In [ ]:
```
import itertools

from tqdm import tqdm
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split

import torch
import torch.nn as nn
```

Question 1

(a)

In [ ]:
```
import pickle
from torch.utils.data import Dataset, DataLoader


class MnistDataset():
    def __init__(self, X, y, transform_X=lambda x: x):
        assert X.shape[0] == y.shape[0]
        self.X = transform_X(X)
        self.y = y

    def __len__(self):
        return len(self.y)

    def __getitem__(self, idx):
        return self.X[idx], self.y[idx]


def load_mnist(path):
    with open(path, 'rb') as f:
        train_data, test_data = pickle.load(f)

    X_train = torch.tensor(train_data[0], dtype=torch.float).unsqueeze(1)
    y_train = torch.tensor(train_data[1], dtype=torch.long)
    X_test = torch.tensor(test_data[0], dtype=torch.float).unsqueeze(1)
    y_test = torch.tensor(test_data[1], dtype=torch.long)
    return X_train, y_train, X_test, y_test
```

In [ ]:
```
# load data and normalize by dividing the maximum value
X_train, y_train, X_test, y_test = load_mnist('mnist.pkl')
X_train /= torch.max(X_train)
X_test /= torch.max(X_test)
```

In [ ]:
```
# further split the train to train/validation with 80/20
X_further_train, X_val, y_further_train, y_val = train_test_split(X_train, y

# use MnistDataset class to handle the data
```

```
train_data = MnistDataset(X_further_train, y_further_train)
val_data = MnistDataset(X_val, y_val)
test_data = MnistDataset(X_test, y_test)
```

(b)

In [ ]:

```
class VAE(nn.Module):
    def __init__(self, in_channels=1, z_dim=32):
        super().__init__()
        self.encoder = nn.Sequential(
            # conv1, input_channel -> 4
            nn.Conv2d(in_channels, 4, kernel_size=4, padding=1, stride=2),
            nn.ReLU(), # relu
            # conv2, channel 4 -> 8
            nn.Conv2d(4, 8, kernel_size=4, padding=1, stride=2),
            nn.ReLU(), # relu
            nn.Conv2d(8, 16, kernel_size=4, padding=1, stride=2),  # conv3,
            nn.ReLU(), # relu
            nn.Conv2d(16, 32, kernel_size=4, padding=1, stride=2), # conv4,
            nn.ReLU(), # relu
            nn.Flatten(), # flatten
        )

        # manually calculate the dimension after all convolutions
        dim_after_conv = 2
        hidden_dim = 32 * dim_after_conv * dim_after_conv

        # Readout layer is mu
        self.readout_mu = nn.Linear(hidden_dim, z_dim)
        # Readout layer
        self.readout_sigma = nn.Linear(hidden_dim, z_dim)

        # You can use nn.ConvTranspose2d to decode
        self.decoder = nn.Sequential(
            nn.Linear(z_dim, hidden_dim),
            nn.Unflatten(1, (32, dim_after_conv, dim_after_conv)),
            nn.ConvTranspose2d(32, 16, kernel_size=4, stride=2, padding=1),
            nn.ReLU(), # relu
            nn.ConvTranspose2d(16, 8, kernel_size=4, stride=2, padding=1), #
            nn.ReLU(), # relu
            nn.ConvTranspose2d(8, 4, kernel_size=4, stride=2, padding=1), #
            nn.ReLU(), # relu
            nn.ConvTranspose2d(4, in_channels, kernel_size=4, stride=2, padd
            nn.Sigmoid(), # use a sigmoid activation to squeeze the outputs
        )

    def reparameterize(self, mu, sigma):
        """
        Reparameterize, i.e. generate a z ~ N(\mu, \sigma)
        """
        # generate epsilon ~ N(0, I)
        # hint: use torch.randn or torch.randn_like
        epsilon = torch.randn_like(sigma)
        # z = \mu + \sigma * \epsilon
```

```
        z = mu + sigma * epsilon
        return z

    def encode(self, x):
        # call the encoder to map input to a hidden state vector
        h = self.encoder(x)
        # use the "readout" layer to get \mu and \sigma
        mu = self.readout_mu(h)
        sigma = self.readout_sigma(h)
        return mu, sigma

    def decode(self, z):
        # call the decoder to map z back to x
        return self.decoder(z)

    def forward(self, x):
        mu, sigma = self.encode(x)
        z = self.reparameterize(mu, sigma)
        x_recon = self.decode(z)
        return x_recon, mu, sigma
```

(c)

For debugging: The `test_kld_loss_func` should output 1.3863

In [ ]:

```
def kld_loss_func(mu, sigma):
    """
    KL-Divergence: KLD = 0.5 * sum(\mu^2 + \sigma^2 - ln(\sigma^2) - 1)

    Parameters
    ----------
    mu: torch.Tensor
        Mean vector in the VAE bottleneck region
    sigma: torch.Tensor
        Standard Deviation vector in the VAE bottleneck region

    Return
    ------
    kld: torch.Tensor
        KL-Divegence loss (a scalar)
    """
    return 0.5 * torch.sum(mu.pow(2) + sigma.pow(2) - torch.log(sigma.pow(2)


def vae_loss_func(recon_x, x, mu, sigma):

    bce_loss = nn.BCELoss(reduction='sum')(recon_x, x)
    kld_loss = kld_loss_func(mu, sigma)

    return bce_loss + kld_loss


def test_kld_loss_func():
    mu = torch.tensor([0.5, 0.5, 1.0])
```

```
    sigma = torch.tensor([1.0, 0.5, 0.5])
    print(kld_loss_func(mu, sigma))

test_kld_loss_func()
```

```
tensor(1.3863)
```

In [ ]:
```
import torch.nn.functional as F

class VAETrainer:

    def __init__(self, model, learning_rate, batch_size, 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.optimizer = torch.optim.Adam(model.parameters(), learning_rate,

        self.epoch = epoch
        self.batch_size = batch_size



    def train(self, train_data, val_data, early_stop=True, verbose=True, dra
        train_loader = DataLoader(train_data, batch_size=self.batch_size, sh

        train_loss_list = []
        val_loss_list = []

        weights = self.model.state_dict()
        lowest_val_loss = np.inf

        for n in tqdm(range(self.epoch), leave=False):
            self.model.train()
            epoch_loss = 0.0
            for X_batch, y_batch in train_loader:
                batch_importance = 1 / len(train_data)
                # call the model
                X_batch_recon, mu, sigma = self.model(X_batch)
                batch_loss = vae_loss_func(X_batch_recon, X_batch, mu, sigma

                self.optimizer.zero_grad()
                batch_loss.backward()
                self.optimizer.step()

                epoch_loss += batch_loss.detach().cpu().item() * batch_impor

            train_loss_list.append(epoch_loss)

            val_loss = self.evaluate(val_data, print_loss=False)
            val_loss_list.append(val_loss)

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

```
        if draw_curve:
            x_axis = np.arange(self.epoch)
            fig, ax = plt.subplots(1, 1, figsize=(5, 4))
            ax.plot(x_axis, train_loss_list, label="Train")
            ax.plot(x_axis, val_loss_list, label="Validation")
            ax.set_title("Total Loss")
            ax.set_xlabel("# Epoch")

        if early_stop:
            self.model.load_state_dict(weights)

        return {
            "train_loss_list": train_loss_list,
            "val_loss_list": val_loss_list,
        }

    def evaluate(self, data, print_loss=True):
        self.model.eval()
        loader = DataLoader(data, batch_size=self.batch_size)
        total_loss = 0.0
        for X_batch, y_batch in loader:
            with torch.no_grad():
                batch_importance = 1 / len(data)
                X_batch_recon, mu, sigma = self.model(X_batch)
                batch_loss = vae_loss_func(X_batch_recon, X_batch, mu, sigma
                total_loss += batch_loss.detach().cpu().item() * batch_impor
        if print_loss:
            print(f"Total Loss: {total_loss}")
        return total_loss
```

In [ ]:

```
train_loader = DataLoader(train_data, batch_size=128, shuffle=True)
for X_batch, y_batch in train_loader:
    print(X_batch.shape)
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torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
torch.Size([128, 1, 32, 32])
```

In [ ]:
```
x, y = next(iter(train_loader))
```

In [ ]:
```
y.shape
```

Out[ ]:
```
torch.Size([128])
```

In [ ]:
```
x.shape
```

Out[ ]:
```
torch.Size([128, 1, 32, 32])
```

In [ ]:
```
vae = VAE()
```

In [ ]:
```
vae(x)
```

Out[ ]:
```
(tensor([[[[0.5465, 0.5466, 0.5461,  ..., 0.5467, 0.5459, 0.5462],
           [0.5431, 0.5441, 0.5418,  ..., 0.5430, 0.5411, 0.5471],
           [0.5462, 0.5461, 0.5440,  ..., 0.5463, 0.5431, 0.5472],
           ...,
           [0.5431, 0.5445, 0.5424,  ..., 0.5439, 0.5422, 0.5468],
           [0.5462, 0.5462, 0.5440,  ..., 0.5469, 0.5421, 0.5468],
           [0.5446, 0.5432, 0.5440,  ..., 0.5433, 0.5442, 0.5450]]],


         [[[0.5465, 0.5465, 0.5461,  ..., 0.5467, 0.5459, 0.5462],
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           [0.5462, 0.5462, 0.5440,  ..., 0.5463, 0.5431, 0.5472],
           ...,
           [0.5431, 0.5445, 0.5423,  ..., 0.5439, 0.5422, 0.5468],
           [0.5462, 0.5462, 0.5440,  ..., 0.5469, 0.5421, 0.5468],
           [0.5446, 0.5432, 0.5440,  ..., 0.5434, 0.5442, 0.5450]]],


         [[[0.5465, 0.5465, 0.5461,  ..., 0.5467, 0.5459, 0.5462],
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           [0.5462, 0.5462, 0.5440,  ..., 0.5463, 0.5431, 0.5472],
           ...,
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           [0.5446, 0.5432, 0.5440,  ..., 0.5433, 0.5442, 0.5450]]],


         ...,


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           ...,
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           [0.5446, 0.5432, 0.5440,  ..., 0.5433, 0.5442, 0.5450]]],


         [[[0.5465, 0.5466, 0.5461,  ..., 0.5467, 0.5459, 0.5462],
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           ...,
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         [[[0.5465, 0.5465, 0.5461,  ..., 0.5467, 0.5459, 0.5462],
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           ...,
           [0.5431, 0.5445, 0.5424,  ..., 0.5439, 0.5422, 0.5468],
           [0.5462, 0.5462, 0.5440,  ..., 0.5469, 0.5421, 0.5468],
           [0.5446, 0.5432, 0.5440,  ..., 0.5434, 0.5442, 0.5450]]]],
        grad_fn=<SigmoidBackward0>),
```

```
tensor([[-0.0063,  0.0882,  0.0155,  ..., -0.0328,  0.0110, -0.0878],
        [-0.0067,  0.0876,  0.0164,  ..., -0.0327,  0.0111, -0.0903],
        [-0.0060,  0.0866,  0.0179,  ..., -0.0334,  0.0124, -0.0885],
        ...,
        [-0.0091,  0.0878,  0.0183,  ..., -0.0336,  0.0114, -0.0815],
        [-0.0089,  0.0875,  0.0205,  ..., -0.0341,  0.0110, -0.0853],
        [-0.0068,  0.0873,  0.0178,  ..., -0.0346,  0.0101, -0.0884]],
       grad_fn=<AddmmBackward0>),
tensor([[ 0.0068,  0.0253,  0.0311,  ...,  0.0323,  0.0757, -0.0555],
        [ 0.0057,  0.0251,  0.0289,  ...,  0.0334,  0.0748, -0.0554],
        [ 0.0035,  0.0267,  0.0292,  ...,  0.0345,  0.0760, -0.0548],
        ...,
        [ 0.0020,  0.0261,  0.0306,  ...,  0.0363,  0.0740, -0.0537],
        [ 0.0047,  0.0252,  0.0276,  ...,  0.0314,  0.0759, -0.0552],
        [ 0.0063,  0.0269,  0.0267,  ...,  0.0357,  0.0750, -0.0543]],
       grad_fn=<AddmmBackward0>))
```

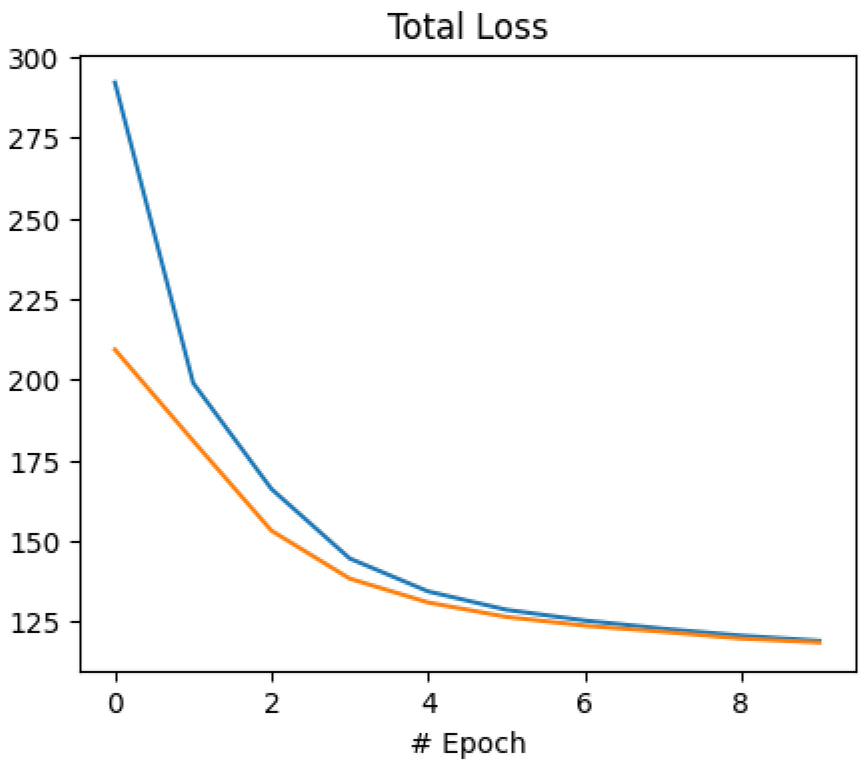
In [ ]:

```python
vae = VAE()
trainer = VAETrainer(vae, 1e-3, 128, 10, 1e-5)
# train
trainer.train(train_data, val_data)
```

```
VAE - Number of parameters: 34201
```

Out[ ]:

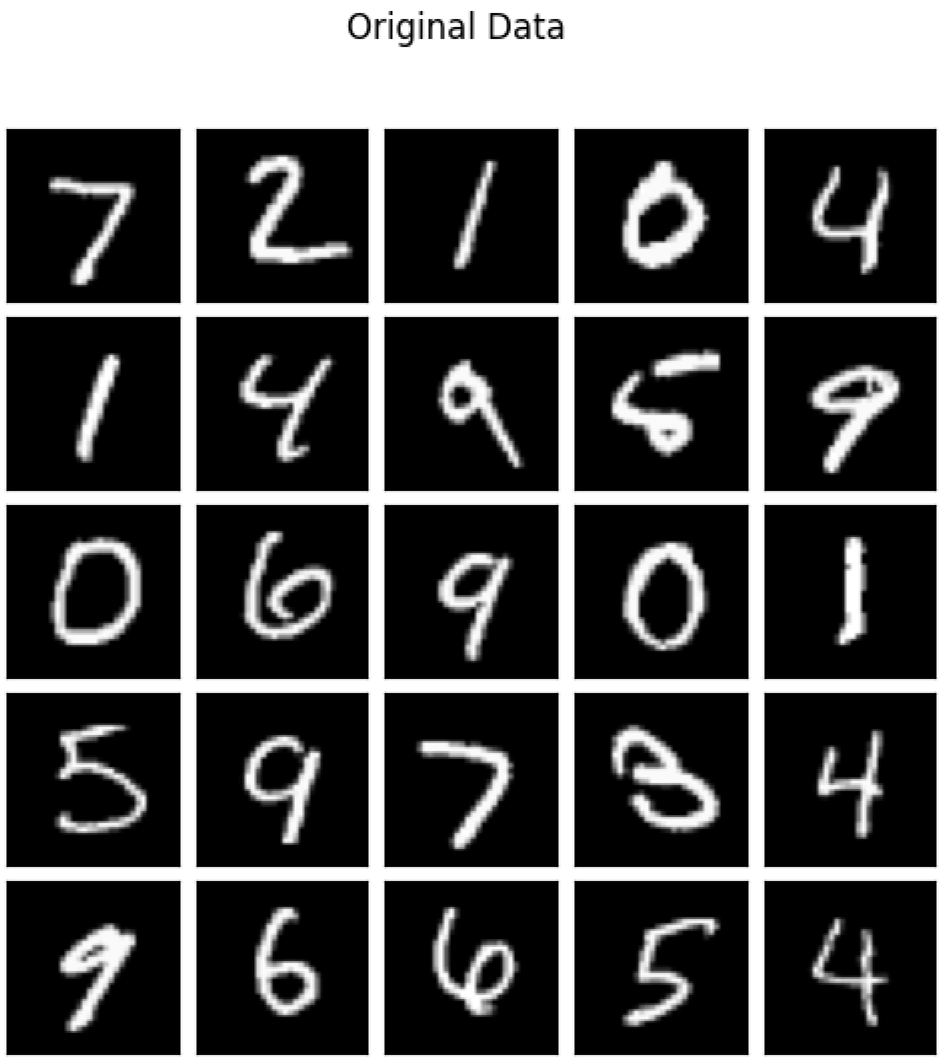
```
{'train_loss_list': [292.1656652832029,
  198.88523193359373,
  166.01494095865885,
  144.44174377441396,
  134.2405961710612,
  128.53765653483072,
  125.20061944580074,
  122.6587432657878,
  120.50614562988284,
  118.90336954752603],
 'val_loss_list': [209.27612076822913,
  180.93946402994783,
  153.07922412109372,
  138.20236848958334,
  130.80785856119792,
  126.32972094726566,
  123.6293977050781,
  121.72244881184905,
  119.62093229166669,
  118.39482324218758]}
```

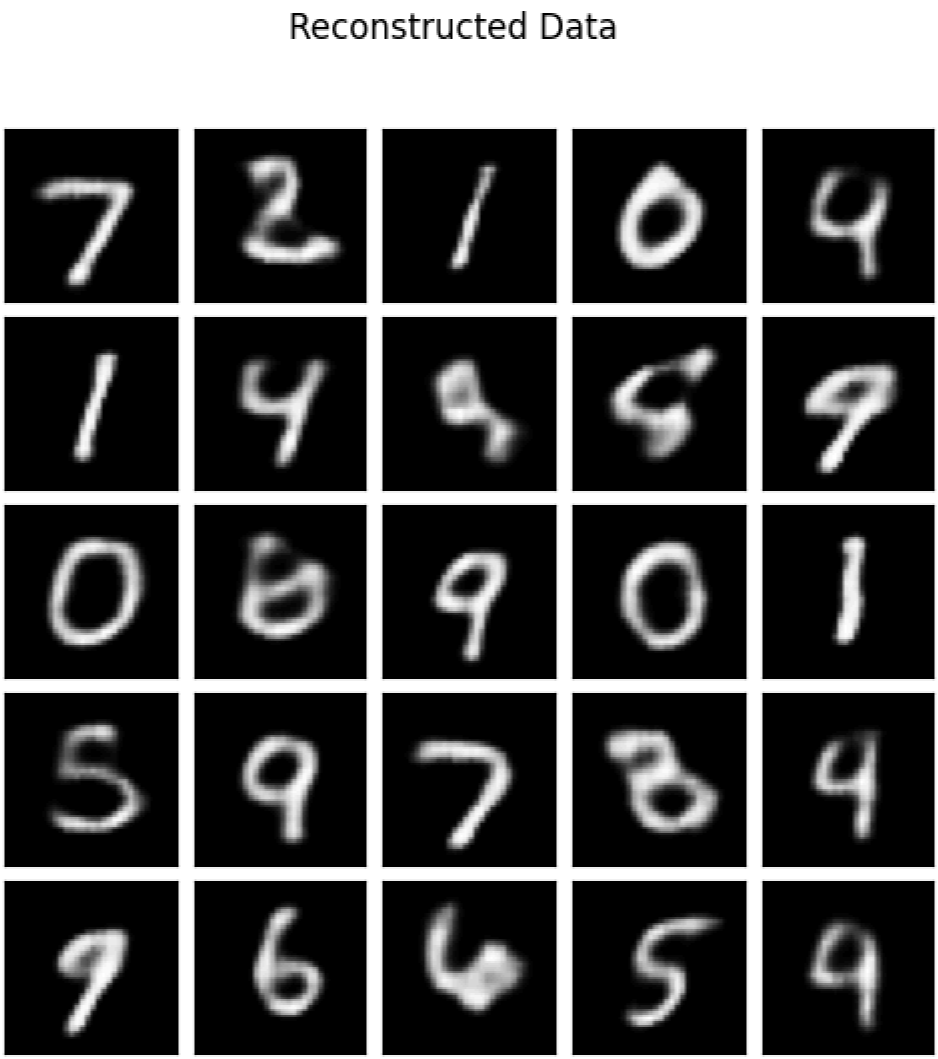


In [ ]:
```
# evaulate the qualitiy of reconstruction
def plot_digits(data, title):
    fig, axes = plt.subplots(5, 5, figsize=(6, 6))
    fig.subplots_adjust(hspace=0.1, wspace=0.1)
    fig.suptitle(title)
    for i, ax in enumerate(axes.flatten()):
        im = ax.imshow(data[i].reshape(32, 32), cmap='gray')
        ax.set_xticks([])
        ax.set_yticks([])

def compare_reconstruct(model, X):
    plot_digits(X, "Original Data")
    with torch.no_grad():
        X_recon, _, _ = model(X)
    plot_digits(X_recon, "Reconstructed Data")


compare_reconstruct(trainer.model, X_test[:100])
```


Original Data



Reconstruction worked well! If I had more time to train on additional epochs, then reconstruction could potentially look even better!

Question 2

In [ ]:
```
from torch_geometric.datasets import QM9
from torch_geometric.loader import DataLoader as GraphDataLoader
from torch_geometric.utils import scatter
```

(a)

In [ ]:
```
def load_qm9(path="./QM9"):
    def transform(data):
        edge_index = torch.tensor(
            list(itertools.permutations(range(data.x.shape[0]), 2)),
            dtype=torch.long
        ).T
        edge_feature = 1 / torch.sqrt(
            torch.sum(
```

```
                (data.pos[edge_index[0]] - data.pos[edge_index[1]]) ** 2,
                axis=1, keepdim=True
            )
        )
        data.edge_index = edge_index
        data.edge_attr = edge_feature
        data.y = data.y[:, [-7]]
        return data

    qm9 = QM9(path, transform=transform)
    return qm9

qm9 = load_qm9("./QM9")
train_data, test_data = train_test_split(qm9, train_size=0.8, test_size=0.2)
```

In [ ]:
```
qm9[0].x.shape
```

Out[ ]: torch.Size([5, 11])

In [ ]:
```
qm9[0].edge_attr.shape
```

Out[ ]: torch.Size([20, 1])

In [ ]:
```
# find out the dimension of node input features
node_input_dim = 11
edge_input_dim = 1
```

(b)

In [ ]:
```
class Layer(nn.Module):
    """
    Basic layer, a linear layer with a ReLU activation
    """
    def __init__(self, in_dim, out_dim):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(in_dim, out_dim), # linear layer
            nn.ReLU() # relu
        )

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


class MessagePassingLayer(nn.Module):
    """
    A message passing layer that updates nodes/edge features
    """
    def __init__(self, node_hidden_dim, edge_hidden_dim):
        super().__init__()
        # figure out the input/output dimension
        self.edge_net = Layer(2*node_hidden_dim + edge_hidden_dim, edge_hidd
        # figure out the input/output dimension
```

```
        self.node_net = Layer(node_hidden_dim + edge_hidden_dim, node_hidder

    def forward(self, node_features, edge_features, edge_index):
        """
        Update node and edge features

        Parameters
        ----------
        node_features: torch.Tensor
            Node features from the previous layer
        edge_features: torch.Tensor
            Edge features from the previous layer
        edge_index: torch.Tensor
            A sparse matrix (n_edge, 2) in which each column denotes node ir
        """
        # concatnate previous edge features with node features forming the e
        # hint: use edge_features[edge_index[0(or 1)]] to get node features
        concate_edge_features = torch.cat([
            node_features[edge_index[0]], # features of one node
            node_features[edge_index[1]], # features of the other node
            edge_features # previous edge features
        ], dim=1)

        # pass through the "edge_net" to map it back to the original dimensi
        updated_edge_features = self.edge_net(concate_edge_features)


        # use scatter to aggrate the edge features to nodes
        aggr_edge_features = scatter(updated_edge_features, edge_index[0])
        # concatenate it with previous node features
        concate_node_features = torch.cat([aggr_edge_features, node_features
        # pass through the "node_net" to map it back to the original dimensi
        updated_node_features = self.node_net(concate_node_features)

        return updated_node_features, updated_edge_features


class GraphNet(nn.Module):
    def __init__(self, node_input_dim, edge_input_dim, node_hidden_dim, edge
        super().__init__()
        # embed the input node features
        self.node_embed = Layer(node_input_dim, node_hidden_dim)
        # embed the input edge features
        self.edge_embed = Layer(edge_input_dim, edge_hidden_dim)
        # message passing layer
        self.message_passing = MessagePassingLayer(node_hidden_dim, edge_hic
        # use a linear layer as readout to get the "atomic" energy contribut
        self.readout = Layer(node_hidden_dim, 1)


    def forward(self, node_features, edge_features, edge_index, batch):
        """
        Update node and edge features

        Parameters
        ----------
```

```
        node_features: torch.Tensor
            Node features from the previous layer
        edge_features: torch.Tensor
            Edge features from the previous layer
        edge_index: torch.Tensor
            A sparse matrix (n_edges, 2) in which each column denotes node i
        batch: torch.Tensor
            A 1-D tensor (n_nodes,) that tells you each node belongs to whic
        """
        node_hidden = self.node_embed(node_features) # call the node embeddi
        edge_hidden = self.edge_embed(edge_features) # call the edge embeddi
        updated_node_hidden, updated_edge_hidden = self.message_passing(node
        readout = self.readout(updated_node_hidden) # use the readout layer
        out = scatter(readout, batch) # use the scatter function to aggregat
        return out
```

In [ ]:

```
class GNNTrainer:
    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

    def train(self, dataset, draw_curve=True):
        self.model.train()
        loader = GraphDataLoader(dataset, batch_size=self.batch_size, shuffl

        loss_func = nn.MSELoss()
        batch_loss_list = []
        for i in range(self.epoch):
            print(f"Epoch: {i}")
            for batch_data in tqdm(loader, leave=False):
                batch_size = batch_data.y.shape[0]
                batch_pred = self.model(batch_data.x, batch_data.edge_attr,
                batch_loss = loss_func(batch_pred, batch_data.y)

                self.optimizer.zero_grad()
                batch_loss.backward()
                self.optimizer.step()

                batch_loss_list.append(batch_loss.detach().numpy())

        if draw_curve:
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            ax.set_yscale("log")
            ax.plot(np.arange(len(batch_loss_list)), batch_loss_list)
            ax.set_xlabel("# Batch")
            ax.set_ylabel("Loss")

        return batch_loss_list

    def evaluate(self, dataset, draw_curve=True):
```

```
        self.model.eval()
        loader = GraphDataLoader(dataset, batch_size=self.batch_size)
        y_true, y_pred = [], []
        with torch.no_grad():
            for batch_data in tqdm(loader, leave=False):
                batch_pred = self.model(batch_data.x, batch_data.edge_attr,
                y_pred.append(batch_pred.detach().numpy().flatten())
                y_true.append(batch_data.y.detach().numpy().flatten())

        y_true = np.concatenate(y_true)
        y_pred = np.concatenate(y_pred)
        mse = np.mean((y_true - y_pred) ** 2)

        if draw_curve:
            fig, ax = plt.subplots(1, 1, figsize=(5, 4), constrained_layout=
            ax.scatter(y_true, y_pred, label=f"MSE: {mse:.2f}", s=2)
            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 mse
```

(c)

In [ ]:
```
node_hidden_dim = 64
edge_hidden_dim = 64

net = GraphNet(node_input_dim, edge_input_dim, node_hidden_dim, edge_hidden_
```

In [ ]:
```
loader = GraphDataLoader(test_data, batch_size=512)
loader_iter = iter(loader)
```

In [ ]:
```
batch_data = next(loader_iter)
batch_data.y
```

Out[ ]:
```
tensor([[ -70.4864],
        [ -75.7974],
        [ -79.6356],
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        [ -78.8615],
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```

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```

```
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In [ ]:
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In [ ]:

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loss_func = nn.MSELoss()
loss_func(batch_pred, batch_data.y)
```

Out[ ]:

```
tensor(9634.5879, grad_fn=<MseLossBackward0>)
```

In [ ]:

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# 1e-3, 128, 10, 1e-5

# train
learning_rate = 1e-3
n_epoch = 3
batch_size = 512
l2 = 1e-5

trainer = GNNTrainer(net, batch_size, learning_rate, n_epoch, l2)
trainer.train(train_data)
```

```
GraphNet - Number of parameters: 21569
Epoch: 0

Epoch: 1

Epoch: 2
```

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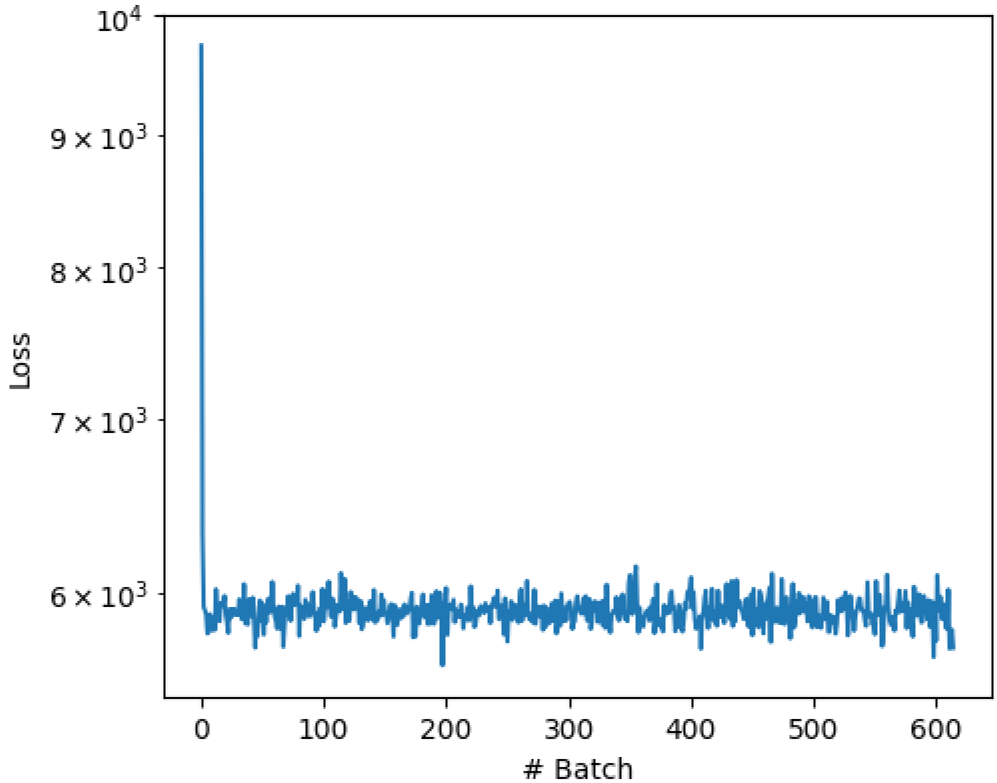
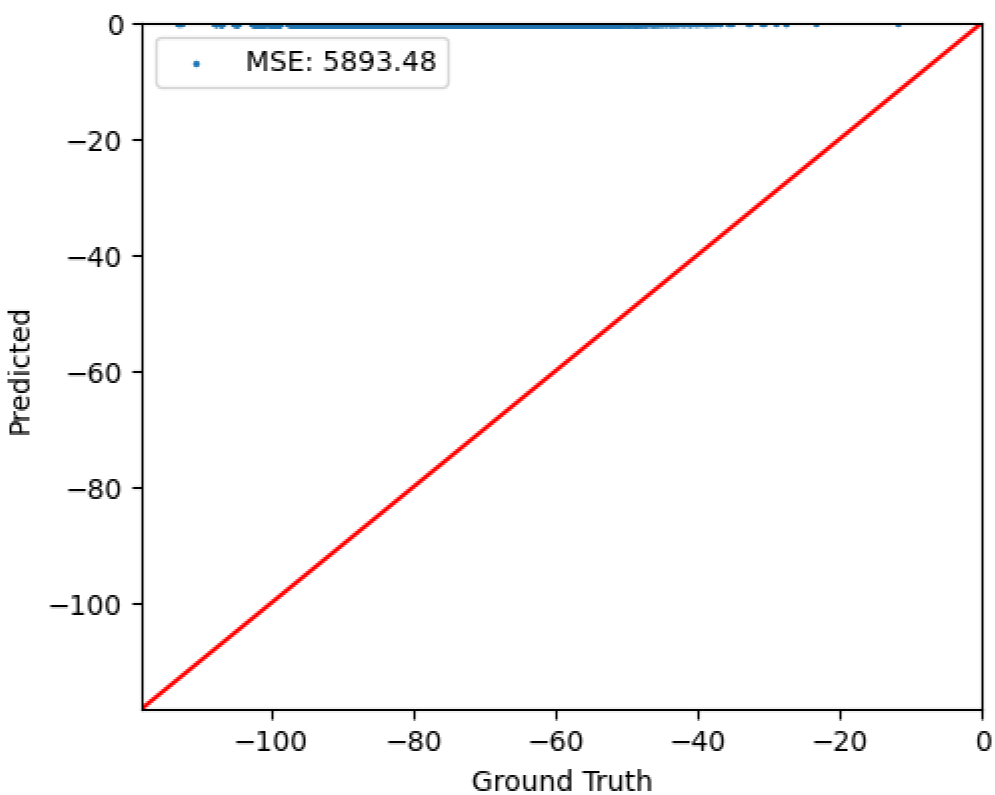
                 array(6032.544, dtype=float32),
                 array(5949.9043, dtype=float32),
                 array(5879.146, dtype=float32),
                 array(5944.947, dtype=float32),
                 array(5992.7407, dtype=float32),
                 array(5880.576, dtype=float32),
                 array(5844.6533, dtype=float32),
                 array(5848.64, dtype=float32),
                 array(5983.8257, dtype=float32),
                 array(5906.478, dtype=float32),
                 array(5952.6504, dtype=float32),
                 array(5860.211, dtype=float32),
                 array(5960.6523, dtype=float32),
                 array(5820.9834, dtype=float32),
                 array(5855.7983, dtype=float32),
                 array(5952.442, dtype=float32),
                 array(5667.8994, dtype=float32),
                 array(5918.335, dtype=float32),
                 array(5750.4834, dtype=float32),
                 array(6094.6396, dtype=float32),
                 array(5907.0166, dtype=float32),
                 array(5980.665, dtype=float32),
                 array(5972.9824, dtype=float32),
                 array(5859.949, dtype=float32),
                 array(5911.221, dtype=float32),
                 array(5939.78, dtype=float32),
                 array(5818.5376, dtype=float32),
                 array(5810.804, dtype=float32),
                 array(6017.117, dtype=float32),
                 array(5710.3623, dtype=float32),
                 array(5783.8438, dtype=float32),
                 array(5806.9355, dtype=float32),
                 array(5714.5273, dtype=float32)]
```



In [ ]:
```
# evaulate
trainer.evaluate(test_data)
```

Out[ ]: 5893.482



It appears that the MSE is quite large, as we are always predicting a slightly positive enthalpy of formation, versus the true enthalpy of formations being negative.