TensorAlloy

TensorAlloy is a TensorFlow based machine learning framework for alloys.

1. Requirements

- Python>=3.7.0
- TensorFlow==1.14.0
- scikit-learn
- scipy
- numpy
- ase>=3.18.0
- matplotlib>=3.0.0
- atsim.potentials>=0.2.1
- toml==0.10.0
- joblib
- pandas

`ase`, `toml` and `joblib` can be installed with `pip` easily. Other packages may be installed with Anaconda3. However, the performance of conda-provided tensorflow may not be that good. Natively compiled TensorFlow, with all CPU features (SSE, AVX, etc.) enabled, is highly recommended.

2. Installation

This package can be installed with `pip` or `python`:

```
cd tensoralloy
pip install .
```

or

```
cd tensoralloy
python setup.py install
```

A command-line interface `tensoralloy` will also be installed.

3. Training

3.1 Usage

TOML is the configuration file format used by TensorAlloy. All the necessary keys are included in the two examples. Default keys and values can be found in default.toml.

To run a training experiment, the easiest way is using the command-line program `tensoralloy`. Here are some key commands:

- `tensoralloy build database [extxyz]`: build a database from an `extxyz` file.
- `tensoralloy run [input.toml]`: run an experiment from a `toml` input file.
- `tensoralloy print [logfile]`: read the evaluation results from a logfile and print these results to a csv file.
- `tensoralloy --help`: print the help messages.

3.2 Output

After the training, a binary `pb` file (the trained model) will be exported to the `model_dir` specified in the input toml file. This exported `pb` file can be used by the ASE-style `TensorAlloyCalculator`.

For pair styles `eam/alloy`, `eam/fs` and `eam/adp`, the corresponding LAMMPS potential file will also be exported.

We provide three examples as well as their optimized potentials:

- Ni: `eam/alloy`
- Mo: `eam/adp`
- MoNi: `eam/adp`

The corresponding symmetry function based atomistic neural network potentials for these systems can be found on our previous work

4. Prediction

The ASE-style calculator, `TensorAlloyCalculator`, shall be used to make predicitons.

```
#!coding=utf-8
""" Simple usage. """
from tensoralloy.calculator import TensorAlloyCalculator
from ase.build import bulk
from ase.units import GPa

calc = TensorAlloyCalculator("examples/Ni/Ni.pb")
atoms = bulk("Ni", cubic=True)
atoms.calc = calc
print(atoms.get_total_energy())
print(atoms.get_forces())
print(atoms.get_stress() / GPa)
```

5. Input

In this section we will introduce the options and values of the input file. Options marked **[required]** must be set manually in the input file.

TensorAlloy uses TOML files as inputs. The following section demonstrates how to write a toml file.

TOML

In the toml file, there are two ways to set a nested key-value pair `A.B.C="x"`:

```
[A.B]
C="X"
```

or

```
A.B.C="x"
```

In this guide, all options are expressed in the second style for simplicity. But in the input file, either can be used.

5.1 Root

- `precision`: `medium` (float32) or `high` (float64). Default is `medium`.
- `seed`: the global seed, default is 611.
- `pair_style` **[required]**: the potential style to use:
  - eam/alloy: embedded-atom method
  - eam/adp: angular-dependent potential
  - atomic/sf: symmetry function based atomistic neural network potential
- `rcut`: the cutoff radius in angstroms. Default is 6.5.

5.2 Dataset

- `dataset.sqlite3` **[required]**: a string, the ASE Sqlite3 Database to use.
- `dataset.name` **[required]**: a string, the name of this experiment.
- `dataset.tfrecords_dir`: a string, the directory to save/load tfrecords files.
- `dataset.test_size`: an integer, the number of examples for evaluation.
- `dataset.serial`: a boolean. Default is `false`. Typically this should be false so that structures in the sqlite3 database can be written to tfrecords in parallel. For some old Linux systems or debugging, this can be set to `true`.

5.3 NN

This section defines the potential model parameters.

General options

- `nn.minimize`: a list of string, the properties to minimize. Some examples: `["energy", "forces"]`, `["energy", "stress"]`
- `nn.export`: a list of string, the properties that the exported model should predict. This option has the same format with `nn.minimize`.

5.3.1 Atomic

This section defines parameters for pair style `atomic/sf`.

- `nn.atomic.kernel_initializer`: a string, the initialization method.
- `nn.atomic.use_atomic_static_energy`: a boolean. If True, a bias unit will be added to the output layer acting as the elemental static energy. Section 3.7 of tensoralloy paper describes this residual model in detail.
- `nn.atomic.fixed_atomic_static_energy`: a boolean. If True, the elementary static energy parameters will be kept fixed.
- `nn.atomic.minmax_scale`: a boolean. If True, min-max normalization (section 3.6 of tensoralloy) will be applied to the descriptors.
- `nn.activation`: a string, the activation function to use. Options are: `elu`, `leaky_relu`, `softplus`, `softsign`, `tanh`, `sigmoid`. Default is `softplus`.

Hidden layers

Neural network hidden layers are set under scope `nn.atomic.layers`. This block is optional. The default setting for arbitrary type of element is `[64, 32]`.

```
[nn.atomic.layers]
Mo = [128, 64, 32]
Ni = [64, 64]
```

Symmetry function atomistic neural network parameters

This section describes the specific parameters for the symmetry function based atomistic neural network potential.

- `nn.atomic.sf.eta`: a list of float, the eta values for radial symmetry functions. Default is `[0.01, 0.1, 0.5, 1.0, 4.0]`.
- `nn.atomic.sf.omega`: a list of float, the omega values for radial symmetry functions. Default is `[0.0]`.
- `nn.atomic.sf.beta`: a list of float, the beta values for angular symmetry functions. Defaults is `[0.005]`.
- `nn.atomic.sf.gamma`: a list of float, the gamma values for angular symmetry functions. Default is `[1.0, -1.0]`.
- `nn.atomic.sf.zeta`: a list of float, the zeta values for angular symmetry functions. Default is `[1.0, 4.0]`.
- `nn.atomic.sf.angular`: a boolean. If true, angular symmetry functions will be used. Otherwise `gamma`, `zeta` and `beta` will be ignored.
- `nn.atomic.sf.cutoff_function`: a string selecting the cutoff function to use, `cosine` (default) or `polynomial`.

5.3.2 EAM/ADP

This section describes the options for pair styles under `eam`.

Functions

`rho`, `phi`, `embed`, `dipole` and `quadrupole` functions are all defined in the similar way.

```
[nn.eam.rho]
Ni = "zjw04xc"

[nn.eam.dipole]
NiNi = "mishinh"
```

The block above sets the rho function of **Ni** to `zjw04xc` and the dipole function of **Ni-Ni** to `mishinh`.

Built-in functions:

```
available_potentials = {
    'sutton90': AgSutton90,
    'zjw04': Zjw04,
    'zjw04xc': Zjw04xc,
    'zjw04uxc': Zjw04uxc,
    'zjw04xcp': Zjw04xcp,
    'msah11': AlFeMsah11,
    "mishinh": MishinH,
}
```

Customized functions

`zjw04` represents the original functions proposed by Zhou, Johnson and Wadley in 2004. `zjw04xc`, `zjw04uxc` and `zjw04xcp` are all customized implementations.

The dict `available_potentials` must be set in order to make customized functions usable.

SetFL

EAM and ADP will be exported to LAMMPS SetFL potential files. This block defines the related parameters.

```
[nn.eam.setfl]
nr = 10000
dr = 0.00065
nrho = 10000
drho = 0.01
```

`nrho` and `nr` are the number of tabulated values in the subsequent arrays, `drho` and `dr` are the spacing in density and distance space for the values in those arrays. See Lammps manual for more information.

5.3.3 Loss options

This section describes the options for computing the total loss.

Energy

- `nn.loss.energy.weight`: a float, the weight of the energy loss. Default is 1.
- `nn.loss.energy.per_atom_loss`: a boolean. If true, per-atom energy loss will be used. Default is false.
- `nn.loss.energy.method`: a string, `"rmse"` or `"logcosh"`.

Forces

- `nn.loss.forces.weight`: a float, the weight of the force loss. Default is 1.
- `nn.loss.forces.method`: a string, `"rmse"` or `"logcosh"`.

Stress

- `nn.loss.stress.weight`: a float, the weight of the force loss. Default is 1.
- `nn.loss.stress.method`: a string, `"rmse"` or `"logcosh"`.

L2 regularization

- `nn.loss.l2.weight`: a float, the weight of the L2 regularization. Default is 1.0. **Note: adaptive optimizers (adam, nadam, etc) are not compatible with L2. If you use any adaptive optimizer, please set this to 0.**
- `nn.loss.l2.decayed`: a boolean. If True, the L2 weight will decay exponentially.
- `nn.loss.l2.decay_rate`: a float controls the decay rate.
- `nn.loss.l2.decay_steps`: an integer.

Structural toml file

Mo.dft.toml is a structural toml file defining essential parameters for physical constraints.

```
name = "Mo"
file = "Mo.dft.cif"
format = "cif"
phase = "bcc"
bulk_modulus = 263.0

c11 = 472
c12 = 158
c44 = 106
```

- `name`: a string, the name of this material.
- `file`: a string, the structure file.
- `format`: the format of this file, must be recognized by `ase.io.read`. Generally, **cif** and **extxyz** are recommended.
- `phase`: a string, the phase of this structure.

- `bulk_modulus`: a float, the bulk modulus (GPa) of this material.
- `c11, c12, c44, ...`: float numbers, the elastic constants (GPa).

Built-in crystals

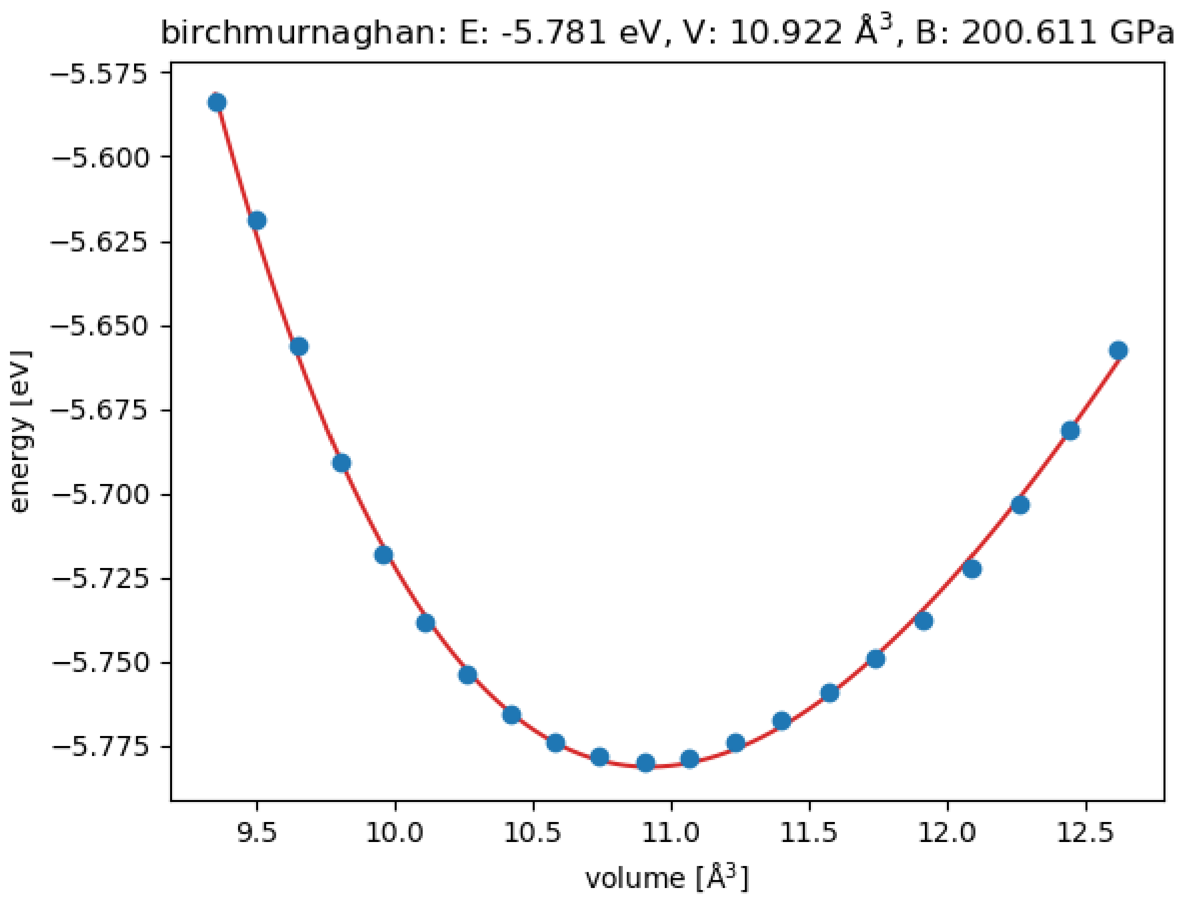
TensorAlloy has several built-in crystals (Ni, Mo, etc). See this file for more information.

Rose EOS

This section defines parameters of the Rose constraint.

- `nn.loss.rose.crystals`: a list of string, the names or files of crystals for constructing Rose EOS constraints. As an example, `["Ni", "Mo.dft.toml"]` means the built-in crystal `Ni` and the crystal specified in `Mo.dft.toml` will be used.
- `nn.loss.rose.weight`: a float, the weight of Rose constraints.
- `nn.loss.rose.beta`: a list of float, the beta values for each crystal. The size of this list must be equal to the size of `nn.loss.rose.crystals`.

`nn.loss.rose.dx` and `nn.loss.rose.delta` controls the number of points to fit EOS curves. `nn.loss.rose.delta` is the limit of the isotropic scaling factor. The volume will range from `(1 - delta)**3` to `(1 + delta)**3` of the equilibrium volume.



The figure above shows the fitted EOS of fcc Ni.

Elastic Tensor

This section defines parameters of the elastic tensor constraint.

- `nn.loss.elastic.crystals`: a list of string, the names or files of crystals to use.
- `nn.loss.elasitc.weight`: a float, the weight of elastic constraints.

When computing the elastic constants, the crystals should be close to their equilibrium structure. In other words, the norms of forces and stress tensor should be close to zero. `nn.loss.elastic.constraint.forces_weight` and `nn.loss.elastic.constraint.stress_weight` are used to define the weights of the norms of forces and stress tensor.

`nn.loss.elastic.constraint.tau` corresponds to the tau value (unit is GPa) of equation 32 in the paper.

5.4 Opt

- `opt.method`: a string, the optimizer to used. Options are: `adam`, `nadam`, `sgd`, `adadelta`, `rmsprop`. Default is `adam`.
- `opt.learning_rate`: a float, the initial learning rate. Default is 0.01.
- `opt.decay_function`: a string, the decay function to use. Options are: `exponential`, `inverse_time`, `natural_exp`. Default is `false` which means learning rate decay is disabled.
- `opt.decay_rate`: a float, the decay rate.
- `opt.decay_steps`: an integer, the decay step.
- `opt.staircase`: a boolean.

5.5 Train

- `train.reset_global_step`: a boolean. If True, the global step will be set to 0 by force. If you want to continue a previous training, this should be changed to `false`.

- `train.batch_size`: an integer, the batch size. Default is 50.

- `train.shuffle`: a boolean. If True, the input dataset will be shuffled. In most cases this should be true.

- `train.model_dir`: a string, the working directory for this experiment.

- `train.max_checkpoints_to_keep`: an integer, the maximum number of checkpoint files to keep in the model dir.

- `train.train_steps`: an integer, the maximum training steps.

- `train.eval_steps`: an integer, the intervals between two evaluations.

- `train.summary_steps`: an integer, the intervals between two writing summary operations.

- `train.log_steps`: an integer, the intervals between two logging operations.

- `train.profile_steps`: an integer, the intervals between two performance profiling operations. Set this to 0 to disable profiling.

- `train.ckpt.checkpoint_filename`: a string, the previous checkpoint file to read. Default is `false`.

- `train.ckpt.use_ema_variables`: a boolean. If `train.ckpt.checkpoint_filename` is provided, the moving average variables will be loaded if this is true.
- `train.ckpt.restore_all_variables`: a boolean. It only works when `train.ckpt.checkpoint_filename` is provided. If this is true, all variables (including the optimizer-specific variables) will be loaded. If false, only model variables will be used. Typically, if you want to continue a previous training with exactly the same settings but more training steps, set `train.reset_global_step` to false and this option to true. If you want to use the checkpoint values as initial guesses, this option shall be false.

6. Licenses

TensorAlloy

This TensorAlloy program is licensed under GNU Lesser General Public License v3.0. For more information please read LICENSE.

SNAP

The SNAP database and its subsets SNAP-Ni and SNAP-Mo are published by Shyue Ping Ong. The original JSON files can be obtained from GitHub freely. The original dataset is also licensed under BSD-3.