CS182 project - Deliver ideas of CGCNN

General Explanation

The key idea of CGCNN is to represent crystal structure by a crystal graph, which encodes not only the atomic information but also bonding information between atoms based on the distance. Here we will let each atomic feature vector as vi, which encodes the property of the atom corresponding to node i. The edge feature vector is represented as u(i,j)k, which encodes k-th bond connecting atom i, j. Note that there can be several bonds between atoms, which originate from the periodic nature of crystals.
Obviously, there are many ways to encode atomic and bond data. For the sake of simplicity, we will follow the methods used in the CGCNN paper, which used a pre-defined encoding vector to change atoms into vectors. These vectors have 92 dimensions, and for 100 atoms in the periodic table, they have different encodings which consist of 0 and 1. For the edge feature vectors, there also can be many ways to encode bond information; bond length, angle, and covalency. However, we will only use bond-length information between nearest neighbors, by applying a Gaussian kernel to change it to encoding vectors. One can follow the homework notebook on how this embedding is done to NaCl(salt) Crystal.

Encoding Crystal into Crystal Graph

In [3]:
```
# Note: Need pymatgen
```

In [2]:
```
# Uncommnet this to install pymatgen
#!pip install pymatgen
```

In [ ]:
```
import os
import sys
import csv
import json
import torch
import torch.nn as nn
import random
import warnings
warnings.filterwarnings('ignore')
import functools
import sklearn
import numpy as np
import networkx as nx
import matplotlib.pyplot as plt
from matplotlib.colors import to_rgba_array

from pymatgen.core.structure import Structure
from pymatgen.analysis.graphs import StructureGraph
from pymatgen.analysis.local_env import CrystalNN
from torch.utils.data import Dataset, DataLoader
from torch.utils.data.dataloader import default_collate
from torch.utils.data.sampler import SubsetRandomSampler
import torch.optim as optim
from torch.optim.lr_scheduler import MultiStepLR
```

```
from data_utils import CIFData
from data_utils import AtomCustomJSONInitializer
from data_utils import AtomInitializer
from data_utils import GaussianDistance
```

In [4]:
```
# Uncomment this to extract data
# !unzip cgcnn_data.zip
# !unzip hw_data.zip
```

Let's convert salt (NaCl) to crystadddl graph.
You can use print method to see the lattice and position of Na, Cl atoms in the cell.
We will also visualize it to a graph. Each node of graph is atom in the crystal, and edge is bonds that have distance as information.

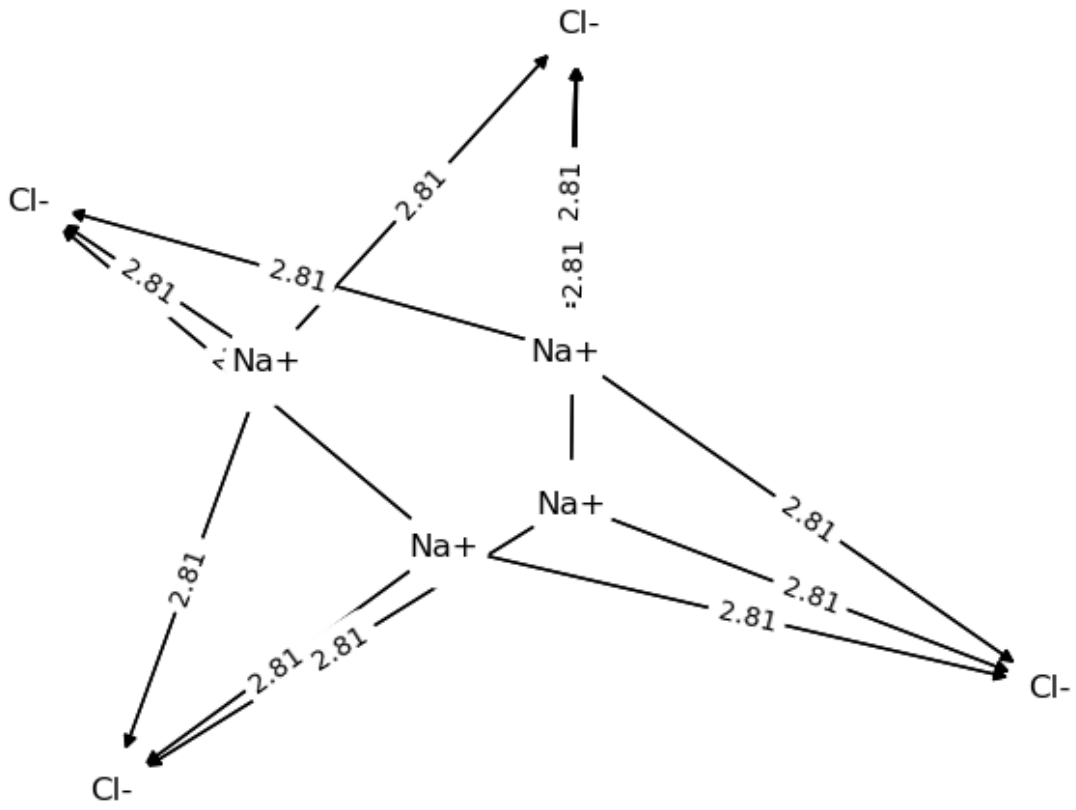
Note that we will use pymatgen package (Python Materials Genomics) which is an open source Python library for materials analysis. But you don't need to worry about that too much. Only important class is 'Structure' class, which can load structure data of materials by Structure.from_file method. After you load it, you can get the site information using Structure_object[index_want_to_check], and this Site object has some useful attributes, such as specie. You can check what specie is in the site by using Structure_object[index].specie

In [5]:
```
# Load structure from CIF file
nacl = Structure.from_file('hw_data/sample_regression/1000041.cif')
print(nacl)
```

```
Full Formula (Na4 Cl4)
Reduced Formula: NaCl
abc   :   5.620000   5.620000   5.620000
angles:  90.000000  90.000000  90.000000
pbc   :        True       True       True
Sites (8)
  #  SP      a    b    c
---  ----  ---  ---  ---
  0  Na+   0    0    0
  1  Na+   0    0.5  0.5
  2  Na+   0.5  0    0.5
  3  Na+   0.5  0.5  0
  4  Cl-   0.5  0.5  0.5
  5  Cl-   0.5  0    0
  6  Cl-   0    0.5  0
  7  Cl-   0    0    0.5
```

In [6]:
```
# Visualization of the structure using the CIF file
crystal = CrystalNN()

sg = StructureGraph.with_local_env_strategy(nacl, crystal)

node_labels = {}
for i, site in enumerate(nacl):
    label = "{}".format(site.specie)
    node_labels[i] = label

edge_weights = {}
for edge in sg.graph.edges():
    dist = nacl.get_distance(edge[0], edge[1])
    edge_weights[edge] = dist

pos = nx.spring_layout(sg.graph)
```

```
nx.draw(sg.graph, pos, with_labels=True, labels=node_labels, font_size=12, node_
nx.draw_networkx_edge_labels(sg.graph, pos, edge_labels=edge_weights, font_size=
plt.axis("off")
plt.show()
```



Next we will encode atoms in the node to atomistic feature vectors using pre-difined atom embedding.

atom_init.json is containing vector embedding of atoms, where key (1, 2, 3, ..., 100) represent atomic number and values are encoding vectors.

You can try different atom embedding too if you want.

In [ ]:

```
# Load embedding file.
element_embedding_file = 'hw_data/sample_regression/atom_init.json'
with open(element_embedding_file) as f:
    elem_embedding = json.load(f)
elem_embedding = {int(key): value for key, value
                  in elem_embedding.items()}

atom_fea = None
################################################################################
# TODO: Encode crsytal data to atomistic features.
# (Hint: Use np.vstack and elem_embedding to join all embedded specie numbers of
# Also, check out pymatgen.core.structure.specie.number attribute.
# nacl[i].specie will give you what kind of specie it is,
# And number attribute will give atomic number of that specie.)
# Atom_feature shd have shape of (# of atoms, len(embedding vector))

# YOUR CODE HERE
```

```
# Solution
atom_fea = np.vstack([elem_embedding[nacl[i].specie.number]
                      for i in range(len(nacl))])
#############################################################################
assert atom_fea is not None
atom_fea = torch.Tensor(atom_fea)


assert atom_fea.shape == (8, 92)
```

Next, we will get neighbor information from each atoms in the cell. We will get help from pymatgen package. get_all_neighbor function of structure object returns atoms within the input radius. Note that here len(all_nbrs) is 8 since there are 8 atoms (4 Na+, 4 Cl-) in the cell. Each list contain the neighbor atom information considering periodicity. We will use 12 nearest neighbors after sorting with distance.

In [8]:

```
all_nbrs = nacl.get_all_neighbors(r = 8, include_index=True)
all_nbrs = [sorted(nbrs, key=lambda x: x[1]) for nbrs in all_nbrs]

assert len(all_nbrs) == 8

nbr_fea_idx, nbr_fea = [], []
for nbr in all_nbrs:
    # Note: x[1] returns distance to neighbors.
    # Note: x[2] returns index of original structure object
    nbr_fea_idx.append(list(map(lambda x: x[2],
                                nbr[:12])))
    nbr_fea.append(list(map(lambda x: x[1],
                            nbr[:12])))

# nbr_fea_idx contain information of nearest neighbor atoms
# from ith row (ith atom in the cell)
# For example, 0th atom (Na+ (0.0000, 0.0000, 0.0000)) is neighbored
# with 5th, 6th, 7th, etc...
# nbr_fea contain information of nearest neighbot distance.
nbr_fea_idx, nbr_fea = np.array(nbr_fea_idx), np.array(nbr_fea)
nbr_fea_idx = torch.LongTensor(nbr_fea_idx)

nbr_fea_idx_standard = torch.LongTensor([[5, 6, 7, 7, 6, 5, 2, 1, 2, 1, 3, 3],
                                         [4, 7, 6, 7, 6, 4, 2, 0, 3, 2, 3, 3],
                                         [4, 7, 5, 7, 5, 4, 0, 3, 1, 3, 3, 1],
                                         [4, 6, 5, 6, 5, 4, 2, 1, 1, 2, 0, 0],
                                         [3, 1, 2, 3, 2, 1, 6, 5, 6, 5, 7, 7],
                                         [2, 3, 0, 3, 0, 2, 4, 4, 6, 6, 4, 7],
                                         [1, 3, 0, 3, 0, 1, 4, 4, 5, 5, 5, 4],
                                         [2, 1, 0, 2, 1, 0, 4, 5, 5, 4, 6, 6]])

assert torch.equal(nbr_fea_idx, nbr_fea_idx_standard)
```

Now we have two features, atomic feature and neighbor feature. Note that neighbor feature is discontionous information with respect to the distance. Therefore we will expand (which means we will stack data based on the current discontinous distance value) neighbor feature using Gaussian Kernel (or Gaussian filter) https://en.wikipedia.org/wiki/Gaussian_filter
While expanding the neighbor feature, one can set the distance range and step. Here we will use minimum distance 0, maximum distance 12, and step size of 0.2, which will expanded to dimension size of 61.

In [9]:
```
dmin = 0
dmax = 12
step = 0.2
var = step
filter_step = np.arange(dmin, dmax+step, step)

def expand(distances):
    ###############################################################################
    # TODO: Implement the expand function using a Gaussian kernel.
    # raise NotImplementedError()

    # Solution
    return np.exp(-(distances[..., np.newaxis] - filter_step)**2 / var**2)
    ###############################################################################


nbr_fea_gaussian = expand(nbr_fea)
```

In [10]:
```
gdf = GaussianDistance(dmin=0, dmax=12, step=0.2)
nbr_fea = gdf.expand(nbr_fea)
```

In [11]:
```
assert np.array_equal(nbr_fea_gaussian, nbr_fea)
```

Build a Model

After building the crystal graph, the convolutional neural network act on top of the graph, and consecutive fully connected networks and pooling layer are used to predict the property of crystals. The convolution layer iteratively updates the atom feature vector v_i by message passing with surrounding atoms and bonds with a non-linear graph convolution function:

$$v_i^{(t+1)} = Conv(v_i^{(t)}, v_j^{(t)}, u_{(i,j)_k}), (i,j)_k \in G$$

And then consequetive pooling layer and hidden fully connected layer will generate output of model:

$$v_c = Pool(v_0^{(0)}, v_1^{(0)}, \ldots, v_N^{(0)}, \ldots, v_N^{(R)})$$

Note that we can use any Convolution and Pooling layer if we maintain the permutation invariance. Here we will try two different convolution layer. Try to implement WeightShareConvLayer in the TODO section of model_hw.py. We will offer solution for the ConvLayer. Note that we will do not change pooling layer, and you can use any activation function you use. But try to use sigmoid function here. After you implement WeightShareConvLayer, try to implement CrystalGraphConvNet by filling in the TODO section of model_hw.py. You can find a detailed explanation there.

1. WeightShareConvLayer; This is a Convolution weight matrix is shared by all neighbors.
   $v_i^{(t+1)} = g[(\sum_{j,k} v_j^{(t)} \oplus u_{(i,j)_k})W_c^{(t)} + v_i^{(t)}W_s^{(t)} + b^{(t)}]$
   Here W_c, W_s, and b are the convolution weight matrix, self-weight matrix, and bias.

1. ConvLayer; This is a Convolution weight matrix is differentiated at all neighbor pairs.
   $v_i^{(t+1)} = v_i^{(t+1)} + \sum_{j,k} \sigma(z_{(i,j)_k}^{(t)} W_f^{(t)} + b_f^{(t)}) \odot g(z_{(i,j)_k}^{(t)} W_s^{(t)} + b_s^{(t)})$
   Here $z_{(i,j)_k} = v_i \oplus v_j \oplus u_{(i,j)_k}$, $\odot$ denotes element-wise multiplication and σ denotes a sigmoid function.

In [12]:
```
from model_hw import CrystalGraphConvNet
from model_hw import ConvLayer
from model_hw import WeightShareConvLayer
```

In [13]:
```
# For testing purpose
data_dir = './cgcnn_data/sample-regression'
test = CIFData(data_dir)
(atom_fea, nbr_fea, nbr_fea_idx), target, cif_id = test[-1]
structures, _, _ = test[-1]
orig_atom_fea_len = structures[0].shape[-1]
nbr_fea_len = structures[1].shape[-1]
```

In [14]:
```
torch.manual_seed(123)

convlayer_test = ConvLayer(92, 41)
convlayer_test_result = convlayer_test.forward(atom_fea, nbr_fea, nbr_fea_idx)

################################################################################
# TODO: Implement the WeightShareConvLayer model in model_hw.py
################################################################################

weightshare_test = WeightShareConvLayer(92, 41)
weightshare_test_result = weightshare_test.forward(atom_fea, nbr_fea, nbr_fea_id

assert convlayer_test_result.shape == (8, 92)
assert weightshare_test_result.shape == (8, 92)
```

In [15]:
```
# Simple test
# Set seed using manual_seed
# TODO explanation about crystal_atom_idx
torch.manual_seed(123)
crystal_atom_idx = [torch.Tensor([0, 1, 2, 3, 4, 5, 6, 7]).long()]
################################################################################
# TODO: Implement the CrystalGraphConvNet model in model_hw.py
################################################################################

model1 = CrystalGraphConvNet(orig_atom_fea_len, nbr_fea_len, option='C')
out = model1.forward(atom_fea, nbr_fea, nbr_fea_idx, crystal_atom_idx)
assert (out.item() - 0.6627038) < 1e-6

model2 = CrystalGraphConvNet(orig_atom_fea_len, nbr_fea_len, option='WC')
out = model2.forward(atom_fea, nbr_fea, nbr_fea_idx, crystal_atom_idx)
assert (out.item() - -0.5442343) < 1e-6
```

Training

Now we are all set to test our model. We will train our model to simplified dataset, which consists of ~700 Perovskite materials. We will predict the energy (which is calculated already with DFT, unit is eV) of Perovskites, and see how the model performs. After run the following

section, try to anser the question. Note that you can find your prediction and corresponding structures in test_result.csv file.

Q. If you built a model, let's train and visualize it. What is the difference between two models? Which one performs better and why do you think so?
Based on what you observed, can you make a convolution layer that performs better?

Hint: Among two convolution layers, ConvLayer performs better in general. This is because the local environments can always change, so maintaining same weights to all local environments makes prediction worse. However, you can see that in Perovskite dataset, WeightShareConvLayer performs better because Perovskite all have similar symmetry, and local environments of them are not much different

In [16]:
```
from data_utils import collate_pool, get_train_val_test_loader
from train_utils import Normalizer, train, validate, save_checkpoint
from model_hw import CrystalGraphConvNet
from random import sample
```

In [17]:
```
torch.manual_seed(123)

# set parameters
data_dir = './hw_data/perovskite_energy'
batch_size = 8
train_ratio, val_ratio, test_ratio = 0.8, 0.1, 0.1

# get dataset

dataset = CIFData(data_dir)
collate_fn = collate_pool
train_loader, val_loader, test_loader = get_train_val_test_loader(
    dataset=dataset,
    collate_fn=collate_fn,
    batch_size=batch_size,
    train_ratio=train_ratio,
    val_ratio=val_ratio,
    test_ratio=test_ratio,
    return_test=True)
```

In [18]:
```
# normalize target

if len(dataset) < 500:
    warnings.warn('Dataset has less than 500 data points. '
                  'Lower accuracy is expected. ')
    sample_data_list = [dataset[i] for i in range(len(dataset))]
else:
    sample_data_list = [dataset[i] for i in
                        sample(range(len(dataset)), 500)]
_, sample_target, _ = collate_pool(sample_data_list)
normalizer = Normalizer(sample_target)
```

In [19]:
```
# build model
structures, _, _ = dataset[0]
orig_atom_fea_len = structures[0].shape[-1]
nbr_fea_len = structures[1].shape[-1]
#################################################################################
```

```
# TODO: Tune the following parameters and model to optimize performance.
# Note: You can change your convolution layer with option argument in
# CrystalGraphConvNet. C is ConvLayer, WC is WeightShareConvLayer.
#############################################################################
# number of hidden atom features in conv layers
atom_fea_len = 64
# number of hidden features after pooling
h_fea_len = 128
# number of conv layers
n_conv = 3
# number of hidden layers after pooling
n_h = 1

model = CrystalGraphConvNet(orig_atom_fea_len, nbr_fea_len,
                            atom_fea_len=atom_fea_len,
                            n_conv=n_conv,
                            h_fea_len=h_fea_len,
                            n_h=n_h, option='C')
```

In [20]:
```
# set hyperparameters, change the parameters to get better results
epochs = 15
criterion = nn.MSELoss()
lr = 0.01
momentum = 0.9
weight_decay = 0

optimizer = optim.SGD(model.parameters(), lr,
                              momentum=momentum,
                              weight_decay=weight_decay)

# optimizer = optim.Adam(model.parameters(), lr,
#                            weight_decay=weight_decay)
lr_milestones = [100]
scheduler = MultiStepLR(optimizer, milestones=lr_milestones,
                            gamma=0.1)
```

In [21]:
```
running_record = {'train_loss': [], 'train_mae': [],
                  'val_loss': [], 'val_mae': []}

for epoch in range(epochs):
    print('Epoch {}/{}'.format(epoch, epochs - 1))
    print('-' * 10)

    best_mae_error = 1e10
    # train for one epoch
    train_loss, train_mae = train(train_loader, model, criterion, optimizer, epo

    # evaluate on validation set
    val_loss, val_mae = validate(val_loader, model, criterion, normalizer)

    # append loss and mae to running record. Convert tensor to float if necessar
    running_record['train_loss'].append(train_loss)
    running_record['train_mae'].append(train_mae)
    running_record['val_loss'].append(val_loss)
    running_record['val_mae'].append(val_mae)


    if val_mae != val_mae:
        print('Exit due to NaN')
        sys.exit(1)
```

```
    scheduler.step()

    # remember the best mae_eror and save checkpoint
    is_best = val_mae < best_mae_error
    best_mae_error = min(val_mae, best_mae_error)

    save_checkpoint({
        'epoch': epoch + 1,
        'state_dict': model.state_dict(),
        'best_mae_error': best_mae_error,
        'optimizer': optimizer.state_dict(),
        'normalizer': normalizer.state_dict(),
    }, is_best)
```

```
Epoch 0/14
----------
100%|████████████████████████████████████████| 67/67 [00:21<00:00,  3.12it/s]
Train:  Time 0.246      Data 0.168      Loss 1.0064     MAE 54.459
100%|████████████████████████████████████████| 9/9 [00:08<00:00,  1.03it/s]
Test:   Time 0.412      Loss 0.4892     MAE 40.253
Epoch 1/14
----------
100%|████████████████████████████████████████| 67/67 [00:19<00:00,  3.40it/s]
Train:  Time 0.220      Data 0.152      Loss 0.6307     MAE 39.189
100%|████████████████████████████████████████| 9/9 [00:08<00:00,  1.04it/s]
Test:   Time 0.405      Loss 0.8308     MAE 51.584
Epoch 2/14
----------
100%|████████████████████████████████████████| 67/67 [00:18<00:00,  3.54it/s]
Train:  Time 0.208      Data 0.150      Loss 0.6201     MAE 38.471
100%|████████████████████████████████████████| 9/9 [00:08<00:00,  1.04it/s]
Test:   Time 0.406      Loss 0.4942     MAE 35.135
Epoch 3/14
----------
100%|████████████████████████████████████████| 67/67 [00:19<00:00,  3.49it/s]
Train:  Time 0.212      Data 0.149      Loss 0.5625     MAE 36.203
100%|████████████████████████████████████████| 9/9 [00:13<00:00,  1.46s/it]
Test:   Time 0.904      Loss 0.5425     MAE 40.618
Epoch 4/14
----------
100%|████████████████████████████████████████| 67/67 [00:19<00:00,  3.50it/s]
Train:  Time 0.211      Data 0.150      Loss 0.6808     MAE 43.837
100%|████████████████████████████████████████| 9/9 [00:08<00:00,  1.06it/s]
Test:   Time 0.389      Loss 0.4754     MAE 41.545
Epoch 5/14
----------
100%|████████████████████████████████████████| 67/67 [00:19<00:00,  3.36it/s]
Train:  Time 0.223      Data 0.156      Loss 0.5892     MAE 37.267
100%|████████████████████████████████████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.395      Loss 0.4730     MAE 44.930
Epoch 6/14
----------
100%|████████████████████████████████████████| 67/67 [00:19<00:00,  3.46it/s]
Train:  Time 0.214      Data 0.153      Loss 0.4989     MAE 34.168
100%|████████████████████████████████████████| 9/9 [00:09<00:00,  1.01s/it]
Test:   Time 0.458      Loss 0.6255     MAE 43.454
Epoch 7/14
----------
```

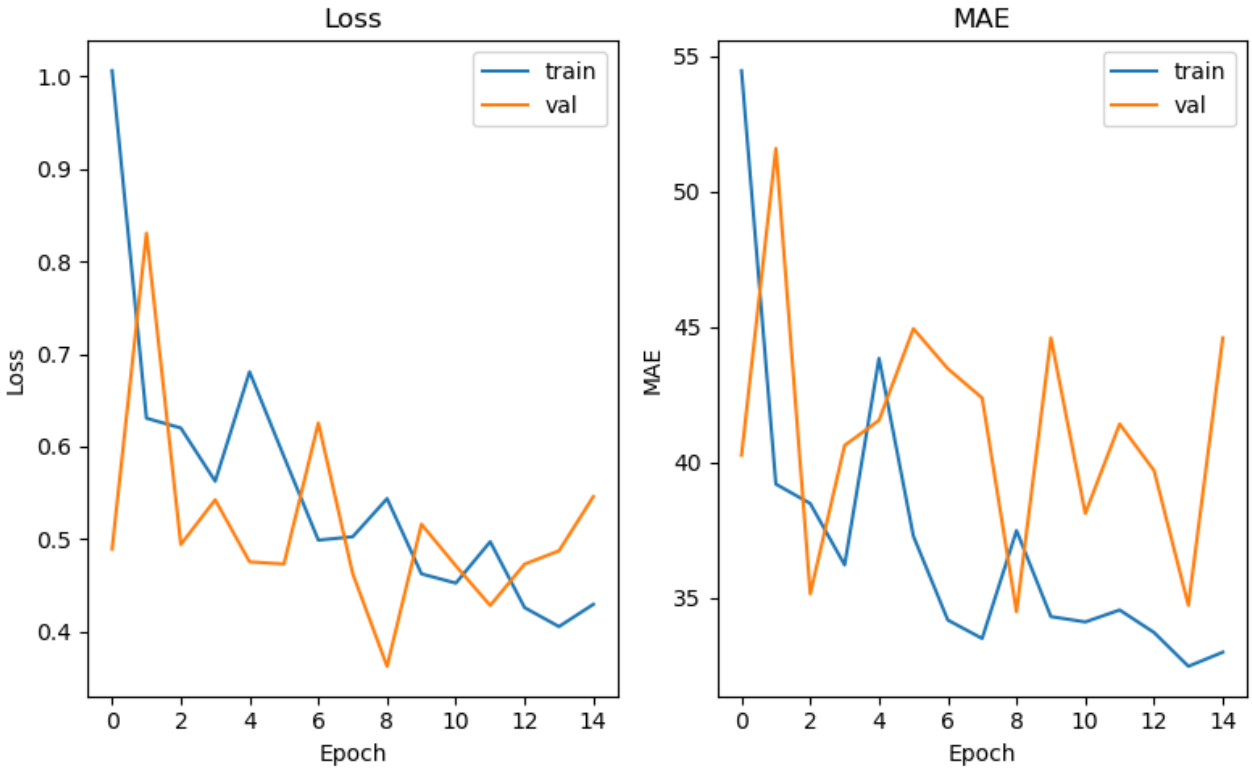
```
100%|██████████| 67/67 [00:19<00:00,  3.51it/s]
Train:  Time 0.210      Data 0.151      Loss 0.5025     MAE 33.486
100%|██████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.405      Loss 0.4627     MAE 42.372
Epoch 8/14
----------
100%|██████████| 67/67 [00:18<00:00,  3.56it/s]
Train:  Time 0.206      Data 0.149      Loss 0.5437     MAE 37.471
100%|██████████| 9/9 [00:09<00:00,  1.04s/it]
Test:   Time 0.484      Loss 0.3625     MAE 34.471
Epoch 9/14
----------
100%|██████████| 67/67 [00:18<00:00,  3.55it/s]
Train:  Time 0.207      Data 0.149      Loss 0.4624     MAE 34.295
100%|██████████| 9/9 [00:08<00:00,  1.06it/s]
Test:   Time 0.393      Loss 0.5161     MAE 44.592
Epoch 10/14
----------
100%|██████████| 67/67 [00:18<00:00,  3.62it/s]
Train:  Time 0.202      Data 0.142      Loss 0.4524     MAE 34.097
100%|██████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.401      Loss 0.4711     MAE 38.106
Epoch 11/14
----------
100%|██████████| 67/67 [00:20<00:00,  3.35it/s]
Train:  Time 0.224      Data 0.159      Loss 0.4972     MAE 34.538
100%|██████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.401      Loss 0.4282     MAE 41.408
Epoch 12/14
----------
100%|██████████| 67/67 [00:18<00:00,  3.59it/s]
Train:  Time 0.204      Data 0.147      Loss 0.4259     MAE 33.707
100%|██████████| 9/9 [00:08<00:00,  1.06it/s]
Test:   Time 0.392      Loss 0.4729     MAE 39.691
Epoch 13/14
----------
100%|██████████| 67/67 [00:19<00:00,  3.52it/s]
Train:  Time 0.209      Data 0.149      Loss 0.4054     MAE 32.458
100%|██████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.399      Loss 0.4873     MAE 34.707
Epoch 14/14
----------
100%|██████████| 67/67 [00:18<00:00,  3.64it/s]
Train:  Time 0.200      Data 0.138      Loss 0.4295     MAE 32.980
100%|██████████| 9/9 [00:08<00:00,  1.05it/s]
Test:   Time 0.398      Loss 0.5460     MAE 44.589
```

In [22]:

```
# test best model
print('---------Evaluate Model on Test Set---------------')
best_checkpoint = torch.load('model_best.pth.tar')
model.load_state_dict(best_checkpoint['state_dict'])
_, l=validate(test_loader, model, criterion, normalizer, test=True)
```

```
---------Evaluate Model on Test Set---------------
100%|██████████| 9/9 [00:09<00:00,  1.01s/it]
Test:   Time 0.459      Loss 1.2363     MAE 53.165
```

In [23]:
```
# visualize the training and val loss
# visualize the training and val mae
import matplotlib.pyplot as plt
from matplotlib.ticker import MaxNLocator

fig, ax = plt.subplots(1, 2, figsize=(8, 5))
ax[0].plot(running_record['train_loss'], label='train')
ax[0].plot(running_record['val_loss'], label='val')
ax[0].set_xlabel('Epoch')
ax[0].set_ylabel('Loss')
ax[0].legend()
ax[0].set_title('Loss')
# set x axis to be integer
ax[0].xaxis.set_major_locator(MaxNLocator(integer=True))

ax[1].plot(running_record['train_mae'], label='train')
ax[1].plot(running_record['val_mae'], label='val')
ax[1].set_xlabel('Epoch')
ax[1].set_ylabel('MAE')
ax[1].legend()
ax[1].set_title('MAE')
# set x axis to be integer
ax[1].xaxis.set_major_locator(MaxNLocator(integer=True))

plt.tight_layout()
plt.show()
```



In [ ]:
```
```