TorchANI Worknotes

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1 Installation

Prerequisites: PyTorch

Recommendation: install to user directory.

The usual steps are applicable:

- `python setup.py build`
- `python setup.py install --user`

TorchANI will be installed at (for example, the version number may vary):

```
$HOME/.local/lib/python3.8/site-packages/torchani-2.1.2-py3.8.egg/
```

To check the installation, go to directory examples and run the `energy_force.py` example. TorchANI will download the necessary files (paramaters for the neural network) so the script might run slowly in the first call. The parameters will put under the `resources` subdirectory of TorchANI.

There is warning when using Torch v-1.6:

```
/home/efefer/.local/lib/python3.8/site-packages/torchani-2.1.2.dev12+g42442af-py3.8.egg/torchani/aev.py:
↪  UserWarning: This overload of nonzero is deprecated:
        nonzero()
Consider using one of the following signatures instead:
        nonzero(*, bool as_tuple) (Triggered internally at
        ↪  /opt/conda/conda-bld/pytorch_1595629395347/work/torch/csrc/utils/python_arg_parser.cpp:766.)
in_cutoff = (distances <= cutoff).nonzero()
```

The fix seems to be:

```
in_cutoff = torch.nonzero(distances <= cutoff, as_tuple=False)
```