Final Project

This notebook is adapted from here:
https://aiqm.github.io/torchani/examples/nnp_training.html

Checkpoint 1: Data preparation

1. Create a working directory: `/global/scratch/users/[USER_NAME]/[DIR_NAME]`. Replace the [USER_NAME] with yours and specify a [DIR_NAME] you like.
2. Copy this Jupyter Notebook to the working directory
3. Download the ANI dataset `ani_dataset_gdb_s01_to_s04.h5` from bCourses and upload it to the working directory
4. Complete this notebook (can be worked on with your laptop, but **must be run on the cluster** for the final outputs)

Hint: You can use ? to learn more about any python function, e.g. ?torch.nn.Linear

In [ ]:
```
!pwd
```

```
/Users/chu/Documents/Class/MSSE_Spring2024/Chem277B/Final_Project
```

In [ ]:
```
import warnings
warnings.filterwarnings("ignore", category=UserWarning)
import numpy as np
from tqdm import tqdm
import torch
from torch.utils.data import DataLoader
import torch.nn as nn
import torchani
import torchani.data
import matplotlib.pyplot as plt
import time
```

Use GPU

In [ ]:
```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)
```

```
cpu
```

Savio Cluster!

In [ ]:
```
torch.version.cuda
```

In [ ]:
```
torch.cuda.is_available()
```

Out[ ]: True

In [ ]:
```
torch.cuda.current_device()
```

Out[ ]: 0

In [ ]:
```
# Now running on SAVIO Cluster!

device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)
```

```
cuda
```

Set up AEV computer

AEV: Atomic Environment Vector (atomic features)

Ref: Chem. Sci., 2017, 8, 3192

In [ ]:
```
def init_aev_computer():
    Rcr = 5.2
    Rca = 3.5
    EtaR = torch.tensor([16], dtype=torch.float, device=device)
    ShfR = torch.tensor([
        0.900000, 1.168750, 1.437500, 1.706250,
        1.975000, 2.243750, 2.512500, 2.781250,
        3.050000, 3.318750, 3.587500, 3.856250,
        4.125000, 4.393750, 4.662500, 4.931250
    ], dtype=torch.float, device=device)


    EtaA = torch.tensor([8], dtype=torch.float, device=device)
    Zeta = torch.tensor([32], dtype=torch.float, device=device)
    ShfA = torch.tensor([0.90, 1.55, 2.20, 2.85], dtype=torch.float, device=
    ShfZ = torch.tensor([
        0.19634954, 0.58904862, 0.9817477, 1.37444680,
        1.76714590, 2.15984490, 2.5525440, 2.94524300
    ], dtype=torch.float, device=device)

    num_species = 4
    aev_computer = torchani.AEVComputer(
        Rcr, Rca, EtaR, ShfR, EtaA, Zeta, ShfA, ShfZ, num_species
    )
    return aev_computer

aev_computer = init_aev_computer()
aev_dim = aev_computer.aev_length
print(aev_dim)
```

```
384
```

Prepare dataset & split

In [ ]:
```
def load_ani_dataset(dspath):
    self_energies = torch.tensor([
        0.500607632585, -37.8302333826,
        -54.5680045287, -75.0362229210
    ], dtype=torch.float, device=device)
    energy_shifter = torchani.utils.EnergyShifter(None)
    species_order = ['H', 'C', 'N', 'O']

    dataset = torchani.data.load(dspath)
    dataset = dataset.subtract_self_energies(energy_shifter, species_order)
    dataset = dataset.species_to_indices(species_order)
    dataset = dataset.shuffle()
    return dataset

dataset = load_ani_dataset("ani_gdb_s01_to_s04.h5")
```

In [ ]:
```
# Use dataset.split method to do split
train_data, val_data, test_data = dataset.split(0.8, 0.1, None)

# Show amount of training data vs total data
print("Training data size:", len(train_data))
print("Validation data size:", len(val_data))
print("Test data size:", len(test_data))
print("Total data size:", len(dataset))
# assert(len(dataset) == len(val_data) + len(test_data) + len(train_data))
print(691918 + 86489 * 2)
```

```
Training data size: 691918
Validation data size: 86489
Test data size: 86491
Total data size: 864898
864896
```

Batching

In [ ]:
```
batch_size = 8192
# use dataset.collate(...).cache() method to do batching

train_data_loader = train_data.collate(batch_size).cache()
val_data_loader = val_data.collate(batch_size).cache()
test_data_loader = test_data.collate(batch_size).cache()
```

In [ ]:
```
# Show that batching is working correctly
train_data_loader_list = list(train_data_loader)
# train_data_loader_list
```

In [ ]:
```
print(len(train_data_loader_list))
assert(len(train_data_loader_list) == len(train_data) // batch_size + 1)
```

```
85
```

The appropriate number of batches were created. For a dataset of size 691918, a total of 85 batches should be created and that is what is observed

In [ ]:
```
display(len(train_data_loader_list[0]['species']))
display(len(train_data_loader_list[0]['coordinates']))
display(len(train_data_loader_list[0]['energies']))
```

```
8192
8192
8192
```

Batching is appropriately creating batches of size 8192. Each batch of the ANI dataset is of a dictionary with species, coordinates, and energies all stored in corresponding tensors.

In [ ]:
```
# Training Data Batches
for i, batch in enumerate(train_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 8192
Batch # 11 is of size: 8192
Batch # 12 is of size: 8192
Batch # 13 is of size: 8192
Batch # 14 is of size: 8192
Batch # 15 is of size: 8192
Batch # 16 is of size: 8192
Batch # 17 is of size: 8192
Batch # 18 is of size: 8192
Batch # 19 is of size: 8192
Batch # 20 is of size: 8192
Batch # 21 is of size: 8192
Batch # 22 is of size: 8192
Batch # 23 is of size: 8192
Batch # 24 is of size: 8192
Batch # 25 is of size: 8192
Batch # 26 is of size: 8192
Batch # 27 is of size: 8192
Batch # 28 is of size: 8192
Batch # 29 is of size: 8192
Batch # 30 is of size: 8192
Batch # 31 is of size: 8192
Batch # 32 is of size: 8192
Batch # 33 is of size: 8192
Batch # 34 is of size: 8192
Batch # 35 is of size: 8192
Batch # 36 is of size: 8192
Batch # 37 is of size: 8192
Batch # 38 is of size: 8192
Batch # 39 is of size: 8192
Batch # 40 is of size: 8192
Batch # 41 is of size: 8192
Batch # 42 is of size: 8192
Batch # 43 is of size: 8192
Batch # 44 is of size: 8192
Batch # 45 is of size: 8192
Batch # 46 is of size: 8192
Batch # 47 is of size: 8192
Batch # 48 is of size: 8192
Batch # 49 is of size: 8192
Batch # 50 is of size: 8192
Batch # 51 is of size: 8192
Batch # 52 is of size: 8192
Batch # 53 is of size: 8192
Batch # 54 is of size: 8192
Batch # 55 is of size: 8192
```

```
Batch # 56 is of size: 8192
Batch # 57 is of size: 8192
Batch # 58 is of size: 8192
Batch # 59 is of size: 8192
Batch # 60 is of size: 8192
Batch # 61 is of size: 8192
Batch # 62 is of size: 8192
Batch # 63 is of size: 8192
Batch # 64 is of size: 8192
Batch # 65 is of size: 8192
Batch # 66 is of size: 8192
Batch # 67 is of size: 8192
Batch # 68 is of size: 8192
Batch # 69 is of size: 8192
Batch # 70 is of size: 8192
Batch # 71 is of size: 8192
Batch # 72 is of size: 8192
Batch # 73 is of size: 8192
Batch # 74 is of size: 8192
Batch # 75 is of size: 8192
Batch # 76 is of size: 8192
Batch # 77 is of size: 8192
Batch # 78 is of size: 8192
Batch # 79 is of size: 8192
Batch # 80 is of size: 8192
Batch # 81 is of size: 8192
Batch # 82 is of size: 8192
Batch # 83 is of size: 8192
Batch # 84 is of size: 3790
```

In [ ]:
```python
# Test Data Batches
for i, batch in enumerate(test_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 4571
```

In [ ]:
```python
# Val Data Batches
for i, batch in enumerate(val_data_loader):
    species = batch['species']
    print(f'Batch # {i} is of size: { len(species) }')
```

```
Batch # 0 is of size: 8192
Batch # 1 is of size: 8192
Batch # 2 is of size: 8192
Batch # 3 is of size: 8192
Batch # 4 is of size: 8192
Batch # 5 is of size: 8192
Batch # 6 is of size: 8192
Batch # 7 is of size: 8192
Batch # 8 is of size: 8192
Batch # 9 is of size: 8192
Batch # 10 is of size: 4569
```

All the batching works well! Appropriate number of batches all of size 8192 except for the last batch were created

Torchani API

In [ ]:
```
class AtomicNet(nn.Module):
    def __init__(self):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(384, 128),
            nn.ReLU(),
            nn.Linear(128, 1)
        )

    def forward(self, x):
        return self.layers(x)

net_H = AtomicNet()
net_C = AtomicNet()
net_N = AtomicNet()
net_O = AtomicNet()

# ANI model requires a network for each atom type
# use torchani.ANIModel() to compile atomic networks
ani_net = torchani.ANIModel([net_H, net_C, net_N, net_O])
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)
```

In [ ]:
```
train_data_batch = next(iter(train_data_loader))

loss_func = nn.MSELoss()
species = train_data_batch['species'].to(device)
coords = train_data_batch['coordinates'].to(device)
true_energies = train_data_batch['energies'].to(device).float()
_, pred_energies = model((species, coords))
loss = loss_func(true_energies, pred_energies)
print(loss)
```

```
tensor(0.2936, device='cuda:0', grad_fn=<MseLossBackward0>)
```

Checkpoint 2

In [ ]:
```
def timeit(f):
    def timed(*args, **kw):
        ts = time.time()
        result = f(*args, **kw)
        te = time.time()
        print(f'func: {f.__name__} took: {te-ts:.4f} sec on {device}')
        return result
    return timed

class ANITrainer:
    def __init__(self, model, batch_size, learning_rate, epoch, l2):
        self.model = model

        num_params = sum(item.numel() for item in model.parameters())
        print(f"{model.__class__.__name__} - Number of parameters: {num_para

        self.batch_size = batch_size
        self.optimizer = torch.optim.Adam(model.parameters(), learning_rate,
        self.epoch = epoch
        # definition of loss function: MSE is a good choice!
        self.loss_function = nn.MSELoss()

    @timeit
    def train(self, train_data, val_data,
              early_stop=True, draw_curve=True, verbose=True):
        self.model.train()

        # init data loader
        print("Initialize training data...")
        train_data_loader = train_data.collate(batch_size).cache()

        # record epoch losses
        train_loss_list = []
        val_loss_list = []
        lowest_val_loss = np.inf

        if verbose:
            iterator = range(self.epoch)
        else:
            iterator = tqdm(range(self.epoch), leave=True)

        for i in iterator:
            train_epoch_loss = 0.0
            for train_data_batch in train_data_loader:

                species = train_data_batch['species'].to(device)
                coords = train_data_batch['coordinates'].to(device)
                true_energies = train_data_batch['energies'].to(device).floa

                # compute energies
                _, pred_energies = self.model((species, coords))
```

```
                # compute loss
                # loss = loss_func(true_energies, pred_energies)
                batch_loss = self.loss_function(true_energies, pred_energies

                # do a step
                self.optimizer.zero_grad()
                batch_loss.backward()
                self.optimizer.step()

                batch_importance = train_data_batch['species'].shape[0] / le
                train_epoch_loss += batch_loss.detach().cpu().item() * batch

            # use the self.evaluate to get loss/MAE/RMSE on the validation s
            val_epoch_loss, mae, rmse = self.evaluate(val_data)

            # append the losses
            train_loss_list.append(train_epoch_loss)
            val_loss_list.append(val_epoch_loss)

            if early_stop:
                if val_epoch_loss < lowest_val_loss:
                    lowest_val_loss = val_epoch_loss
                    weights = self.model.state_dict()

        if draw_curve:
            # Plot train loss and validation loss
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            # If you used MSELoss above to compute the loss
            # Calculate the RMSE for plotting
            x_axis = np.arange(self.epoch)
            train_loss_rmse = np.sqrt(train_loss_list)
            val_loss_rmse = np.sqrt(val_loss_list)
            ax.plot(x_axis, train_loss_rmse, label='Train Loss (RMSE)')
            ax.plot(x_axis, val_loss_rmse, label='Validation Loss (RMSE)')
            # ax.plot(np.arange(len(train_loss_rmse))+1, train_loss_rmse, la
            # ax.plot(np.arange(len(val_loss_rmse))+1, val_loss_rmse, label=
            ax.legend()
            ax.set_xlabel("Epoch")
            ax.set_ylabel("RMSE")

        if early_stop:
            self.model.load_state_dict(weights)

        return train_loss_list, val_loss_list


    def evaluate(self, data, draw_plot=False):

        # init data loader
        data_loader = data.collate(batch_size).cache()
        total_loss = 0.0

        # init energies containers
        true_energies_all = []
        pred_energies_all = []
```

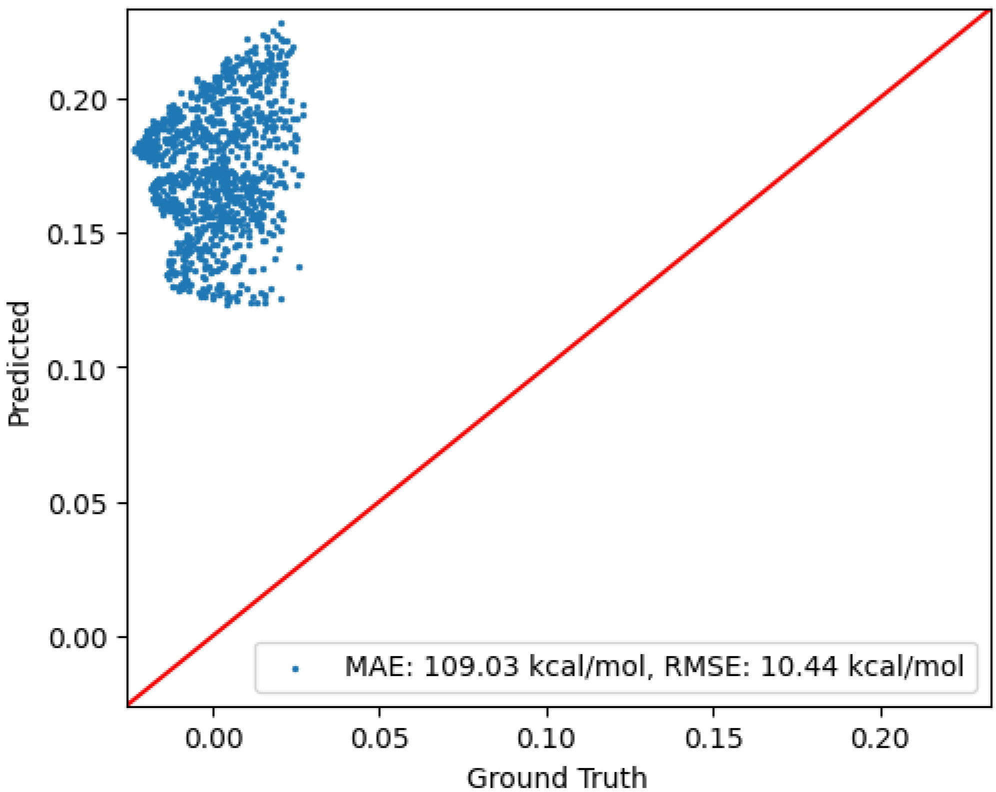
```
        with torch.no_grad():
            for batch_data in data_loader:

                # compute energies
                species = batch_data['species'].to(device)
                coords = batch_data['coordinates'].to(device)
                true_energies = batch_data['energies'].to(device).float()

                # compute energies
                _, pred_energies = self.model((species, coords))

                # compute loss
                batch_loss = self.loss_function(true_energies, pred_energies

                batch_importance = batch_data['species'].shape[0] / len(data
                total_loss += batch_loss.detach().cpu().item() * batch_impor

                # store true and predicted energies
                true_energies_all.append(true_energies.detach().cpu().numpy(
                pred_energies_all.append(pred_energies.detach().cpu().numpy(
        true_energies_all = np.concatenate(true_energies_all)
        pred_energies_all = np.concatenate(pred_energies_all)

        # Report the mean absolute error (MAE) and root mean square error (R
        # The unit of energies in the dataset is hartree
        # please convert it to kcal/mol when reporting
        # 1 hartree = 627.5094738898777 kcal/mol
        # MAE = mean(|true - pred|)
        # RMSE = sqrt(mean( (true-pred)^2 ))
        hartree2kcalmol = 627.5094738898777
        mae = np.mean(np.abs(true_energies_all - pred_energies_all)) * hartr
        rmse = np.sqrt(mae)

        if draw_plot:
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            ax.scatter(true_energies_all, pred_energies_all, label=f"MAE: {m
            ax.set_xlabel("Ground Truth")
            ax.set_ylabel("Predicted")
            xmin, xmax = ax.get_xlim()
            ymin, ymax = ax.get_ylim()
            vmin, vmax = min(xmin, ymin), max(xmax, ymax)
            ax.set_xlim(vmin, vmax)
            ax.set_ylim(vmin, vmax)
            ax.plot([vmin, vmax], [vmin, vmax], color='red')
            ax.legend()

        return total_loss, mae, rmse
```

1 heavy atom

In [ ]:
```
# Load dataset with 1 heavy atom
# Then do a train/val/test = 80/10/10 split
dataset = load_ani_dataset("ani_gdb_s01.h5")
```

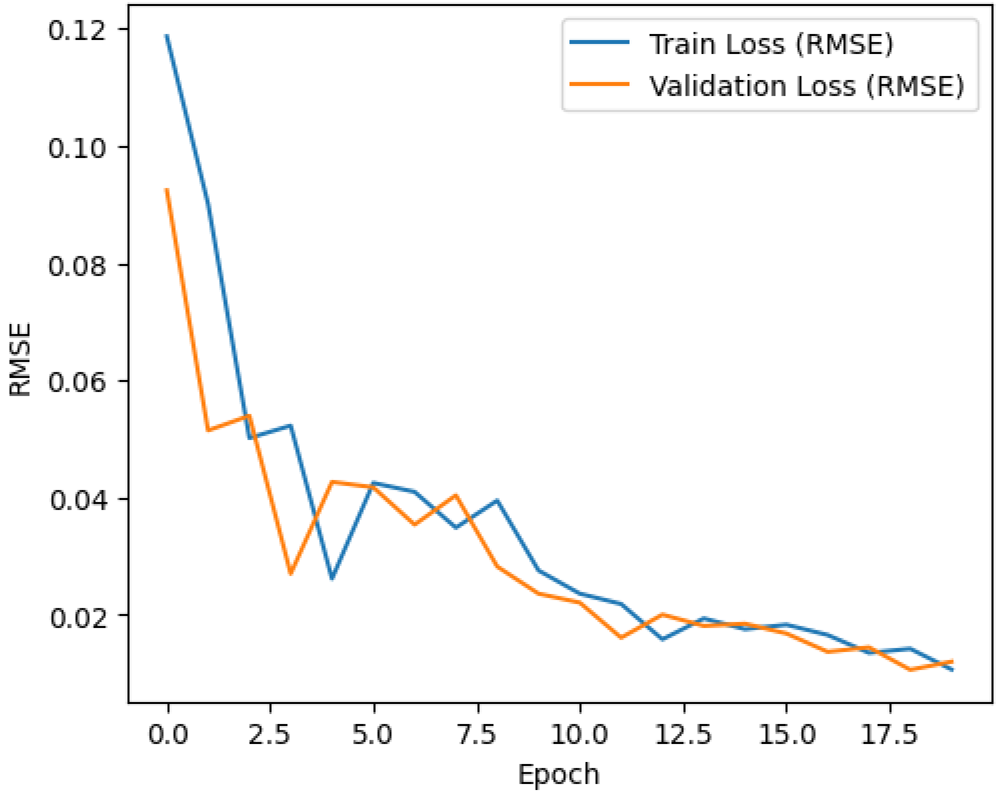
```
train_data, val_data, test_data = dataset.split(0.8, 0.1, 0.1)
print(f'Train/Total: {len(train_data)}/{len(dataset)}')

# Define the model
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)

# Initiate the trainer and evaluate on test_dataset with draw_plot=True
trainer = ANITrainer(model=model, batch_size=8192, learning_rate=1e-3, epoch
loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

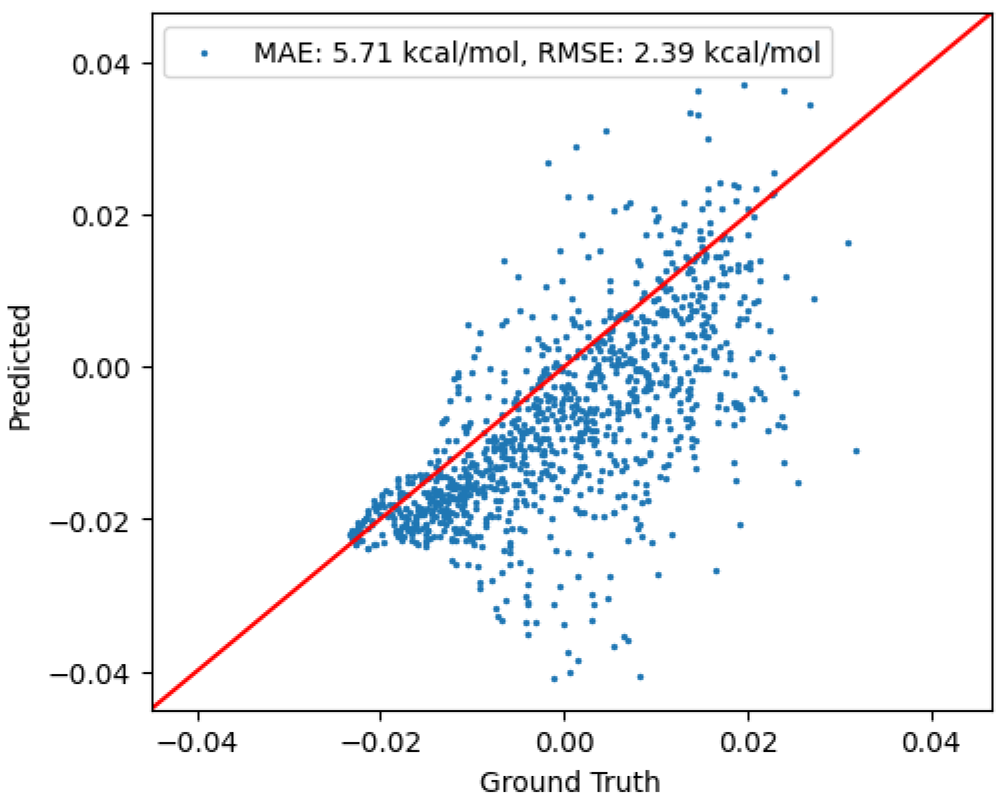
```
Train/Total: 8640/10800
Sequential - Number of parameters: 197636
```



In [ ]:
```
# Run on CPU
# Perform training and re-evaluate on test_dataset with draw_plot=True
train_losses, val_losses = trainer.train(train_data, val_data, verbose=True)
loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

```
Initialize training data...
func: train took: 3.3006 sec on cpu
```



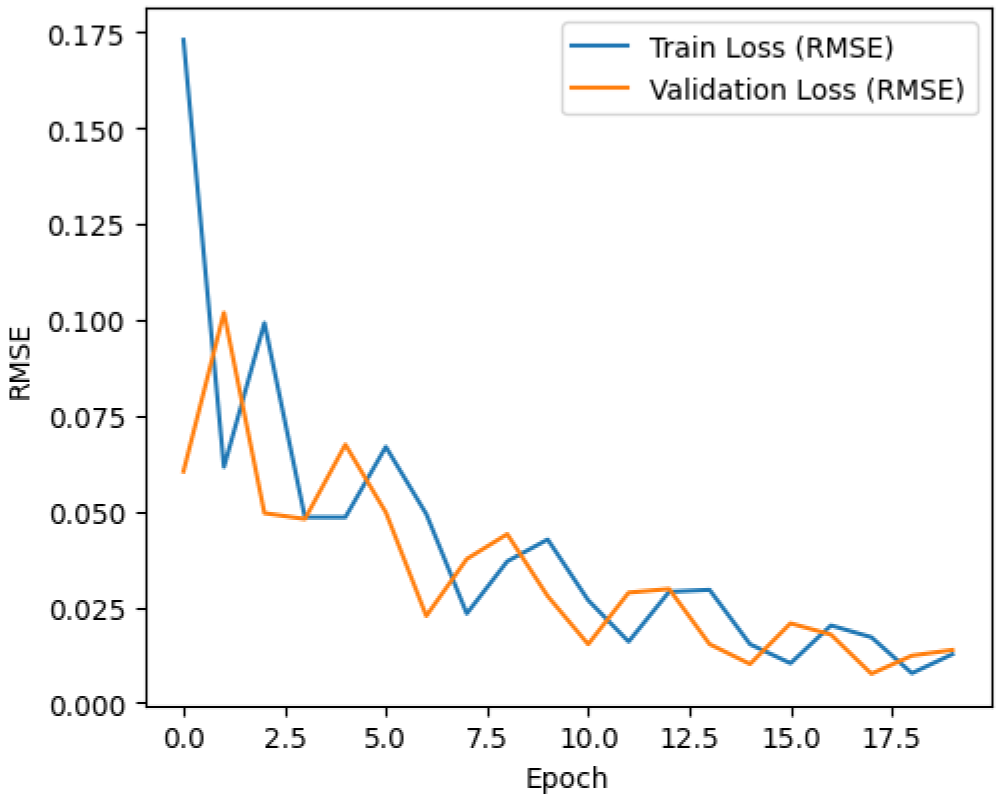


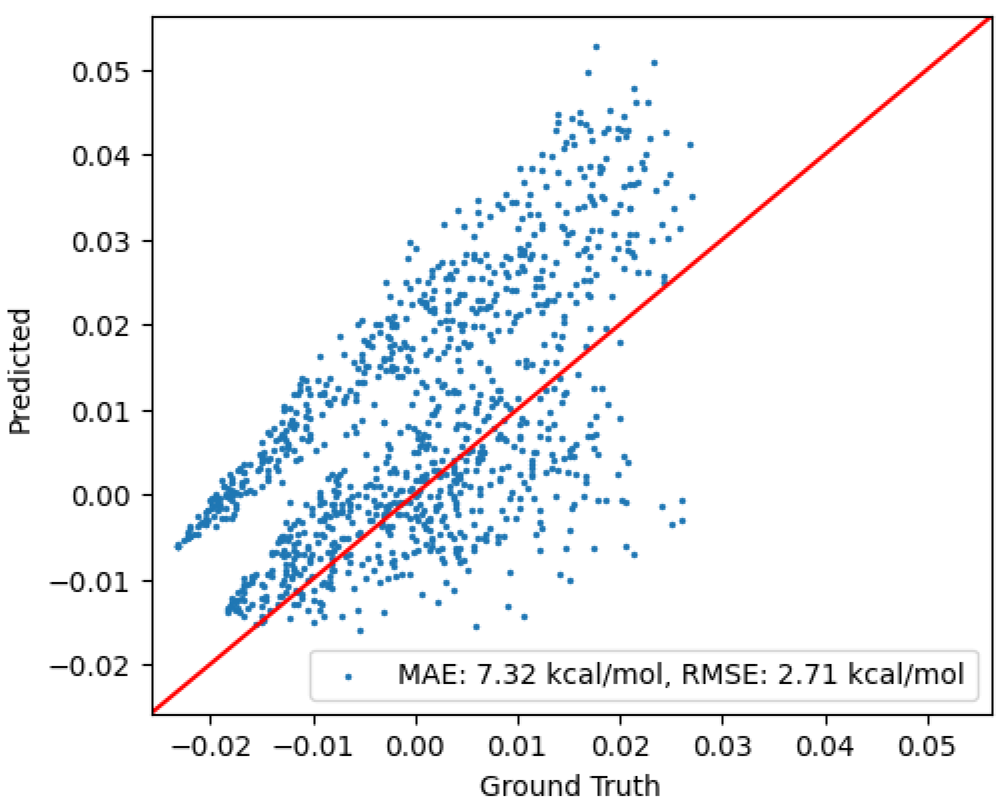
In [ ]:
```
# Now running on SAVIO Cluster!

device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)
```

```
cuda
```

```
In [ ]: # Run on GPU
        # Perform training and re-evaluate on test_dataset with draw_plot=True
        train_losses, val_losses = trainer.train(train_data, val_data, verbose=True)
        loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

```
Initialize training data...
func: train took: 4.1930 sec on cuda
```

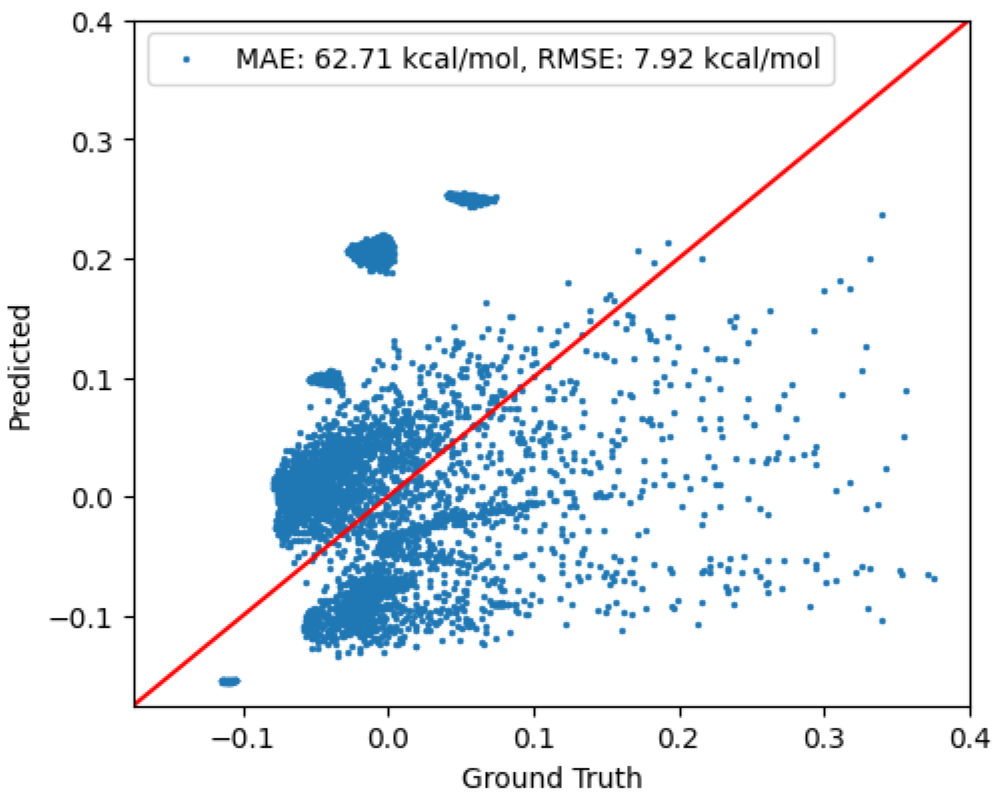




n heavy atoms

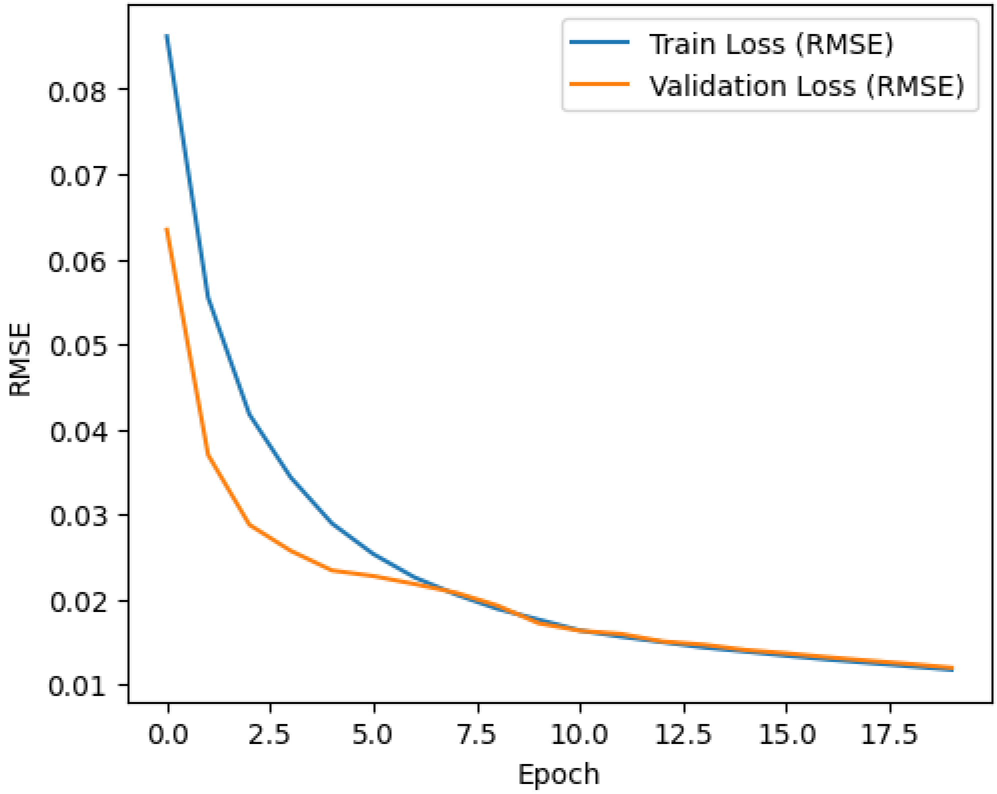
In [ ]:
```
# Load dataset with n (different from 1) heavy atom
# Then do a train/val/test = 80/10/10 split
dataset = load_ani_dataset("ani_gdb_s02.h5")
train_data, val_data, test_data = dataset.split(0.8, 0.1, 0.1)
print(f'Train/Total: {len(train_data)}/{len(dataset)}')

# Define the model
model = nn.Sequential(
    aev_computer,
    ani_net
).to(device)

# Initiate the trainer and evaluate on test_dataset with draw_plot=True
trainer = ANITrainer(model=model, batch_size=8192, learning_rate=1e-3, epoch
loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

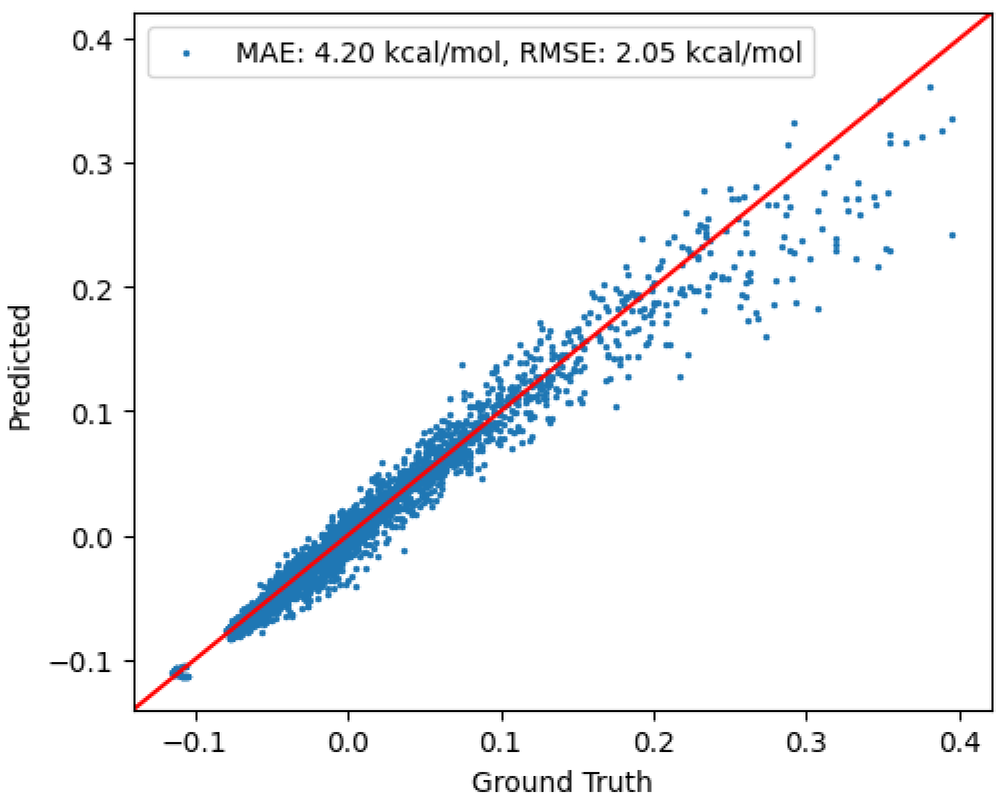
```
Train/Total: 40769/50962
Sequential - Number of parameters: 197636
```



In [ ]:
```
# Run on CPU
# Perform training and re-evaluate on test_dataset with draw_plot=True
train_losses, val_losses = trainer.train(train_data, val_data, verbose=True)
loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

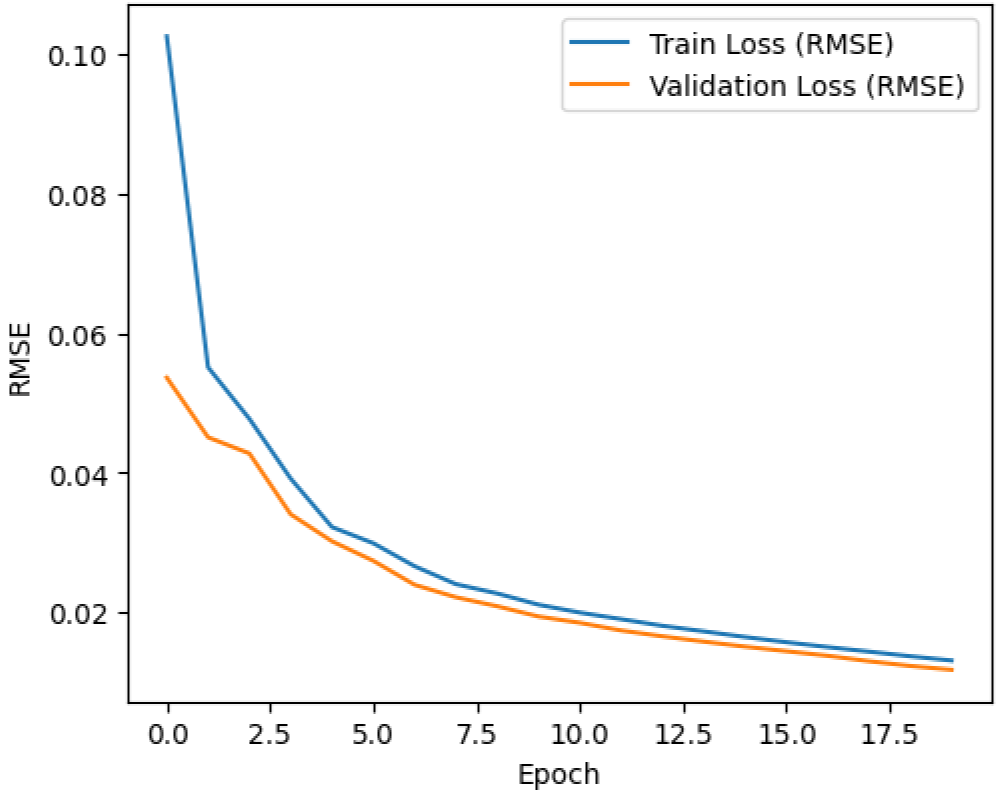
```
Initialize training data...
func: train took: 18.0796 sec on cpu
```

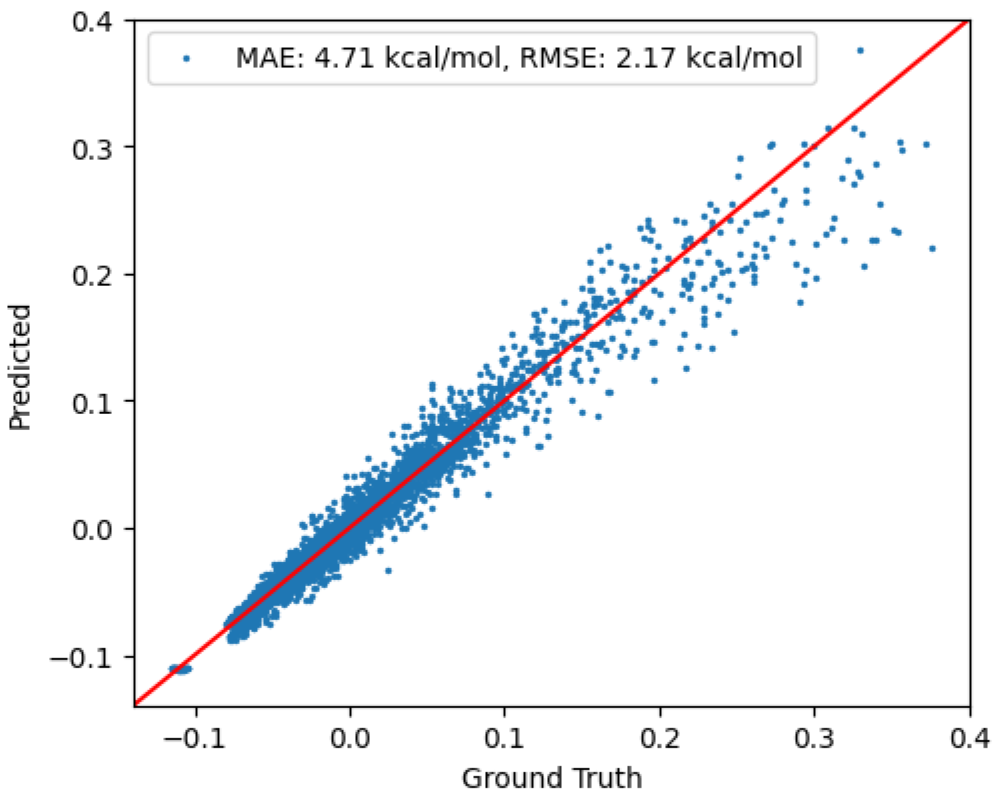




In [ ]:
```
# Run on GPU
# Perform training and re-evaluate on test_dataset with draw_plot=True
train_losses, val_losses = trainer.train(train_data, val_data, verbose=True)
loss, mae, rmse = trainer.evaluate(test_data, draw_plot=True)
```

```
Initialize training data...
func: train took: 9.9976 sec on cuda
```





For more atoms, utilizing the GPU has significant improvements in time! For the single atom, using the CPU is actually faster, but this initial overhang gets rapidly overshadowed by how fast GPUs are at parallelizing processes.

```
In [ ]:
```