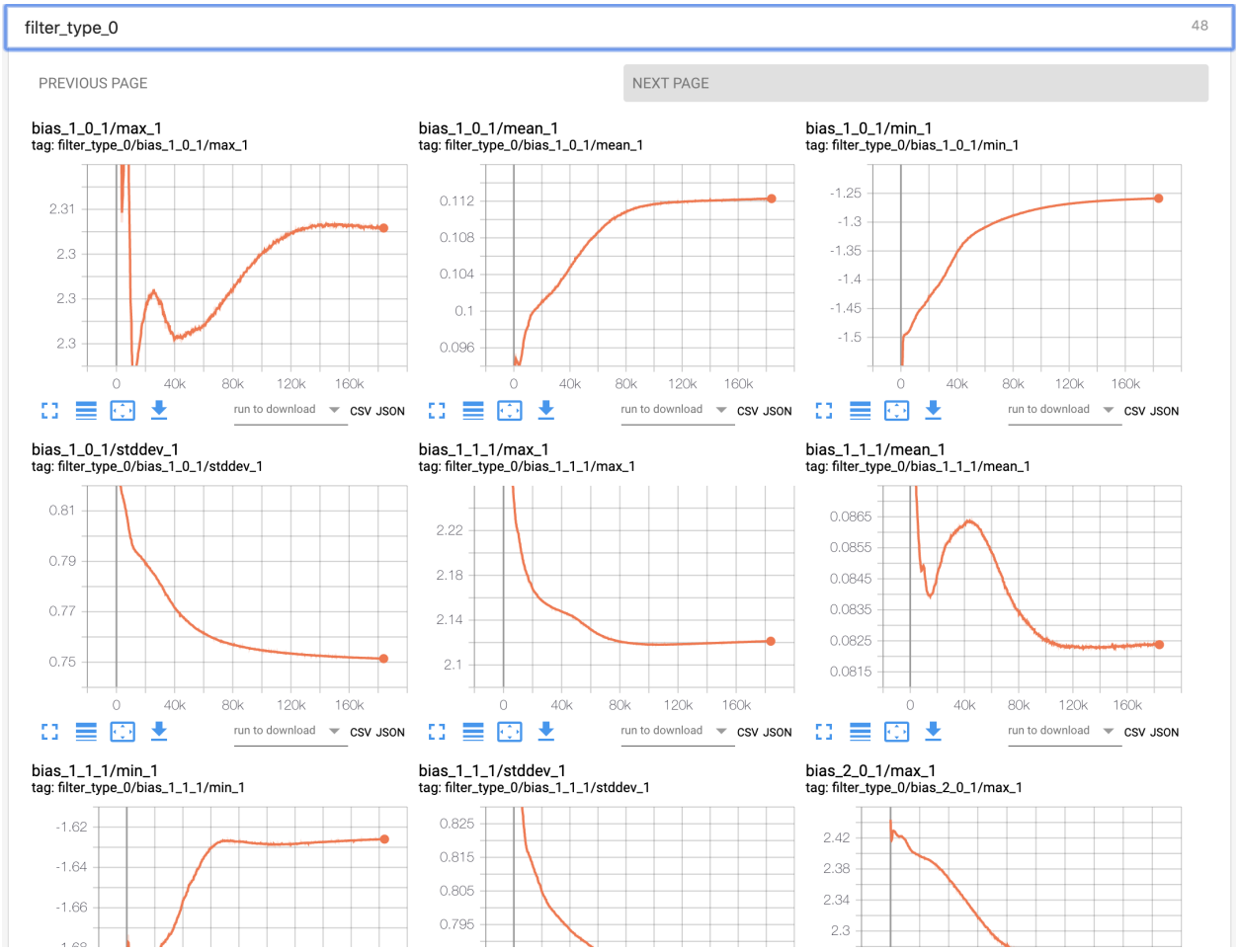
filter_type_0/matrix_1_1_1/histogram train



filter_type_0/matrix_2_0_1/histogram train



Viewing summaries of trainable variables



5.5.4 Attention

Allowing the tensorboard analysis will takes extra execution time.(eg, 15% increasing @Nvidia GTX 1080Ti double precision with default water sample)

TensorBoard can be used in Google Chrome or Firefox. Other browsers might work, but there may be bugs or performance issues.

5.6 Known limitations of using GPUs

If you use deepmd-kit in a GPU environment, the acceptable value range of some variables are additionally restricted compared to the CPU environment due to the software's GPU implementations:

1. The number of atom type of a given system must be less than 128.
2. The maximum distance between an atom and it's neighbors must be less than 128. It can be controlled by setting the rcut value of training parameters.
3. Theoretically, the maximum number of atoms that a single GPU can accept is about 10,000,000. However, this value is actually limited by the GPU memory size currently, usually within 1000,000 atoms even at the model

compression mode.

4. The total sel value of training parameters(in model/descriptor section) must be less than 4096.
5. The size of the last layer of embedding net must be less than 1024 during the model compression process.

CHAPTER

SIX

FREEZE AND COMPRESS

6.1 Freeze a model

The trained neural network is extracted from a checkpoint and dumped into a database. This process is called "freezing" a model. The idea and part of our code are from Morgan. To freeze a model, typically one does

```
$ dp freeze -o graph.pb
```

in the folder where the model is trained. The output database is called `graph.pb`.

6.2 Compress a model

Once the frozen model is obtained from deepmd-kit, we can get the neural network structure and its parameters (weights, biases, etc.) from the trained model, and compress it in the following way:

```
dp compress -i graph.pb -o graph-compress.pb
```

where `-i` gives the original frozen model, `-o` gives the compressed model. Several other command line options can be passed to `dp compress`, which can be checked with

```
$ dp compress --help
```

An explanation will be provided

```
usage: dp compress [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}] [-l LOG_PATH]
                   [-m {master,collect,workers}] [-i INPUT] [-o OUTPUT]
                   [-s STEP] [-e EXTRAPOLATE] [-f FREQUENCY]
                   [-c CHECKPOINT_FOLDER]

optional arguments:
  -h, --help            show this help message and exit
  -v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}, --log-level {DEBUG,3,INFO,2,WARNING,1,ERROR,0}
                        set verbosity level by string or number, 0=ERROR,
                        1=WARNING, 2=INFO and 3=DEBUG (default: INFO)
  -l LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to disk, if not
                        specified, the logs will only be output to console
                        (default: None)
  -m {master,collect,workers}, --mpi-log {master,collect,workers}
```

(continues on next page)

(continued from previous page)

```
                      Set the manner of logging when running with MPI.
                      'master' logs only on main process, 'collect'
                      broadcasts logs from workers to master and 'workers'
                      means each process will output its own log (default:
                      master)
-i INPUT, --input INPUT
                      The original frozen model, which will be compressed by
                      the code (default: frozen_model.pb)
-o OUTPUT, --output OUTPUT
                      The compressed model (default:
                      frozen_model_compressed.pb)
-s STEP, --step STEP  Model compression uses fifth-order polynomials to
                      interpolate the embedding-net. It introduces two
                      tables with different step size to store the
                      parameters of the polynomials. The first table covers
                      the range of the training data, while the second table
                      is an extrapolation of the training data. The domain
                      of each table is uniformly divided by a given step
                      size. And the step(parameter) denotes the step size of
                      the first table and the second table will use 10 *
                      step as it's step size to save the memory. Usually the
                      value ranges from 0.1 to 0.001. Smaller step means
                      higher accuracy and bigger model size (default: 0.01)
-e EXTRAPOLATE, --extrapolate EXTRAPOLATE
                      The domain range of the first table is automatically
                      detected by the code: [d_low, d_up]. While the second
                      table ranges from the first table's upper
                      boundary(d_up) to the extrapolate(parameter) * d_up:
                      [d_up, extrapolate * d_up] (default: 5)
-f FREQUENCY, --frequency FREQUENCY
                      The frequency of tabulation overflow check(Whether the
                      input environment matrix overflow the first or second
                      table range). By default do not check the overflow
                      (default: -1)
-c CHECKPOINT_FOLDER, --checkpoint-folder CHECKPOINT_FOLDER
                      path to checkpoint folder (default: .)
-t TRAINING_SCRIPT, --training-script TRAINING_SCRIPT
                      The training script of the input frozen model
                      (default: None)
```

Parameter explanation

Model compression, which including tabulating the embedding-net. The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first sub-table takes the stride(parameter) as it's uniform stride, while the second sub-table takes 10 * stride as it's uniform stride. The range of the first table is automatically detected by deepmd-kit, while the second table ranges from the first table's upper boundary(upper) to the extrapolate(parameter) * upper. Finally, we added a check frequency parameter. It indicates how often the program checks for overflow(if the input environment matrix overflow the first or second table range) during the MD inference.

Justification of model compression

Model compression, with little loss of accuracy, can greatly speed up MD inference time. According to different simulation systems and training parameters, the speedup can reach more than 10 times at both CPU and GPU devices. At the same time, model compression can greatly change the memory usage, reducing as much as 20 times under the

same hardware conditions.

Acceptable original model version

The model compression interface requires the version of deepmd-kit used in original model generation should be `2.0.0-alpha.0` or above. If one has a frozen 1.2 or 1.3 model, one can upgrade it through the `dp convert-from` interface.(eg: `dp convert-from 1.2/1.3 -i old_frozen_model.pb -o new_frozen_model.pb`)

CHAPTER

SEVEN

TEST

7.1 Test a model

The frozen model can be used in many ways. The most straightforward test can be performed using `dp test`. A typical usage of `dp test` is

```
dp test -m graph.pb -s /path/to/system -n 30
```

where `-m` gives the tested model, `-s` the path to the tested system and `-n` the number of tested frames. Several other command line options can be passed to `dp test`, which can be checked with

```
$ dp test --help
```

An explanation will be provided

```
usage: dp test [-h] [-m MODEL] [-s SYSTEM] [-S SET_PREFIX] [-n NUMB_TEST]
               [-r RAND_SEED] [--shuffle-test] [-d DETAIL_FILE]

optional arguments:
  -h, --help            show this help message and exit
  -m MODEL, --model MODEL
                        Frozen model file to import
  -s SYSTEM, --system SYSTEM
                        The system dir
  -S SET_PREFIX, --set-prefix SET_PREFIX
                        The set prefix
  -n NUMB_TEST, --numb-test NUMB_TEST
                        The number of data for test
  -r RAND_SEED, --rand-seed RAND_SEED
                        The random seed
  --shuffle-test        Shuffle test data
  -d DETAIL_FILE, --detail-file DETAIL_FILE
                        The file containing details of energy force and virial
                        accuracy
```

7.2 Calculate Model Deviation

One can also use a subcommand to calculate deviation of prediced forces or virials for a bunch of models in the following way:

```
dp model-devi -m graph.000.pb graph.001.pb graph.002.pb graph.003.pb -s ./data -o model_
↪devi.out
```

where `-m` specifies graph files to be calculated, `-s` gives the data to be evaluated, `-o` the file to which model deviation results is dumped. Here is more information on this sub-command:

```
usage: dp model-devi [-h] [-v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}]
                     [-l LOG_PATH] [-m MODELS [MODELS ...]] [-s SYSTEM]
                     [-S SET_PREFIX] [-o OUTPUT] [-f FREQUENCY] [-i ITEMS]

optional arguments:
  -h, --help            show this help message and exit
  -v {DEBUG,3,INFO,2,WARNING,1,ERROR,0}, --log-level {DEBUG,3,INFO,2,WARNING,1,ERROR,0}
                        set verbosity level by string or number, 0=ERROR,
                        1=WARNING, 2=INFO and 3=DEBUG (default: INFO)
  -l LOG_PATH, --log-path LOG_PATH
                        set log file to log messages to disk, if not
                        specified, the logs will only be output to console
                        (default: None)
  -m MODELS [MODELS ...], --models MODELS [MODELS ...]
                        Frozen models file to import (default:
                        ['graph.000.pb', 'graph.001.pb', 'graph.002.pb',
                        'graph.003.pb'])
  -s SYSTEM, --system SYSTEM
                        The system directory, not support recursive detection.
                        (default: .)
  -S SET_PREFIX, --set-prefix SET_PREFIX
                        The set prefix (default: set)
  -o OUTPUT, --output OUTPUT
                        The output file for results of model deviation
                        (default: model_devi.out)
  -f FREQUENCY, --frequency FREQUENCY
                        The trajectory frequency of the system (default: 1)
```

For more details with respect to definition of model deviation and its application, please refer to Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang, Han Wang, and Weinan E, DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models, Computer Physics Communications, 2020, 253, 107206.

CHAPTER

EIGHT

INFERENCE

Note that the model for inference is required to be compatible with the DeePMD-kit package. See Model compatibility for details.

8.1 Python interface

One may use the python interface of DeePMD-kit for model inference, an example is given as follows

```
from deepmd.infer import DeepPot
import numpy as np
dp = DeepPot('graph.pb')
coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
cell = np.diag(10 * np.ones(3)).reshape([1, -1])
atype = [1,0,1]
e, f, v = dp.eval(coord, cell, atype)
```

where `e`, `f` and `v` are predicted energy, force and virial of the system, respectively.

Furthermore, one can use the python interface to calulate model deviation.

```
from deepmd.infer import calc_model_devi
from deepmd.infer import DeepPot as DP
import numpy as np

coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
cell = np.diag(10 * np.ones(3)).reshape([1, -1])
atype = [1,0,1]
graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
model_devi = calc_model_devi(coord, cell, atype, graphs)
```

8.2 C++ interface

The C++ interface of DeePMD-kit is also avaiable for model interface, which is considered faster than Python interface. An example `infer_water.cpp` is given below:

```
#include "deepmd/DeepPot.h"

int main(){
```

(continues on next page)

(continued from previous page)

```
  deepmd::DeepPot dp ("graph.pb");
  std::vector<double > coord = {1., 0., 0., 0., 0., 1.5, 1. ,0. ,3.};
  std::vector<double > cell = {10., 0., 0., 0., 10., 0., 0., 0., 10.};
  std::vector<int > atype = {1, 0, 1};
  double e;
  std::vector<double > f, v;
  dp.compute (e, f, v, coord, atype, cell);
}
```

where `e`, `f` and `v` are predicted energy, force and virial of the system, respectively.

You can compile `infer_water.cpp` using `gcc`:

```
gcc infer_water.cpp -D HIGH_PREC -L $deepmd_root/lib -L $tensorflow_root/lib -I $deepmd_
↪root/include -I $tensorflow_root/include -Wl,--no-as-needed -ldeepmd_cc -lstdc++ -Wl,-
↪rpath=$deepmd_root/lib -Wl,-rpath=$tensorflow_root/lib -o infer_water
```

and then run the program:

```
./infer_water
```

CHAPTER

NINE

INTEGRATE WITH THIRD-PARTY PACKAGES

Note that the model for inference is required to be compatible with the DeePMD-kit package. See Model compatibility for details.

9.1 Use deep potential with ASE

Deep potential can be set up as a calculator with ASE to obtain potential energies and forces.

```
from ase import Atoms
from deepmd.calculator import DP

water = Atoms('H2O',
              positions=[(0.7601, 1.9270, 1),
                         (1.9575, 1, 1),
                         (1., 1., 1.)],
              cell=[100, 100, 100],
              calculator=DP(model="frozen_model.pb"))
print(water.get_potential_energy())
print(water.get_forces())
```

Optimization is also available:

```
from ase.optimize import BFGS
dyn = BFGS(water)
dyn.run(fmax=1e-6)
print(water.get_positions())
```

9.2 Run MD with LAMMPS

Running an MD simulation with LAMMPS is simpler. In the LAMMPS input file, one needs to specify the pair style as follows

```
pair_style      deepmd graph.pb
pair_coeff      * *
```

where `graph.pb` is the file name of the frozen model. It should be noted that LAMMPS counts atom types starting from 1, therefore, all LAMMPS atom type will be firstly subtracted by 1, and then passed into the DeePMD-kit engine to compute the interactions.

9.3 LAMMPS commands

9.3.1 Enable DeePMD-kit plugin (plugin mode)

If you are using the plugin mode, enable DeePMD-kit package in LAMMPS with `plugin` command:

```
plugin load libdeepmd_lmp.so
```

The built-in mode doesn't need this step.

9.3.2 pair_style deepmd

The DeePMD-kit package provides the pair_style `deepmd`

```
pair_style deepmd models ... keyword value ...
```

- deepmd = style of this pair_style
- models = frozen model(s) to compute the interaction. If multiple models are provided, then only the first model serves to provide energy and force prediction for each timestep of molecular dynamics, and the model deviation will be computed among all models every `out_freq` timesteps.
- keyword = *out_file* or *out_freq* or *fparam* or *atomic* or *relative*

Examples

```
pair_style deepmd graph.pb
pair_style deepmd graph.pb fparam 1.2
pair_style deepmd graph_0.pb graph_1.pb graph_2.pb out_file md.out out_freq 10 atomic␣
↪relative 1.0
```

Description

Evaluate the interaction of the system by using Deep Potential or Deep Potential Smooth Edition. It is noticed that deep potential is not a "pairwise" interaction, but a multi-body interaction.

This pair style takes the deep potential defined in a model file that usually has the .pb extension. The model can be trained and frozen by package DeePMD-kit.

The model deviation evalulate the consistency of the force predictions from multiple models. By default, only the maximal, minimal and averge model deviations are output. If the key `atomic` is set, then the model deviation of force prediction of each atom will be output.

By default, the model deviation is output in absolute value. If the keyword `relative` is set, then the relative model deviation will be output. The relative model deviation of the force on atom `i` is defined by

```
           |Df_i|
Ef_i = -------------
       |f_i| + level
```

where `Df_i` is the absolute model deviation of the force on atom `i`, `|f_i|` is the norm of the the force and `level` is provided as the parameter of the keyword `relative`.

Restrictions

- The `deepmd` pair style is provided in the USER-DEEPMD package, which is compiled from the DeePMD-kit, visit the DeePMD-kit website for more information.

9.3.3 Compute tensorial properties

The DeePMD-kit package provide the compute `deeptensor/atom` for computing atomic tensorial properties.

```
compute ID group-ID deeptensor/atom model_file
```

- ID: user-assigned name of the computation
- group-ID: ID of the group of atoms to compute
- deeptensor/atom: the style of this compute
- model_file: the name of the binary model file.

Examples

```
compute         dipole all deeptensor/atom dipole.pb
```

The result of the compute can be dump to trajctory file by

```
dump            1 all custom 100 water.dump id type c_dipole[1] c_dipole[2] c_dipole[3]
```

Restrictions

- The `deeptensor/atom` compute is provided in the USER-DEEPMD package, which is compiled from the DeePMD-kit, visit the DeePMD-kit website for more information.

9.3.4 Long-range interaction

The reciprocal space part of the long-range interaction can be calculated by LAMMPS command `kspace_style`. To use it with DeePMD-kit, one writes

```
pair_style        deepmd graph.pb
pair_coeff
kspace_style        pppm 1.0e-5
kspace_modify        gewald 0.45
```

Please notice that the DeePMD does nothing to the direct space part of the electrostatic interaction, because this part is assumed to be fitted in the DeePMD model (the direct space cut-off is thus the cut-off of the DeePMD model). The splitting parameter `gewald` is modified by the `kspace_modify` command.

9.3.5 Use of the centroid/stress/atom to get the full 3x3 "atomic-virial"

The DeePMD-kit allows also the computation of per-atom stress tensor defined as:

Where is the atomic position of nth atom, velocity of atom and the derivative of the atomic energy.

In LAMMPS one can get the per-atom stress using the command `centroid/stress/atom`:

```
compute ID group-ID centroid/stress/atom NULL virial
```

see LAMMPS doc page for more detailes on the meaning of the keywords.

Examples

In order of computing the 9-component per-atom stress

```
compute stress all centroid/stress/atom NULL virial
```

Thus `c_stress` is an array with 9 component in the order `xx,yy,zz,xy,xz,yz,yx,zx,zy`.

If you use this feature please cite D. Tisi, L. Zhang, R. Bertossa, H. Wang, R. Car, S. Baroni - arXiv preprint arXiv:2108.10850, 2021

9.3.6 Computation of heat flux

Using per-atom stress tensor one can, for example, compute the heat flux defined as:

to compute the heat flux with LAMMPS:

```
compute ke_ID all ke/atom
compute pe_ID all pe/atom
compute stress_ID group-ID centroid/stress/atom NULL virial
compute flux_ID all heat/flux ke_ID pe_ID stress_ID
```

Examples

```
compute ke all ke/atom
compute pe all pe/atom
compute stress all centroid/stress/atom NULL virial
compute flux all heat/flux ke pe stress
```

`c_flux` is a global vector of length 6. The first three components are the `x`, `y` and `z` components of the full heat flux vector. The others are the components of the so-called convective portion, see LAMMPS doc page for more detailes.

If you use these features please cite D. Tisi, L. Zhang, R. Bertossa, H. Wang, R. Car, S. Baroni - arXiv preprint arXiv:2108.10850, 2021

9.4 Run path-integral MD with i-PI

The i-PI works in a client-server model. The i-PI provides the server for integrating the replica positions of atoms, while the DeePMD-kit provides a client named `dp_ipi` (or `dp_ipi_low` for low precision) that computes the interactions (including energy, force and virial). The server and client communicates via the Unix domain socket or the Internet socket. Installation instructions of i-PI can be found *here*. The client can be started by

```
i-pi input.xml &
dp_ipi water.json
```

It is noted that multiple instances of the client is allow for computing, in parallel, the interactions of multiple replica of the path-integral MD.

`water.json` is the parameter file for the client `dp_ipi`, and an example is provided:

```
{
    "verbose":                false,
    "use_unix":                true,
    "port":                  31415,
    "host":                  "localhost",
    "graph_file":          "graph.pb",
    "coord_file":          "conf.xyz",
    "atom_type" : {
        "OW":                  0,
        "HW1":                 1,
        "HW2":                 1
    }
}
```

The option **`use_unix`** is set to `true` to activate the Unix domain socket, otherwise, the Internet socket is used.

The option **`port`** should be the same as that in input.xml:

```
<port>31415</port>
```

The option **`graph_file`** provides the file name of the frozen model.

The `dp_ipi` gets the atom names from an XYZ file provided by **`coord_file`** (meanwhile ignores all coordinates in it), and translates the names to atom types by rules provided by **`atom_type`**.

9.5 Running MD with GROMACS

9.5.1 DP/MM Simulation

This part gives a simple tutorial on how to run a DP/MM simulation for methane in water, which means using DP for methane and TIP3P for water. All relevant files can be found in `examples/methane`.

Topology Preparation

Similar to QM/MM simulation, the internal interactions (including bond, angle, dihedrals, LJ, Columb) of the region descibed by a neural network potential (NNP) have to be **turned off**. In GROMACS, bonded interactions can be turned off by modifying `[ bonds ]`, `[ angles ]`, `[ dihedrals ]` and `[ pairs ]` sections. And LJ and Columb interactions must be turned off by `[ exclusions ]` section.

For example, if one wants to simulate ethane in water, using DeepPotential for methane and TIP3P for water, the topology of methane should be like the following (as presented in `examples/methane/methane.itp`):

```
[ atomtypes ]
;name btype  mass  charge ptype    sigma  epsilon
  c3    c3   0.0     0.0     A 0.339771 0.451035
  hc    hc   0.0     0.0     A 0.260018 0.087027

[ moleculetype ]
;name            nrexcl
 methane          3

[ atoms ]
; nr type  resnr residue atom  cgnr  charge   mass
  1   c3      1     MOL   C1     1 -0.1068 12.010
  2   hc      1     MOL   H1     2  0.0267  1.008
  3   hc      1     MOL   H2     3  0.0267  1.008
  4   hc      1     MOL   H3     4  0.0267  1.008
  5   hc      1     MOL   H4     5  0.0267  1.008

[ bonds ]
; i  j  func  b0  kb
 1  2     5
 1  3     5
 1  4     5
 1  5     5

[ exclusions ]
; ai  aj1  aj2  aj3  aj4
  1    2    3    4    5
  2    1    3    4    5
  3    1    2    4    5
  4    1    2    3    5
  5    1    2    3    4
```

For comparsion, the original topology file genearted by `acpype` will be:

```
; methane_GMX.itp created by acpype (v: 2021-02-05T22:15:50CET) on Wed Sep  8 01:21:53␣
↪2021

[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 c3       c3          0.00000  0.00000   A     3.39771e-01   4.51035e-01 ; 1.91  0.1078
 hc       hc          0.00000  0.00000   A     2.60018e-01   8.70272e-02 ; 1.46  0.0208

[ moleculetype ]
;name            nrexcl
```

(continues on next page)

(continued from previous page)

```
 methane          3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1   c3     1   MOL    C1    1    -0.106800     12.01000 ; qtot -0.107
     2   hc     1   MOL    H1    2     0.026700      1.00800 ; qtot -0.080
     3   hc     1   MOL    H2    3     0.026700      1.00800 ; qtot -0.053
     4   hc     1   MOL    H3    4     0.026700      1.00800 ; qtot -0.027
     5   hc     1   MOL    H4    5     0.026700      1.00800 ; qtot 0.000

[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.0970e-01    3.1455e+05 ;     C1 - H1
     1      3   1    1.0970e-01    3.1455e+05 ;     C1 - H2
     1      4   1    1.0970e-01    3.1455e+05 ;     C1 - H3
     1      5   1    1.0970e-01    3.1455e+05 ;     C1 - H4

[ angles ]
;   ai     aj     ak    funct   theta         cth
     2      1      3      1    1.0758e+02    3.2635e+02 ;     H1 - C1     - H2
     2      1      4      1    1.0758e+02    3.2635e+02 ;     H1 - C1     - H3
     2      1      5      1    1.0758e+02    3.2635e+02 ;     H1 - C1     - H4
     3      1      4      1    1.0758e+02    3.2635e+02 ;     H2 - C1     - H3
     3      1      5      1    1.0758e+02    3.2635e+02 ;     H2 - C1     - H4
     4      1      5      1    1.0758e+02    3.2635e+02 ;     H3 - C1     - H4
```

DeepMD Settings

Before running simulation, we need to tell GROMACS to use DeepPotential by setting environment variable `GMX_DEEPMD_INPUT_JSON`:

```
export GMX_DEEPMD_INPUT_JSON=input.json
```

Then, in your working directories, we have to write `input.json` file:

```
{
    "graph_file": "/path/to/graph.pb",
    "type_file": "type.raw",
    "index_file": "index.raw",
    "lambda": 1.0,
    "pbc": false
}
```

Here is an explanation for these settings:

- `graph_file` : The graph file (with suffix .pb) generated by `dp freeze` command
- `type_file` : File to specify DP atom types (in space-sepreated format). Here, `type.raw` looks like

```
1 0 0 0 0
```

- `index_file` : File containing indices of DP atoms (in space-seperated format), which should be in consistent with indices' order in .gro file but **starting from zero**. Here, `index.raw` looks like

```
0 1 2 3 4
```

- `lambda`: Optional, default 1.0. Used in alchemical calculations.
- `pbc`: Optional, default true. If true, the GROMACS peroidic condition is passed to DeepMD.

Run Simulation

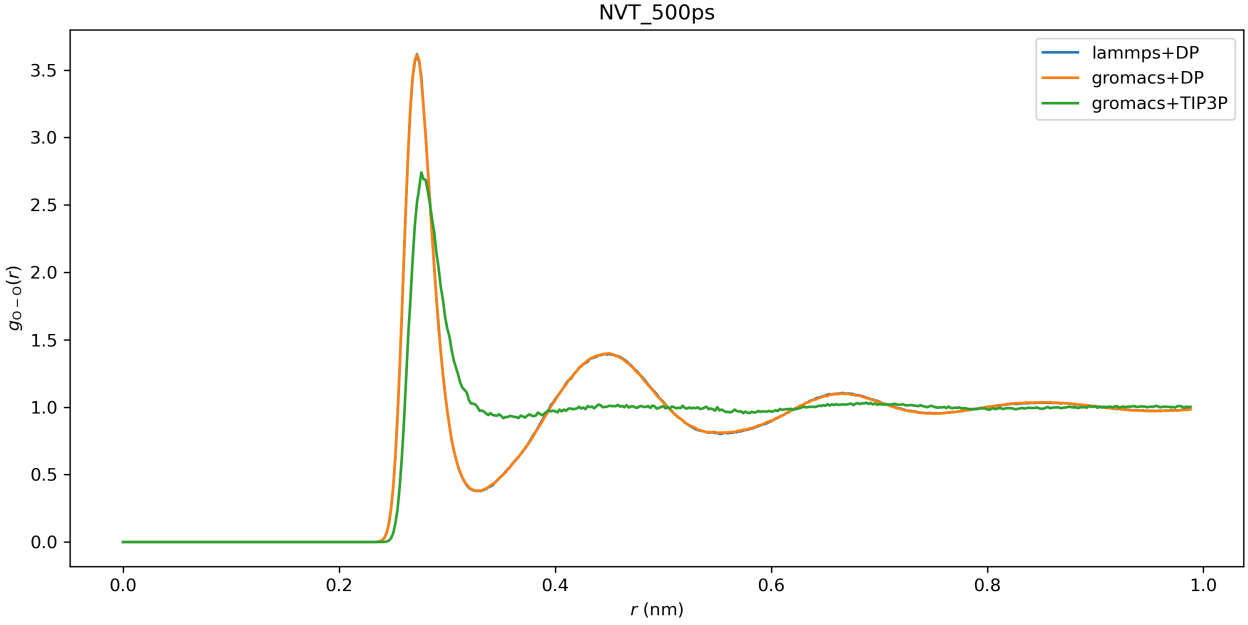
Finally, you can run GROMACS using `gmx mdrun` as usual.

9.5.2 All-atom DP Simulation

This part gives an example on how to run a simulation with all atoms described by a DeepPotential with Gromacs, taking water as an example. Instead of using `[ exclusions ]` to turn off the non-bonded energies, we can simply do this by setting LJ parameters (i.e. epsilon and sigma) and partial charges to 0, as shown in `examples/water/gmx/water.top`:

```
[ atomtypes ]
; name      at.num  mass     charge ptype  sigma       epsilon
HW           1       1.008   0.0000  A   0.00000e+00  0.00000e+00
OW           8      16.00    0.0000  A   0.00000e+00  0.00000e+00
```

As mentioned in the above section, `input.json` and relevant files (`index.raw`, `type.raw`) should also be created. Then, we can start the simulation under NVT ensemble and plot the radial distribution function (RDF) by `gmx rdf` command. We can see that the RDF given by Gromacs+DP matches perfectly with Lammps+DP, which further provides an evidence on the validity of our simulation.



However, we still recommend you run all-atom DP simulation using LAMMPS since it is more stable and efficient.

CHAPTER

TEN

FAQS

In consequence of various differences of computers or systems, problems may occur. Some common circumstances are listed as follows. In addition, some frequently asked questions about parameters setting are listed as follows. If other unexpected problems occur, you're welcome to contact us for help.

10.1 How to tune Fitting/embedding-net size ?

Here are some test forms on fitting-net size tuning or embedding-net size tuning performed on several different systems.

10.1.1 Al2O3

Fitting net size tuning form on Al2O3: (embedding-net size: [25,50,100])

Fitting-net size	Energy L2err(eV)	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[240,240,240]	1.742252e-02	7.259383e-05	4.014115e-02
[80,80,80]	1.799349e-02	7.497287e-05	4.042977e-02
[40,40,40]	1.799036e-02	7.495984e-05	4.068806e-02
[20,20,20]	1.834032e-02	7.641801e-05	4.094784e-02
[10,10,10]	1.913058e-02	7.971073e-05	4.154775e-02
[5,5,5]	1.932914e-02	8.053808e-05	4.188052e-02
[4,4,4]	1.944832e-02	8.103467e-05	4.217826e-02
[3,3,3]	2.068631e-02	8.619296e-05	4.300497e-02
[2,2,2]	2.267962e-02	9.449840e-05	4.413609e-02
[1,1,1]	2.813596e-02	1.172332e-04	4.781115e-02
[]	3.135002e-02	1.306251e-04	5.373120e-02

[] means no hidden layer, but there is still a linear output layer. This situation is equal to the linear regression.

Embedding net size tuning form on Al2O3: (Fitting-net size: [240,240,240])

Embedding-net size	Energy L2err(eV)	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[25,50,100]	1.742252e-02	7.259383e-05	4.014115e-02
[10,20,40]	2.909990e-02	1.212496e-04	4.734667e-02
[5,10,20]	3.357767e-02	1.399070e-04	5.706385e-02
[4,8,16]	6.060367e-02	2.525153e-04	7.333304e-02
[3,6,12]	5.656043e-02	2.356685e-04	7.793539e-02
[2,4,8]	5.277023e-02	2.198759e-04	7.459995e-02
[1,2,4]	1.302282e-01	5.426174e-04	9.672238e-02

10.1.2 Cu

Fitting net size tuning form on Cu: (embedding-net size: [25,50,100])

Fitting-net size	Energy L2err(eV)	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[240,240,240]	4.135548e-02	1.615449e-04	8.940946e-02
[20,20,20]	4.323858e-02	1.689007e-04	8.955762e-02
[10,10,10]	4.399364e-02	1.718502e-04	8.962891e-02
[5,5,5]	4.468404e-02	1.745470e-04	8.970111e-02
[4,4,4]	4.463580e-02	1.743586e-04	8.972011e-02
[3,3,3]	4.493758e-02	1.755374e-04	8.971303e-02
[2,2,2]	4.500736e-02	1.758100e-04	8.973878e-02
[1,1,1]	4.542073e-02	1.774247e-04	8.964761e-02
[]	4.545168e-02	1.775456e-04	8.983201e-02

Embedding net size tuning form on Cu: (Fitting-net size: [240,240,240])

Embedding-net size	Energy L2err(eV)	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[25,50,100]	4.135548e-02	1.615449e-04	8.940946e-02
[20,40,80]	4.203562e-02	1.642016e-04	8.925881e-02
[15,30,60]	4.146672e-02	1.619794e-04	8.936911e-02
[10,20,40]	4.263060e-02	1.665258e-04	8.955818e-02
[5,10,20]	4.994913e-02	1.951138e-04	9.007786e-02
[4,8,16]	1.022157e-01	3.992802e-04	9.532119e-02
[3,9,12]	1.362098e-01	5.320695e-04	1.073860e-01
[2,4,8]	7.061800e-02	2.758515e-04	9.126418e-02
[1,2,4] && seed = 1	9.843161e-02	3.844985e-04	9.348505e-02
[1,2,4] && seed = 2	9.404335e-02	3.673568e-04	9.304089e-02
[1,2,4] && seed = 3	1.508016e-01	5.890688e-04	1.382356e-01
[1,2,4] && seed = 4	9.686949e-02	3.783965e-04	9.294820e-02

10.1.3 Water

Fitting net size tuning form on water: (embedding-net size: [25,50,100])

Fitting-net size	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[240,240,240]	9.1589E-04	5.1540E-02
[200,200,200]	9.3221E-04	5.2366E-02
[160,160,160]	9.4274E-04	5.3403E-02
[120,120,120]	9.5407E-04	5.3093E-02
[80,80,80]	9.4605E-04	5.3402E-02
[40,40,40]	9.8533E-04	5.5790E-02
[20,20,20]	1.0057E-03	5.8232E-02
[10,10,10]	1.0466E-03	6.2279E-02
[5,5,5]	1.1154E-03	6.7994E-02
[4,4,4]	1.1289E-03	6.9613E-02
[3,3,3]	1.2368E-03	7.9786E-02
[2,2,2]	1.3558E-03	9.7042E-02
[1,1,1]	1.4633E-03	1.1265E-01
[]	1.5193E-03	1.2136E-01

Embedding net size tuning form on water: (Fitting-net size: [240,240,240])

Embedding-net size	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[25,50,100]	9.1589E-04	5.1540E-02
[20,40,80]	9.5080E-04	5.3593E-02
[15,30,60]	9.7996E-04	5.6338E-02
[10,20,40]	1.0353E-03	6.2776E-02
[5,10,20]	1.1254E-03	7.3195E-02
[4,8,16]	1.2495E-03	8.0371E-02
[3,6,12]	1.3604E-03	9.9883E-02
[2,4,8]	1.4358E-03	9.7389E-02
[1,2,4]	2.1765E-03	1.7276E-01

10.1.4 Mg-Al

Fitting net size tuning form on Mg-Al: (embedding-net size: [25,50,100])

Fitting-net size	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[240,240,240]	3.9606e-03	1.6289e-02
[200,200,200]	3.9449e-03	1.6471e-02
[160,160,160]	4.0947e-03	1.6413e-02
[120,120,120]	3.9234e-03	1.6283e-02
[80,80,80]	3.9758e-03	1.6506e-02
[40,40,40]	3.9142e-03	1.6348e-02
[20,20,20]	4.1302e-03	1.7006e-02
[10,10,10]	4.3433e-03	1.7524e-02
[5,5,5]	5.3154e-03	1.9716e-02
[4,4,4]	5.4210e-03	1.9710e-02
[2,2,2]	6.2667e-03	2.2568e-02
[1,1,1]	7.3676e-03	2.6375e-02
[]	7.3999e-03	2.6097e-02

Embedding net size tuning form on Mg-Al: (Fitting-net size: [240,240,240])

Embedding-net size	Energy L2err/Natoms(eV)	Force L2err(eV/Angstrom)
[25,50,100]	3.9606e-03	1.6289e-02
[20,40,80]	4.0292e-03	1.6555e-02
[15,30,60]	4.1743e-03	1.7026e-02
[10,20,40]	4.8138e-03	1.8516e-02
[5,10,20]	5.6052e-03	2.0709e-02
[4,8,16]	6.1335e-03	2.1450e-02
[3,6,12]	6.6469e-03	2.3003e-02
[2,4,8]	6.8222e-03	2.6318e-02
[1,2,4]	1.0678e-02	3.9559e-02

10.2 How to control the number of nodes used by a job ?

Set the number of CPU nodes used by DP algorithms with:

```
mpirun -np $num_nodes dp
```

Set the number of threads used by DP algorithms with:

```
export OMP_NUM_THREADS=$num_threads
```

Set the number of CPU nodes used by TF kernels with:

```
export TF_INTRA_OP_PARALLELISM_THREADS=$num_nodes
export TF_INTER_OP_PARALLELISM_THREADS=$num_nodes
```

10.3 Do we need to set rcut < half boxsize ?

When seeking the neighbors of atom i under periodic boundary condition, deepmd-kit considers all j atoms within cutoff rcut from atom i in all mirror cells.

So, so there is no limitation on the setting of rcut.

PS: The reason why some softwares require rcut < half boxsize is that they only consider the nearest mirrors from the center cell. Deepmd-kit is totally different from them.

10.4 How to set sel ?

`sel` is short for "selected number of atoms in `rcut`".

`sel_a[i]` is a list of integers. The length of the list should be the same as the number of atom types in the system.

`sel_a[i]` gives the number of selected number of type `i` neighbors within `rcut`. To ensure that the results are strictly accurate, `sel_a[i]` should be larger than the largest number of type `i` neighbors in the `rcut`.

However, the computation overhead increases with `sel_a[i]`, therefore, `sel_a[i]` should be as small as possible.

The setting of `sel_a[i]` should balance the above two considerations.

10.5 Installation

10.5.1 Inadequate versions of gcc/g++

Sometimes you may use a gcc/g++ of version < 4.8. In this way, you can still compile all the parts of TensorFlow and most of the parts of DeePMD-kit, but i-Pi and GROMACS plugin will be disabled automatically. Or if you have a gcc/g++ of version > 4.8, say, 7.2.0, you may choose to use it by doing

```
export CC=/path/to/gcc-7.2.0/bin/gcc
export CXX=/path/to/gcc-7.2.0/bin/g++
```

10.5.2 Build files left in DeePMD-kit

When you try to build a second time when installing DeePMD-kit, files produced before may contribute to failure. Thus, you may clear them by

```
cd build
rm -r *
```

and redo the `cmake` process.

10.6 The temperature undulates violently during early stages of MD

This is probably because your structure is too far from the equlibrium configuration.

Although, to make sure the potential model is truly accurate, we recommend to check model deviation.

10.7 MD: cannot run LAMMPS after installing a new version of DeePMD-kit

This typically happens when you install a new version of DeePMD-kit and copy directly the generated `USER-DEEPMD` to a LAMMPS source code folder and re-install LAMMPS.

To solve this problem, it suffices to first remove `USER-DEEPMD` from LAMMPS source code by

```
make no-user-deepmd
```

and then install the new `USER-DEEPMD`.

If this does not solve your problem, try to decompress the LAMMPS source tarball and install LAMMPS from scratch again, which typically should be very fast.

10.8 Model compatibility

When the version of DeePMD-kit used to training model is different from the that of DeePMD-kit running MDs, one has the problem of model compatibility.

DeePMD-kit guarantees that the codes with the same major and minor revisions are compatible. That is to say v0.12.5 is compatible to v0.12.0, but is not compatible to v0.11.0 nor v1.0.0.

One can execute `dp convert-from` to convert an old model to a new one.

Model version	v0.12	v1.0	v1.1	v1.2	v1.3	v2.0
Compatibility						

Legend:

- : The model is compatible with the DeePMD-kit package.
- : The model is incompatible with the DeePMD-kit package, but one can execute `dp convert-from` to convert an old model to v2.0.
- : The model is incompatible with the DeePMD-kit package, and there is no way to convert models.

CHAPTER

ELEVEN

CODING CONVENTIONS

11.1 Preface

The aim of these coding standards is to help create a codebase with defined and consistent coding style that every contributor can get easily familiar with. This will in enhance code readability as there will be no different coding styles from different contributors and everything will be documented. Also PR diffs will be smaller because of unified coding style. Finally static typing will help in hunting down potential bugs before the code is even run.

Contributed code will not be refused merely because it does not strictly adhere to these conditions; as long as it's internally consistent, clean, and correct, it probably will be accepted. But don't be surprised if the "offending" code gets fiddled over time to conform to these conventions.

There are also github actions CI checks for python code style which will annotate the PR diff for you to see the areas where your code is lacking compared to the set standard.

11.2 Rules

The code must be compatible with the oldest supported version of python which is 3.6

The project follows the generic coding conventions as specified in the Style Guide for Python Code, Docstring Conventions and Typing Conventions PEPs, clarified and extended as follows:

- Do not use "*" imports such as `from module import *`. Instead, list imports explicitly.
- Use 4 spaces per indentation level. No tabs.
- No one-liner compound statements (i.e., no `if x: return`: use two lines).
- Maximum line length is 88 characters as recomended by black wich is less strict than Docstring Conventions suggests.
- Use "StudlyCaps" for class names.
- Use "lowercase" or "lowercase_with_underscores" for function, method, variable names and module names. For short names, joined lowercase may be used (e.g. "tagname"). Choose what is most readable.
- No single-character variable names, except indices in loops that encompass a very small number of lines (`for i in range(5): ...`).
- Avoid lambda expressions. Use named functions instead.
- Avoid functional constructs (filter, map, etc.). Use list comprehensions instead.
- Use `"double quotes"` for string literals, and `"""triple double quotes"""` for docstring's. Single quotes are OK for something like

```
f"something {'this' if x else 'that'}"
```

- Use f-strings `s = f"{x:.2f}"` instead of old style formating with `"%f" % x`. string format method `"{x:.2f}".format()` may be used sparsely where it is more convenient than f-strings.

11.3 Whitespace

Python is not C/C++ so whitespace should be used sparingly to maintain code readability

- Read the *Whitespace in Expressions and Statements* section of PEP8.
- Avoid trailing whitespaces.
- Do not use excessive whitespace in your expressions and statements.
- You should have blank spaces after commas, colons, and semi-colons if it isn't trailing next to the end of a bracket, brace, or parentheses.
- With any operators you should use a space in on both sides of the operator.
- Colons for slicing are considered a binary operator, and should not have any spaces between them.
- You should have parentheses with no space, directly next to the function when calling functions `function()`.
- When indexing or slicing the brackets should be directly next to the collection with no space `collection["index"]`.
- Whitespace used to line up variable values is not recommended.
- Make sure you are consistent with the formats you choose when optional choices are available.

11.4 General advice

- Get rid of as many `break` and `continue` statements as possible.
- Write short functions. All functions should fit within a standard screen.
- Use descriptive variable names.

11.5 Writing documentation in the code

Here is an example of how to write good docstrings:

> https://github.com/numpy/numpy/blob/master/doc/example.py

The numpy doctring documentation can be found here

It is a good practice to run pydocstyle check on your code or use a text editor that does it automatically):

```
$ pydocstyle filename.py
```

11.6 Run pycodestyle on your code

It's a good idea to run pycodestyle on your code (or use a text editor that does it automatically):

```
$ pycodestyle filename.py
```

11.7 Run mypy on your code

It's a good idea to run mypy on your code (or use a text editor that does it automatically):

```
$ mypy filename.py
```

11.8 Run pydocstyle on your code

It's a good idea to run pycodestyle on your code (or use a text editor that does it automatically):

```
$ pycodestyle filename.py --max-line-length=88
```

11.9 Run black on your code

Another method of enforcing PEP8 is using a tool such as black. These tools tend to be very effective at cleaning up code, but should be used carefully and code should be retested after cleaning it. Try:

```
$ black --help
```

CHAPTER

TWELVE

CREATE A MODEL

If you'd like to create a new model that isn't covered by the existing DeePMD-kit library, but reuse DeePMD-kit's other efficient module such as data processing, trainner, etc, you may want to read this section.

To incorporate your custom model you'll need to:

1. Register and implement new components (e.g. descriptor) in a Python file. You may also want to regiester new TensorFlow OPs if necessary.
2. Register new arguments for user inputs.
3. Package new codes into a Python package.
4. Test new models.

12.1 Design a new component

When creating a new component, take descriptor as the example, you should inherit *deepmd.descriptor.descriptor.Descriptor* class and override several methods. Abstract methods such as *deepmd.descriptor.descriptor.Descriptor.build* must be implemented and others are not. You should keep arguments of these methods unchanged.

After implementation, you need to register the component with a key:

```
from deepmd.descriptor import Descriptor

@Descriptor.register("some_descrpt")
class SomeDescript(Descriptor):
    def __init__(self, arg1: bool, arg2: float) -> None:
        pass
```

12.2 Register new arguments

To let some one uses your new component in their input file, you need to create a new methods that returns some `Argument` of your new component, and then register new arguments. For example, the code below

```
from typing import List

from dargs import Argument
from deepmd.utils.argcheck import descrpt_args_plugin
```

(continues on next page)

(continued from previous page)

```
@descrpt_args_plugin.register("some_descrpt")
def descrpt_some_args() -> List[Argument]:
    return [
        Argument("arg1", bool, optional=False, doc="balabala"),
        Argument("arg2", float, optional=True, default=6.0, doc="haha"),
    ]
```

allows one to use your new descriptor as below:

```
"descriptor" :{
    "type": "some_descrpt",
    "arg1": true,
    "arg2": 6.0
}
```

The arguments here should be consistent with the class arguments of your new componenet.

12.3 Package new codes

You may use `setuptools` to package new codes into a new Python package. It's crirical to add your new component to `entry_points['deepmd']` in `setup.py`:

```
    entry_points={
        'deepmd': [
            'some_descrpt=deepmd_some_descrtpt:SomeDescript',
        ],
    },
```

where `deepmd_some_descrtpt` is the module of your codes. It is equivalent to `from deepmd_some_descrtpt import SomeDescript`.

If you place `SomeDescript` and `descrpt_some_args` into different modules, you are also expected to add `descrpt_some_args` to `entry_points`.

After you install your new package, you can now use `dp train` to run your new model.

CHAPTER

THIRTEEN

ATOM TYPE EMBEDDING

13.1 Overview

Here is an overview of the deepmd-kit algorithm. Given a specific centric atom, we can obtain the matrix describing its local environment, named as `R`. It is consist of the distance between centric atom and its neighbors, as well as a direction vector. We can embed each distance into a vector of M1 dimension by a `embedding net`, so the environment matrix `R` can be embed into matrix `G`. We can thus extract a descriptor vector (of M1*M2 dim) of the centric atom from the `G` by some matrix multiplication, and put the descriptor into `fitting net` to get predicted energy `E`. The vanilla version of deepmd-kit build `embedding net` and `fitting net` relying on the atom type, resulting in O(N) memory usage. After applying atom type embedding, in deepmd-kit v2.0, we can share one `embedding net` and one `fitting net` in total, which decline training complexity largely.

13.2 Preliminary

In the following chart, you can find the meaning of symbols used to clarify the atom type embedding algorithm.

Symbol	Meaning
i	Type of centric atom
j	Type of neighbor atom
s_ij	Distance between centric atom and neighbor atom
G_ij(·)	Origin embedding net, take s_ij as input and output embedding vector of M1 dim
G(·)	Shared embedding net
Multi(·)	Matrix multiplication and flattening, output the descriptor vector of M1*M2 dim
F_i(·)	Origin fitting net, take the descriptor vector as input and output energy
F(·)	Shared fitting net
A(·)	Atom type embedding net, input is atom type, output is type embedding vector of dim `nchanl`

So, we can formulate the training process as follows. Vanilla deepmd-kit algorithm:

```
Energy = F_i( Multi( G_ij( s_ij ) ) )
```

Deepmd-kit applying atom type embedding:

```
Energy = F( [ Multi( G( [s_ij, A(i), A(j)] ) ), A(j)] )
```

or

```
Energy = F( [ Multi( G( [s_ij, A(j)] ) ), A(j)] )
```

The difference between two variants above is whether using the information of centric atom when generating the descriptor. Users can choose by modifying the `type_one_side` hyper-parameter in the input json file.

13.3 How to use

A detailed introduction can be found at `se_e2_a_tebd`. Looking for a fast start up, you can simply add a `type_embedding` section in the input json file as displayed in the following, and the algorithm will adopt atom type embedding algorithm automatically. An example of `type_embedding` is like

```
    "type_embedding":{
       "neuron":    [2, 4, 8],
       "resnet_dt": false,
       "seed":      1
    }
```

13.4 Code Modification

Atom type embedding can be applied to varied `embedding net` and `fitting net`, as a result we build a class `TypeEmbedNet` to support this free combination. In the following, we will go through the execution process of the code to explain our code modification.

13.4.1 trainer (train/trainer.py)

In trainer.py, it will parse the parameter from the input json file. If a `type_embedding` section is detected, it will build a `TypeEmbedNet`, which will be later input in the `model`. `model` will be built in the function `_build_network`.

13.4.2 model (model/ener.py)

When building the operation graph of the `model` in `model.build`. If a `TypeEmbedNet` is detected, it will build the operation graph of `type embed net`, `embedding net` and `fitting net` by order. The building process of `type embed net` can be found in `TypeEmbedNet.build`, which output the type embedding vector of each atom type (of [ntypes * nchanl] dimension). We then save the type embedding vector into `input_dict`, so that they can be fetched later in `embedding net` and `fitting net`.

13.4.3 embedding net (descriptor/se*.py)

In `embedding net`, we shall take local environment `R` as input and output matrix `G`. Functions called in this process by order is

```
build -> _pass_filter -> _filter -> _filter_lower
```

- `_pass_filter`: It will first detect whether an atom type embedding exists, if so, it will apply atom type embedding algorithm and doesn't divide the input by type.
- `_filter`: It will call `_filter_lower` function to obtain the result of matrix multiplication (`G^T·R`), do further multiplication involved in Multi(·), and finally output the result of descriptor vector of M1*M2 dim.

- `_filter_lower`: The main function handling input modification. If type embedding exists, it will call `_concat_type_embedding` function to concat the first column of input `R` (the column of s_ij) with the atom type embedding information. It will decide whether using the atom type embedding vector of centric atom according to the value of `type_one_side` (if set **True**, then we only use the vector of the neighbor atom). The modified input will be put into the `fitting net` to get `G` for further matrix multiplication stage.

13.4.4 fitting net (fit/ener.py)

In `fitting net`, it take the descriptor vector as input, whose dimension is [natoms, (M1*M2)]. Because we need to involve information of centric atom in this step, we need to generate a matrix named as `atype_embed` (of dim [natoms, nchanl]), in which each row is the type embedding vector of the specific centric atom. The input is sorted by type of centric atom, we also know the number of a particular atom type (stored in `natoms[2+i]`), thus we get the type vector of centric atom. In the build phrase of fitting net, it will check whether type embedding exist in `input_dict` and fetch them. After that calling `embed_atom_type` function to lookup embedding vector for type vector of centric atom to obtain `atype_embed`, and concat input with it ([input, atype_embed]). The modified input go through `fitting net` to get predicted energy.

P.S.: You can't apply compression method while using atom type embedding

CHAPTER

FOURTEEN

PYTHON API

14.1 deepmd package

Root of the deepmd package, exposes all public classes and submodules.

class deepmd.**DeepEval**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*, *auto_batch_size: Union[bool, int,* deepmd.utils.batch_size.AutoBatchSize*] = False*)

Bases: object

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size [bool or int or AutomaticBatchSize, default: False] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

load_prefix: str

make_natoms_vec(*atom_types: numpy.ndarray*) → numpy.ndarray

Make the natom vector used by deepmd-kit.

Parameters

atom_types The type of atoms

Returns

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

property model_type: str
Get type of model.

:type:str

property model_version: str
Get version of model.

Returns

str version of model

static reverse_map(*vec: numpy.ndarray*, *imap: List[int]*) → numpy.ndarray
Reverse mapping of a vector according to the index map

Parameters

vec Input vector. Be of shape [nframes, natoms, -1]

imap Index map. Be of shape [natoms]

Returns

vec_out Reverse mapped vector.

static sort_input(*coord: numpy.ndarray*, *atom_type: numpy.ndarray*, *sel_atoms: Optional[List[int]] = None*)
Sort atoms in the system according their types.

Parameters

coord The coordinates of atoms. Should be of shape [nframes, natoms, 3]

atom_type The type of atoms Should be of shape [natoms]

sel_atom The selected atoms by type

Returns

coord_out The coordinates after sorting

atom_type_out The atom types after sorting

idx_map The index mapping from the input to the output. For example coord_out = coord[:,idx_map,:]

sel_atom_type Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

deepmd.**DeepPotential**(*model_file: Union[str, pathlib.Path]*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*) → Union[*deepmd.infer.deep_dipole.DeepDipole*, *deepmd.infer.deep_polar.DeepGlobalPolar*, *deepmd.infer.deep_polar.DeepPolar*, *deepmd.infer.deep_pot.DeepPot*, *deepmd.infer.deep_wfc.DeepWFC*]
Factory function that will inialize appropriate potential read from *model_file*.

Parameters

model_file: str The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Returns

Union[DeepDipole, DeepGlobalPolar, DeepPolar, DeepPot, DeepWFC] one of the available potentials

Raises

RuntimeError if model file does not correspond to any implementd potential

class deepmd.DipoleChargeModifier(*model_name: str*, *model_charge_map: List[float]*, *sys_charge_map: List[float]*, *ewald_h: float = 1*, *ewald_beta: float = 1*)

Bases: *deepmd.infer.deep_dipole.DeepDipole*

Parameters

model_name The model file for the DeepDipole model

model_charge_map Gives the amount of charge for the wfcc

sys_charge_map Gives the amount of charge for the real atoms

ewald_h Grid spacing of the reciprocal part of Ewald sum. Unit: A

ewald_beta Splitting parameter of the Ewald sum. Unit: A^{-1}

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

build_fv_graph()	Build the computational graph for the force and virial inference.
eval(coord, box, atype[, eval_fv])	Evaluate the modification
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
modify_data(data)	Modify data.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

build_fv_graph() → tensorflow.python.framework.ops.Tensor
Build the computational graph for the force and virial inference.

eval(*coord: numpy.ndarray*, *box: numpy.ndarray*, *atype: numpy.ndarray*, *eval_fv: bool = True*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]
Evaluate the modification

Parameters

coord The coordinates of atoms

box The simulation region. PBC is assumed

atype The atom types

eval_fv Evaluate force and virial

Returns

tot_e The energy modification

tot_f The force modification

tot_v The virial modification

load_prefix: str

modify_data(*data: dict*) → None
Modify data.

Parameters

data Internal data of DeepmdData. Be a dict, has the following keys - coord coordinates - box simulation box - type atom types - find_energy tells if data has energy - find_force tells if data has force - find_virial tells if data has virial - energy energy - force force - virial virial

14.1.1 Subpackages

deepmd.cluster package

Module that reads node resources, auto detects if running local or on SLURM.

deepmd.cluster.**get_resource**() → Tuple[str, List[str], Optional[List[int]]]
Get local or slurm resources: nodename, nodelist, and gpus.

Returns

Tuple[str, List[str], Optional[List[int]]] nodename, nodelist, and gpus

Submodules

deepmd.cluster.local module

Get local GPU resources.

deepmd.cluster.local.**get_gpus**()
Get available IDs of GPU cards at local. These IDs are valid when used as the TensorFlow device ID.

Returns

Optional[List[int]] List of available GPU IDs. Otherwise, None.

deepmd.cluster.local.**get_resource**() → Tuple[str, List[str], Optional[List[int]]]
Get local resources: nodename, nodelist, and gpus.

Returns

`Tuple[str, List[str], Optional[List[int]]]` nodename, nodelist, and gpus

deepmd.cluster.slurm module

MOdule to get resources on SLURM cluster.

References

https://github.com/deepsense-ai/tensorflow_on_slurm ####

deepmd.cluster.slurm.**get_resource**() → Tuple[str, List[str], Optional[List[int]]]
Get SLURM resources: nodename, nodelist, and gpus.

Returns

`Tuple[str, List[str], Optional[List[int]]]` nodename, nodelist, and gpus

Raises

`RuntimeError` if number of nodes could not be retrieved

`ValueError` list of nodes is not of the same length sa number of nodes

`ValueError` if current nodename is not found in node list

deepmd.descriptor package

Submodules

deepmd.descriptor.descriptor module

class deepmd.descriptor.descriptor.**Descriptor**(**args*, ***kwargs*)
Bases: *deepmd.utils.plugin.PluginVariant*

The abstract class for descriptors. All specific descriptors should be based on this class.

The descriptor $\mathcal{D}$ describes the environment of an atom, which should be a function of coordinates and types of its neighbour atoms.

Notes

Only methods and attributes defined in this class are generally public, that can be called by other classes.

Examples

```
>>> descript = Descriptor(type="se_e2_a", rcut=6., rcut_smth=0.5, sel=[50])
>>> type(descript)
<class 'deepmd.descriptor.se_a.DescrptSeA'>
```

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor.
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor.
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	Returns neighbor information.
get_ntypes()	Returns the number of atom types.
get_rcut()	Returns the cut-off radius.
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(*tensors)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial.
register(key)	Regiester a descriptor plugin.

abstract build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: Dict[str, Any]*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor.

Parameters

coord_ [tf.Tensor] The coordinate of atoms

atype_ [tf.Tensor] The type of atoms

natoms [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

box [tf.Tensor] The box of frames

mesh [tf.Tensor] For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict [dict[str, Any]] Dictionary for additional inputs

reuse [bool, optional] The weights in the networks should be reused when get the variable.

suffix [str, optional] Name suffix to identify this descriptor

Returns

descriptor: `tf.Tensor` The output descriptor

Notes

This method must be implemented, as it's called by other classes.

abstract compute_input_stats(*data_coord: List[numpy.ndarray]*, *data_box: List[numpy.ndarray]*, *data_atype: List[numpy.ndarray]*, *natoms_vec: List[numpy.ndarray]*, *mesh: List[numpy.ndarray]*, *input_dict: Dict[str, List[numpy.ndarray]]*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord [list[np.ndarray]] The coordinates. Can be generated by *deepmd.model.model_stat.make_stat_input()*

data_box [list[np.ndarray]] The box. Can be generated by *deepmd.model.model_stat.make_stat_input()*

data_atype [list[np.ndarray]] The atom types. Can be generated by *deepmd.model.model_stat.make_stat_input()*

natoms_vec [list[np.ndarray]] The vector for the number of atoms of the system and different types of atoms. Can be generated by *deepmd.model.model_stat.make_stat_input()*

mesh [list[np.ndarray]] The mesh for neighbor searching. Can be generated by *deepmd.model.model_stat.make_stat_input()*

input_dict [dict[str, list[np.ndarray]]] Dictionary for additional input

Notes

This method must be implemented, as it's called by other classes.

enable_compression(*min_nbor_dist: float*, *model_file: str = 'frozon_model.pb'*, *table_extrapolate: float = 5.0*, *table_stride_1: float = 0.01*, *table_stride_2: float = 0.1*, *check_frequency: int = -1*, *suffix: str = ''*) → None

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist [float] The nearest distance between atoms

model_file [str, default: 'frozon_model.pb'] The original frozen model, which will be compressed by the program

table_extrapolate [float, default: 5.] The scale of model extrapolation

table_stride_1 [float, default: 0.01] The uniform stride of the first table

table_stride_2 [float, default: 0.1] The uniform stride of the second table

check_frequency [int, default: -1] The overflow check frequency

suffix [str, optional] The suffix of the scope

Notes

This method is called by others when the descriptor supported compression.

abstract get_dim_out() → int
Returns the output dimension of this descriptor.

Returns

int the output dimension of this descriptor

Notes

This method must be implemented, as it's called by other classes.

get_dim_rot_mat_1() → int
Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3

Returns

int the first dimension of the rotation matrix

get_feed_dict(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*) → Dict[str, tensorflow.python.framework.ops.Tensor]
Generate the feed_dict for current descriptor

Parameters

coord_ [tf.Tensor] The coordinate of atoms

atype_ [tf.Tensor] The type of atoms

natoms [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

box [tf.Tensor] The box. Can be generated by deepmd.model.make_stat_input

mesh [tf.Tensor] For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

Returns

feed_dict [dict[str, tf.Tensor]] The output feed_dict of current descriptor

get_nlist() → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]
Returns neighbor information.

Returns

nlist [tf.Tensor] Neighbor list

rij [tf.Tensor] The relative distance between the neighbor and the center atom.

sel_a [list[int]] The number of neighbors with full information

sel_r [list[int]] The number of neighbors with only radial information

abstract get_ntypes() → int
Returns the number of atom types.

Returns

`int` the number of atom types

Notes

This method must be implemented, as it's called by other classes.

abstract get_rcut() → float
Returns the cut-off radius.

Returns

`float` the cut-off radius

Notes

This method must be implemented, as it's called by other classes.

get_tensor_names(*suffix: str = ''*) → Tuple[str]
Get names of tensors.

Parameters

suffix [`str`] The suffix of the scope

Returns

`Tuple[str]` Names of tensors

init_variables(*model_file: str*, *suffix: str = ''*) → None
Init the embedding net variables with the given dict

Parameters

model_file [`str`] The input model file

suffix [`str`, `optional`] The suffix of the scope

Notes

This method is called by others when the descriptor supported initialization from the given variables.

pass_tensors_from_frz_model(**tensors: tensorflow.python.framework.ops.Tensor*) → None
Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def

Parameters

***tensors** [`tf.Tensor`] passed tensors

Notes

The number of parameters in the method must be equal to the numbers of returns in *get_tensor_names()*.

abstract prod_force_virial(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]

Compute force and virial.

Parameters

atom_ener [tf.Tensor] The atomic energy

natoms [tf.Tensor] The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force [tf.Tensor] The force on atoms

virial [tf.Tensor] The total virial

atom_virial [tf.Tensor] The atomic virial

static register(*key: str*) → *deepmd.descriptor.descriptor.Descriptor*

Regiester a descriptor plugin.

Parameters

key [str] the key of a descriptor

Returns

Descriptor the regiestered descriptor

Examples

```
>>> @Descriptor.register("some_descrpt")
    class SomeDescript(Descriptor):
        pass
```

deepmd.descriptor.hybrid module

class deepmd.descriptor.hybrid.**DescrptHybrid**(**args*, ***kwargs*)

Bases: *deepmd.descriptor.descriptor.Descriptor*

Concate a list of descriptors to form a new descriptor.

Parameters

list [list] Build a descriptor from the concatenation of the list of descriptors.

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	Returns neighbor information.
get_nlist_i(ii)	Get the neighbor information of the ii-th descriptor
get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radius
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(*tensors)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord: list*, *data_box: list*, *data_atype: list*, *natoms_vec: list*, *mesh: list*, *input_dict: dict*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

enable_compression(*min_nbor_dist: float*, *model_file: str = 'frozon_model.pb'*, *table_extrapolate: float = 5.0*, *table_stride_1: float = 0.01*, *table_stride_2: float = 0.1*, *check_frequency: int = -1*, *suffix: str = ''*) → None

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist [float] The nearest distance between atoms

model_file [str, default: 'frozon_model.pb'] The original frozen model, which will be compressed by the program

table_extrapolate [float, default: 5.] The scale of model extrapolation

table_stride_1 [float, default: 0.01] The uniform stride of the first table

table_stride_2 [float, default: 0.1] The uniform stride of the second table

check_frequency [int, default: -1] The overflow check frequency

suffix [str, optional] The suffix of the scope

get_dim_out() → int

Returns the output dimension of this descriptor

get_nlist_i(*ii: int*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]

Get the neighbor information of the ii-th descriptor

Parameters

ii [int] The index of the descriptor

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

get_ntypes() → int

Returns the number of atom types

get_rcut() → float

Returns the cut-off radius

get_tensor_names(*suffix: str = ''*) → Tuple[str]

Get names of tensors.

Parameters

suffix [str] The suffix of the scope

Returns

`Tuple[str]` Names of tensors

`init_variables`(*model_file: str*, *suffix: str = ''*) → None
Init the embedding net variables with the given dict

Parameters

model_file [`str`] The input frozen model file

suffix [`str`, `optional`] The suffix of the scope

`pass_tensors_from_frz_model`(**tensors: tensorflow.python.framework.ops.Tensor*) → None
Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def

Parameters

***tensors** [`tf.Tensor`] passed tensors

`prod_force_virial`(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]
Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

deepmd.descriptor.loc_frame module

`class deepmd.descriptor.loc_frame.DescrptLocFrame`(**args*, ***kwargs*)
Bases: *deepmd.descriptor.descriptor.Descriptor*

Defines a local frame at each atom, and the compute the descriptor as local coordinates under this frame.

Parameters

rcut The cut-off radius

sel_a [`list[str]`] The length of the list should be the same as the number of atom types in the system. *sel_a[i]* gives the selected number of type-i neighbors. The full relative coordinates of the neighbors are used by the descriptor.

sel_r [`list[str]`] The length of the list should be the same as the number of atom types in the system. *sel_r[i]* gives the selected number of type-i neighbors. Only relative distance of the neighbors are used by the descriptor. sel_a[i] + sel_r[i] is recommended to be larger than the maximally possible number of type-i neighbors in the cut-off radius.

axis_rule: list[int] The length should be 6 times of the number of types. - axis_rule[i*6+0]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.

- axis_rule[i*6+1]: type of the atom defining the first axis of type-i atom.
- axis_rule[i*6+2]: index of the axis atom defining the first axis. Note that the neighbors with the same class and type are sorted according to their relative distance.
- axis_rule[i*6+3]: class of the atom defining the first axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.
- axis_rule[i*6+4]: type of the atom defining the second axis of type-i atom.
- axis_rule[i*6+5]: class of the atom defining the second axis of type-i atom. 0 for neighbors with full coordinates and 1 for neighbors only with relative distance.

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radisu
get_rot_mat()	Get rotational matrix
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(*tensors)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord: list*, *data_box: list*, *data_atype: list*, *natoms_vec: list*, *mesh: list*, *input_dict: dict*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

get_dim_out() → int

Returns the output dimension of this descriptor

get_nlist() → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

get_ntypes() → int

Returns the number of atom types

get_rcut() → float

Returns the cut-off radisu

get_rot_mat() → tensorflow.python.framework.ops.Tensor

Get rotational matrix

prod_force_virial(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]

Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

deepmd.descriptor.se module

class deepmd.descriptor.se.**DescrptSe**(**args*, ***kwargs*)

Bases: *deepmd.descriptor.descriptor.Descriptor*

A base class for smooth version of descriptors.

Notes

All of these descriptors have an environmental matrix and an embedding network (*deepmd.utils.network.embedding_net()*), so they can share some similiar methods without defining them twice.

Attributes

embedding_net_variables [dict] initial embedding network variables

descrpt_reshape [tf.Tensor] the reshaped descriptor

descrpt_deriv [tf.Tensor] the descriptor derivative

rij [tf.Tensor] distances between two atoms

nlist [tf.Tensor] the neighbor list

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor.
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor.
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	Returns neighbor information.
get_ntypes()	Returns the number of atom types.
get_rcut()	Returns the cut-off radius.
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict

continues on next page

Table 6 – continued from previous page

pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial.
register(key)	Regiester a descriptor plugin.

get_tensor_names(*suffix: str = ''*) → Tuple[str]
Get names of tensors.

Parameters

suffix [str] The suffix of the scope

Returns

Tuple[str] Names of tensors

init_variables(*model_file: str*, *suffix: str = ''*) → None
Init the embedding net variables with the given dict

Parameters

model_file [str] The input frozen model file

suffix [str, optional] The suffix of the scope

pass_tensors_from_frz_model(*descrpt_reshape: tensorflow.python.framework.ops.Tensor*, *descrpt_deriv: tensorflow.python.framework.ops.Tensor*, *rij: tensorflow.python.framework.ops.Tensor*, *nlist: tensorflow.python.framework.ops.Tensor*)
Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def

Parameters

descrpt_reshape The passed descrpt_reshape tensor

descrpt_deriv The passed descrpt_deriv tensor

rij The passed rij tensor

nlist The passed nlist tensor

deepmd.descriptor.se_a module

class deepmd.descriptor.se_a.**DescrptSeA**(**args*, ***kwargs*)
Bases: *deepmd.descriptor.se.DescrptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations. The embedding takes the distance between atoms as input.

The descriptor $\mathcal{D}^i \in \mathcal{R}^{M_1 \times M_2}$ is given by [1]

$$\mathcal{D}^i = (\mathcal{G}^i)^T \mathcal{R}^i (\mathcal{R}^i)^T \mathcal{G}^i_<$$

where $\mathcal{R}^i \in \mathbb{R}^{N \times 4}$ is the coordinate matrix, and each row of $\mathcal{R}^i$ can be constructed as follows

$$(\mathcal{R}^i)_j = [\begin{array}{c} s(r_{ji}) \\ \frac{s(r_{ji}) x_{ji}}{r_{ji}} \\ \frac{s(r_{ji}) y_{ji}}{r_{ji}} \\ \frac{s(r_{ji}) z_{ji}}{r_{ji}} \end{array}]$$

where $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i = (x_{ji}, y_{ji}, z_{ji})$ is the relative coordinate and $r_{ji} = \|\mathbf{R}_{ji}\|$ is its norm. The switching function $s(r)$ is defined as:

$$s(r) = \begin{cases} \frac{1}{r}, & r < r_s \\ \frac{1}{r}\{(\frac{r-r_s}{r_c-r_s})^3(-6(\frac{r-r_s}{r_c-r_s})^2 + 15\frac{r-r_s}{r_c-r_s} - 10) + 1\}, & r_s \leq r < r_c \\ 0, & r \geq r_c \end{cases}$$

Each row of the embedding matrix $\mathcal{G}^i \in \mathbb{R}^{N \times M_1}$ consists of outputs of a embedding network $\mathcal{N}$ of $s(r_{ji})$:

$$(\mathcal{G}^i)_j = \mathcal{N}(s(r_{ji}))$$

$\mathcal{G}^i_< \in \mathbb{R}^{N \times M_2}$ takes first M_2 columns of $\mathcal{G}^i$. The equation of embedding network $\mathcal{N}$ can be found at *deepmd.utils.network.embedding_net()*.

Parameters

rcut The cut-off radius r_c

rcut_smth From where the environment matrix should be smoothed r_s

sel [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron [list[int]] Number of neurons in each hidden layers of the embedding net $\mathcal{N}$

axis_neuron Number of the axis neuron M_2 (number of columns of the sub-matrix of the embedding matrix)

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

type_one_side Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

exclude_types [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

set_davg_zero Set the shift of embedding net input to zero.

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

References

[1]

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radius
get_rot_mat()	Get rotational matrix
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord: list*, *data_box: list*, *data_atype: list*, *natoms_vec: list*, *mesh: list*, *input_dict: dict*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

enable_compression(*min_nbor_dist: float*, *model_file: str = 'frozon_model.pb'*, *table_extrapolate: float = 5*, *table_stride_1: float = 0.01*, *table_stride_2: float = 0.1*, *check_frequency: int = - 1*, *suffix: str = ''*) → None

Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.

Parameters

min_nbor_dist The nearest distance between atoms

model_file The original frozen model, which will be compressed by the program

table_extrapolate The scale of model extrapolation

table_stride_1 The uniform stride of the first table

table_stride_2 The uniform stride of the second table

check_frequency The overflow check frequency

suffix [str, optional] The suffix of the scope

get_dim_out() → int

Returns the output dimension of this descriptor

get_dim_rot_mat_1() → int

Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3

get_nlist() → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

get_ntypes() → int

Returns the number of atom types

get_rcut() → float

Returns the cut-off radius

get_rot_mat() → tensorflow.python.framework.ops.Tensor

Get rotational matrix

prod_force_virial(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]

Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

deepmd.descriptor.se_a_ebd module

class deepmd.descriptor.se_a_ebd.**DescrptSeAEbd**(**args*, ***kwargs*)

Bases: *deepmd.descriptor.se_a.DescrptSeA*

DeepPot-SE descriptor with type embedding approach.

Parameters

rcut The cut-off radius

rcut_smth From where the environment matrix should be smoothed

sel [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron [list[int]] Number of neurons in each hidden layers of the embedding net

axis_neuron Number of the axis neuron (number of columns of the sub-matrix of the embedding matrix)

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

type_one_side Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

type_nchanl Number of channels for type representation

type_nlayer Number of hidden layers for the type embedding net (skip connected).

numb_aparam Number of atomic parameters. If >0 it will be embedded with atom types.

set_davg_zero Set the shift of embedding net input to zero.

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

exclude_types [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radius
get_rot_mat()	Get rotational matrix
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

deepmd.descriptor.se_a_ef module

class deepmd.descriptor.se_a_ef.**DescrptSeAEf**(**args*, ***kwargs*)
Bases: *deepmd.descriptor.descriptor.Descriptor*

Parameters

rcut The cut-off radius

rcut_smth From where the environment matrix should be smoothed

sel [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron [list[int]] Number of neurons in each hidden layers of the embedding net

axis_neuron Number of the axis neuron (number of columns of the sub-matrix of the embedding matrix)

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

type_one_side Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

exclude_types [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

set_davg_zero Set the shift of embedding net input to zero.

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radisu
get_rot_mat()	Get rotational matrix
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict

continues on next page

Table 9 – continued from previous page

pass_tensors_from_frz_model(*tensors)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs. Should have 'efield'.

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord: list*, *data_box: list*, *data_atype: list*, *natoms_vec: list*, *mesh: list*, *input_dict: dict*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

get_dim_out() → int

Returns the output dimension of this descriptor

get_dim_rot_mat_1() → int

Returns the first dimension of the rotation matrix. The rotation is of shape dim_1 x 3

get_nlist() → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

get_ntypes() → int
Returns the number of atom types

get_rcut() → float
Returns the cut-off radisu

get_rot_mat() → tensorflow.python.framework.ops.Tensor
Get rotational matrix

prod_force_virial(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]
Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

class deepmd.descriptor.se_a_ef.**DescrptSeAEfLower**(**args*, ***kwargs*)
Bases: *deepmd.descriptor.se_a.DescrptSeA*

Helper class for implementing DescrptSeAEf

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	**Returns**

continues on next page

Table 10 – continued from previous page

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radius
get_rot_mat()	Get rotational matrix
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_*, *atype_*, *natoms*, *box_*, *mesh*, *input_dict*, *suffix=''*, *reuse=None*)
Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord*, *data_box*, *data_atype*, *natoms_vec*, *mesh*, *input_dict*)
Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

deepmd.descriptor.se_r module

class deepmd.descriptor.se_r.**DescrptSeR**(**args*, ***kwargs*)

Bases: *deepmd.descriptor.se.DescrptSe*

DeepPot-SE constructed from radial information of atomic configurations.

The embedding takes the distance between atoms as input.

Parameters

rcut The cut-off radius

rcut_smth From where the environment matrix should be smoothed

sel [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron [list[int]] Number of neurons in each hidden layers of the embedding net

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

type_one_side Try to build N_types embedding nets. Otherwise, building N_types^2 embedding nets

exclude_types [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radisu
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def

continues on next page

Table 11 – continued from previous page

prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord*, *data_box*, *data_atype*, *natoms_vec*, *mesh*, *input_dict*)

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

get_dim_out()

Returns the output dimension of this descriptor

get_nlist()

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

get_ntypes()
Returns the number of atom types

get_rcut()
Returns the cut-off radisu

prod_force_virial(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]
Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

deepmd.descriptor.se_t module

class deepmd.descriptor.se_t.**DescrptSeT**(**args*, ***kwargs*)
Bases: *deepmd.descriptor.se.DescrptSe*

DeepPot-SE constructed from all information (both angular and radial) of atomic configurations.

The embedding takes angles between two neighboring atoms as input.

Parameters

rcut The cut-off radius

rcut_smth From where the environment matrix should be smoothed

sel [list[str]] sel[i] specifies the maxmum number of type i atoms in the cut-off radius

neuron [list[int]] Number of neurons in each hidden layers of the embedding net

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

set_davg_zero Set the shift of embedding net input to zero.

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(coord_, atype_, natoms, box_, mesh, ...)	Build the computational graph for the descriptor
compute_input_stats(data_coord, data_box, ...)	Compute the statisitcs (avg and std) of the training data.
enable_compression(min_nbor_dist[, ...])	Reveive the statisitcs (distance, max_nbor_size and env_mat_range) of the training data.
get_dim_out()	Returns the output dimension of this descriptor
get_dim_rot_mat_1()	Returns the first dimension of the rotation matrix.
get_feed_dict(coord_, atype_, natoms, box, mesh)	Generate the feed_dict for current descriptor
get_nlist()	

Returns

get_ntypes()	Returns the number of atom types
get_rcut()	Returns the cut-off radisu
get_tensor_names([suffix])	Get names of tensors.
init_variables(model_file[, suffix])	Init the embedding net variables with the given dict
pass_tensors_from_frz_model(descrpt_reshape, ...)	Pass the descrpt_reshape tensor as well as descrpt_deriv tensor from the frz graph_def
prod_force_virial(atom_ener, natoms)	Compute force and virial
register(key)	Regiester a descriptor plugin.

build(*coord_: tensorflow.python.framework.ops.Tensor*, *atype_: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *box_: tensorflow.python.framework.ops.Tensor*, *mesh: tensorflow.python.framework.ops.Tensor*, *input_dict: dict*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for the descriptor

Parameters

coord_ The coordinate of atoms

atype_ The type of atoms

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

mesh For historical reasons, only the length of the Tensor matters. if size of mesh == 6, pbc is assumed. if size of mesh == 0, no-pbc is assumed.

input_dict Dictionary for additional inputs

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

descriptor The output descriptor

compute_input_stats(*data_coord: list*, *data_box: list*, *data_atype: list*, *natoms_vec: list*, *mesh: list*, *input_dict: dict*) → None

Compute the statisitcs (avg and std) of the training data. The input will be normalized by the statistics.

Parameters

data_coord The coordinates. Can be generated by deepmd.model.make_stat_input

data_box The box. Can be generated by deepmd.model.make_stat_input

data_atype The atom types. Can be generated by deepmd.model.make_stat_input

natoms_vec The vector for the number of atoms of the system and different types of atoms. Can be generated by deepmd.model.make_stat_input

mesh The mesh for neighbor searching. Can be generated by deepmd.model.make_stat_input

input_dict Dictionary for additional input

`get_dim_out()` → int
Returns the output dimension of this descriptor

`get_nlist()` → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, List[int], List[int]]

Returns

nlist Neighbor list

rij The relative distance between the neighbor and the center atom.

sel_a The number of neighbors with full information

sel_r The number of neighbors with only radial information

`get_ntypes()` → int
Returns the number of atom types

`get_rcut()` → float
Returns the cut-off radisu

`prod_force_virial`(*atom_ener: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*) → Tuple[tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor, tensorflow.python.framework.ops.Tensor]
Compute force and virial

Parameters

atom_ener The atomic energy

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

Returns

force The force on atoms

virial The total virial

atom_virial The atomic virial

deepmd.entrypoints package

Submodule that contains all the DeePMD-Kit entry point scripts.

deepmd.entrypoints.**compress**(*, *input: str*, *output: str*, *extrapolate: int*, *step: float*, *frequency: str*, *checkpoint_folder: str*, *training_script: str*, *mpi_log: str*, *log_path: Optional[str]*, *log_level: int*, ***kwargs*)

Compress model.

The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the step parameter as the domain's uniform step size, while the second table takes 10 * step as it's uniform step size. The range of the first table is automatically detected by the code, while the second table ranges from the first table's upper boundary(upper) to the extrapolate(parameter) * upper.

Parameters

input [str] frozen model file to compress

output [str] compressed model filename

extrapolate [int] scale of model extrapolation

step [float] uniform step size of the tabulation's first table

frequency [str] frequency of tabulation overflow check

checkpoint_folder [str] trining checkpoint folder for freezing

training_script [str] training script of the input frozen model

mpi_log [str] mpi logging mode for training

log_path [Optional[str]] if speccified log will be written to this file

log_level [int] logging level

deepmd.entrypoints.**config**(*, *output: str*, ***kwargs*)

Auto config file generator.

Parameters

output: str file to write config file

Raises

RuntimeError if user does not input any systems

ValueError if output file is of wrong type

deepmd.entrypoints.**convert**(*, *FROM: str*, *input_model: str*, *output_model: str*, ***kwargs*)

deepmd.entrypoints.**doc_train_input**(*, *out_type: str = 'rst'*, ***kwargs*)

Print out trining input arguments to console.

deepmd.entrypoints.**freeze**(*, *checkpoint_folder: str*, *output: str*, *node_names: Optional[str] = None*, ***kwargs*)

Freeze the graph in supplied folder.

Parameters

checkpoint_folder [str] location of the folder with model

output [str] output file name

node_names [Optional[str], optional] names of nodes to output, by default None

deepmd.entrypoints.**make_model_devi**(*, *models: list*, *system: str*, *set_prefix: str*, *output: str*, *frequency: int*, ***kwargs*)

Make model deviation calculation

Parameters

models: list A list of paths of models to use for making model deviation

system: str The path of system to make model deviation calculation

set_prefix: str The set prefix of the system

output: str The output file for model deviation results

frequency: int The number of steps that elapse between writing coordinates in a trajectory by a MD engine (such as Gromacs / Lammps). This paramter is used to determine the index in the output file.

deepmd.entrypoints.**test**(*, *model: str*, *system: str*, *set_prefix: str*, *numb_test: int*, *rand_seed: Optional[int]*, *shuffle_test: bool*, *detail_file: str*, *atomic: bool*, ***kwargs*)

Test model predictions.

Parameters

model [str] path where model is stored

system [str] system directory

set_prefix [str] string prefix of set

numb_test [int] munber of tests to do

rand_seed [Optional[int]] seed for random generator

shuffle_test [bool] whether to shuffle tests

detail_file [Optional[str]] file where test details will be output

atomic [bool] whether per atom quantities should be computed

Raises

RuntimeError if no valid system was found

deepmd.entrypoints.**train_dp**(*, *INPUT: str*, *init_model: Optional[str]*, *restart: Optional[str]*, *output: str*, *init_frz_model: str*, *mpi_log: str*, *log_level: int*, *log_path: Optional[str]*, *is_compress: bool = False*, ***kwargs*)

Run DeePMD model training.

Parameters

INPUT [str] json/yaml control file

init_model [Optional[str]] path to checkpoint folder or None

restart [Optional[str]] path to checkpoint folder or None

output [str] path for dump file with arguments

init_frz_model [str] path to frozen model or None

mpi_log [str] mpi logging mode

log_level [int] logging level defined by int 0-3

log_path [Optional[str]] logging file path or None if logs are to be output only to stdout

is_compress: bool indicates whether in the model compress mode

Raises

`RuntimeError` if distributed training job nem is wrong

`deepmd.entrypoints.transfer(*, old_model: str, raw_model: str, output: str, **kwargs)`
Transfer operation from old fron graph to new prepared raw graph.

Parameters

old_model [`str`] frozen old graph model

raw_model [`str`] new model that will accept ops from old model

output [`str`] new model with transfered parameters will be saved to this location

Submodules

deepmd.entrypoints.compress module

Compress a model, which including tabulating the embedding-net.

`deepmd.entrypoints.compress.compress(*, input: str, output: str, extrapolate: int, step: float, frequency: str, checkpoint_folder: str, training_script: str, mpi_log: str, log_path: Optional[str], log_level: int, **kwargs)`
Compress model.

The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the step parameter as the domain's uniform step size, while the second table takes 10 * step as it's uniform step size. The range of the first table is automatically detected by the code, while the second table ranges from the first table's upper boundary(upper) to the extrapolate(parameter) * upper.

Parameters

input [`str`] frozen model file to compress

output [`str`] compressed model filename

extrapolate [`int`] scale of model extrapolation

step [`float`] uniform step size of the tabulation's first table

frequency [`str`] frequency of tabulation overflow check

checkpoint_folder [`str`] trining checkpoint folder for freezing

training_script [`str`] training script of the input frozen model

mpi_log [`str`] mpi logging mode for training

log_path [`Optional[str]`] if speccified log will be written to this file

log_level [`int`] logging level

deepmd.entrypoints.config module

Quickly create a configuration file for smooth model.

deepmd.entrypoints.config.**config**(*, *output: str*, ***kwargs*)
Auto config file generator.

Parameters

output: str file to write config file

Raises

`RuntimeError` if user does not input any systems

`ValueError` if output file is of wrong type

deepmd.entrypoints.convert module

deepmd.entrypoints.convert.**convert**(*, *FROM: str*, *input_model: str*, *output_model: str*, ***kwargs*)

deepmd.entrypoints.doc module

Module that prints train input arguments docstrings.

deepmd.entrypoints.doc.**doc_train_input**(*, *out_type: str = 'rst'*, ***kwargs*)
Print out trining input arguments to console.

deepmd.entrypoints.freeze module

Script for freezing TF trained graph so it can be used with LAMMPS and i-PI.

References

https://blog.metaflow.fr/tensorflow-how-to-freeze-a-model-and-serve-it-with-a-python-api-d4f3596b3adc

deepmd.entrypoints.freeze.**freeze**(*, *checkpoint_folder: str*, *output: str*, *node_names: Optional[str] = None*, ***kwargs*)
Freeze the graph in supplied folder.

Parameters

checkpoint_folder [`str`] location of the folder with model

output [`str`] output file name

node_names [`Optional`[`str`], `optional`] names of nodes to output, by default None

deepmd.entrypoints.main module

DeePMD-Kit entry point module.

deepmd.entrypoints.main.**get_ll**(*log_level: str*) → int
Convert string to python logging level.

Parameters

log_level [str] allowed input values are: DEBUG, INFO, WARNING, ERROR, 3, 2, 1, 0

Returns

int one of python logging module log levels - 10, 20, 30 or 40

deepmd.entrypoints.main.**main**()
DeePMD-Kit entry point.

Raises

RuntimeError if no command was input

deepmd.entrypoints.main.**parse_args**(*args: Optional[List[str]] = None*)
DeePMD-Kit commandline options argument parser.

Parameters

args: List[str] list of command line arguments, main purpose is testing default option None takes arguments from sys.argv

deepmd.entrypoints.test module

Test trained DeePMD model.

deepmd.entrypoints.test.**test**(*, *model: str*, *system: str*, *set_prefix: str*, *numb_test: int*, *rand_seed: Optional[int]*, *shuffle_test: bool*, *detail_file: str*, *atomic: bool*, **kwargs*)
Test model predictions.

Parameters

model [str] path where model is stored

system [str] system directory

set_prefix [str] string prefix of set

numb_test [int] munber of tests to do

rand_seed [Optional[int]] seed for random generator

shuffle_test [bool] whether to shuffle tests

detail_file [Optional[str]] file where test details will be output

atomic [bool] whether per atom quantities should be computed

Raises

RuntimeError if no valid system was found

deepmd.entrypoints.train module

DeePMD training entrypoint script.

Can handle local or distributed training.

deepmd.entrypoints.train.**train**(*, *INPUT: str*, *init_model: Optional[str]*, *restart: Optional[str]*, *output: str*, *init_frz_model: str*, *mpi_log: str*, *log_level: int*, *log_path: Optional[str]*, *is_compress: bool = False*, ***kwargs*)

Run DeePMD model training.

Parameters

INPUT [str] json/yaml control file

init_model [Optional[str]] path to checkpoint folder or None

restart [Optional[str]] path to checkpoint folder or None

output [str] path for dump file with arguments

init_frz_model [str] path to frozen model or None

mpi_log [str] mpi logging mode

log_level [int] logging level defined by int 0-3

log_path [Optional[str]] logging file path or None if logs are to be output only to stdout

is_compress: bool indicates whether in the model compress mode

Raises

RuntimeError if distributed training job nem is wrong

deepmd.entrypoints.transfer module

Module used for transfering parameters between models.

deepmd.entrypoints.transfer.**transfer**(*, *old_model: str*, *raw_model: str*, *output: str*, ***kwargs*)

Transfer operation from old fron graph to new prepared raw graph.

Parameters

old_model [str] frozen old graph model

raw_model [str] new model that will accept ops from old model

output [str] new model with transfered parameters will be saved to this location

deepmd.fit package

Submodules

deepmd.fit.dipole module

class deepmd.fit.dipole.**DipoleFittingSeA**

Bases: object

Fit the atomic dipole with descriptor se_a

Parameters

descrpt [tf.Tensor] The descrptor

neuron [List[int]] Number of neurons in each hidden layer of the fitting net

resnet_dt [bool] Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

sel_type [List[int]] The atom types selected to have an atomic dipole prediction. If is None, all atoms are selected.

seed [int] Random seed for initializing the network parameters.

activation_function [str] The activation function in the embedding net. Supported options are {0}

precision [str] The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(input_d, rot_mat, natoms[, reuse, suffix])	Build the computational graph for fitting net
get_out_size()	Get the output size.
get_sel_type()	Get selected type

build(*input_d: tensorflow.python.framework.ops.Tensor*, *rot_mat: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for fitting net

Parameters

input_d The input descriptor

rot_mat The rotation matrix from the descriptor.

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

dipole The atomic dipole.

get_out_size() → int

Get the output size. Should be 3

get_sel_type() → int

Get selected type

deepmd.fit.ener module

class deepmd.fit.ener.**EnerFitting**

Bases: object

Fitting the energy of the system. The force and the virial can also be trained.

The potential energy E is a fitting network function of the descriptor $\mathcal{D}$:

$$E(\mathcal{D}) = \mathcal{L}^{(n)} \circ \mathcal{L}^{(n-1)} \circ \cdots \circ \mathcal{L}^{(1)} \circ \mathcal{L}^{(0)}$$

The first n hidden layers $\mathcal{L}^{(0)}, \cdots, \mathcal{L}^{(n-1)}$ are given by

$$\mathbf{y} = \mathcal{L}(\mathbf{x}; \mathbf{w}, \mathbf{b}) = \boldsymbol{\phi}(\mathbf{x}^T\mathbf{w} + \mathbf{b})$$

where $\mathbf{x} \in \mathbb{R}^{N_1}$ is the input vector and $\mathbf{y} \in \mathbb{R}^{N_2}$ is the output vector. $\mathbf{w} \in \mathbb{R}^{N_1 \times N_2}$ and $\mathbf{b} \in \mathbb{R}^{N_2}$ are weights and biases, respectively, both of which are trainable if *trainable[i]* is *True*. $\boldsymbol{\phi}$ is the activation function.

The output layer $\mathcal{L}^{(n)}$ is given by

$$\mathbf{y} = \mathcal{L}^{(n)}(\mathbf{x}; \mathbf{w}, \mathbf{b}) = \mathbf{x}^T\mathbf{w} + \mathbf{b}$$

where $\mathbf{x} \in \mathbb{R}^{N_{n-1}}$ is the input vector and $\mathbf{y} \in \mathbb{R}$ is the output scalar. $\mathbf{w} \in \mathbb{R}^{N_{n-1}}$ and $\mathbf{b} \in \mathbb{R}$ are weights and bias, respectively, both of which are trainable if *trainable[n]* is *True*.

Parameters

descrpt The descrptor $\mathcal{D}$

neuron Number of neurons N in each hidden layer of the fitting net

resnet_dt Time-step *dt* in the resnet construction: $y = x + dt * \phi(Wx + b)$

numb_fparam Number of frame parameter

numb_aparam Number of atomic parameter

rcond The condition number for the regression of atomic energy.

tot_ener_zero Force the total energy to zero. Useful for the charge fitting.

trainable If the weights of fitting net are trainable. Suppose that we have N_l hidden layers in the fitting net, this list is of length $N_l + 1$, specifying if the hidden layers and the output layer are trainable.

seed Random seed for initializing the network parameters.

atom_ener Specifying atomic energy contribution in vacuum. The *set_davg_zero* key in the descrptor should be set.

activation_function The activation function $\boldsymbol{\phi}$ in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(inputs, natoms[, input_dict, reuse, ...])	Build the computational graph for fitting net
compute_input_stats(all_stat[, protection])	Compute the input statistics
compute_output_stats(all_stat)	Compute the ouput statistics
get_numb_aparam()	Get the number of atomic parameters
get_numb_fparam()	Get the number of frame parameters
init_variables(fitting_net_variables)	Init the fitting net variables with the given dict

build(*inputs: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *input_dict: dict = {}*, *reuse: Optional[bool] = None*, *suffix: str = ''*) → tensorflow.python.framework.ops.Tensor

Build the computational graph for fitting net

Parameters

inputs The input descriptor

input_dict Additional dict for inputs. if numb_fparam > 0, should have input_dict['fparam'] if numb_aparam > 0, should have input_dict['aparam']

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

ener The system energy

compute_input_stats(*all_stat: dict*, *protection: float = 0.01*) → None

Compute the input statistics

Parameters

all_stat if numb_fparam > 0 must have all_stat['fparam'] if numb_aparam > 0 must have all_stat['aparam'] can be prepared by model.make_stat_input

protection Divided-by-zero protection

compute_output_stats(*all_stat: dict*) → None

Compute the ouput statistics

Parameters

all_stat must have the following components: all_stat['energy'] of shape n_sys x n_batch x n_frame can be prepared by model.make_stat_input

get_numb_aparam() → int

Get the number of atomic parameters

get_numb_fparam() → int

Get the number of frame parameters

init_variables(*fitting_net_variables: dict*) → None

Init the fitting net variables with the given dict

Parameters

fitting_net_variables The input dict which stores the fitting net variables

deepmd.fit.polar module

class deepmd.fit.polar.**GlobalPolarFittingSeA**
Bases: object

Fit the system polarizability with descriptor se_a

Parameters

descrpt [tf.Tensor] The descrptor

neuron [List[int]] Number of neurons in each hidden layer of the fitting net

resnet_dt [bool] Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

sel_type [List[int]] The atom types selected to have an atomic polarizability prediction

fit_diag [bool] Fit the diagonal part of the rotational invariant polarizability matrix, which will be converted to normal polarizability matrix by contracting with the rotation matrix.

scale [List[float]] The output of the fitting net (polarizability matrix) for type i atom will be scaled by scale[i]

diag_shift [List[float]] The diagonal part of the polarizability matrix of type i will be shifted by diag_shift[i]. The shift operation is carried out after scale.

seed [int] Random seed for initializing the network parameters.

activation_function [str] The activation function in the embedding net. Supported options are {0}

precision [str] The precision of the embedding net parameters. Supported options are {1}

Methods

build(input_d, rot_mat, natoms[, reuse, suffix])	Build the computational graph for fitting net
get_out_size()	Get the output size.
get_sel_type()	Get selected atom types

build(*input_d*, *rot_mat*, *natoms*, *reuse=None*, *suffix=''*) → tensorflow.python.framework.ops.Tensor
Build the computational graph for fitting net

Parameters

input_d The input descriptor

rot_mat The rotation matrix from the descriptor.

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

polar The system polarizability

get_out_size() → int
Get the output size. Should be 9

get_sel_type() → int
Get selected atom types

class deepmd.fit.polar.**PolarFittingLocFrame**(*jdata*, *descrpt*)
Bases: object

Fitting polarizability with local frame descriptor.

Deprecated since version 2.0.0: This class is not supported any more.

Methods

build	
get_out_size	
get_sel_type	

build(*input_d*, *rot_mat*, *natoms*, *reuse=None*, *suffix=''*)

get_out_size()

get_sel_type()

class deepmd.fit.polar.**PolarFittingSeA**
Bases: object

Fit the atomic polarizability with descriptor se_a

Methods

build(input_d, rot_mat, natoms[, reuse, suffix])	Build the computational graph for fitting net
compute_input_stats(all_stat[, protection])	Compute the input statistics
get_out_size()	Get the output size.
get_sel_type()	Get selected atom types

build(*input_d: tensorflow.python.framework.ops.Tensor*, *rot_mat: tensorflow.python.framework.ops.Tensor*, *natoms: tensorflow.python.framework.ops.Tensor*, *reuse: Optional[bool] = None*, *suffix: str = ''*)
Build the computational graph for fitting net

Parameters

input_d The input descriptor

rot_mat The rotation matrix from the descriptor.

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

atomic_polar The atomic polarizability

compute_input_stats(*all_stat*, *protection=0.01*)
Compute the input statistics

Parameters

all_stat Dictionary of inputs. can be prepared by model.make_stat_input

protection Divided-by-zero protection

get_out_size() → int
Get the output size. Should be 9

get_sel_type() → List[int]
Get selected atom types

deepmd.fit.wfc module

class deepmd.fit.wfc.**WFCFitting**(*jdata*, *descrpt*)
Bases: object

Fitting Wannier function centers (WFCs) with local frame descriptor.

Deprecated since version 2.0.0: This class is not supported any more.

Methods

build	
get_out_size	
get_sel_type	
get_wfc_numb	

build(*input_d*, *rot_mat*, *natoms*, *reuse=None*, *suffix=''*)

get_out_size()

get_sel_type()

get_wfc_numb()

deepmd.infer package

Submodule containing all the implemented potentials.

class deepmd.infer.**DeepDipole**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)
Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

class deepmd.infer.**DeepEval**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*, *auto_batch_size: Union[bool, int, deepmd.utils.batch_size.AutoBatchSize] = False*)

Bases: object

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size [bool or int or AutomaticBatchSize, default: False] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

load_prefix: *str*

make_natoms_vec(*atom_types: numpy.ndarray*) → numpy.ndarray
Make the natom vector used by deepmd-kit.

Parameters

atom_types The type of atoms

Returns

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

property model_type: *str*
Get type of model.

:type:str

property model_version: *str*
Get version of model.

Returns

str version of model

static reverse_map(*vec: numpy.ndarray*, *imap: List[int]*) → numpy.ndarray
Reverse mapping of a vector according to the index map

Parameters

vec Input vector. Be of shape [nframes, natoms, -1]

imap Index map. Be of shape [natoms]

Returns

vec_out Reverse mapped vector.

static sort_input(*coord: numpy.ndarray*, *atom_type: numpy.ndarray*, *sel_atoms: Optional[List[int]] = None*)
Sort atoms in the system according their types.

Parameters

coord The coordinates of atoms. Should be of shape [nframes, natoms, 3]

atom_type The type of atoms Should be of shape [natoms]

sel_atom The selected atoms by type

Returns

coord_out The coordinates after sorting

atom_type_out The atom types after sorting

idx_map The index mapping from the input to the output. For example coord_out = coord[:,idx_map,:]

sel_atom_type Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

class deepmd.infer.**DeepGlobalPolar**(*model_file: str*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [str] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

eval(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = False*, *fparam: Optional[numpy.ndarray] = None*, *aparam: Optional[numpy.ndarray] = None*, *efield: Optional[numpy.ndarray] = None*) → numpy.ndarray

Evaluate the model.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic Not used in this model

fparam Not used in this model

aparam Not used in this model

efield Not used in this model

Returns

tensor The returned tensor If atomic == False then of size nframes x variable_dof else of size nframes x natoms x variable_dof

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

class deepmd.infer.**DeepPolar**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)
Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.

continues on next page

Table 20 – continued from previous page

get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

class deepmd.infer.**DeepPot**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*, *auto_batch_size: Union[bool, int,* deepmd.utils.batch_size.AutoBatchSize*] = True*)

Bases: *deepmd.infer.deep_eval.DeepEval*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size [bool or int or AutomaticBatchSize, default: True] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Examples

```
>>> from deepmd.infer import DeepPot
>>> import numpy as np
>>> dp = DeepPot('graph.pb')
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> e, f, v = dp.eval(coord, cell, atype)
```

where e, f and v are predicted energy, force and virial of the system, respectively.

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the energy, force and virial by using this DP.
get_dim_aparam()	Get the number (dimension) of atomic parameters of this DP.
get_dim_fparam()	Get the number (dimension) of frame parameters of this DP.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Unsupported in this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

eval(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = False*, *fparam: Optional[numpy.ndarray] = None*, *aparam: Optional[numpy.ndarray] = None*, *efield: Optional[numpy.ndarray] = None*) → Tuple[numpy.ndarray, ...]

Evaluate the energy, force and virial by using this DP.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic Calculate the atomic energy and virial

fparam The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield The external field on atoms. The array should be of size nframes x natoms x 3

Returns

energy The system energy.

force The force on each atom

virial The virial

atom_energy The atomic energy. Only returned when atomic == True

atom_virial The atomic virial. Only returned when atomic == True

get_dim_aparam() → int

Get the number (dimension) of atomic parameters of this DP.

get_dim_fparam() → int

Get the number (dimension) of frame parameters of this DP.

get_ntypes() → int
Get the number of atom types of this model.

get_rcut() → float
Get the cut-off radius of this model.

get_sel_type() → List[int]
Unsupported in this model.

get_type_map() → List[int]
Get the type map (element name of the atom types) of this model.

load_prefix: str

deepmd.infer.**DeepPotential**(*model_file: Union[str, pathlib.Path]*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*) → Union[*deepmd.infer.deep_dipole.DeepDipole*, *deepmd.infer.deep_polar.DeepGlobalPolar*, *deepmd.infer.deep_polar.DeepPolar*, *deepmd.infer.deep_pot.DeepPot*, *deepmd.infer.deep_wfc.DeepWFC*]

Factory function that will inialize appropriate potential read from *model_file*.

Parameters

model_file: str The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Returns

Union[*DeepDipole*, *DeepGlobalPolar*, *DeepPolar*, *DeepPot*, *DeepWFC*] one of the available potentials

Raises

RuntimeError if model file does not correspond to any implementd potential

class deepmd.infer.**DeepWFC**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

class deepmd.infer.**DipoleChargeModifier**(*model_name: str*, *model_charge_map: List[float]*, *sys_charge_map: List[float]*, *ewald_h: float = 1*, *ewald_beta: float = 1*)

Bases: *deepmd.infer.deep_dipole.DeepDipole*

Parameters

model_name The model file for the DeepDipole model

model_charge_map Gives the amount of charge for the wfcc

sys_charge_map Gives the amount of charge for the real atoms

ewald_h Grid spacing of the reciprocal part of Ewald sum. Unit: A

ewald_beta Splitting parameter of the Ewald sum. Unit: A^{-1}

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

build_fv_graph()	Build the computational graph for the force and virial inference.
eval(coord, box, atype[, eval_fv])	Evaluate the modification
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.

continues on next page

Table 23 – continued from previous page

get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
modify_data(data)	Modify data.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

build_fv_graph() → tensorflow.python.framework.ops.Tensor
Build the computational graph for the force and virial inference.

eval(*coord: numpy.ndarray*, *box: numpy.ndarray*, *atype: numpy.ndarray*, *eval_fv: bool = True*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]
Evaluate the modification

Parameters

coord The coordinates of atoms

box The simulation region. PBC is assumed

atype The atom types

eval_fv Evaluate force and virial

Returns

tot_e The energy modification

tot_f The force modification

tot_v The virial modification

load_prefix: str

modify_data(*data: dict*) → None
Modify data.

Parameters

data Internal data of DeepmdData. Be a dict, has the following keys - coord coordinates - box simulation box - type atom types - find_energy tells if data has energy - find_force tells if data has force - find_virial tells if data has virial - energy energy - force force - virial virial

class deepmd.infer.**EwaldRecp**(*hh*, *beta*)
Bases: object

Evaluate the reciprocal part of the Ewald sum

Methods

eval(coord, charge, box)	Evaluate

eval(*coord: numpy.ndarray*, *charge: numpy.ndarray*, *box: numpy.ndarray*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]
Evaluate

Parameters

coord The coordinates of atoms

charge The atomic charge

box The simulation region. PBC is assumed

Returns

e The energy

f The force

v The virial

deepmd.infer.**calc_model_devi**(*coord*, *box*, *atype*, *models*, *fname=None*, *frequency=1*, *nopbc=True*)
Python interface to calculate model deviation

Parameters

coord [numpy.ndarray, *n_frames x n_atoms x 3*] Coordinates of system to calculate

box [numpy.ndarray or None, *n_frames x 3 x 3*] Box to specify periodic boundary condition. If None, no pbc will be used

atype [numpy.ndarray, *n_atoms x 1*] Atom types

models [list of *DeepPot* models] Models used to evaluate deviation

fname [str or None] File to dump results, default None

frequency [int] Steps between frames (if the system is given by molecular dynamics engine), default 1

nopbc [bool] Whether to use pbc conditions

Returns

model_devi [numpy.ndarray, *n_frames x 7*] Model deviation results. The first column is index of steps, the other 6 columns are max_devi_v, min_devi_v, avg_devi_v, max_devi_f, min_devi_f, avg_devi_f.

Examples

```
>>> from deepmd.infer import calc_model_devi
>>> from deepmd.infer import DeepPot as DP
>>> import numpy as np
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
>>> model_devi = calc_model_devi(coord, cell, atype, graphs)
```

Submodules

deepmd.infer.data_modifier module

class deepmd.infer.data_modifier.**DipoleChargeModifier**(*model_name: str*, *model_charge_map: List[float]*, *sys_charge_map: List[float]*, *ewald_h: float = 1*, *ewald_beta: float = 1*)

Bases: *deepmd.infer.deep_dipole.DeepDipole*

Parameters

model_name The model file for the DeepDipole model

model_charge_map Gives the amount of charge for the wfcc

sys_charge_map Gives the amount of charge for the real atoms

ewald_h Grid spacing of the reciprocal part of Ewald sum. Unit: A

ewald_beta Splitting parameter of the Ewald sum. Unit: A^{-1}

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

build_fv_graph()	Build the computational graph for the force and virial inference.
eval(coord, box, atype[, eval_fv])	Evaluate the modification
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
modify_data(data)	Modify data.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

build_fv_graph() → tensorflow.python.framework.ops.Tensor
Build the computational graph for the force and virial inference.

eval(*coord: numpy.ndarray*, *box: numpy.ndarray*, *atype: numpy.ndarray*, *eval_fv: bool = True*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]
Evaluate the modification

Parameters

coord The coordinates of atoms

box The simulation region. PBC is assumed

atype The atom types

eval_fv Evaluate force and virial

Returns

tot_e The energy modification

tot_f The force modification

tot_v The virial modification

load_prefix: str

modify_data(*data: dict*) → None
Modify data.

Parameters

data Internal data of DeepmdData. Be a dict, has the following keys - coord coordinates - box simulation box - type atom types - find_energy tells if data has energy - find_force tells if data has force - find_virial tells if data has virial - energy energy - force force - virial virial

deepmd.infer.deep_dipole module

class deepmd.infer.deep_dipole.**DeepDipole**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

deepmd.infer.deep_eval module

class deepmd.infer.deep_eval.**DeepEval**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*, *auto_batch_size: Union[bool, int, deepmd.utils.batch_size.AutoBatchSize] = False*)

Bases: object

Common methods for DeepPot, DeepWFC, DeepPolar, ...

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size [bool or int or AutomaticBatchSize, default: False] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

load_prefix: str

make_natoms_vec(*atom_types: numpy.ndarray*) → numpy.ndarray
Make the natom vector used by deepmd-kit.

Parameters

atom_types The type of atoms

Returns

natoms The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

property model_type: str
Get type of model.

:type:str

property model_version: str
Get version of model.

Returns

str version of model

static reverse_map(*vec: numpy.ndarray*, *imap: List[int]*) → numpy.ndarray
Reverse mapping of a vector according to the index map

Parameters

vec Input vector. Be of shape [nframes, natoms, -1]

imap Index map. Be of shape [natoms]

Returns

vec_out Reverse mapped vector.

static sort_input(*coord: numpy.ndarray*, *atom_type: numpy.ndarray*, *sel_atoms: Optional[List[int]] = None*)
Sort atoms in the system according their types.

Parameters

coord The coordinates of atoms. Should be of shape [nframes, natoms, 3]

atom_type The type of atoms Should be of shape [natoms]

sel_atom The selected atoms by type

Returns

coord_out The coordinates after sorting

atom_type_out The atom types after sorting

idx_map The index mapping from the input to the output. For example coord_out = coord[:,idx_map,:]

sel_atom_type Only output if sel_atoms is not None The sorted selected atom types

sel_idx_map Only output if sel_atoms is not None The index mapping from the selected atoms to sorted selected atoms.

deepmd.infer.deep_polar module

class deepmd.infer.deep_polar.**DeepGlobalPolar**(*model_file: str*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [str] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

eval(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = False*, *fparam: Optional[numpy.ndarray] = None*, *aparam: Optional[numpy.ndarray] = None*, *efield: Optional[numpy.ndarray] = None*) → numpy.ndarray

Evaluate the model.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic Not used in this model

fparam Not used in this model

aparam Not used in this model

efield Not used in this model

Returns

tensor The returned tensor If atomic == False then of size nframes x variable_dof else of size nframes x natoms x variable_dof

`get_dim_aparam`() → int
Unsupported in this model.

`get_dim_fparam`() → int
Unsupported in this model.

`load_prefix: str`

class deepmd.infer.deep_polar.**DeepPolar**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.

continues on next page

Table 29 – continued from previous page

get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

deepmd.infer.deep_pot module

class deepmd.infer.deep_pot.**DeepPot**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*, *auto_batch_size: Union[bool, int, deepmd.utils.batch_size.AutoBatchSize] = True*)

Bases: *deepmd.infer.deep_eval.DeepEval*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

auto_batch_size [bool or int or AutomaticBatchSize, default: True] If True, automatic batch size will be used. If int, it will be used as the initial batch size.

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Examples

```
>>> from deepmd.infer import DeepPot
>>> import numpy as np
>>> dp = DeepPot('graph.pb')
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> e, f, v = dp.eval(coord, cell, atype)
```

where e, f and v are predicted energy, force and virial of the system, respectively.

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the energy, force and virial by using this DP.
get_dim_aparam()	Get the number (dimension) of atomic parameters of this DP.
get_dim_fparam()	Get the number (dimension) of frame parameters of this DP.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Unsupported in this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

eval(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = False*, *fparam: Optional[numpy.ndarray] = None*, *aparam: Optional[numpy.ndarray] = None*, *efield: Optional[numpy.ndarray] = None*) → Tuple[numpy.ndarray, ...]

Evaluate the energy, force and virial by using this DP.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic Calculate the atomic energy and virial

fparam The frame parameter. The array can be of size : - nframes x dim_fparam. - dim_fparam. Then all frames are assumed to be provided with the same fparam.

aparam The atomic parameter The array can be of size : - nframes x natoms x dim_aparam. - natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. - dim_aparam. Then all frames and atoms are provided with the same aparam.

efield The external field on atoms. The array should be of size nframes x natoms x 3

Returns

energy The system energy.

force The force on each atom

virial The virial

atom_energy The atomic energy. Only returned when atomic == True

atom_virial The atomic virial. Only returned when atomic == True

get_dim_aparam() → int

Get the number (dimension) of atomic parameters of this DP.

get_dim_fparam() → int
Get the number (dimension) of frame parameters of this DP.

get_ntypes() → int
Get the number of atom types of this model.

get_rcut() → float
Get the cut-off radius of this model.

get_sel_type() → List[int]
Unsupported in this model.

get_type_map() → List[int]
Get the type map (element name of the atom types) of this model.

load_prefix: str

deepmd.infer.deep_tensor module

class deepmd.infer.deep_tensor.**DeepTensor**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_eval.DeepEval*

Evaluates a tensor model.

Parameters

model_file: str The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Get the number (dimension) of atomic parameters of this DP.
get_dim_fparam()	Get the number (dimension) of frame parameters of this DP.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map

continues on next page

Table 31 – continued from previous page

`sort_input`(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

eval(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = True*, *fparam: Optional[numpy.ndarray] = None*, *aparam: Optional[numpy.ndarray] = None*, *efield: Optional[numpy.ndarray] = None*) → numpy.ndarray

Evaluate the model.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic If True (default), return the atomic tensor Otherwise return the global tensor

fparam Not used in this model

aparam Not used in this model

efield Not used in this model

Returns

tensor The returned tensor If atomic == False then of size nframes x output_dim else of size nframes x natoms x output_dim

eval_full(*coords: numpy.ndarray*, *cells: numpy.ndarray*, *atom_types: List[int]*, *atomic: bool = False*, *fparam: Optional[numpy.array] = None*, *aparam: Optional[numpy.array] = None*, *efield: Optional[numpy.array] = None*) → Tuple[numpy.ndarray, ...]

Evaluate the model with interface similar to the energy model. Will return global tensor, component-wise force and virial and optionally atomic tensor and atomic virial.

Parameters

coords The coordinates of atoms. The array should be of size nframes x natoms x 3

cells The cell of the region. If None then non-PBC is assumed, otherwise using PBC. The array should be of size nframes x 9

atom_types The atom types The list should contain natoms ints

atomic Whether to calculate atomic tensor and virial

fparam Not used in this model

aparam Not used in this model

efield Not used in this model

Returns

tensor The global tensor. shape: [nframes x nout]

force The component-wise force (negative derivative) on each atom. shape: [nframes x nout x natoms x 3]

virial The component-wise virial of the tensor. shape: [nframes x nout x 9]

atom_tensor The atomic tensor. Only returned when atomic == True shape: [nframes x natoms x nout]

atom_virial The atomic virial. Only returned when atomic == True shape: [nframes x nout x natoms x 9]

get_dim_aparam() → int
Get the number (dimension) of atomic parameters of this DP.

get_dim_fparam() → int
Get the number (dimension) of frame parameters of this DP.

get_ntypes() → int
Get the number of atom types of this model.

get_rcut() → float
Get the cut-off radius of this model.

get_sel_type() → List[int]
Get the selected atom types of this model.

get_type_map() → List[int]
Get the type map (element name of the atom types) of this model.

load_prefix: str

tensors = {'t_box': 't_box:0', 't_coord': 't_coord:0', 't_mesh': 't_mesh:0', 't_natoms': 't_natoms:0', 't_ntypes': 'descrpt_attr/ntypes:0', 't_ouput_dim': 'model_attr/output_dim:0', 't_rcut': 'descrpt_attr/rcut:0', 't_sel_type': 'model_attr/sel_type:0', 't_tmap': 'model_attr/tmap:0', 't_type': 't_type:0'}

deepmd.infer.deep_wfc module

class deepmd.infer.deep_wfc.**DeepWFC**(*model_file: Path*, *load_prefix: str = 'load'*, *default_tf_graph: bool = False*)

Bases: *deepmd.infer.deep_tensor.DeepTensor*

Constructor.

Parameters

model_file [Path] The name of the frozen model file.

load_prefix: str The prefix in the load computational graph

default_tf_graph [bool] If uses the default tf graph, otherwise build a new tf graph for evaluation

Warning: For developers: *DeepTensor* initializer must be called at the end after *self.tensors* are modified because it uses the data in *self.tensors* dict. Do not chanage the order!

Attributes

model_type Get type of model.

model_version Get version of model.

Methods

eval(coords, cells, atom_types[, atomic, ...])	Evaluate the model.
eval_full(coords, cells, atom_types[, ...])	Evaluate the model with interface similar to the energy model.
get_dim_aparam()	Unsupported in this model.
get_dim_fparam()	Unsupported in this model.
get_ntypes()	Get the number of atom types of this model.
get_rcut()	Get the cut-off radius of this model.
get_sel_type()	Get the selected atom types of this model.
get_type_map()	Get the type map (element name of the atom types) of this model.
make_natoms_vec(atom_types)	Make the natom vector used by deepmd-kit.
reverse_map(vec, imap)	Reverse mapping of a vector according to the index map
sort_input(coord, atom_type[, sel_atoms])	Sort atoms in the system according their types.

get_dim_aparam() → int
Unsupported in this model.

get_dim_fparam() → int
Unsupported in this model.

load_prefix: str

deepmd.infer.ewald_recp module

class deepmd.infer.ewald_recp.**EwaldRecp**(*hh*, *beta*)
Bases: object

Evaluate the reciprocal part of the Ewald sum

Methods

eval(coord, charge, box)	Evaluate

eval(*coord: numpy.ndarray*, *charge: numpy.ndarray*, *box: numpy.ndarray*) → Tuple[numpy.ndarray, numpy.ndarray, numpy.ndarray]
Evaluate

Parameters

coord The coordinates of atoms

charge The atomic charge

box The simulation region. PBC is assumed

Returns

e The energy

f The force

v The virial

deepmd.infer.model_devi module

deepmd.infer.model_devi.**calc_model_devi**(*coord*, *box*, *atype*, *models*, *fname=None*, *frequency=1*, *nopbc=True*)

Python interface to calculate model deviation

Parameters

coord [numpy.ndarray, *n_frames x n_atoms x 3*] Coordinates of system to calculate

box [numpy.ndarray or None, *n_frames x 3 x 3*] Box to specify periodic boundary condition. If None, no pbc will be used

atype [numpy.ndarray, *n_atoms x 1*] Atom types

models [list of DeepPot models] Models used to evaluate deviation

fname [str or None] File to dump results, default None

frequency [int] Steps between frames (if the system is given by molecular dynamics engine), default 1

nopbc [bool] Whether to use pbc conditions

Returns

model_devi [numpy.ndarray, *n_frames x 7*] Model deviation results. The first column is index of steps, the other 6 columns are max_devi_v, min_devi_v, avg_devi_v, max_devi_f, min_devi_f, avg_devi_f.

Examples

```
>>> from deepmd.infer import calc_model_devi
>>> from deepmd.infer import DeepPot as DP
>>> import numpy as np
>>> coord = np.array([[1,0,0], [0,0,1.5], [1,0,3]]).reshape([1, -1])
>>> cell = np.diag(10 * np.ones(3)).reshape([1, -1])
>>> atype = [1,0,1]
>>> graphs = [DP("graph.000.pb"), DP("graph.001.pb")]
>>> model_devi = calc_model_devi(coord, cell, atype, graphs)
```

deepmd.infer.model_devi.**calc_model_devi_e**(*es: numpy.ndarray*)

Parameters

es [numpy.ndarray] size of `n_models x n_frames x n_atoms

deepmd.infer.model_devi.**calc_model_devi_f**(*fs: numpy.ndarray*)

Parameters

fs [numpy.ndarray] size of *n_models x n_frames x n_atoms x 3*

deepmd.infer.model_devi.**calc_model_devi_v**(*vs: numpy.ndarray*)

Parameters

vs [numpy.ndarray] size of *n_models x n_frames x 9*

deepmd.infer.model_devi.**make_model_devi**(*, *models: list*, *system: str*, *set_prefix: str*, *output: str*, *frequency: int*, ***kwargs*)

Make model deviation calculation

Parameters

models: list A list of paths of models to use for making model deviation

system: str The path of system to make model deviation calculation

set_prefix: str The set prefix of the system

output: str The output file for model deviation results

frequency: int The number of steps that elapse between writing coordinates in a trajectory by a MD engine (such as Gromacs / Lammps). This paramter is used to determine the index in the output file.

deepmd.infer.model_devi.**write_model_devi_out**(*devi: numpy.ndarray*, *fname: str*)

Parameters

devi [numpy.ndarray] the first column is the steps index

fname [str] the file name to dump

deepmd.loggers package

Module taking care of logging duties.

deepmd.loggers.**set_log_handles**(*level: int*, *log_path: Optional[Path] = None*, *mpi_log: Optional[str] = None*)

Set desired level for package loggers and add file handlers.

Parameters

level: int logging level

log_path: Optional[str] path to log file, if None logs will be send only to console. If the parent directory does not exist it will be automatically created, by default None

mpi_log [Optional[str], optional] mpi log type. Has three options. *master* will output logs to file and console only from rank==0. *collect* will write messages from all ranks to one file opened under rank==0 and to console. *workers* will open one log file for each worker designated by its rank, console behaviour is the same as for *collect*. If this argument is specified, package 'mpi4py' must be already installed. by default None

Raises

RuntimeError If the argument *mpi_log* is specified, package *mpi4py* is not installed.

Notes

Logging levels:

	our notation	python logging	tensorflow cpp	OpenMP
debug	10	10	0	1/on/true/yes
info	20	20	1	0/off/false/no
warning	30	30	2	0/off/false/no
error	40	40	3	0/off/false/no

References

https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U https://stackoverflow.com/questions/35869137/avoid-tensorflow-print-on-standard-error https://stackoverflow.com/questions/56085015/suppress-openmp-debug-messages-when-running-tensorflow-on-cpu

Submodules

deepmd.loggers.loggers module

Logger initialization for package.

`deepmd.loggers.loggers.`**`set_log_handles`**(*level: int*, *log_path: Optional[Path] = None*, *mpi_log: Optional[str] = None*)

Set desired level for package loggers and add file handlers.

Parameters

level: int logging level

log_path: Optional[str] path to log file, if None logs will be send only to console. If the parent directory does not exist it will be automatically created, by default None

mpi_log [`Optional`[`str`], `optional`] mpi log type. Has three options. *master* will output logs to file and console only from rank==0. *collect* will write messages from all ranks to one file opened under rank==0 and to console. *workers* will open one log file for each worker designated by its rank, console behaviour is the same as for *collect*. If this argument is specified, package 'mpi4py' must be already installed. by default None

Raises

`RuntimeError` If the argument *mpi_log* is specified, package *mpi4py* is not installed.

Notes

Logging levels:

	our notation	python logging	tensorflow cpp	OpenMP
debug	10	10	0	1/on/true/yes
info	20	20	1	0/off/false/no
warning	30	30	2	0/off/false/no
error	40	40	3	0/off/false/no

References

https://groups.google.com/g/mpi4py/c/SaNzc8bdj6U https://stackoverflow.com/questions/35869137/avoid-tensorflow-print-on-standard-error https://stackoverflow.com/questions/56085015/suppress-openmp-debug-messages-when-running-tensorflow-on-cpu

deepmd.loss package

Submodules

deepmd.loss.ener module

class deepmd.loss.ener.**EnerDipoleLoss**(*starter_learning_rate: float*, *start_pref_e: float = 0.1*, *limit_pref_e: float = 1.0*, *start_pref_ed: float = 1.0*, *limit_pref_ed: float = 1.0*)

Bases: object

Methods

build	
eval	
print_header	
print_on_training	

build(*learning_rate*, *natoms*, *model_dict*, *label_dict*, *suffix*)

eval(*sess*, *feed_dict*, *natoms*)

static **print_header**()

print_on_training(*tb_writer*, *cur_batch*, *sess*, *natoms*, *feed_dict_test*, *feed_dict_batch*)

class deepmd.loss.ener.**EnerStdLoss**(*starter_learning_rate: float*, *start_pref_e: float = 0.02*, *limit_pref_e: float = 1.0*, *start_pref_f: float = 1000*, *limit_pref_f: float = 1.0*, *start_pref_v: float = 0.0*, *limit_pref_v: float = 0.0*, *start_pref_ae: float = 0.0*, *limit_pref_ae: float = 0.0*, *start_pref_pf: float = 0.0*, *limit_pref_pf: float = 0.0*, *relative_f: Optional[float] = None*)

Bases: object

Standard loss function for DP models

Methods

build	
eval	
print_header	
print_on_training	

build(*learning_rate*, *natoms*, *model_dict*, *label_dict*, *suffix*)

eval(*sess*, *feed_dict*, *natoms*)

print_header()

print_on_training(*tb_writer*, *cur_batch*, *sess*, *natoms*, *feed_dict_test*, *feed_dict_batch*)

deepmd.loss.tensor module

class deepmd.loss.tensor.**TensorLoss**(*jdata*, ***kwarg*)

Bases: object

Loss function for tensorial properties.

Methods

build	
eval	
print_header	
print_on_training	

build(*learning_rate*, *natoms*, *model_dict*, *label_dict*, *suffix*)

eval(*sess*, *feed_dict*, *natoms*)

print_header()

print_on_training(*tb_writer*, *cur_batch*, *sess*, *natoms*, *feed_dict_test*, *feed_dict_batch*)

deepmd.model package

Submodules

deepmd.model.ener module

class deepmd.model.ener.**EnerModel**(*descrpt*, *fitting*, *typeebd=None*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*, *use_srtab: Optional[str] = None*, *smin_alpha: Optional[float] = None*, *sw_rmin: Optional[float] = None*, *sw_rmax: Optional[float] = None*)

Bases: object

Energy model.

Parameters

descrpt Descriptor

fitting Fitting net

type_map Mapping atom type to the name (str) of the type. For example *type_map[1]* gives the name of the type 1.

data_stat_nbatch Number of frames used for data statistic

data_stat_protect Protect parameter for atomic energy regression

use_srtab The table for the short-range pairwise interaction added on top of DP. The table is a text data file with (N_t + 1) * N_t / 2 + 1 columes. The first colume is the distance between atoms. The second to the last columes are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columes from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

smin_alpha The short-range tabulated interaction will be swithed according to the distance of the nearest neighbor. This distance is calculated by softmin. This parameter is the decaying parameter in the softmin. It is only required when *use_srtab* is provided.

sw_rmin The lower boundary of the interpolation between short-range tabulated interaction and DP. It is only required when *use_srtab* is provided.

sw_rmin The upper boundary of the interpolation between short-range tabulated interaction and DP. It is only required when *use_srtab* is provided.

Methods

build	
data_stat	
get_ntypes	
get_rcut	
get_type_map	

build(*coord_*, *atype_*, *natoms*, *box*, *mesh*, *input_dict*, *frz_model=None*, *suffix=''*, *reuse=None*)

data_stat(*data*)

get_ntypes()

get_rcut()

get_type_map()

model_type = 'ener'

deepmd.model.model_stat module

deepmd.model.model_stat.**make_stat_input**(*data*, *nbatches*, *merge_sys=True*)
pack data for statistics Parameters ———- data:

The data

merge_sys: bool (True) Merge system data

all_stat: A dictionary of list of list storing data for stat. if merge_sys == False data can be accessed by all_stat[key][sys_idx][batch_idx][frame_idx]

else merge_sys == True can be accessed by all_stat[key][batch_idx][frame_idx]

deepmd.model.model_stat.**merge_sys_stat**(*all_stat*)

deepmd.model.tensor module

class deepmd.model.tensor.**DipoleModel**(*descrpt*, *fitting*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*)
Bases: *deepmd.model.tensor.TensorModel*

Methods

build	
data_stat	
get_ntypes	
get_out_size	
get_rcut	
get_sel_type	
get_type_map	

class deepmd.model.tensor.**GlobalPolarModel**(*descrpt*, *fitting*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*)
Bases: *deepmd.model.tensor.TensorModel*

Methods

build	
data_stat	
get_ntypes	
get_out_size	
get_rcut	
get_sel_type	
get_type_map	

class deepmd.model.tensor.**PolarModel**(*descrpt*, *fitting*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*)

Bases: *deepmd.model.tensor.TensorModel*

Methods

build	
data_stat	
get_ntypes	
get_out_size	
get_rcut	
get_sel_type	
get_type_map	

class deepmd.model.tensor.**TensorModel**(*tensor_name: str*, *descrpt*, *fitting*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*)

Bases: object

Tensor model.

Parameters

tensor_name Name of the tensor.

descrpt Descriptor

fitting Fitting net

type_map Mapping atom type to the name (str) of the type. For example *type_map[1]* gives the name of the type 1.

data_stat_nbatch Number of frames used for data statistic

data_stat_protect Protect parameter for atomic energy regression

Methods

build	
data_stat	
get_ntypes	
get_out_size	
get_rcut	
get_sel_type	
get_type_map	

build(*coord_*, *atype_*, *natoms*, *box*, *mesh*, *input_dict*, *frz_model=None*, *suffix=''*, *reuse=None*)

data_stat(*data*)

get_ntypes()

get_out_size()

get_rcut()

get_sel_type()

get_type_map()

class deepmd.model.tensor.**WFCModel**(*descrpt*, *fitting*, *type_map: Optional[List[str]] = None*, *data_stat_nbatch: int = 10*, *data_stat_protect: float = 0.01*)

Bases: *deepmd.model.tensor.TensorModel*

Methods

build	
data_stat	
get_ntypes	
get_out_size	
get_rcut	
get_sel_type	
get_type_map	

deepmd.op package

This module will house cust Tf OPs after CMake installation.

deepmd.op.**import_ops**()
Import all custom TF ops that are present in this submodule.

deepmd.utils package

Submodules

deepmd.utils.argcheck module

class deepmd.utils.argcheck.**ArgsPlugin**
Bases: object

Methods

get_all_argument()	Get all arguments.
register(name[, alias])	Regiester a descriptor argument plugin.

get_all_argument() → List[dargs.dargs.Argument]
Get all arguments.

Returns

List[Argument] all arguments

register(*name: str*, *alias: Optional[List[str]] = None*) → Callable[[], List[dargs.dargs.Argument]]
Regiester a descriptor argument plugin.

Parameters

name [str] the name of a descriptor

alias [List[str], optional] the list of aliases of this descriptor

Returns

Callable[[], List[Argument]] the regiestered descriptor argument method

Examples

```
>>> some_plugin = ArgsPlugin()
>>> @some_plugin.register("some_descrpt")
    def descrpt_some_descrpt_args():
        return []
```

deepmd.utils.argcheck.**descrpt_hybrid_args**()

deepmd.utils.argcheck.**descrpt_local_frame_args**()

deepmd.utils.argcheck.**descrpt_se_a_args**()

deepmd.utils.argcheck.**descrpt_se_a_tpe_args**()

deepmd.utils.argcheck.**descrpt_se_r_args**()

deepmd.utils.argcheck.**descrpt_se_t_args**()

deepmd.utils.argcheck.**descrpt_variant_type_args**()

deepmd.utils.argcheck.**fitting_dipole**()

deepmd.utils.argcheck.**fitting_ener**()

deepmd.utils.argcheck.**fitting_polar**()

deepmd.utils.argcheck.**fitting_variant_type_args**()

deepmd.utils.argcheck.**gen_doc**(*, *make_anchor=True*, *make_link=True*, ***kwargs*)

deepmd.utils.argcheck.**gen_json**(***kwargs*)

deepmd.utils.argcheck.**learning_rate_args**()

deepmd.utils.argcheck.**learning_rate_exp**()

deepmd.utils.argcheck.**learning_rate_variant_type_args**()

deepmd.utils.argcheck.**limit_pref**(*item*)

deepmd.utils.argcheck.**list_to_doc**(*xx*)

deepmd.utils.argcheck.**loss_args**()

deepmd.utils.argcheck.**loss_ener**()

deepmd.utils.argcheck.**loss_tensor**()

deepmd.utils.argcheck.**loss_variant_type_args**()

deepmd.utils.argcheck.**make_index**(*keys*)

deepmd.utils.argcheck.**make_link**(*content*, *ref_key*)

deepmd.utils.argcheck.**model_args**()

deepmd.utils.argcheck.**model_compression**()

deepmd.utils.argcheck.**model_compression_type_args**()

deepmd.utils.argcheck.**modifier_dipole_charge**()

deepmd.utils.argcheck.**modifier_variant_type_args**()

deepmd.utils.argcheck.**normalize**(*data*)

deepmd.utils.argcheck.**normalize_hybrid_list**(*hy_list*)

deepmd.utils.argcheck.**start_pref**(*item*)

deepmd.utils.argcheck.**training_args**()

deepmd.utils.argcheck.**training_data_args**()

deepmd.utils.argcheck.**type_embedding_args**()

deepmd.utils.argcheck.**validation_data_args**()

deepmd.utils.batch_size module

class deepmd.utils.batch_size.**AutoBatchSize**(*initial_batch_size: int = 1024*, *factor: float = 2.0*)

Bases: `object`

This class allows DeePMD-kit to automatically decide the maximum batch size that will not cause an OOM error.

Parameters

initial_batch_size [`int`, default: 1024] initial batch size (number of total atoms)

factor [`float`, default: 2.] increased factor

Notes

We assume all OOM error will raise **:metd:`OutOfMemoryError`**.

Attributes

current_batch_size [int] current batch size (number of total atoms)

maximum_working_batch_size [int] maximum working batch size

minimal_not_working_batch_size [int] minimal not working batch size

Methods

execute(callable, start_index, natoms)	Excuate a method with given batch size.
execute_all(callable, total_size, natoms, ...)	Excuate a method with all given data.

execute(*callable: Callable*, *start_index: int*, *natoms: int*) → Tuple[int, tuple]
Excuate a method with given batch size.

Parameters

callable [Callable] The method should accept the batch size and start_index as parameters, and returns executed batch size and data.

start_index [int] start index

natoms [int] natoms

Returns

int executed batch size * number of atoms

tuple result from callable, None if failing to execute

Raises

OutOfMemoryError OOM when batch size is 1

execute_all(*callable: Callable*, *total_size: int*, *natoms: int*, **args*, ***kwargs*) → Tuple[numpy.ndarray]
Excuate a method with all given data.

Parameters

callable [Callable] The method should accept *args and **kwargs as input and return the similiar array.

total_size [int] Total size

natoms [int] The number of atoms

****kwargs** If 2D np.ndarray, assume the first axis is batch; otherwise do nothing.

deepmd.utils.compat module

Module providing compatibility between *0.x.x* and *1.x.x* input versions.

deepmd.utils.compat.**convert_input_v0_v1**(*jdata: Dict[str, Any]*, *warning: bool = True*, *dump: Optional[Union[str, pathlib.Path]] = None*) → Dict[str, Any]

Convert input from v0 format to v1.

Parameters

jdata [Dict[str, Any]] loaded json/yaml file

warning [bool, optional] whether to show deprecation warning, by default True

dump [Optional[Union[str, Path]], optional] whether to dump converted file, by default None

Returns

Dict[str, Any] converted output

deepmd.utils.compat.**convert_input_v1_v2**(*jdata: Dict[str, Any]*, *warning: bool = True*, *dump: Optional[Union[str, pathlib.Path]] = None*) → Dict[str, Any]

deepmd.utils.compat.**remove_decay_rate**(*jdata: Dict[str, Any]*)

convert decay_rate to stop_lr.

Parameters

jdata: Dict[str, Any] input data

deepmd.utils.compat.**updata_deepmd_input**(*jdata: Dict[str, Any]*, *warning: bool = True*, *dump: Optional[Union[str, pathlib.Path]] = None*) → Dict[str, Any]

deepmd.utils.convert module

deepmd.utils.convert.**convert_12_to_20**(*input_model: str*, *output_model: str*)

deepmd.utils.convert.**convert_13_to_20**(*input_model: str*, *output_model: str*)

deepmd.utils.convert.**convert_dp12_to_dp13**(*file*)

deepmd.utils.convert.**convert_dp13_to_dp20**(*fname: str*)

deepmd.utils.convert.**convert_pb_to_pbtxt**(*pbfile: str*, *pbtxtfile: str*)

deepmd.utils.convert.**convert_pbtxt_to_pb**(*pbtxtfile: str*, *pbfile: str*)

deepmd.utils.data module

class deepmd.utils.data.**DataSets**(*sys_path*, *set_prefix*, *seed=None*, *shuffle_test=True*)

Bases: object

Outdated class for one data system.

Deprecated since version 2.0.0: This class is not maintained any more.

Methods

get_batch(batch_size)	returned property prefector [4] in order: energy, force, virial, atom_ener
get_test()	returned property prefector [4] in order: energy, force, virial, atom_ener
load_energy(set_name, nframes, nvalues, ...)	return : coeff_ener, ener, coeff_atom_ener, atom_ener

check_batch_size	
check_test_size	
get_ener	
get_natoms	
get_natoms_2	
get_natoms_vec	
get_numb_set	
get_set	
get_sys_numb_batch	
get_type_map	
load_batch_set	
load_data	
load_set	
load_test_set	
load_type	
load_type_map	
numb_aparam	
numb_fparam	
reset_iter	
set_numb_batch	
stats_energy	

check_batch_size(*batch_size*)

check_test_size(*test_size*)

get_batch(*batch_size*)

returned property prefector [4] in order: energy, force, virial, atom_ener

get_ener()

get_natoms()

get_natoms_2(*ntypes*)

get_natoms_vec(*ntypes*)

get_numb_set()

get_set(*data*, *idx=None*)

get_sys_numb_batch(*batch_size*)

get_test()
returned property prefector [4] in order: energy, force, virial, atom_ener

get_type_map()

load_batch_set(*set_name*)

load_data(*set_name*, *data_name*, *shape*, *is_necessary=True*)

load_energy(*set_name*, *nframes*, *nvalues*, *energy_file*, *atom_energy_file*)
return : coeff_ener, ener, coeff_atom_ener, atom_ener

load_set(*set_name*, *shuffle=True*)

load_test_set(*set_name*, *shuffle_test*)

load_type(*sys_path*)

load_type_map(*sys_path*)

numb_aparam()

numb_fparam()

reset_iter()

set_numb_batch(*batch_size*)

stats_energy()

class deepmd.utils.data.**DeepmdData**(*sys_path: str*, *set_prefix: str = 'set'*, *shuffle_test: bool = True*, *type_map: Optional[List[str]] = None*, *modifier=None*, *trn_all_set: bool = False*)

Bases: object

Class for a data system.

It loads data from hard disk, and mantains the data as a *data_dict*

Parameters

sys_path Path to the data system

set_prefix Prefix for the directories of different sets

shuffle_test If the test data are shuffled

type_map Gives the name of different atom types

modifier Data modifier that has the method *modify_data*

trn_all_set Use all sets as training dataset. Otherwise, if the number of sets is more than 1, the last set is left for test.

Methods

add(key, ndof[, atomic, must, high_prec, ...])	Add a data item that to be loaded
avg(key)	Return the average value of an item.
check_batch_size(batch_size)	Check if the system can get a batch of data with *batch_size* frames.
check_test_size(test_size)	Check if the system can get a test dataset with *test_size* frames.
get_atom_type()	Get atom types
get_batch(batch_size)	Get a batch of data with *batch_size* frames.
get_data_dict()	Get the *data_dict*
get_natoms()	Get number of atoms
get_natoms_vec(ntypes)	Get number of atoms and number of atoms in different types
get_ntypes()	Number of atom types in the system
get_numb_batch(batch_size, set_idx)	Get the number of batches in a set.
get_numb_set()	Get number of training sets
get_sys_numb_batch(batch_size)	Get the number of batches in the data system.
get_test([ntests])	Get the test data with *ntests* frames.
get_type_map()	Get the type map
reduce(key_out, key_in)	Generate a new item from the reduction of another atom

reset_get_batch

add(*key: str*, *ndof: int*, *atomic: bool = False*, *must: bool = False*, *high_prec: bool = False*, *type_sel: Optional[List[int]] = None*, *repeat: int = 1*)
Add a data item that to be loaded

Parameters

key The key of the item. The corresponding data is stored in *sys_path/set.*/key.npy*

ndof The number of dof

atomic The item is an atomic property. If False, the size of the data should be nframes x ndof If True, the size of data should be nframes x natoms x ndof

must The data file *sys_path/set.*/key.npy* must exist. If must is False and the data file does not exist, the *data_dict[find_key]* is set to 0.0

high_prec Load the data and store in float64, otherwise in float32

type_sel Select certain type of atoms

repeat The data will be repeated *repeat* times.

avg(*key*)
Return the average value of an item.

check_batch_size(*batch_size*)
Check if the system can get a batch of data with *batch_size* frames.

check_test_size(*test_size*)
Check if the system can get a test dataset with *test_size* frames.

get_atom_type() → List[int]
Get atom types

get_batch(*batch_size: int*) → dict
Get a batch of data with *batch_size* frames. The frames are randomly picked from the data system.

Parameters

batch_size size of the batch

get_data_dict() → dict
Get the *data_dict*

get_natoms()
Get number of atoms

get_natoms_vec(*ntypes: int*)
Get number of atoms and number of atoms in different types

Parameters

ntypes Number of types (may be larger than the actual number of types in the system).

Returns

natoms natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

get_ntypes() → int
Number of atom types in the system

get_numb_batch(*batch_size: int*, *set_idx: int*) → int
Get the number of batches in a set.

get_numb_set() → int
Get number of training sets

get_sys_numb_batch(*batch_size: int*) → int
Get the number of batches in the data system.

get_test(*ntests: int = - 1*) → dict
Get the test data with *ntests* frames.

Parameters

ntests Size of the test data set. If *ntests* is -1, all test data will be get.

get_type_map() → List[str]
Get the type map

reduce(*key_out: str*, *key_in: str*)
Generate a new item from the reduction of another atom

Parameters

key_out The name of the reduced item

key_in The name of the data item to be reduced

reset_get_batch()

deepmd.utils.data_system module

class deepmd.utils.data_system.**DataSystem**(*systems*, *set_prefix*, *batch_size*, *test_size*, *rcut*, *run_opt=None*)
Bases: object

Outdated class for the data systems.

Deprecated since version 2.0.0: This class is not maintained any more.

Methods

check_type_map_consistency	
compute_energy_shift	
format_name_length	
get_batch	
get_batch_size	
get_nbatches	
get_nsystems	
get_ntypes	
get_sys	
get_test	
get_type_map	
numb_fparam	
print_summary	
process_sys_weights	

check_type_map_consistency(*type_map_list*)

compute_energy_shift()

format_name_length(*name*, *width*)

get_batch(*sys_idx=None*, *sys_weights=None*, *style='prob_sys_size'*)

get_batch_size()

get_nbatches()

get_nsystems()

get_ntypes()

get_sys(*sys_idx*)

get_test(*sys_idx=None*)

get_type_map()

numb_fparam()

print_summary()

process_sys_weights(*sys_weights*)

class deepmd.utils.data_system.**DeepmdDataSystem**(*systems: List[str]*, *batch_size: int*, *test_size: int*, *rcut: float*, *set_prefix: str = 'set'*, *shuffle_test: bool = True*, *type_map: Optional[List[str]] = None*, *modifier=None*, *trn_all_set=False*, *sys_probs=None*, *auto_prob_style='prob_sys_size'*)

Bases: object

Class for manipulating many data systems.

It is implemented with the help of DeepmdData

Methods

add(key, ndof[, atomic, must, high_prec, ...])	Add a data item that to be loaded
add_dict(adict)	Add items to the data system by a *dict*. *adict* should have items like adict[key] = { 'ndof': ndof, 'atomic': atomic, 'must': must, 'high_prec': high_prec, 'type_sel': type_sel, 'repeat': repeat, } For the explaination of the keys see *add*.
get_batch([sys_idx])	Get a batch of data from the data systems
get_batch_size()	Get the batch size
get_nbatches()	Get the total number of batches
get_nsystems()	Get the number of data systems
get_ntypes()	Get the number of types
get_sys(idx)	Get a certain data system
get_sys_ntest([sys_idx])	Get number of tests for the currently selected system,
get_test([sys_idx, n_test])	Get test data from the the data systems.
get_type_map()	Get the type map
reduce(key_out, key_in)	Generate a new item from the reduction of another atom

compute_energy_shift	
get_data_dict	
print_summary	
set_sys_probs	

add(*key: str*, *ndof: int*, *atomic: bool = False*, *must: bool = False*, *high_prec: bool = False*, *type_sel: Optional[List[int]] = None*, *repeat: int = 1*)
Add a data item that to be loaded

Parameters

key The key of the item. The corresponding data is stored in *sys_path/set.*/key.npy*

ndof The number of dof

atomic The item is an atomic property. If False, the size of the data should be nframes x ndof If True, the size of data should be nframes x natoms x ndof

must The data file *sys_path/set.*/key.npy* must exist. If must is False and the data file does not exist, the *data_dict[find_key]* is set to 0.0

high_prec Load the data and store in float64, otherwise in float32

type_sel Select certain type of atoms

repeat The data will be repeated *repeat* times.

add_dict(*adict: dict*) → None
Add items to the data system by a *dict*. *adict* should have items like adict[key] = {

'ndof': ndof, 'atomic': atomic, 'must': must, 'high_prec': high_prec, 'type_sel': type_sel, 'repeat': repeat,

} For the explaination of the keys see *add*

compute_energy_shift(*rcond=0.001*, *key='energy'*)

get_batch(*sys_idx: Optional[int] = None*)
Get a batch of data from the data systems

Parameters

sys_idx: int The index of system from which the batch is get. If sys_idx is not None, *sys_probs* and *auto_prob_style* are ignored If sys_idx is None, automatically determine the system according to *sys_probs* or *auto_prob_style*, see the following.

get_batch_size() → int
Get the batch size

get_data_dict(*ii: int = 0*) → dict

get_nbatches() → int
Get the total number of batches

get_nsystems() → int
Get the number of data systems

get_ntypes() → int
Get the number of types

get_sys(*idx: int*) → *deepmd.utils.data.DeepmdData*
Get a certain data system

get_sys_ntest(*sys_idx=None*)

Get number of tests for the currently selected system, or one defined by sys_idx.

get_test(*sys_idx: Optional[int] = None*, *n_test: int = - 1*)
Get test data from the the data systems.

Parameters

sys_idx The test dat of system with index *sys_idx* will be returned. If is None, the currently selected system will be returned.

n_test Number of test data. If set to -1 all test data will be get.

get_type_map() → List[str]
Get the type map

print_summary(*name*)

reduce(*key_out*, *key_in*)
Generate a new item from the reduction of another atom

Parameters

key_out The name of the reduced item

key_in The name of the data item to be reduced

set_sys_probs(*sys_probs=None*, *auto_prob_style: str = 'prob_sys_size'*)

deepmd.utils.errors module

exception deepmd.utils.errors.**GraphTooLargeError**
Bases: Exception

exception deepmd.utils.errors.**GraphWithoutTensorError**
Bases: Exception

exception deepmd.utils.errors.**OutOfMemoryError**
Bases: Exception

This error is caused by out-of-memory (OOM).

deepmd.utils.graph module

deepmd.utils.graph.**get_embedding_net_nodes**(*model_file: str*, *suffix: str = ''*) → Dict
Get the embedding net nodes with the given frozen model(model_file)

Parameters

model_file The input frozen model path

suffix [str, optional] The suffix of the scope

Returns

Dict The embedding net nodes with the given frozen model

deepmd.utils.graph.**get_embedding_net_nodes_from_graph_def**(*graph_def: tensorflow.core.framework.graph_pb2.GraphDef*, *suffix: str = ''*) → Dict

Get the embedding net nodes with the given tf.GraphDef object

Parameters

graph_def The input tf.GraphDef object

suffix [str, optional] The scope suffix

Returns

Dict The embedding net nodes within the given tf.GraphDef object

deepmd.utils.graph.**get_embedding_net_variables**(*model_file: str*, *suffix: str = ''*) → Dict

Get the embedding net variables with the given frozen model(model_file)

Parameters

model_file The input frozen model path

suffix [str, optional] The suffix of the scope

Returns

Dict The embedding net variables within the given frozen model

deepmd.utils.graph.**get_embedding_net_variables_from_graph_def**(*graph_def: tensorflow.core.framework.graph_pb2.GraphDef*, *suffix: str = ''*) → Dict

Get the embedding net variables with the given tf.GraphDef object

Parameters

graph_def The input tf.GraphDef object

suffix [str, optional] The suffix of the scope

Returns

Dict The embedding net variables within the given tf.GraphDef object

deepmd.utils.graph.**get_fitting_net_nodes**(*model_file: str*) → Dict

Get the fitting net nodes with the given frozen model(model_file)

Parameters

model_file The input frozen model path

Returns

Dict The fitting net nodes with the given frozen model

deepmd.utils.graph.**get_fitting_net_nodes_from_graph_def**(*graph_def: tensorflow.core.framework.graph_pb2.GraphDef*) → Dict

Get the fitting net nodes with the given tf.GraphDef object

Parameters

graph_def The input tf.GraphDef object

Returns

Dict The fitting net nodes within the given tf.GraphDef object

deepmd.utils.graph.**get_fitting_net_variables**(*model_file: str*) → Dict
Get the fitting net variables with the given frozen model(model_file)

Parameters

model_file The input frozen model path

Returns

Dict The fitting net variables within the given frozen model

deepmd.utils.graph.**get_fitting_net_variables_from_graph_def**(*graph_def: tensorflow.core.framework.graph_pb2.GraphDef*) → Dict
Get the fitting net variables with the given tf.GraphDef object

Parameters

graph_def The input tf.GraphDef object

Returns

Dict The fitting net variables within the given tf.GraphDef object

deepmd.utils.graph.**get_tensor_by_name**(*model_file: str*, *tensor_name: str*) → tensorflow.python.framework.ops.Tensor
Load tensor value from the frozen model(model_file)

Parameters

model_file [str] The input frozen model path

tensor_name [str] Indicates which tensor which will be loaded from the frozen model

Returns

tf.Tensor The tensor which was loaded from the frozen model

Raises

GraphWithoutTensorError Whether the tensor_name is within the frozen model

deepmd.utils.graph.**get_tensor_by_name_from_graph**(*graph: tensorflow.python.framework.ops.Graph*, *tensor_name: str*) → tensorflow.python.framework.ops.Tensor
Load tensor value from the given tf.Graph object

Parameters

graph [tf.Graph] The input TensorFlow graph

tensor_name [str] Indicates which tensor which will be loaded from the frozen model

Returns

tf.Tensor The tensor which was loaded from the frozen model

Raises

GraphWithoutTensorError Whether the tensor_name is within the frozen model

deepmd.utils.graph.**get_tensor_by_type**(*node*, *data_type: numpy.dtype*) → tensorflow.python.framework.ops.Tensor
Get the tensor value within the given node according to the input data_type

Parameters

node The given tensorflow graph node

data_type The data type of the node

Returns

`tf.Tensor` The tensor value of the given node

deepmd.utils.graph.**load_graph_def**(*model_file: str*) → Tuple[tensorflow.python.framework.ops.Graph, tensorflow.core.framework.graph_pb2.GraphDef]

Load graph as well as the graph_def from the frozen model(model_file)

Parameters

model_file [`str`] The input frozen model path

Returns

`tf.Graph` The graph loaded from the frozen model

tf.GraphDef The graph_def loaded from the frozen model

deepmd.utils.learning_rate module

class deepmd.utils.learning_rate.**LearningRateExp**(*start_lr: float*, *stop_lr: float = 5e-08*, *decay_steps: int = 5000*, *decay_rate: float = 0.95*)

Bases: `object`

The exponentially decaying learning rate.

The learning rate at step t is given by

$$\alpha(t) = \alpha_0 \lambda^{t/\tau}$$

where α is the learning rate, α_0 is the starting learning rate, λ is the decay rate, and τ is the decay steps.

Parameters

start_lr Starting learning rate α_0

stop_lr Stop learning rate α_1

decay_steps Learning rate decay every this number of steps τ

decay_rate The decay rate λ. If *stop_step* is provided in *build*, then it will be determined automatically and overwritten.

Methods

build(global_step[, stop_step])	Build the learning rate
start_lr()	Get the start lr
value(step)	Get the lr at a certain step

build(*global_step: tensorflow.python.framework.ops.Tensor*, *stop_step: Optional[int] = None*) → tensorflow.python.framework.ops.Tensor

Build the learning rate

Parameters

global_step The tf Tensor prividing the global training step

stop_step The stop step. If provided, the decay_rate will be determined automatically and

overwritten.

Returns

learning_rate The learning rate

start_lr() → float
Get the start lr

value(*step: int*) → float
Get the lr at a certain step

deepmd.utils.neighbor_stat module

class deepmd.utils.neighbor_stat.**NeighborStat**(*ntypes: int*, *rcut: float*)
Bases: object

Class for getting training data information.

It loads data from DeepmdData object, and measures the data info, including neareest nbor distance between atoms, max nbor size of atoms and the output data range of the environment matrix.

Parameters

ntypes The num of atom types

rcut The cut-off radius

Methods

get_stat(data)	get the data statistics of the training data, including nearest nbor distance between atoms, max nbor size of atoms

get_stat(*data: deepmd.utils.data_system.DeepmdDataSystem*) → Tuple[float, List[int]]
get the data statistics of the training data, including nearest nbor distance between atoms, max nbor size of atoms

Parameters

data Class for manipulating many data systems. It is implemented with the help of DeepmdData.

Returns

min_nbor_dist The nearest distance between neighbor atoms

max_nbor_size A list with ntypes integers, denotes the actual achieved max sel

deepmd.utils.network module

deepmd.utils.network.**embedding_net**(*xx*, *network_size*, *precision*, *activation_fn=<function tanh>*, *resnet_dt=False*, *name_suffix=''*, *stddev=1.0*, *bavg=0.0*, *seed=None*, *trainable=True*, *uniform_seed=False*, *initial_variables=None*)

The embedding network.

The embedding network function $\mathcal{N}$ is constructed by is the composition of multiple layers $\mathcal{L}^{(i)}$:

$$\mathcal{N} = \mathcal{L}^{(n)} \circ \mathcal{L}^{(n-1)} \circ \cdots \circ \mathcal{L}^{(1)}$$

A layer $\mathcal{L}$ is given by one of the following forms, depending on the number of nodes: [1]

$$\mathbf{y} = \mathcal{L}(\mathbf{x}; \mathbf{w}, \mathbf{b}) = \begin{cases} \boldsymbol{\phi}(\mathbf{x}^T\mathbf{w} + \mathbf{b}) + \mathbf{x}, & N_2 = N_1 \\ \boldsymbol{\phi}(\mathbf{x}^T\mathbf{w} + \mathbf{b}) + (\mathbf{x}, \mathbf{x}), & N_2 = 2N_1 \\ \boldsymbol{\phi}(\mathbf{x}^T\mathbf{w} + \mathbf{b}), & \text{otherwise} \end{cases}$$

where $\mathbf{x} \in \mathbb{R}^{N_1}$ is the input vector and $\mathbf{y} \in \mathbb{R}^{N_2}$ is the output vector. $\mathbf{w} \in \mathbb{R}^{N_1 \times N_2}$ and $\mathbf{b} \in \mathbb{R}^{N_2}$ are weights and biases, respectively, both of which are trainable if *trainable* is *True*. $\boldsymbol{\phi}$ is the activation function.

Parameters

xx [Tensor] Input tensor $\mathbf{x}$ of shape [-1,1]

network_size: list of int Size of the embedding network. For example [16,32,64]

precision: Precision of network weights. For example, tf.float64

activation_fn: Activation function $\boldsymbol{\phi}$

resnet_dt: boolean Using time-step in the ResNet construction

name_suffix: str The name suffix append to each variable.

stddev: float Standard deviation of initializing network parameters

bavg: float Mean of network intial bias

seed: int Random seed for initializing network parameters

trainable: boolean If the network is trainable

uniform_seed [bool] Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

initial_variables [dict] The input dict which stores the embedding net variables

References

[1]

deepmd.utils.network.**embedding_net_rand_seed_shift**(*network_size*)

deepmd.utils.network.**one_layer**(*inputs*, *outputs_size*, *activation_fn=<function tanh>*, *precision=tf.float64*, *stddev=1.0*, *bavg=0.0*, *name='linear'*, *reuse=None*, *seed=None*, *use_timestep=False*, *trainable=True*, *useBN=False*, *uniform_seed=False*, *initial_variables=None*)

deepmd.utils.network.**one_layer_rand_seed_shift**()

deepmd.utils.network.**variable_summaries**(*var: tensorflow.python.ops.variables.VariableV1*, *name: str*)
Attach a lot of summaries to a Tensor (for TensorBoard visualization).

Parameters

var [tf.Variable] [description]

name [str] variable name

deepmd.utils.pair_tab module

class deepmd.utils.pair_tab.**PairTab**(*filename: str*)
Bases: object

Parameters

filename File name for the short-range tabulated potential. The table is a text data file with (N_t + 1) * N_t / 2 + 1 columes. The first colume is the distance between atoms. The second to the last columes are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columes from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

Methods

get()	Get the serialized table.
reinit(filename)	Initialize the tabulated interaction

get() → Tuple[numpy.array, numpy.array]
Get the serialized table.

reinit(*filename: str*) → None
Initialize the tabulated interaction

Parameters

filename File name for the short-range tabulated potential. The table is a text data file with (N_t + 1) * N_t / 2 + 1 columes. The first colume is the distance between atoms. The second to the last columes are energies for pairs of certain types. For example we have two atom types, 0 and 1. The columes from 2nd to 4th are for 0-0, 0-1 and 1-1 correspondingly.

deepmd.utils.path module

class deepmd.utils.path.**DPH5Path**(*path: str*)
Bases: *deepmd.utils.path.DPPath*

The path class to data system (DeepmdData) for HDF5 files.

Parameters

path [str] path

Notes

OS - HDF5 relationship: directory - Group file - Dataset

Methods

glob(pattern)	Search path using the glob pattern.
is_dir()	Check if self is directory.
is_file()	Check if self is file.
load_numpy()	Load NumPy array.
load_txt([dtype])	Load NumPy array from text.
rglob(pattern)	This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

glob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
Search path using the glob pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

is_dir() → bool
Check if self is directory.

is_file() → bool
Check if self is file.

load_numpy() → numpy.ndarray
Load NumPy array.

Returns

np.ndarray loaded NumPy array

load_txt(*dtype: Optional[numpy.dtype] = None*, ***kwargs*) → numpy.ndarray
Load NumPy array from text.

Returns

np.ndarray loaded NumPy array

rglob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

class deepmd.utils.path.**DPOSPath**(*path: str*)
Bases: *deepmd.utils.path.DPPath*

The OS path class to data system (DeepmdData) for real directories.

Parameters

path [str] path

Methods

glob(pattern)	Search path using the glob pattern.
is_dir()	Check if self is directory.
is_file()	Check if self is file.
load_numpy()	Load NumPy array.
load_txt(**kwargs)	Load NumPy array from text.
rglob(pattern)	This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

glob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
Search path using the glob pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

is_dir() → bool
Check if self is directory.

is_file() → bool
Check if self is file.

load_numpy() → numpy.ndarray
Load NumPy array.

Returns

np.ndarray loaded NumPy array

load_txt(**kwargs*) → numpy.ndarray
Load NumPy array from text.

Returns

np.ndarray loaded NumPy array

rglob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

class deepmd.utils.path.**DPPath**(*path: str*)
Bases: abc.ABC

The path class to data system (DeepmdData).

Parameters

path [str] path

Methods

glob(pattern)	Search path using the glob pattern.
is_dir()	Check if self is directory.
is_file()	Check if self is file.
load_numpy()	Load NumPy array.
load_txt(**kwargs)	Load NumPy array from text.
rglob(pattern)	This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

abstract glob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
Search path using the glob pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

abstract is_dir() → bool
Check if self is directory.

abstract is_file() → bool
Check if self is file.

abstract load_numpy() → numpy.ndarray
Load NumPy array.

Returns

np.ndarray loaded NumPy array

abstract load_txt(**kwargs*) → numpy.ndarray
Load NumPy array from text.

Returns

np.ndarray loaded NumPy array

abstract rglob(*pattern: str*) → List[*deepmd.utils.path.DPPath*]
This is like calling **:metd:`DPPath.glob()`** with **/ added in front of the given relative pattern.

Parameters

pattern [str] glob pattern

Returns

List[*DPPath*] list of paths

deepmd.utils.plugin module

Base of plugin systems.

class deepmd.utils.plugin.**Plugin**
Bases: object

A class to register and restore plugins.

Examples

```
>>> plugin = Plugin()
>>> @plugin.register("xx")
    def xxx():
        pass
>>> print(plugin.plugins['xx'])
```

Attributes

plugins [Dict[str, object]] plugins

Methods

get_plugin(key)	Visit a plugin by key.
register(key)	Register a plugin.

get_plugin(*key*) → object
Visit a plugin by key.

Parameters

key **str** key of the plugin

Returns

object the plugin

register(*key: str*) → Callable[[object], object]
Register a plugin.

Returns

Callable[[object], object] decorator

class deepmd.utils.plugin.**PluginVariant**(**args*, ***kwargs*)
Bases: object

A class to remove *type* from input arguments.

class deepmd.utils.plugin.**VariantABCMeta**(*name*, *bases*, *namespace*, ***kwargs*)
Bases: *deepmd.utils.plugin.VariantMeta*, abc.ABCMeta

Methods

`__call__`(*args, **kwargs)	Remove *type* and keys that starts with underline.
`mro`(/)	Return a type's method resolution order.
`register`(subclass)	Register a virtual subclass of an ABC.

class deepmd.utils.plugin.**VariantMeta**

Bases: `object`

Methods

`__call__`(*args, **kwargs)	Remove *type* and keys that starts with underline.

deepmd.utils.random module

deepmd.utils.random.**choice**(*a: numpy.ndarray*, *p: Optional[numpy.ndarray] = None*)

Generates a random sample from a given 1-D array.

Parameters

a [np.ndarray] A random sample is generated from its elements.

p [np.ndarray] The probabilities associated with each entry in a.

Returns

np.ndarray arrays with results and their shapes

deepmd.utils.random.**random**(*size=None*)

Return random floats in the half-open interval [0.0, 1.0).

Parameters

size Output shape.

Returns

np.ndarray Arrays with results and their shapes.

deepmd.utils.random.**seed**(*val: Optional[int] = None*)

Seed the generator.

Parameters

val [int] Seed.

deepmd.utils.random.**shuffle**(*x: numpy.ndarray*)

Modify a sequence in-place by shuffling its contents.

Parameters

x [np.ndarray] The array or list to be shuffled.

deepmd.utils.sess module

deepmd.utils.sess.**run_sess**(*sess: tensorflow.python.client.session.Session*, **args*, ***kwargs*)
Run session with erorrs caught.

Parameters

sess: tf.Session TensorFlow Session

Returns

the result of sess.run()

deepmd.utils.tabulate module

class deepmd.utils.tabulate.**DPTabulate**(*model_file: str*, *type_one_side: bool = False*, *exclude_types: List[List[int]] = []*, *activation_fn: Callable[[tensorflow.python.framework.ops.Tensor], tensorflow.python.framework.ops.Tensor] = <function tanh>*, *suffix: str = ''*)
Bases: object

Class for tabulation.

Compress a model, which including tabulating the embedding-net. The table is composed of fifth-order polynomial coefficients and is assembled from two sub-tables. The first table takes the stride(parameter) as it's uniform stride, while the second table takes 10 * stride as its uniform stride The range of the first table is automatically detected by deepmd-kit, while the second table ranges from the first table's upper boundary(upper) to the extrapolate(parameter) * upper.

Parameters

model_file The frozen model

type_one_side Try to build N_types tables. Otherwise, building N_types^2 tables

exclude_types [List[List[int]]] The excluded pairs of types which have no interaction with each other. For example, *[[0, 1]]* means no interaction between type 0 and type 1.

activation_function The activation function in the embedding net. Supported options are {"tanh","gelu"} in common.ACTIVATION_FN_DICT.

suffix [str, optional] The suffix of the scope

Methods

build(min_nbor_dist, extrapolate, stride0, ...)	Build the tables for model compression

build(*min_nbor_dist: float*, *extrapolate: float*, *stride0: float*, *stride1: float*) → Tuple[int, int]
Build the tables for model compression

Parameters

min_nbor_dist The nearest distance between neighbor atoms

extrapolate The scale of model extrapolation

stride0 The uniform stride of the first table

stride1 The uniform stride of the second table

Returns

lower The lower boundary of environment matrix

upper The upper boundary of environment matrix

deepmd.utils.type_embed module

class deepmd.utils.type_embed.**TypeEmbedNet**
Bases: object

Parameters

neuron [list[int]] Number of neurons in each hidden layers of the embedding net

resnet_dt Time-step *dt* in the resnet construction: y = x + dt * phi (Wx + b)

activation_function The activation function in the embedding net. Supported options are {0}

precision The precision of the embedding net parameters. Supported options are {1}

trainable If the weights of embedding net are trainable.

seed Random seed for initializing the network parameters.

uniform_seed Only for the purpose of backward compatibility, retrieves the old behavior of using the random seed

Methods

build(ntypes[, reuse, suffix])	Build the computational graph for the descriptor

build(*ntypes: int*, *reuse=None*, *suffix=''*)
Build the computational graph for the descriptor

Parameters

ntypes Number of atom types.

reuse The weights in the networks should be reused when get the variable.

suffix Name suffix to identify this descriptor

Returns

embedded_types The computational graph for embedded types

deepmd.utils.type_embed.**embed_atom_type**(*ntypes: int*, *natoms: tensorflow.python.framework.ops.Tensor*, *type_embedding: tensorflow.python.framework.ops.Tensor*)
Make the embedded type for the atoms in system. The atoms are assumed to be sorted according to the type, thus their types are described by a *tf.Tensor* natoms, see explanation below.

Parameters

ntypes: Number of types.

natoms: The number of atoms. This tensor has the length of Ntypes + 2 natoms[0]: number of local atoms natoms[1]: total number of atoms held by this processor natoms[i]: 2 <= i < Ntypes+2, number of type i atoms

type_embedding: The type embedding. It has the shape of [ntypes, embedding_dim]

Returns

atom_embedding The embedded type of each atom. It has the shape of [numb_atoms, embedding_dim]

deepmd.utils.weight_avg module

deepmd.utils.weight_avg.**weighted_average**(*errors: List[Dict[str, Tuple[float, float]]]*) → Dict

Compute wighted average of prediction errors for model.

Parameters

errors [List[Dict[str, Tuple[float, float]]]] List: the error of systems Dict: the error of quantities, name given by the key Tuple: (error, weight)

Returns

Dict weighted averages

14.1.2 Submodules

14.1.3 deepmd.calculator module

ASE calculator interface module.

class deepmd.calculator.**DP**(*model: Union[str, pathlib.Path]*, *label: str = 'DP'*, *type_dict: Optional[Dict[str, int]] = None*, ***kwargs*)

Bases: ase.calculators.calculator.Calculator

Implementation of ASE deepmd calculator.

Implemented propertie are *energy*, *forces* and *stress*

Parameters

model [Union[str, Path]] path to the model

label [str, optional] calculator label, by default "DP"

type_dict [Dict[str, int], optional] mapping of element types and their numbers, best left None and the calculator will infer this information from model, by default None

Examples

Compute potential energy

```
>>> from ase import Atoms
>>> from deepmd.calculator import DP
>>> water = Atoms('H2O',
>>>               positions=[(0.7601, 1.9270, 1),
>>>                          (1.9575, 1, 1),
>>>                          (1., 1., 1.)],
>>>               cell=[100, 100, 100],
>>>               calculator=DP(model="frozen_model.pb"))
>>> print(water.get_potential_energy())
>>> print(water.get_forces())
```

Run BFGS structure optimization

```
>>> from ase.optimize import BFGS
>>> dyn = BFGS(water)
>>> dyn.run(fmax=1e-6)
>>> print(water.get_positions())
```

Attributes

directory

label

Methods

band_structure()	Create band-structure object for plotting.
calculate([atoms, properties, system_changes])	Run calculation with deepmd model.
calculate_numerical_forces(atoms[, d])	Calculate numerical forces using finite difference.
calculate_numerical_stress(atoms[, d, voigt])	Calculate numerical stress using finite difference.
calculate_properties(atoms, properties)	This method is experimental; currently for internal use.
check_state(atoms[, tol])	Check for any system changes since last calculation.
get_magnetic_moments([atoms])	Calculate magnetic moments projected onto atoms.
get_property(name[, atoms, allow_calculation])	Get the named property.
get_stresses([atoms])	the calculator should return intensive stresses, i.e., such that stresses.sum(axis=0) == stress
read(label)	Read atoms, parameters and calculated properties from output file.
reset()	Clear all information from old calculation.
set(**kwargs)	Set parameters like set(key1=value1, key2=value2, ...).
set_label(label)	Set label and convert label to directory and prefix.

calculation_required	
export_properties	
get_atoms	
get_charges	
get_default_parameters	
get_dipole_moment	
get_forces	
get_magnetic_moment	
get_potential_energies	
get_potential_energy	
get_stress	
read_atoms	
todict	

calculate(*atoms: Optional[Atoms] = None*, *properties: List[str] = ['energy', 'forces', 'virial']*, *system_changes: List[str] = ['positions', 'numbers', 'cell', 'pbc', 'initial_charges', 'initial_magmoms']*)

Run calculation with deepmd model.

Parameters

atoms [Optional[Atoms], optional] atoms object to run the calculation on, by default None

properties [List[str], optional] unused, only for function signature compatibility, by default ["energy", "forces", "stress"]

system_changes [List[str], optional] unused, only for function signature compatibility, by default all_changes

implemented_properties: List[str] = ['energy', 'forces', 'virial', 'stress']
Properties calculator can handle (energy, forces, ...)

name = 'DP'

14.1.4 deepmd.common module

Collection of functions and classes used throughout the whole package.

class deepmd.common.**ClassArg**
Bases: object

Class that take care of input json/yaml parsing.

The rules for parsing are defined by the *add* method, than *parse* is called to process the supplied dict

Attributes

arg_dict: Dict[str, Any] dictionary containing parsing rules

alias_map: Dict[str, Any] dictionary with keyword aliases

Methods

add(key, types_[, alias, default, must])	Add key to be parsed.
get_dict()	Get dictionary built from rules defined by add method.
parse(jdata)	Parse input dictionary, use the rules defined by add method.

add(*key: str*, *types_: Union[type, List[type]]*, *alias: Optional[Union[str, List[str]]] = None*, *default: Optional[Any] = None*, *must: bool = False*) → *deepmd.common.ClassArg*
Add key to be parsed.

Parameters

key [str] key name

types_ [Union[type, List[type]]] list of allowed key types

alias [Optional[Union[str, List[str]]], optional] alias for the key, by default None

default [Any, optional] default value for the key, by default None

must [bool, optional] if the key is mandatory, by default False

Returns

ClassArg instance with added key

get_dict() → Dict[str, Any]
Get dictionary built from rules defined by add method.

Returns

Dict[str, Any] settings dictionary with default values

parse(*jdata: Dict[str, Any]*) → Dict[str, Any]
Parse input dictionary, use the rules defined by add method.

Parameters

jdata [Dict[str, Any]] loaded json/yaml data

Returns

Dict[str, Any] parsed dictionary

deepmd.common.**add_data_requirement**(*key: str*, *ndof: int*, *atomic: bool = False*, *must: bool = False*, *high_prec: bool = False*, *type_sel: Optional[bool] = None*, *repeat: int = 1*)
Specify data requirements for training.

Parameters

key [str] type of data stored in corresponding **.npy* file e.g. *forces* or *energy*

ndof [int] number of the degrees of freedom, this is tied to *atomic* parameter e.g. forces have *atomic=True* and *ndof=3*

atomic [bool, optional] specifies whwther the *ndof* keyworrd applies to per atom quantity or not, by default False

must [bool, optional] specifi if the **.npy* data file must exist, by default False

high_prec [bool, optional] if tru load data to *np.float64* else *np.float32*, by default False

type_sel [bool, optional] select only certain type of atoms, by default None

repeat [int, optional] if specify repaeat data *repeat* times, by default 1

deepmd.common.**docstring_parameter**(**sub: Tuple[str, ...]*)
Add parameters to object docstring.

Parameters

sub: Tuple[str, ...] list of strings that will be inserted into prepared locations in docstring.

deepmd.common.**expand_sys_str**(*root_dir: Union[str, pathlib.Path]*) → List[str]
Recursively iterate over directories taking those that contain *type.raw* file.

Parameters

root_dir [Union[str, Path]] starting directory

Returns

List[str] list of string pointing to system directories

deepmd.common.**gelu**(*x: tensorflow.python.framework.ops.Tensor*) → tensorflow.python.framework.ops.Tensor
Gaussian Error Linear Unit.

This is a smoother version of the RELU.

Parameters

x [tf.Tensor] float Tensor to perform activation

Returns

x with the GELU activation applied

References

Original paper https://arxiv.org/abs/1606.08415

deepmd.common.**get_activation_func**(*activation_fn: _ACTIVATION*) → Callable[[tensorflow.python.framework.ops.Tensor], tensorflow.python.framework.ops.Tensor]

Get activation function callable based on string name.

Parameters

activation_fn [_ACTIVATION] one of the defined activation functions

Returns

Callable[[tf.Tensor], tf.Tensor] correspondingg TF callable

Raises

RuntimeError if unknown activation function is specified

deepmd.common.**get_np_precision**(*precision: _PRECISION*) → numpy.dtype

Get numpy precision constant from string.

Parameters

precision [_PRECISION] string name of numpy constant or default

Returns

np.dtype numpy presicion constant

Raises

RuntimeError if string is invalid

deepmd.common.**get_precision**(*precision: _PRECISION*) → Any

Convert str to TF DType constant.

Parameters

precision [_PRECISION] one of the allowed precisions

Returns

tf.python.framework.dtypes.DType appropriate TF constant

Raises

RuntimeError if supplied precision string does not have acorresponding TF constant

deepmd.common.**j_loader**(*filename: Union[str, pathlib.Path]*) → Dict[str, Any]

Load yaml or json settings file.

Parameters

filename [Union[str, Path]] path to file

Returns

Dict[str, Any] loaded dictionary

Raises

TypeError if the supplied file is of unsupported type

deepmd.common.**j_must_have**(*jdata: Dict[str, _DICT_VAL]*, *key: str*, *deprecated_key: List[str] = []*) → _DICT_VAL

Assert that supplied dictionary conaines specified key.

Returns

_DICT_VAL value that was store unde supplied key

Raises

RuntimeError if the key is not present

deepmd.common.**make_default_mesh**(*test_box: numpy.ndarray*, *cell_size: float = 3.0*) → numpy.ndarray

Get number of cells of size=`cell_size` fit into average box.

Parameters

test_box [np.ndarray] numpy array with cells of shape Nx9

cell_size [float, optional] length of one cell, by default 3.0

Returns

np.ndarray mesh for supplied boxes, how many cells fit in each direction

deepmd.common.**select_idx_map**(*atom_types: numpy.ndarray*, *select_types: numpy.ndarray*) → numpy.ndarray

Build map of indices for element supplied element types from all atoms list.

Parameters

atom_types [np.ndarray] array specifing type for each atoms as integer

select_types [np.ndarray] types of atoms you want to find indices for

Returns

np.ndarray indices of types of atoms defined by *select_types* in *atom_types* array

Warning: *select_types* array will be sorted before finding indices in *atom_types*

14.1.5 deepmd.env module

Module that sets tensorflow working environment and exports inportant constants.

deepmd.env.**GLOBAL_ENER_FLOAT_PRECISION**

alias of numpy.float64

deepmd.env.**GLOBAL_NP_FLOAT_PRECISION**

alias of numpy.float64

deepmd.env.**global_cvt_2_ener_float**(*xx: tensorflow.python.framework.ops.Tensor*) → tensorflow.python.framework.ops.Tensor

Cast tensor to globally set energy precision.

Parameters

xx [tf.Tensor] input tensor

Returns

tf.Tensor output tensor cast to *GLOBAL_ENER_FLOAT_PRECISION*

deepmd.env.**global_cvt_2_tf_float**(*xx: tensorflow.python.framework.ops.Tensor*) → tensorflow.python.framework.ops.Tensor

Cast tensor to globally set TF precision.

Parameters

xx [tf.Tensor] input tensor

Returns

tf.Tensor output tensor cast to *GLOBAL_TF_FLOAT_PRECISION*

deepmd.env.**reset_default_tf_session_config**(*cpu_only: bool*)

Limit tensorflow session to CPU or not.

Parameters

cpu_only [bool] If enabled, no GPU device is visible to the TensorFlow Session.

CHAPTER

FIFTEEN

C++ API

15.1 Class Hierarchy

- *Namespace deepmd*
  - *Struct NeighborListData*
  - *Struct tf_exception*
  - *Template Class AtomMap*
  - *Class DeepPot*
  - *Class DeepPotModelDevi*
  - *Class DeepTensor*
  - *Class DipoleChargeModifier*
- *Struct InputNlist*
- *Struct DeviceFunctor*

15.2 File Hierarchy

- **dir_source**
  - **dir_source_api_cc**
    - **dir_source_api_cc_include**
      - file_source_api_cc_include_AtomMap.h
      - file_source_api_cc_include_common.h
      - file_source_api_cc_include_custom_op.h
      - file_source_api_cc_include_DataModifier.h
      - file_source_api_cc_include_DeepPot.h
      - file_source_api_cc_include_DeepTensor.h

15.3 Full API

15.3.1 Namespaces

Namespace deepmd

Contents

Classes

Functions

- *Template Function deepmd::session_get_vector*
- *Function deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, const VALUETYPE&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap<VALUETYPE>&, const std::string)*
- *Function deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, InputNlist&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap<VALUETYPE>&, const int, const int, const std::string)*

Typedefs

- *Typedef deepmd::ENERGYTYPE*
- *Typedef deepmd::STRINGTYPE*
- *Typedef deepmd::VALUETYPE*

Namespace std

Namespace tensorflow

15.3.2 Classes and Structs

Struct InputNlist

- Defined in file_source_api_cc_include_common.h

Struct Documentation

struct **deepmd::InputNlist**
Construct *InputNlist* with the input LAMMPS nbor list info.

Public Functions

inline **InputNlist**()

inline **InputNlist**(int inum_, int *ilist_, int *numneigh_, int **firstneigh_)

inline **~InputNlist**()

Public Members

int **inum**
Number of core region atoms.

int ***ilist**
Array stores the core region atom's index.

int ***numneigh**
Array stores the core region atom's neighbor atom number.

int ****firstneigh**
Array stores the core region atom's neighbor index.

Struct NeighborListData

- Defined in file_source_api_cc_include_common.h

Struct Documentation

struct `deepmd::NeighborListData`

Public Functions

void **copy_from_nlist**(const *InputNlist* &inlist)

void **shuffle**(const std::vector<int> &fwd_map)

void **shuffle**(const deepmd::*AtomMap*<*VALUETYPE*> &map)

void **shuffle_exclude_empty**(const std::vector<int> &fwd_map)

void **make_inlist**(*InputNlist* &inlist)

Public Members

std::vector<int> **ilist**
Array stores the core region atom's index.

std::vector<std::vector<int>> **jlist**
Array stores the core region atom's neighbor index.

std::vector<int> **numneigh**
Array stores the number of neighbors of core region atoms.

std::vector<int*> **firstneigh**
Array stores the the location of the first neighbor of core region atoms.

Struct tf_exception

- Defined in file_source_api_cc_include_common.h

Inheritance Relationships

Base Type

- `public std::exception`

Struct Documentation

struct **tf_exception** : public std::exception

Struct DeviceFunctor

- Defined in file_source_api_cc_include_custom_op.h

Struct Documentation

struct **DeviceFunctor**

Public Functions

inline void **operator()**(std::string &device, const *CPUDevice* &d)

Template Class AtomMap

- Defined in file_source_api_cc_include_AtomMap.h

Class Documentation

template<typename **VALUETYPE**>

class deepmd::**AtomMap**

Public Functions

AtomMap()

AtomMap(const std::vector<int>::const_iterator in_begin, const std::vector<int>::const_iterator in_end)

void **forward**(typename std::vector<*VALUETYPE*>::iterator out, const typename std::vector<*VALUETYPE*>::const_iterator in, const int stride = 1) const

void **backward**(typename std::vector<*VALUETYPE*>::iterator out, const typename std::vector<*VALUETYPE*>::const_iterator in, const int stride = 1) const

inline const std::vector<int> &**get_type**() const

inline const std::vector<int> &**get_fwd_map**() const

inline const std::vector<int> &**get_bkw_map**() const

Class DeepPot

- Defined in file_source_api_cc_include_DeepPot.h

Class Documentation

class deepmd::**DeepPot**
Deep Potential.

Public Functions

DeepPot()
DP constructor without initialization.

~DeepPot()

DeepPot(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")
DP constructor with initialization.

Parameters

- **model** – **[in]** The name of the frozen model file.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &file_content = "")
Initialize the DP.

Parameters

- **model** – **[in]** The name of the frozen model file.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **print_summary**(const std::string &pre) const
Print the DP summary to the screen.

Parameters **pre** – **[in]** The prefix to each line.

void **compute**(*ENERGYTYPE* &ener, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())
Evaluate the energy, force and virial by using this DP.

Parameters

- **ener** – **[out]** The system energy.
- **force** – **[out]** The force on each atom.
- **virial** – **[out]** The virial.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

void **compute**(*ENERGYTYPE* &ener, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &inlist, const int &ago, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())
Evaluate the energy, force and virial by using this DP.

Parameters

- **ener** – **[out]** The system energy.
- **force** – **[out]** The force on each atom.
- **virial** – **[out]** The virial.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **nghost** – **[in]** The number of ghost atoms.

- **inlist** – **[in]** The input neighbour list.
- **ago** – **[in]** Update the internal neighbour list if ago is 0.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

void **compute**(*ENERGYTYPE* &ener, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, std::vector<*VALUETYPE*> &atom_energy, std::vector<*VALUETYPE*> &atom_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP.

Parameters

- **ener** – **[out]** The system energy.
- **force** – **[out]** The force on each atom.
- **virial** – **[out]** The virial.
- **atom_energy** – **[out]** The atomic energy.
- **atom_virial** – **[out]** The atomic virial.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

void **compute**(*ENERGYTYPE* &ener, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, std::vector<*VALUETYPE*> &atom_energy, std::vector<*VALUETYPE*> &atom_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &lmp_list, const int &ago, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())

Evaluate the energy, force, virial, atomic energy, and atomic virial by using this DP.

Parameters

- **ener** – **[out]** The system energy.
- **force** – **[out]** The force on each atom.
- **virial** – **[out]** The virial.
- **atom_energy** – **[out]** The atomic energy.

- **atom_virial** – **[out]** The atomic virial.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **nghost** – **[in]** The number of ghost atoms.
- **lmp_list** – **[in]** The input neighbour list.
- **ago** – **[in]** Update the internal neighbour list if ago is 0.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

inline *VALUETYPE* **cutoff**() const
Get the cutoff radius.

Returns The cutoff radius.

inline int **numb_types**() const
Get the number of types.

Returns The number of types.

inline int **dim_fparam**() const
Get the dimension of the frame parameter.

Returns The dimension of the frame parameter.

inline int **dim_aparam**() const
Get the dimension of the atomic parameter.

Returns The dimension of the atomic parameter.

void **get_type_map**(std::string &type_map)
Get the type map (element name of the atom types) of this model.

Parameters **type_map** – **[out]** The type map of this model.

Class DeepPotModelDevi

- Defined in file_source_api_cc_include_DeepPot.h

Class Documentation

class deepmd::**DeepPotModelDevi**

Public Functions

DeepPotModelDevi()
DP model deviation constructor without initialization.

~DeepPotModelDevi()

DeepPotModelDevi(const std::vector<std::string> &models, const int &gpu_rank = 0, const std::vector<std::string> &file_contents = std::vector<std::string>())
DP model deviation constructor with initialization.

Parameters

- **model** – **[in]** The names of the frozen model files.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The contents of the model files. If it is not empty, DP will read from the strings instead of the files.

void **init**(const std::vector<std::string> &models, const int &gpu_rank = 0, const std::vector<std::string> &file_contents = std::vector<std::string>())
Initialize the DP model deviation contrcutor.

Parameters

- **model** – **[in]** The names of the frozen model files.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The contents of the model files. If it is not empty, DP will read from the strings instead of the files.

void **compute**(std::vector<*ENERGYTYPE*> &all_ener, std::vector<std::vector<*VALUETYPE*>> &all_force, std::vector<std::vector<*VALUETYPE*>> &all_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &lmp_list, const int &ago, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())
Evaluate the energy, force and virial by using these DP models.

Parameters

- **all_ener** – **[out]** The system energies of all models.
- **all_force** – **[out]** The forces on each atom of all models.
- **all_virial** – **[out]** The virials of all models.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **nghost** – **[in]** The number of ghost atoms.

- **lmp_list** – **[in]** The input neighbour list.
- **ago** – **[in]** Update the internal neighbour list if ago is 0.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

void **compute**(std::vector<*ENERGYTYPE*> &all_ener, std::vector<std::vector<*VALUETYPE*>> &all_force, std::vector<std::vector<*VALUETYPE*>> &all_virial, std::vector<std::vector<*VALUETYPE*>> &all_atom_energy, std::vector<std::vector<*VALUETYPE*>> &all_atom_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &lmp_list, const int &ago, const std::vector<*VALUETYPE*> &fparam = std::vector<*VALUETYPE*>(), const std::vector<*VALUETYPE*> &aparam = std::vector<*VALUETYPE*>())

Evaluate the energy, force, virial, atomic energy, and atomic virial by using these DP models.

Parameters

- **all_ener** – **[out]** The system energies of all models.
- **all_force** – **[out]** The forces on each atom of all models.
- **all_virial** – **[out]** The virials of all models.
- **all_atom_energy** – **[out]** The atomic energies of all models.
- **all_atom_virial** – **[out]** The atomic virials of all models.
- **coord** – **[in]** The coordinates of atoms. The array should be of size nframes x natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size nframes x 9.
- **nghost** – **[in]** The number of ghost atoms.
- **lmp_list** – **[in]** The input neighbour list.
- **ago** – **[in]** Update the internal neighbour list if ago is 0.
- **fparam** – **[in]** The frame parameter. The array can be of size : nframes x dim_fparam. dim_fparam. Then all frames are assumed to be provided with the same fparam.
- **aparam** – **[in]** The atomic parameter The array can be of size : nframes x natoms x dim_aparam. natoms x dim_aparam. Then all frames are assumed to be provided with the same aparam. dim_aparam. Then all frames and atoms are provided with the same aparam.

inline *VALUETYPE* **cutoff**() const

Get the cutoff radius.

Returns The cutoff radius.

inline int **numb_types**() const

Get the number of types.

Returns The number of types.

inline int **dim_fparam**() const
Get the dimension of the frame parameter.

Returns The dimension of the frame parameter.

inline int **dim_aparam**() const
Get the dimension of the atomic parameter.

Returns The dimension of the atomic parameter.

void **compute_avg**(*ENERGYTYPE* &dener, const std::vector<*ENERGYTYPE*> &all_energy)
Compute the average energy.

Parameters

- **dener** – **[out]** The average energy.
- **all_energy** – **[in]** The energies of all models.

void **compute_avg**(*VALUETYPE* &dener, const std::vector<*VALUETYPE*> &all_energy)
Compute the average energy.

Parameters

- **dener** – **[out]** The average energy.
- **all_energy** – **[in]** The energies of all models.

void **compute_avg**(std::vector<*VALUETYPE*> &avg, const std::vector<std::vector<*VALUETYPE*>> &xx)
Compute the average of vectors.

Parameters

- **avg** – **[out]** The average of vectors.
- **xx** – **[in]** The vectors of all models.

void **compute_std**(*std*::vector<*VALUETYPE*> &std, const *std*::vector<*VALUETYPE*> &avg, const *std*::vector<*std*::vector<*VALUETYPE*>> &xx, const int &stride)
Compute the standard deviation of vectors.

Parameters

- **std** – **[out]** The standard deviation of vectors.
- **avg** – **[in]** The average of vectors.
- **xx** – **[in]** The vectors of all models.
- **stride** – **[in]** The stride to compute the deviation.

void **compute_relative_std**(*std*::vector<*VALUETYPE*> &std, const *std*::vector<*VALUETYPE*> &avg, const *VALUETYPE* eps, const int &stride)
Compute the relative standard deviation of vectors.

Parameters

- **std** – **[out]** The standard deviation of vectors.
- **avg** – **[in]** The average of vectors.
- **eps** – **[in]** The level parameter for computing the deviation.
- **stride** – **[in]** The stride to compute the deviation.

void **compute_std_e**(*std*::vector<*VALUETYPE*> &std, const *std*::vector<*VALUETYPE*> &avg, const *std*::vector<*std*::vector<*VALUETYPE*>> &xx)
Compute the standard deviation of atomic energies.

Parameters

- **std** – **[out]** The standard deviation of atomic energies.
- **avg** – **[in]** The average of atomic energies.
- **xx** – **[in]** The vectors of all atomic energies.

void **compute_std_f**(*std*::vector<*VALUETYPE*> &std, const *std*::vector<*VALUETYPE*> &avg, const *std*::vector<*std*::vector<*VALUETYPE*>> &xx)

Compute the standard deviation of forces.

Parameters

- **std** – **[out]** The standard deviation of forces.
- **avg** – **[in]** The average of forces.
- **xx** – **[in]** The vectors of all forces.

void **compute_relative_std_f**(*std*::vector<*VALUETYPE*> &std, const *std*::vector<*VALUETYPE*> &avg, const *VALUETYPE* eps)

Compute the relative standard deviation of forces.

Parameters

- **std** – **[out]** The relative standard deviation of forces.
- **avg** – **[in]** The relative average of forces.
- **eps** – **[in]** The level parameter for computing the deviation.

Class DeepTensor

- Defined in file_source_api_cc_include_DeepTensor.h

Class Documentation

class deepmd::**DeepTensor**

Deep Tensor.

Public Functions

DeepTensor()

Deep Tensor constructor without initialization.

DeepTensor(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

Deep Tensor constructor with initialization..

Parameters

- **model** – **[in]** The name of the frozen model file.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

Initialize the Deep Tensor.

Parameters

- **model** – **[in]** The name of the frozen model file.
- **gpu_rank** – **[in]** The GPU rank. Default is 0.
- **file_content** – **[in]** The content of the model file. If it is not empty, DP will read from the string instead of the file.

void **print_summary**(const std::string &pre) const
Print the DP summary to the screen.

Parameters **pre** – **[in]** The prefix to each line.

void **compute**(std::vector<*VALUETYPE*> &value, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box)
Evaluate the value by using this model.

Parameters

- **value** – **[out]** The value to evalute, usually would be the atomic tensor.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.

void **compute**(std::vector<*VALUETYPE*> &value, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &inlist)
Evaluate the value by using this model.

Parameters

- **value** – **[out]** The value to evalute, usually would be the atomic tensor.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.
- **nghost** – **[in]** The number of ghost atoms.
- **inlist** – **[in]** The input neighbour list.

void **compute**(std::vector<*VALUETYPE*> &global_tensor, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box)
Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – **[out]** The global tensor to evalute.
- **force** – **[out]** The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – **[out]** The component-wise virial of the global tensor, size odim x 9.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.

void **compute**(std::vector<*VALUETYPE*> &global_tensor, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &inlist)

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – **[out]** The global tensor to evalute.
- **force** – **[out]** The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – **[out]** The component-wise virial of the global tensor, size odim x 9.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.
- **nghost** – **[in]** The number of ghost atoms.
- **inlist** – **[in]** The input neighbour list.

void **compute**(std::vector<*VALUETYPE*> &global_tensor, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, std::vector<*VALUETYPE*> &atom_tensor, std::vector<*VALUETYPE*> &atom_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box)

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – **[out]** The global tensor to evalute.
- **force** – **[out]** The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – **[out]** The component-wise virial of the global tensor, size odim x 9.
- **atom_tensor** – **[out]** The atomic tensor value of the model, size natoms x odim.
- **atom_virial** – **[out]** The component-wise atomic virial of the global tensor, size odim x natoms x 9.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.

void **compute**(std::vector<*VALUETYPE*> &global_tensor, std::vector<*VALUETYPE*> &force, std::vector<*VALUETYPE*> &virial, std::vector<*VALUETYPE*> &atom_tensor, std::vector<*VALUETYPE*> &atom_virial, const std::vector<*VALUETYPE*> &coord, const std::vector<int> &atype, const std::vector<*VALUETYPE*> &box, const int nghost, const *InputNlist* &inlist)

Evaluate the global tensor and component-wise force and virial.

Parameters

- **global_tensor** – **[out]** The global tensor to evalute.
- **force** – **[out]** The component-wise force of the global tensor, size odim x natoms x 3.
- **virial** – **[out]** The component-wise virial of the global tensor, size odim x 9.

- **atom_tensor** – **[out]** The atomic tensor value of the model, size natoms x odim.
- **atom_virial** – **[out]** The component-wise atomic virial of the global tensor, size odim x natoms x 9.
- **coord** – **[in]** The coordinates of atoms. The array should be of size natoms x 3.
- **atype** – **[in]** The atom types. The list should contain natoms ints.
- **box** – **[in]** The cell of the region. The array should be of size 9.
- **nghost** – **[in]** The number of ghost atoms.
- **inlist** – **[in]** The input neighbour list.

inline *VALUETYPE* **cutoff**() const
Get the cutoff radius.

Returns The cutoff radius.

inline int **numb_types**() const
Get the number of types.

Returns The number of types.

inline int **output_dim**() const
Get the output dimension.

Returns The output dimension.

inline const std::vector<int> &**sel_types**() const

Class DipoleChargeModifier

- Defined in file_source_api_cc_include_DataModifier.h

Class Documentation

class deepmd::**DipoleChargeModifier**

Public Functions

DipoleChargeModifier()

DipoleChargeModifier(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

inline **~DipoleChargeModifier**()

void **init**(const std::string &model, const int &gpu_rank = 0, const std::string &name_scope = "")

void **print_summary**(const std::string &pre) const

void **compute**(std::vector<*VALUETYPE*> &dfcorr_, std::vector<*VALUETYPE*> &dvcorr_, const std::vector<*VALUETYPE*> &dcoord_, const std::vector<int> &datype_, const std::vector<*VALUETYPE*> &dbox, const std::vector<std::pair<int, int>> &pairs, const std::vector<*VALUETYPE*> &delef_, const int nghost, const *InputNlist* &lmp_list)

inline *VALUETYPE* **cutoff**() const

inline int **numb_types**() const

inline std::vector<int> **sel_types**() const

15.3.3 Functions

Function deepmd::check_status

- Defined in file_source_api_cc_include_common.h

Function Documentation

void deepmd::**check_status**(const tensorflow::Status &status)
Check TensorFlow status. Exit if not OK.

Parameters **status** – **[in]** TensorFlow status.

Function deepmd::get_env_nthreads

- Defined in file_source_api_cc_include_common.h

Function Documentation

void deepmd::**get_env_nthreads**(int &num_intra_nthreads, int &num_inter_nthreads)
Get the number of threads from the environment variable.

Parameters

- **num_intra_nthreads** – **[out]** The number of intra threads. Read from TF_INTRA_OP_PARALLELISM_THREADS.
- **num_inter_nthreads** – **[out]** The number of inter threads. Read from TF_INTER_OP_PARALLELISM_THREADS.

Function deepmd::model_compatable

- Defined in file_source_api_cc_include_common.h

Function Documentation

bool deepmd::**model_compatable**(std::string &model_version)
Check if the model version is supported.

Parameters **model_version** – **[in]** The model version.

Returns Whether the model is supported (true or false).

Function deepmd::name_prefix

- Defined in file_source_api_cc_include_common.h

Function Documentation

std::string deepmd::**name_prefix**(const std::string &name_scope)

Function deepmd::select_by_type

- Defined in file_source_api_cc_include_common.h

Function Documentation

void deepmd::**select_by_type**(std::vector<int> &fwd_map, std::vector<int> &bkw_map, int &nghost_real, const std::vector<*VALUETYPE*> &dcoord_, const std::vector<int> &datype_, const int &nghost, const std::vector<int> &sel_type_)

Template Function deepmd::select_map(std::vector<VT>&, const std::vector<VT>&, const std::vector<int>&, const int&)

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
void deepmd::**select_map**(std::vector<*VT*> &out, const std::vector<*VT*> &in, const std::vector<int> &fwd_map, const int &stride)

Template Function deepmd::select_map(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&)

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
void `deepmd::select_map`(typename std::vector<*VT*>::iterator out, const typename std::vector<*VT*>::const_iterator in, const std::vector<int> &fwd_map, const int &stride)

Template Function deepmd::select_map_inv(std::vector<VT>&, const std::vector<VT>&, const std::vector<int>&, const int&)

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
void `deepmd::select_map_inv`(std::vector<*VT*> &out, const std::vector<*VT*> &in, const std::vector<int> &fwd_map, const int &stride)

Template Function deepmd::select_map_inv(typename std::vector<VT>::iterator, const typename std::vector<VT>::const_iterator, const std::vector<int>&, const int&)

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
void `deepmd::select_map_inv`(typename std::vector<*VT*>::iterator out, const typename std::vector<*VT*>::const_iterator in, const std::vector<int> &fwd_map, const int &stride)

Function deepmd::select_real_atoms

- Defined in file_source_api_cc_include_common.h

Function Documentation

void deepmd::**select_real_atoms**(std::vector<int> &fwd_map, std::vector<int> &bkw_map, int &nghost_real, const std::vector<*VALUETYPE*> &dcoord_, const std::vector<int> &datype_, const int &nghost, const int &ntypes)

Template Function deepmd::session_get_scalar

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
VT deepmd::**session_get_scalar**(tensorflow::Session *session, const std::string name, const std::string scope = "")

Template Function deepmd::session_get_vector

- Defined in file_source_api_cc_include_common.h

Function Documentation

template<typename **VT**>
void deepmd::**session_get_vector**(std::vector<*VT*> &o_vec, tensorflow::Session *session, const std::string name_, const std::string scope = "")

Function deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, const VALUETYPE&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap<VALUETYPE>&, const std::string)

- Defined in file_source_api_cc_include_common.h

Function Documentation

int deepmd::**session_input_tensors**(std::vector<std::pair<std::string, tensorflow::Tensor>> &input_tensors, const std::vector<*VALUETYPE*> &dcoord_, const int &ntypes, const std::vector<int> &datype_, const std::vector<*VALUETYPE*> &dbox, const *VALUETYPE* &cell_size, const std::vector<*VALUETYPE*> &fparam_, const std::vector<*VALUETYPE*> &aparam_, const deepmd::*AtomMap*<*VALUETYPE*> &atommap, const std::string scope = "")

Function deepmd::session_input_tensors(std::vector<std::pair<std::string, tensorflow::Tensor>>&, const std::vector<VALUETYPE>&, const int&, const std::vector<int>&, const std::vector<VALUETYPE>&, InputNlist&, const std::vector<VALUETYPE>&, const std::vector<VALUETYPE>&, const deepmd::AtomMap<VALUETYPE>&, const int, const int, const std::string)

- Defined in file_source_api_cc_include_common.h

Function Documentation

int deepmd::**session_input_tensors**(std::vector<std::pair<std::string, tensorflow::Tensor>> &input_tensors, const std::vector<*VALUETYPE*> &dcoord_, const int &ntypes, const std::vector<int> &datype_, const std::vector<*VALUETYPE*> &dbox, *InputNlist* &dlist, const std::vector<*VALUETYPE*> &fparam_, const std::vector<*VALUETYPE*> &aparam_, const deepmd::*AtomMap*<*VALUETYPE*> &atommap, const int nghost, const int ago, const std::string scope = "")

15.3.4 Typedefs

Typedef CPUDevice

- Defined in file_source_api_cc_include_custom_op.h

Typedef Documentation

using **CPUDevice** = Eigen::ThreadPoolDevice

Typedef deepmd::ENERGYTYPE

- Defined in file_source_api_cc_include_common.h

Typedef Documentation

typedef double deepmd::**ENERGYTYPE**

Typedef deepmd::STRINGTYPE

- Defined in file_source_api_cc_include_common.h

Typedef Documentation

typedef std::string deepmd::**STRINGTYPE**

Typedef deepmd::VALUETYPE

- Defined in file_source_api_cc_include_common.h

Typedef Documentation

typedef float deepmd::**VALUETYPE**

Typedef GPUDevice

- Defined in file_source_api_cc_include_custom_op.h

Typedef Documentation

using **GPUDevice** = Eigen::GpuDevice

CHAPTER

SIXTEEN

LICENSE

The project DeePMD-kit is licensed under GNU LGPLv3.0.

CHAPTER

SEVENTEEN

AUTHORS AND CREDITS

17.1 Package Contributors

- AnguseZhang
- baohan
- bwang-ecnu
- denghuilu
- frankhan91
- GeiduanLiu
- gzq942560379
- Han Wang
- haidi-ustc
- hlyang1992
- hsulab
- iProzd
- Jiequn Han
- JiabinYang
- jxxiaoshaoye
- Linfeng Zhang
- marian-code
- njzjz
- Nick Lin
- pkulzy
- Shaochen Shi
- tuoping
- wsyxbcl
- Xia, Yu
- Ye Ding
- Yingze Wang

- Yixiao Chen
- YWolfeee
- Zhanlue Yang
- zhouwei25
- ZiyaoLi

17.2 Other Credits

- Zhang ZiXuan for designing the Deepmodeling logo.
- Everyone on the *Deepmodeling mailing list* for contributing to many discussions and decisions!

(If you have contributed to the `deepmd-kit` core package and your name is missing, please send an email to the contributors, or open a pull request in the deepmd-kit repository)

- genindex
- modindex
- search

BIBLIOGRAPHY

[1] Linfeng Zhang, Jiequn Han, Han Wang, Wissam A. Saidi, Roberto Car, and E. Weinan. 2018. End-to-end symmetry preserving inter-atomic potential energy model for finite and extended systems. In Proceedings of the 32nd International Conference on Neural Information Processing Systems (NIPS'18). Curran Associates Inc., Red Hook, NY, USA, 4441–4451.

[1] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Identitymappings in deep residual networks. InComputer Vision – ECCV 2016,pages 630–645. Springer International Publishing, 2016.

PYTHON MODULE INDEX

d

INDEX

D

E

F

G

I

J

L

M

N

O

P

R

S

T

U

V

W