- Costruire un dataset di grafi di spin glass di piccola taglia (# basso di nodi) e studiare come l'apprendimento dell'energia da parte della GNN cambia al variare della connettività del grafo. Ad esempio fissando a 10 il numero di nodi, il numero di edges può essere cambiato da 9 (open spin glass chain) a 45 (fully connected spin glass) , magari provando 9, 15, 25, 45. Si costruiscono 4 dataset e si allena la stessa GNN separatamente su questi dataset in modo supervised per fare poi il confronto. (Livello medio)

In [ ]:
```python
import torch
from torch_geometric.data import Data
from torch_geometric.utils import to_networkx, from_networkx
import networkx as nx
import matplotlib.pyplot as plt
import numpy as np

import seaborn as sns
import matplotlib.pyplot as plt
from matplotlib.offsetbox import AnchoredText

import torch.nn.functional as F
from torch_geometric.profile import get_model_size

from torch.nn import Linear
from torch_geometric.nn import global_max_pool, GraphConv
from torch_geometric.loader import DataLoader

import os
```

In [ ]:
```python
# set standard dimensions for the plots
plt.rcParams['figure.figsize'] = (10, 6)
plt.rcParams['font.size'] = 14
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['axes.titlesize'] = 14
plt.rcParams['xtick.labelsize'] = 14
plt.rcParams['ytick.labelsize'] = 14
plt.rcParams['legend.fontsize'] = 14
```

In [ ]:
```python
def initialize_graph(L, periodic=True, n_dimensions=2):
    """
    Initialize a graph with L nodes
    """
    G = nx.Graph()
    for i in range(L):
        G.add_node(i, spin = np.random.choice([-1, 1]))

    for i in range(L):
        if periodic:
            for j in range(i+1, i+n_dimensions+1):
                G.add_edge(i, j % L, weight = np.random.rand()*2 -1 )
        else:
            for j in range(i+1, i+n_dimensions+1):
                if j < L:
                    G.add_edge(i, j, weight = np.random.rand()*2 -1 )
    return G
```

```
def plot_graph(G, pos=None):
    """
    Plot the graph with nodes colored according to their spin.
    """
    if pos is None:
        pos = nx.circular_layout(G)
    colors = ['blue' if G.nodes[i]["spin"] == 1 else 'red' for i in range
    fig = plt.figure()
    nx.draw(G, pos = pos, node_color=colors, with_labels=True)
    plt.show(fig)
    return fig


def calculate_energy(G, h=0 ):
    """
    Calculate the energy of the graph
    """
    E = 0
    E_h = 0
    for i, j in G.edges:
        E += G[i][j]["weight"] * G.nodes[i]["spin"] * G.nodes[j]["spin"]

    if h != 0:  # exclude the case of h = 0 to avoid floating point error
        E_h = h * np.sum([G.nodes[i]["spin"] for i in G.nodes])


    return -E/2 - E_h  # divide by 2 to avoid double counting

# create a dataset with the energy as label
def create_dataset(n_nodes=10, h=0, periodic= True, n_dimensions=1, n_sam
    dataset = []
    graphs = []

    for i in range(n_samples):
        G = initialize_graph(n_nodes, periodic=periodic, n_dimensions=n_d
        X = torch.tensor([G.nodes[i]["spin"] for i in G.nodes]).float().v

        graphs.append(G)
        dataset.append(
            Data(x = X,
                edge_index = torch.tensor(np.array(G.edges).T, dtype=torc
                edge_weight = torch.tensor([G[i][j]["weight"] for i, j in
                y = torch.tensor([calculate_energy(G, h)], dtype=torch.fl

    return dataset, graphs
```

In [ ]:

```
# GNN model

class GNN(torch.nn.Module):
    def __init__(self,hidden_channels_1=16, hidden_channels_2=16, hidden_
                 lr = 1e-5, weight_decay=1e-3, dropout=0.5, num_node_feat
        super(GNN, self).__init__()
        self.conv1 = GraphConv(num_node_features,hidden_channels_1)
        self.conv2 = GraphConv(hidden_channels_1, hidden_channels_2)
        self.conv3 = GraphConv(hidden_channels_2, hidden_channels_3)
        self.conv4 = GraphConv(hidden_channels_3, hidden_channels_4)

        self.pool = global_max_pool
```

```
        self.linear1 = Linear(hidden_channels_4, hidden_linear)
        self.linear2 = Linear(hidden_linear, num_classes)



        self.dropout = torch.nn.Dropout(dropout)

        # we should consider also batch normalization in case of overfitt



        # Optimizer:
        self.optimizer = torch.optim.Adam(self.parameters(), lr=lr, weigh

        # Loss function:
        self.criterion = torch.nn.MSELoss()



    def forward(self, data):
        x, edge_index, edge_weight = data.x, data.edge_index, data.edge_w
        x = F.leaky_relu(self.conv1(x, edge_index, edge_weight))
        x = F.leaky_relu(self.conv2(x, edge_index, edge_weight))
        x = F.leaky_relu(self.conv3(x, edge_index, edge_weight))
        x = F.leaky_relu(self.conv4(x, edge_index, edge_weight))

        x = self.pool(x, data.batch) # [n_nodes*n_graph_of_the_batch, n_f

        #x = torch.flatten(x) # not needed since we are using global_max_
        #print(x.shape)
        x = self.dropout(x)
        x = F.leaky_relu(self.linear1(x))
        out = self.linear2(x)

        return out



    def train_step(self, data):
        # Reset gradients
        self.optimizer.zero_grad()
        # Passing the node features and the connection info
        prediction = self.forward(data)
        # reshape the prediction to match the shape of the target
        prediction = prediction.view(data.y.shape)
        # Calculating the loss and gradients
        loss = self.criterion(prediction, data.y)
        #print("prediction:",prediction.shape)
        #print("data.y:",data.y.shape)
        loss.backward()
        # Update using the gradients
        self.optimizer.step()

        return loss.item()
```

In [ ]:
```
def plot_loss( train_losses, test_losses):
    fig = plt.figure()
    epoch = range(1, len(train_losses)+1)
    plt.plot(epoch, train_losses, label='Training Loss')
```

```
    plt.plot(epoch, test_losses, label='Test Loss')
    plt.xlabel('Epochs')
    plt.ylabel('Loss')
    plt.title('Losses')
    plt.legend()
    plt.grid(True)
    plt.show()
    return fig


def train_model(model, train_loader, test_loader, num_epochs, patience =

    if device is None:
        device = torch.device('cuda' if torch.cuda.is_available() else 'c

    # parameters for patience
    best_loss = np.inf
    patience_counter = 0


    epochs = range(1, num_epochs+1)
    train_losses, test_losses = [], []

    print('Training ...')

    for epoch in epochs:
        loss_per_epoch = []
        test_loss_per_epoch = []

        for i, mini_batch in enumerate(train_loader):
            mini_batch.to(device)
            train_loss = model.train_step(mini_batch)
            loss_per_epoch.append(train_loss)

        train_losses.append(sum(loss_per_epoch)/len(loss_per_epoch))


        with torch.no_grad():
            """Evaluate the model on test set"""
            for i, mini_batch in enumerate(test_loader):
                mini_batch.to(device)
                prediction = model.forward(mini_batch)
                prediction.to('cpu')
                test_loss = model.criterion(prediction, mini_batch.y).ite
                test_loss_per_epoch.append(test_loss)
            test_losses.append(sum(test_loss_per_epoch)/len(test_loss_per

            if test_losses[-1] < best_loss:
                best_loss = test_losses[-1]
                torch.save(model.state_dict(), model_name + '/model.pth')
                patience_counter = 0
            else:
                patience_counter += 1
                if patience_counter == patience:
                    print(f"Early stopping at epoch {epoch}")
                    break
        if verbose:
            print(f"Ep {epoch} \t| Loss {round(train_losses[-1], 5)} \t|
```

```
    return  train_losses, test_losses
```

In [ ]:
```
# set the model name based on the values
def set_model_name(n_nodes, n_dimensions, h, periodic,n_samples, hidden_c
                   hidden_channels_2, hidden_channels_3, hidden_channels
                   lr, weight_decay, dropout, epochs):
    return f"model_{n_nodes}_{n_dimensions}_{h}_{periodic}_{n_samples}_{h


# translate the model name into values
def print_values_from_model_name(model_name, print_values=True, return_di
    values = model_name.split('_')
    # create a dictionary to store the values
    dict = {"n_nodes": values[1], "n_dimensions": values[2], "h": values[
            "hidden_channels_1": values[6], "hidden_channels_2": values[7
            "lr": values[11], "weight_decay": values[12], "dropout": valu
    if print_values:
        for key, value in dict.items():
            print(f"{key}: {value}")
    if return_dict:
        return dict



def test_trained_model(model_name, test_loader, device = None):

    if device is None:
        device = torch.device('cuda' if torch.cuda.is_available() else 'c

    values = print_values_from_model_name(model_name, print_values=False,

    trained_model = GNN(hidden_channels_1= int(values["hidden_channels_1"
                hidden_channels_2= int(values["hidden_channels_2"]),
                hidden_channels_3= int(values["hidden_channels_3"]),
                hidden_channels_4= int(values["hidden_channels_4"]),
                hidden_linear= int(values["hidden_linear"]),
                lr= float(values["lr"]), weight_decay= float(values["weig

    trained_model.load_state_dict(torch.load(model_name + '/model.pth'))
    trained_model.to(device)

    fig = plt.figure()
    with torch.no_grad():
        predictions = []
        true_values = []
        for i, mini_batch in enumerate(test_loader):
            mini_batch.to(device)
            prediction = trained_model.forward(mini_batch)
            predictions.append(prediction.item())
            true_values.append(mini_batch.y.item())

        # save the mean squared error
        mse = np.mean((np.array(predictions) - np.array(true_values))**2)

        plt.scatter(true_values, predictions)
        plt.plot(true_values, true_values, color='red')
        plt.xlabel('True energy')
        plt.ylabel('Predicted energy')
        plt.title('Predicted vs True energy')
```

```
        at = AnchoredText(f"MSE: {np.round(mse,2)}", frameon=True, loc='u
        plt.gca().add_artist(at)

        # plot a box similar to the legend to show the MSE
        plt.grid(True)
        plt.show()



    return fig, mse
```

In [ ]:
```
# set the device and a random seed
torch.manual_seed(1022000)
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print('Device: ', device)

# set the palette
palette = sns.color_palette("coolwarm", as_cmap=True)
```

```
Device:  cuda
```

In [ ]:
```
# set standard parameters for the model

# parameters for the dataset
n_nodes = 10
h = 0
n_samples = 1000

# parameters for the model
num_epochs = 30
batch_size = 1
lr = 1e-4
weight_decay = 1e-4
dropout = 0.4
patience = 15

# parameters for the layers
hidden_channels_1 = 16
hidden_channels_2 = 32
hidden_channels_3 = 32
hidden_channels_4 = 64
hidden_linear = 32
```

In [ ]:
```
# create the model
starting_model = GNN(hidden_channels_1=hidden_channels_1, hidden_channels
            hidden_channels_4=hidden_channels_4, hidden_linear=hidden_lin

# Model size and number of parameters of the model:
print(44 * '-')
print("Model:")
print("Model size (bytes):\t\t  ", get_model_size(starting_model))
print("Number of parameters:\t\t  ", sum(p.numel() for p in starting_mode
print(44 * '-')
```

```
--------------------------------------------
Model:
Model size (bytes):                43862
Number of parameters:              9457
--------------------------------------------
```

In [ ]:
```
# prepare lists to store the results
list_dimensions = [1,2,3,4,5]
list_periodic = [False, True]
list_datasets = []
list_graphs = []
list_n_connections = []
list_model_names = []
list_train_losses = []
list_test_losses = []
list_fig_losses = []
list_fig_tests = []
list_mse = []
```

In [ ]:
```
for n_dimensions in list_dimensions:
    for periodic in list_periodic:

        # create the dataset
        dataset, graphs = create_dataset(n_nodes=n_nodes, h=h, periodic=p
        list_datasets.append(dataset)
        list_graphs.append(graphs)

        n_connections = len(graphs[0].edges)
        list_n_connections.append(n_connections)

        print(f"n_dimensions: {n_dimensions}, periodic: {periodic}, numbe

        # plot the first graph
        fig = plot_graph(graphs[0])


        # split the dataset into training and test set and create the loa
        train_loader = DataLoader(dataset[:int(0.8*n_samples)], batch_siz
        test_loader = DataLoader(dataset[int(0.8*n_samples):], batch_size

        # copy the model from scratch
        model = GNN(hidden_channels_1=hidden_channels_1, hidden_channels_
            hidden_channels_4=hidden_channels_4, hidden_linear=hidden_lin

        model.to(device)

        # set the model name
        model_name = set_model_name(n_nodes, n_dimensions, h, periodic, n
        list_model_names.append(model_name)

        try:
            os.mkdir(model_name)
        except:
            pass

        # save the graph plot
        fig.savefig(model_name + "/graph.png")

        # train the model
        train_losses, test_losses = train_model(model, train_loader, test
        list_train_losses.append(train_losses)
        list_test_losses.append(test_losses)

        # save train and test losses
        np.save(model_name + '/train_losses.npy', train_losses)
```

```
        np.save(model_name + '/test_losses.npy', test_losses)


        # plot the losses
        fig_losses = plot_loss(train_losses, test_losses)
        fig_losses.savefig(model_name + "/losses.png")
        list_fig_losses.append(fig_losses)

        # test the trained model
        fig, mse = test_trained_model(model_name, test_loader, device=dev
        fig.savefig(model_name + "/test.png")
        list_fig_tests.append(fig)

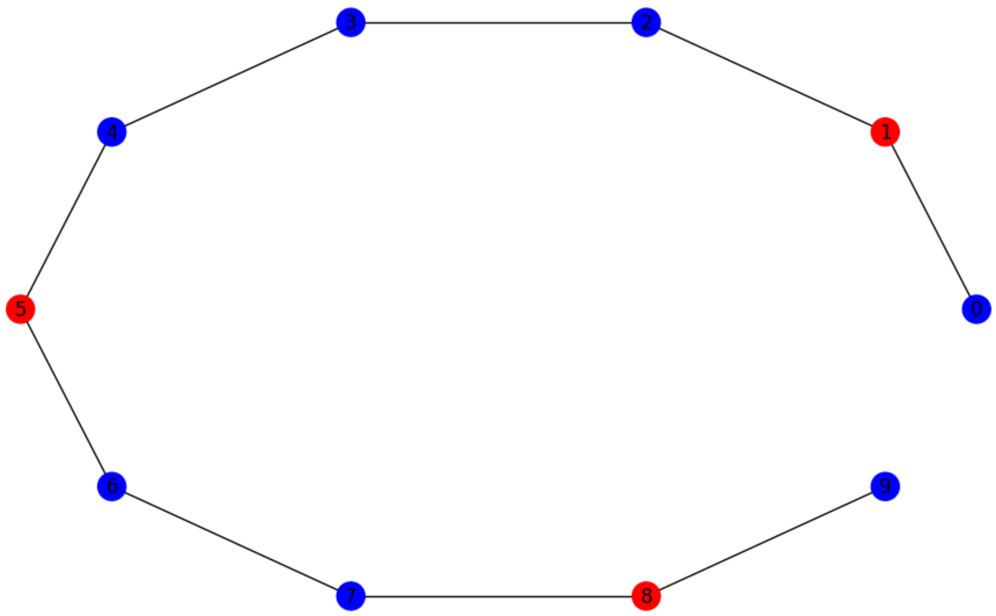
        # store the mse
        list_mse.append(mse)

        print(44 * '-')
        print("\n")

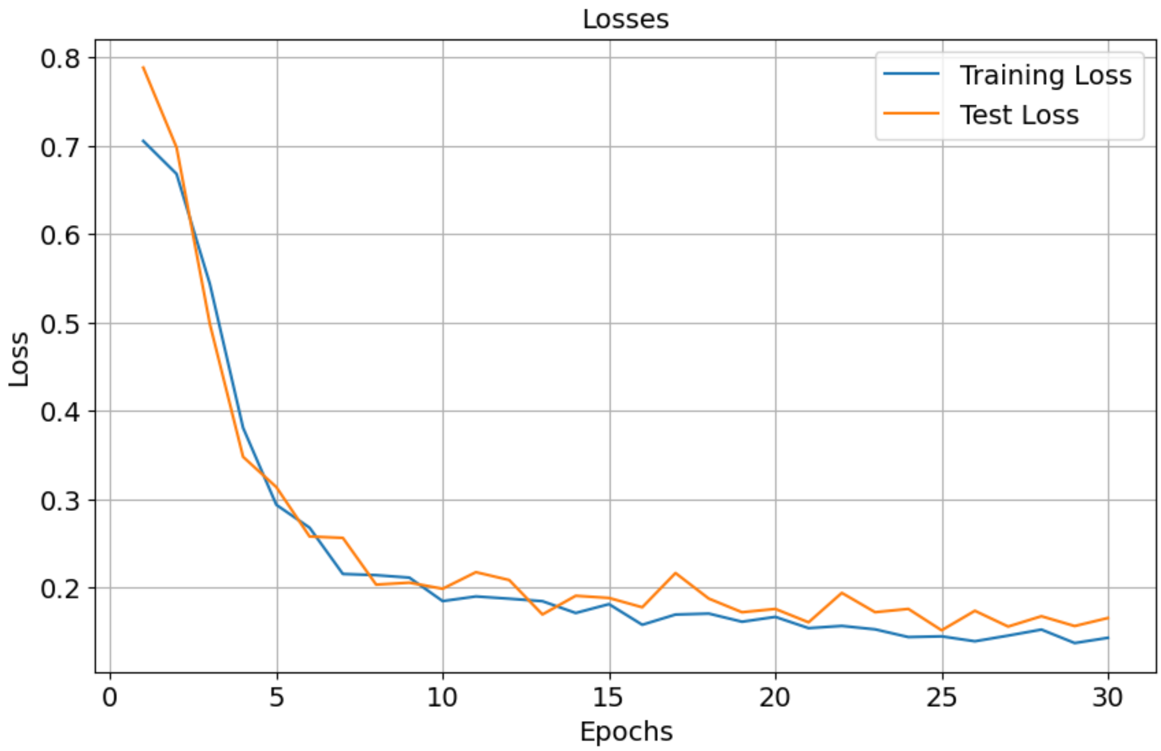
        folder_name = f"n_nodes_{n_nodes}_n_dimensions_{n_dimensions}"
        try: os.mkdir(folder_name)
        except: pass

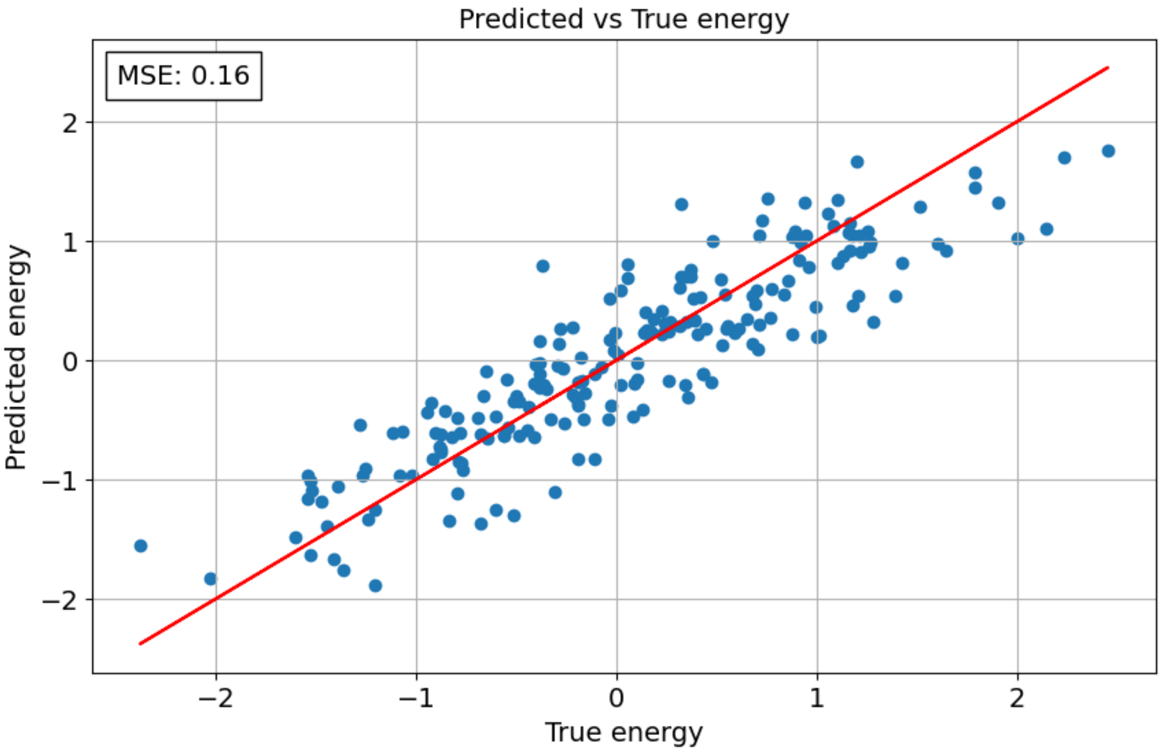
        # move the files to the folder
        os.system(f"mv {model_name} {folder_name}")
```

```
n_dimensions: 1, periodic: False, number of connections: 9
```



```
Training ...
Ep 1     | Loss 0.70537  | Test Loss 0.78843
Ep 2     | Loss 0.6681   | Test Loss 0.69803
Ep 3     | Loss 0.54367  | Test Loss 0.4984
Ep 4     | Loss 0.38067  | Test Loss 0.34783
Ep 5     | Loss 0.29352  | Test Loss 0.31354
Ep 6     | Loss 0.26759  | Test Loss 0.25766
Ep 7     | Loss 0.21526  | Test Loss 0.25608
Ep 8     | Loss 0.2139   | Test Loss 0.20321
Ep 9     | Loss 0.21111  | Test Loss 0.20542
Ep 10    | Loss 0.18454  | Test Loss 0.1985
Ep 11    | Loss 0.1898   | Test Loss 0.21728
Ep 12    | Loss 0.18727  | Test Loss 0.20838
Ep 13    | Loss 0.18443  | Test Loss 0.1694
Ep 14    | Loss 0.17107  | Test Loss 0.19054
Ep 15    | Loss 0.18109  | Test Loss 0.1881
Ep 16    | Loss 0.15774  | Test Loss 0.17754
Ep 17    | Loss 0.16931  | Test Loss 0.2163
Ep 18    | Loss 0.1704   | Test Loss 0.18738
Ep 19    | Loss 0.16119  | Test Loss 0.17191
Ep 20    | Loss 0.16666  | Test Loss 0.17569
Ep 21    | Loss 0.15394  | Test Loss 0.16053
Ep 22    | Loss 0.15644  | Test Loss 0.19382
Ep 23    | Loss 0.15255  | Test Loss 0.17197
Ep 24    | Loss 0.14382  | Test Loss 0.17571
Ep 25    | Loss 0.14463  | Test Loss 0.15147
Ep 26    | Loss 0.13906  | Test Loss 0.17356
Ep 27    | Loss 0.14549  | Test Loss 0.15571
Ep 28    | Loss 0.15229  | Test Loss 0.16741
Ep 29    | Loss 0.13707  | Test Loss 0.15629
Ep 30    | Loss 0.14299  | Test Loss 0.1654
```





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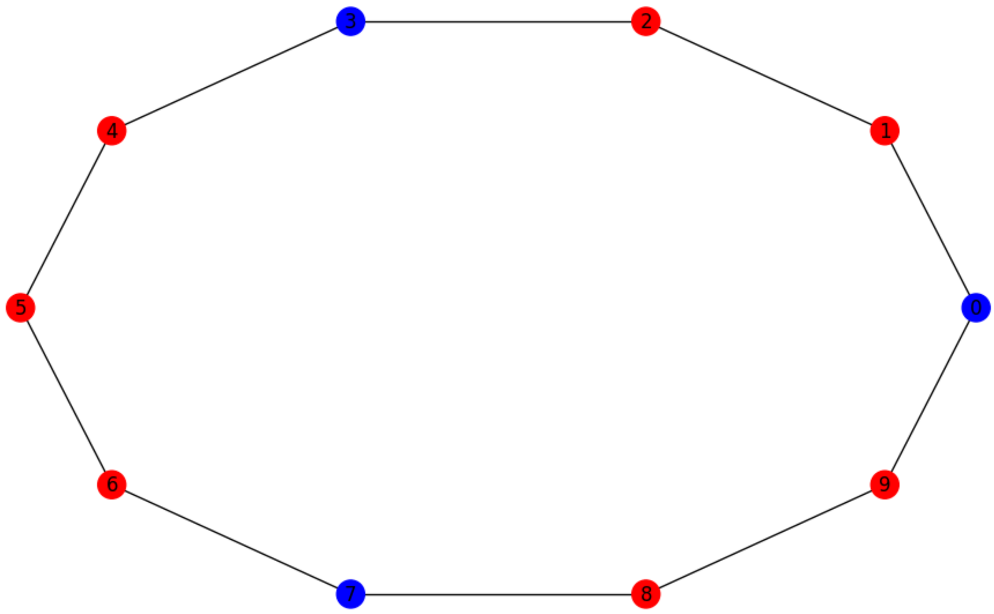
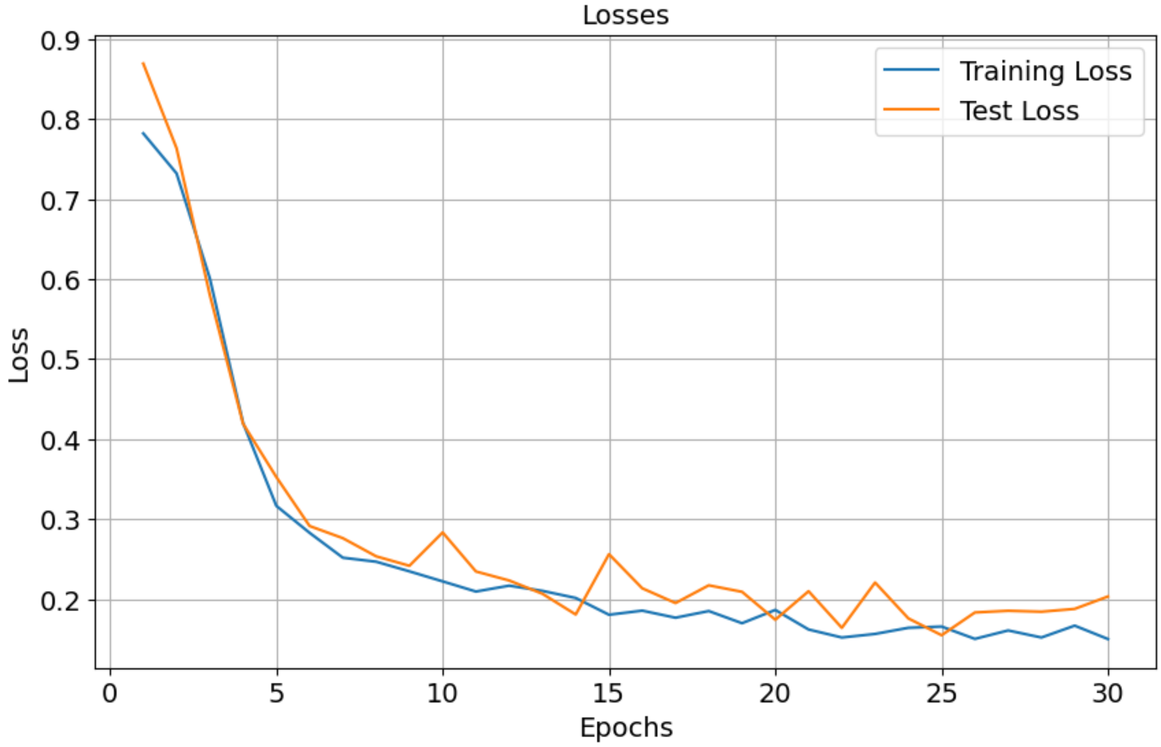
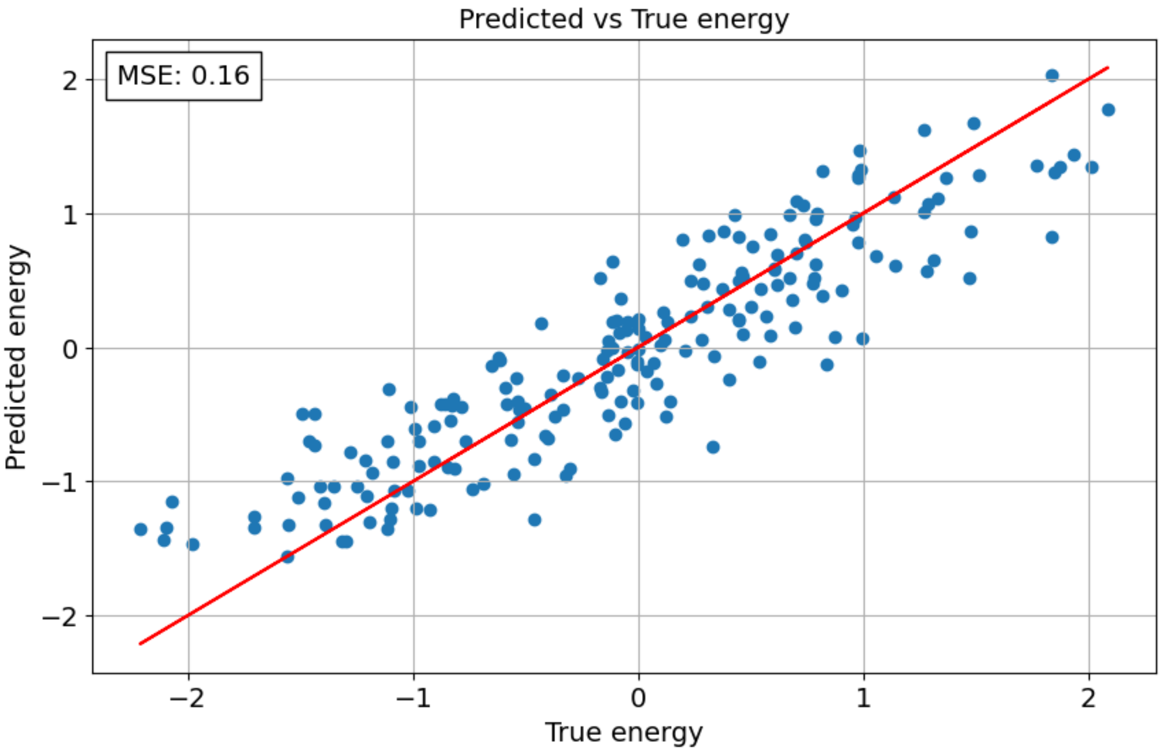
n_dimensions: 1, periodic: True, number of connections: 10



```
Training ...
Ep 1     | Loss 0.78206  | Test Loss 0.86936
Ep 2     | Loss 0.7321   | Test Loss 0.76358
Ep 3     | Loss 0.60101  | Test Loss 0.58025
Ep 4     | Loss 0.42004  | Test Loss 0.41915
Ep 5     | Loss 0.31649  | Test Loss 0.3525
Ep 6     | Loss 0.28277  | Test Loss 0.29132
Ep 7     | Loss 0.25168  | Test Loss 0.27609
Ep 8     | Loss 0.24668  | Test Loss 0.25344
Ep 9     | Loss 0.23463  | Test Loss 0.24159
Ep 10    | Loss 0.2221   | Test Loss 0.28325
Ep 11    | Loss 0.20941  | Test Loss 0.23449
Ep 12    | Loss 0.21674  | Test Loss 0.22319
Ep 13    | Loss 0.21022  | Test Loss 0.20659
Ep 14    | Loss 0.20136  | Test Loss 0.1807
Ep 15    | Loss 0.18039  | Test Loss 0.25609
Ep 16    | Loss 0.18551  | Test Loss 0.21345
Ep 17    | Loss 0.17667  | Test Loss 0.19503
Ep 18    | Loss 0.18501  | Test Loss 0.21717
Ep 19    | Loss 0.1698   | Test Loss 0.20905
Ep 20    | Loss 0.18639  | Test Loss 0.17418
Ep 21    | Loss 0.16196  | Test Loss 0.2098
Ep 22    | Loss 0.15194  | Test Loss 0.16403
Ep 23    | Loss 0.1564   | Test Loss 0.22066
Ep 24    | Loss 0.16406  | Test Loss 0.1758
Ep 25    | Loss 0.16563  | Test Loss 0.15479
Ep 26    | Loss 0.1502   | Test Loss 0.18324
Ep 27    | Loss 0.16076  | Test Loss 0.18534
Ep 28    | Loss 0.15193  | Test Loss 0.18417
Ep 29    | Loss 0.16675  | Test Loss 0.18771
Ep 30    | Loss 0.15003  | Test Loss 0.20319
```





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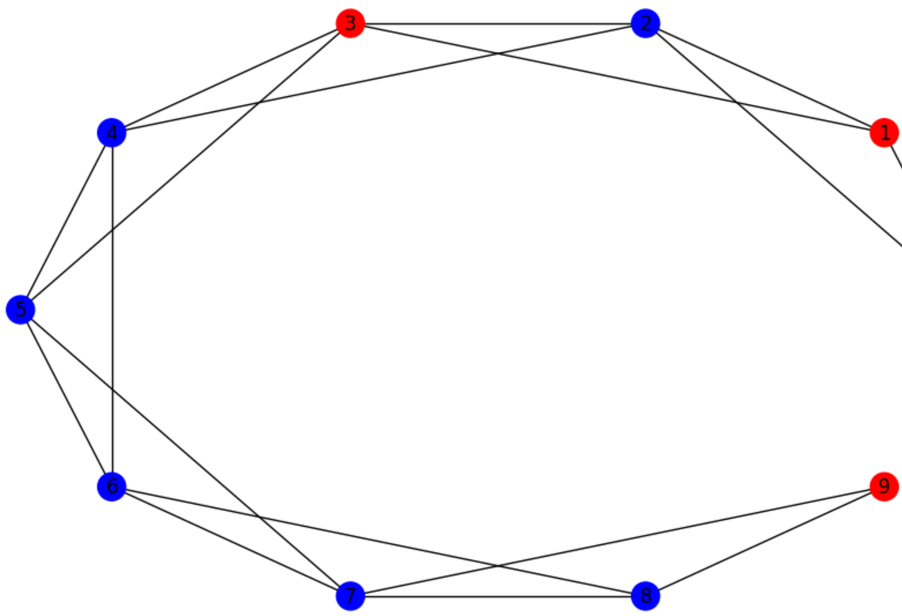
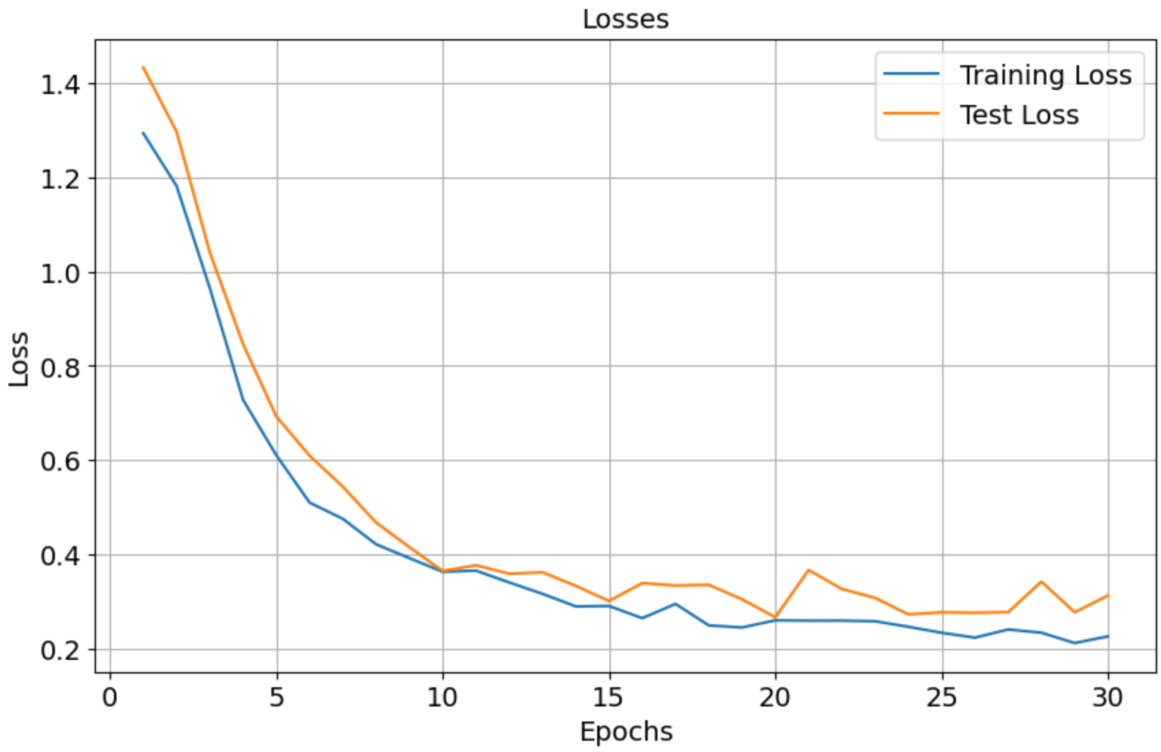
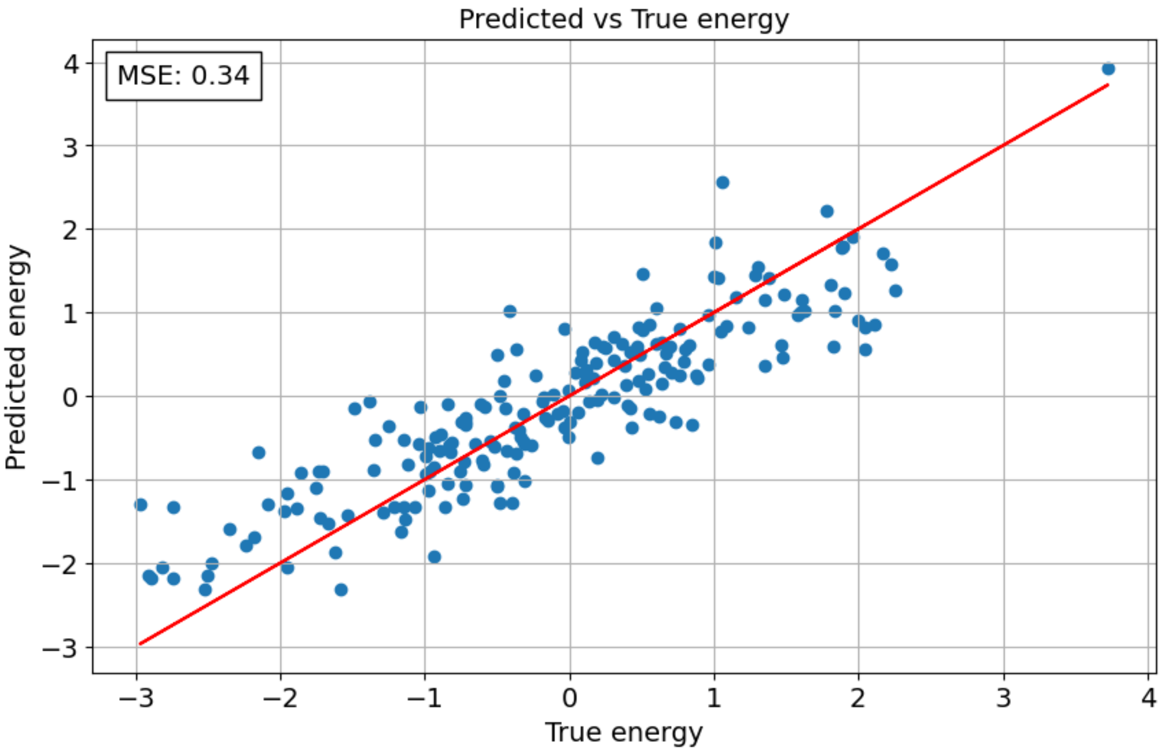
n_dimensions: 2, periodic: False, number of connections: 17



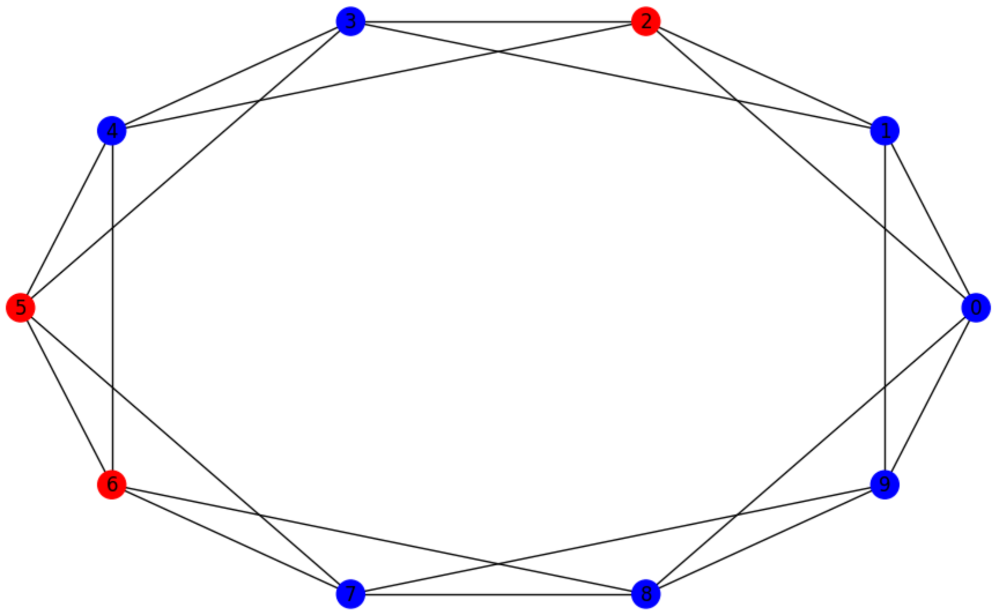
```
Training ...
Ep 1     | Loss 1.29405  | Test Loss 1.43348
Ep 2     | Loss 1.18209  | Test Loss 1.29734
Ep 3     | Loss 0.96527  | Test Loss 1.04082
Ep 4     | Loss 0.72775  | Test Loss 0.84602
Ep 5     | Loss 0.60998  | Test Loss 0.69232
Ep 6     | Loss 0.50955  | Test Loss 0.60914
Ep 7     | Loss 0.47498  | Test Loss 0.54317
Ep 8     | Loss 0.42092  | Test Loss 0.46692
Ep 9     | Loss 0.39152  | Test Loss 0.41481
Ep 10    | Loss 0.36254  | Test Loss 0.36416
Ep 11    | Loss 0.36501  | Test Loss 0.37646
Ep 12    | Loss 0.3399   | Test Loss 0.35845
Ep 13    | Loss 0.3157   | Test Loss 0.3615
Ep 14    | Loss 0.28904  | Test Loss 0.33271
Ep 15    | Loss 0.28988  | Test Loss 0.30049
Ep 16    | Loss 0.264    | Test Loss 0.3385
Ep 17    | Loss 0.29435  | Test Loss 0.33338
Ep 18    | Loss 0.24866  | Test Loss 0.33482
Ep 19    | Loss 0.24426  | Test Loss 0.30401
Ep 20    | Loss 0.25933  | Test Loss 0.26588
Ep 21    | Loss 0.25873  | Test Loss 0.36626
Ep 22    | Loss 0.25883  | Test Loss 0.32601
Ep 23    | Loss 0.25744  | Test Loss 0.30707
Ep 24    | Loss 0.24574  | Test Loss 0.27204
Ep 25    | Loss 0.23291  | Test Loss 0.2765
Ep 26    | Loss 0.22263  | Test Loss 0.27547
Ep 27    | Loss 0.23998  | Test Loss 0.27679
Ep 28    | Loss 0.23314  | Test Loss 0.34158
Ep 29    | Loss 0.2112   | Test Loss 0.27647
Ep 30    | Loss 0.22533  | Test Loss 0.31221
```



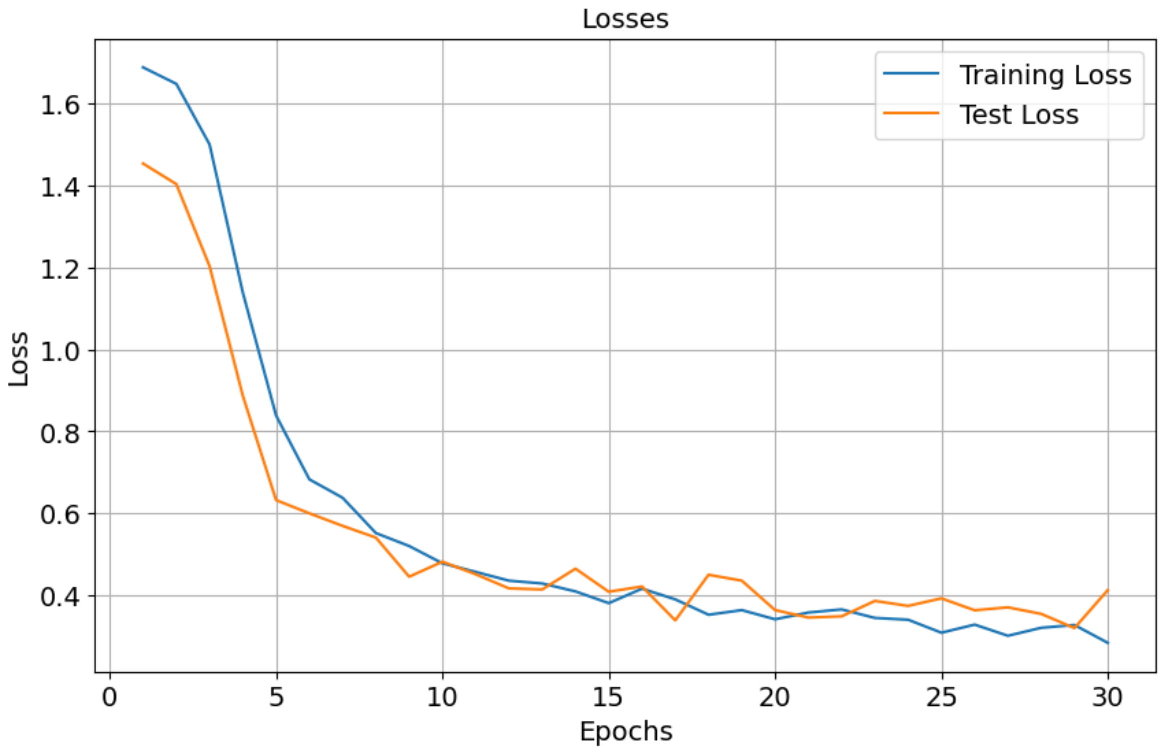


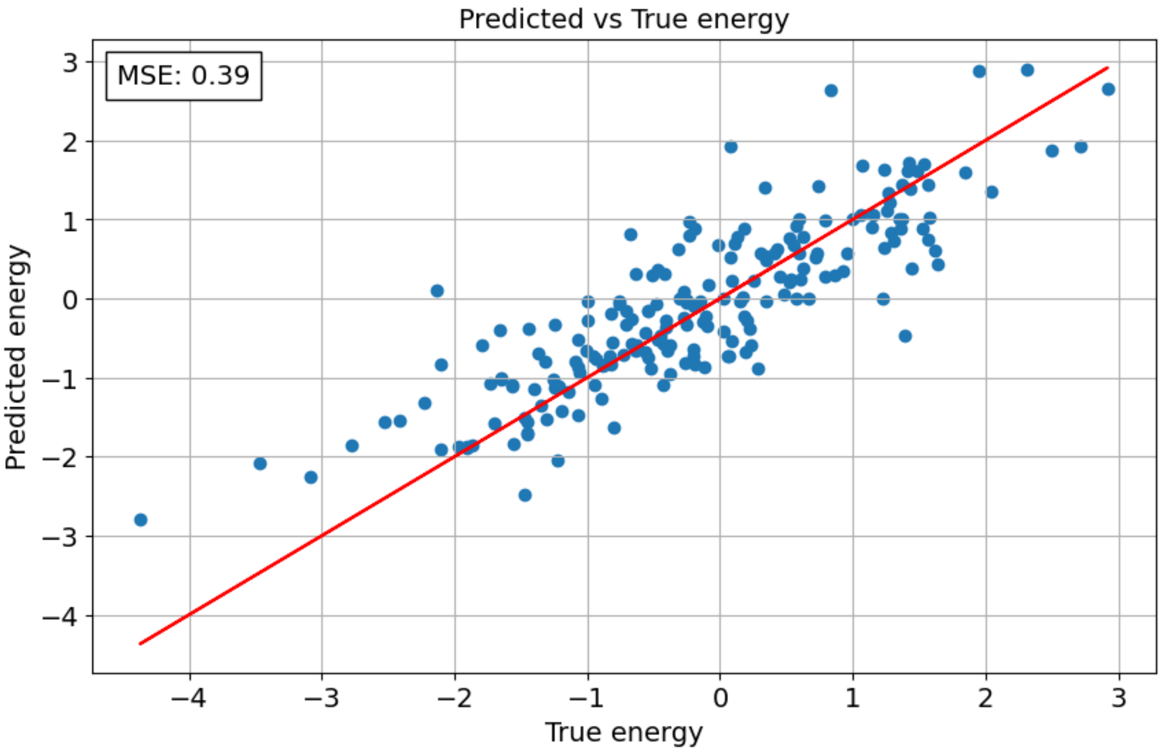

```
--------------------------------------------

n_dimensions: 2, periodic: True, number of connections: 20
```



```
Training ...
Ep 1     | Loss 1.68916  | Test Loss 1.45429
Ep 2     | Loss 1.64887  | Test Loss 1.404
Ep 3     | Loss 1.50092  | Test Loss 1.20358
Ep 4     | Loss 1.13877  | Test Loss 0.88705
Ep 5     | Loss 0.83881  | Test Loss 0.63218
Ep 6     | Loss 0.68285  | Test Loss 0.59988
Ep 7     | Loss 0.63787  | Test Loss 0.56923
Ep 8     | Loss 0.55166  | Test Loss 0.54059
Ep 9     | Loss 0.52003  | Test Loss 0.44516
Ep 10    | Loss 0.47781  | Test Loss 0.48177
Ep 11    | Loss 0.45683  | Test Loss 0.45109
Ep 12    | Loss 0.43542  | Test Loss 0.41655
Ep 13    | Loss 0.42856  | Test Loss 0.41394
Ep 14    | Loss 0.40917  | Test Loss 0.46474
Ep 15    | Loss 0.38051  | Test Loss 0.40835
Ep 16    | Loss 0.41592  | Test Loss 0.42118
Ep 17    | Loss 0.38971  | Test Loss 0.33851
Ep 18    | Loss 0.35222  | Test Loss 0.44988
Ep 19    | Loss 0.36351  | Test Loss 0.43546
Ep 20    | Loss 0.3411   | Test Loss 0.36363
Ep 21    | Loss 0.35766  | Test Loss 0.34532
Ep 22    | Loss 0.36521  | Test Loss 0.34828
Ep 23    | Loss 0.34444  | Test Loss 0.38599
Ep 24    | Loss 0.34002  | Test Loss 0.37388
Ep 25    | Loss 0.30831  | Test Loss 0.39223
Ep 26    | Loss 0.32808  | Test Loss 0.36319
Ep 27    | Loss 0.30084  | Test Loss 0.37029
Ep 28    | Loss 0.32032  | Test Loss 0.35431
Ep 29    | Loss 0.32719  | Test Loss 0.31964
Ep 30    | Loss 0.28372  | Test Loss 0.41222
```





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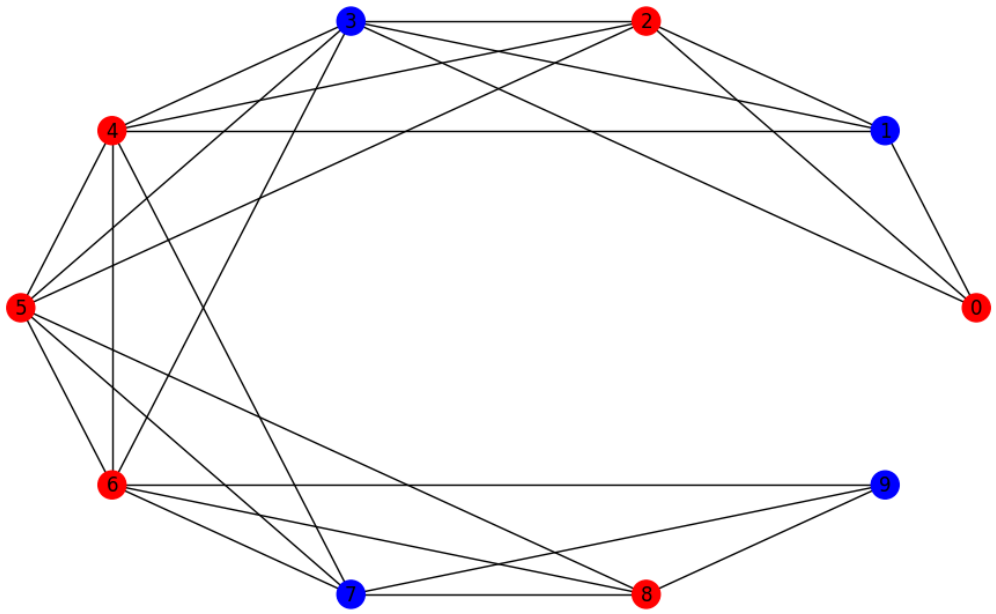
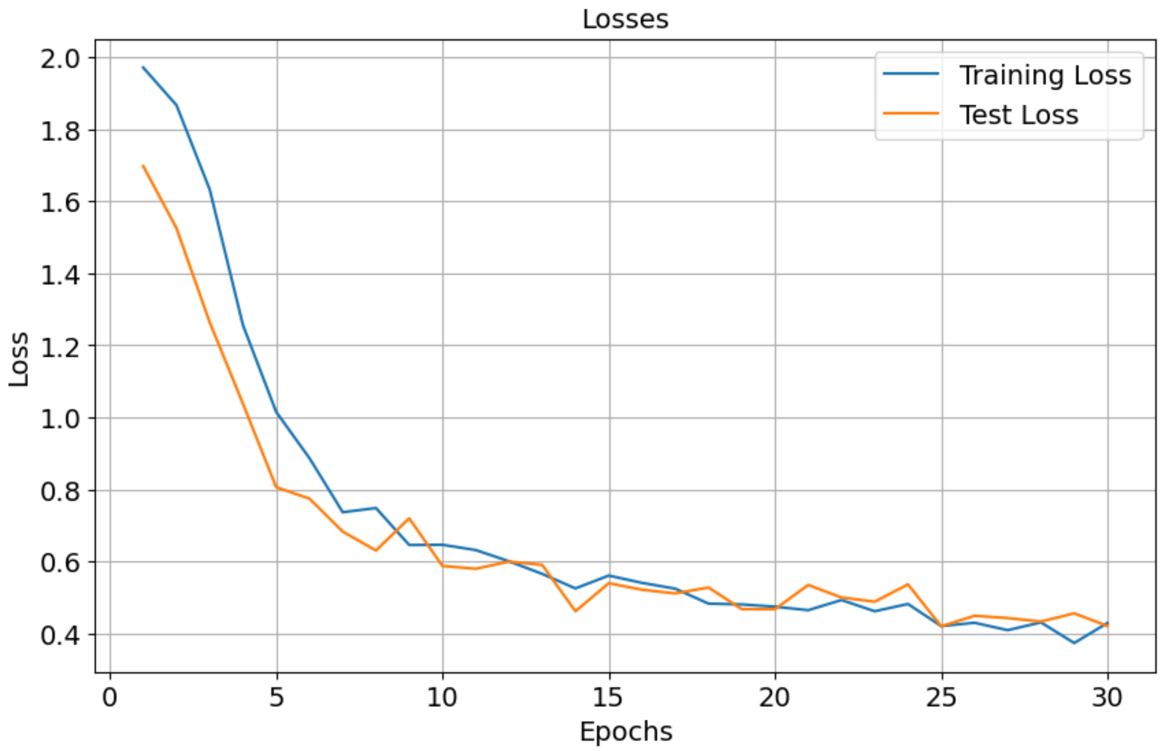
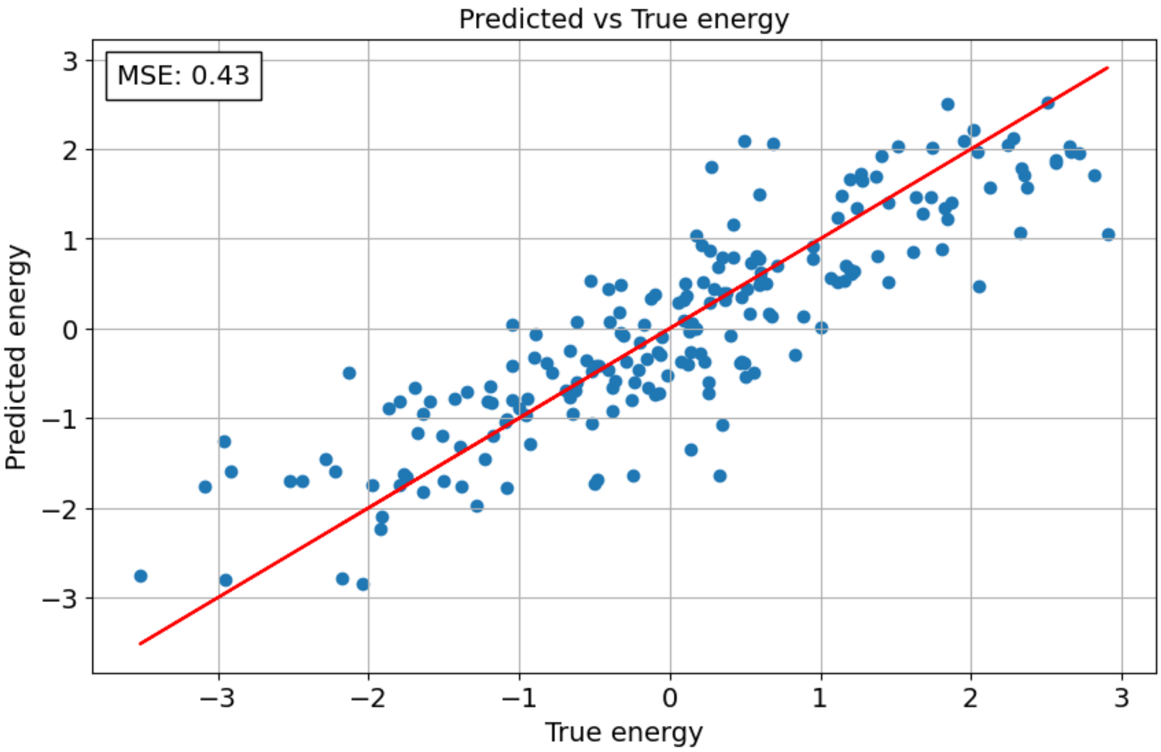
n_dimensions: 3, periodic: False, number of connections: 24



```
Training ...
Ep 1     | Loss 1.97106  | Test Loss 1.69749
Ep 2     | Loss 1.8668   | Test Loss 1.52526
Ep 3     | Loss 1.63256  | Test Loss 1.26374
Ep 4     | Loss 1.25584  | Test Loss 1.03757
Ep 5     | Loss 1.01485  | Test Loss 0.80604
Ep 6     | Loss 0.88672  | Test Loss 0.77442
Ep 7     | Loss 0.73667  | Test Loss 0.68283
Ep 8     | Loss 0.74816  | Test Loss 0.63038
Ep 9     | Loss 0.64555  | Test Loss 0.71961
Ep 10    | Loss 0.64622  | Test Loss 0.58745
Ep 11    | Loss 0.6316   | Test Loss 0.57963
Ep 12    | Loss 0.60041  | Test Loss 0.59947
Ep 13    | Loss 0.56537  | Test Loss 0.59032
Ep 14    | Loss 0.5251   | Test Loss 0.46168
Ep 15    | Loss 0.56075  | Test Loss 0.53962
Ep 16    | Loss 0.5405   | Test Loss 0.52142
Ep 17    | Loss 0.5244   | Test Loss 0.51113
Ep 18    | Loss 0.48286  | Test Loss 0.52762
Ep 19    | Loss 0.48061  | Test Loss 0.46759
Ep 20    | Loss 0.47432  | Test Loss 0.46727
Ep 21    | Loss 0.46466  | Test Loss 0.53468
Ep 22    | Loss 0.49287  | Test Loss 0.49982
Ep 23    | Loss 0.46172  | Test Loss 0.48824
Ep 24    | Loss 0.48188  | Test Loss 0.53621
Ep 25    | Loss 0.42048  | Test Loss 0.41989
Ep 26    | Loss 0.42972  | Test Loss 0.44907
Ep 27    | Loss 0.40911  | Test Loss 0.44268
Ep 28    | Loss 0.43069  | Test Loss 0.43316
Ep 29    | Loss 0.37343  | Test Loss 0.45588
Ep 30    | Loss 0.42908  | Test Loss 0.42072
```






```
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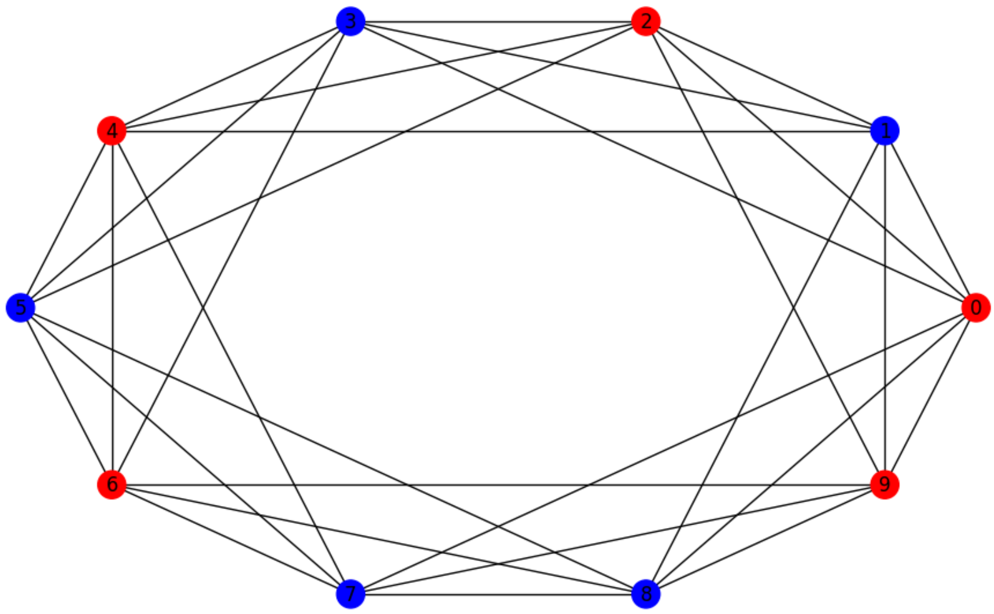
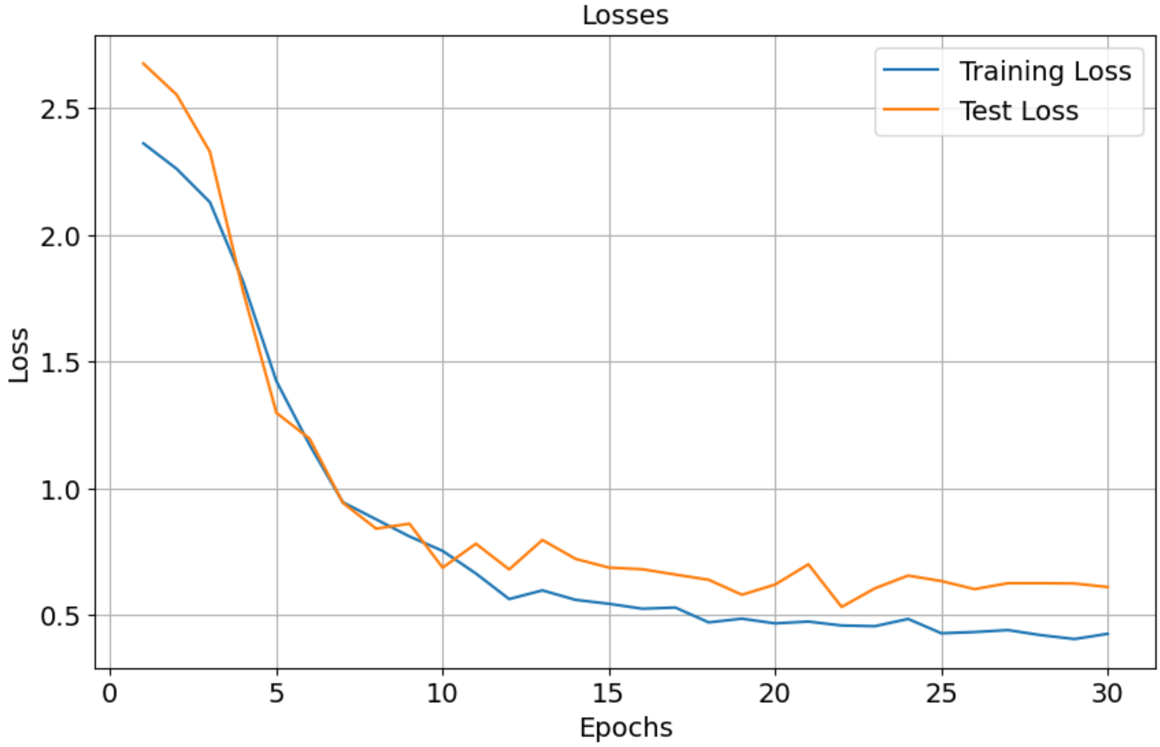
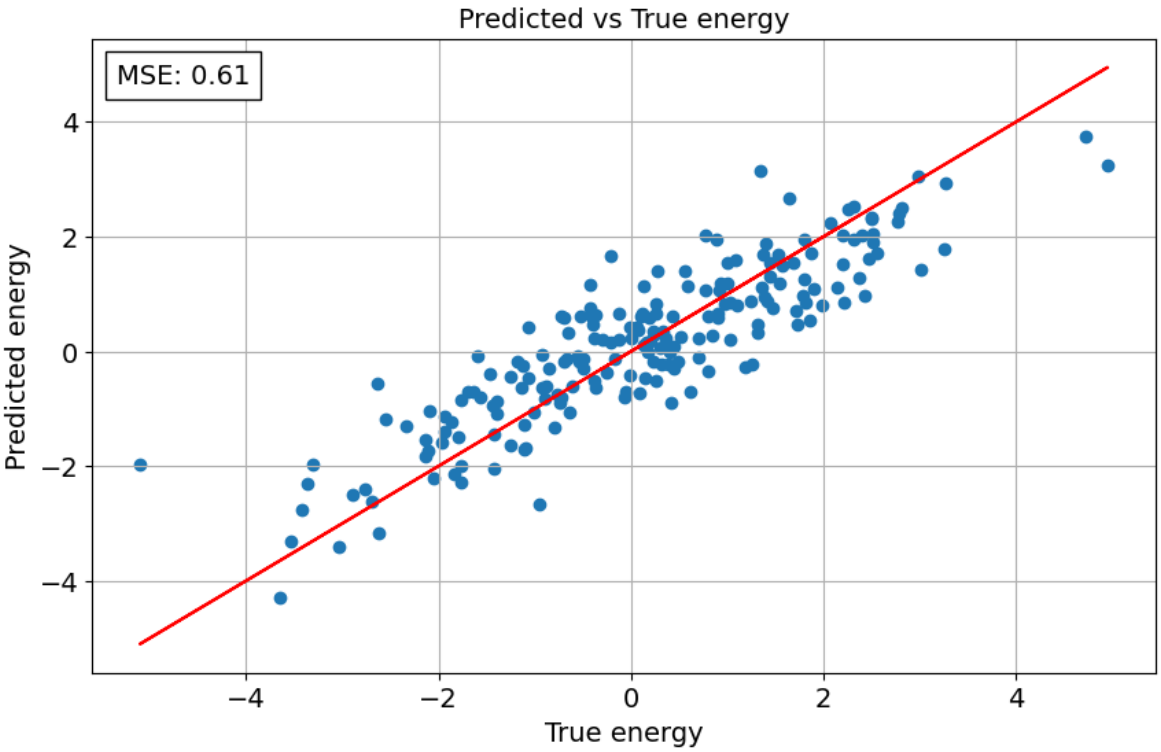
n_dimensions: 3, periodic: True, number of connections: 30
```

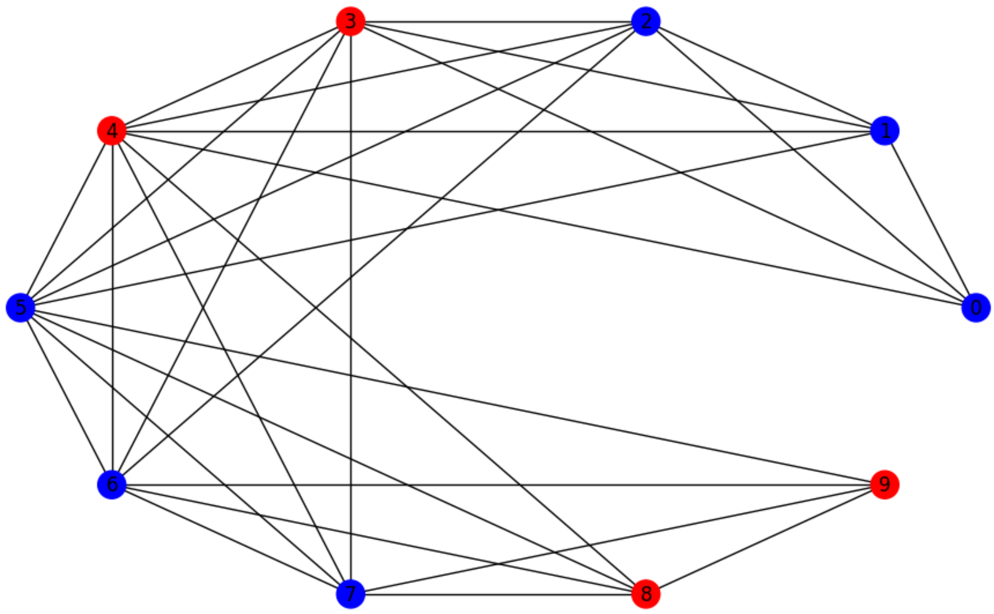


```
Training ...
Ep 1     | Loss 2.36014  | Test Loss 2.67497
Ep 2     | Loss 2.25979  | Test Loss 2.55212
Ep 3     | Loss 2.12817  | Test Loss 2.32695
Ep 4     | Loss 1.81415  | Test Loss 1.77575
Ep 5     | Loss 1.42196  | Test Loss 1.29708
Ep 6     | Loss 1.16985  | Test Loss 1.19485
Ep 7     | Loss 0.94396  | Test Loss 0.94186
Ep 8     | Loss 0.87668  | Test Loss 0.83994
Ep 9     | Loss 0.80946  | Test Loss 0.85959
Ep 10    | Loss 0.75215  | Test Loss 0.68609
Ep 11    | Loss 0.66309  | Test Loss 0.78061
Ep 12    | Loss 0.56218  | Test Loss 0.67915
Ep 13    | Loss 0.5965   | Test Loss 0.79531
Ep 14    | Loss 0.55902  | Test Loss 0.72066
Ep 15    | Loss 0.54356  | Test Loss 0.68636
Ep 16    | Loss 0.52416  | Test Loss 0.67988
Ep 17    | Loss 0.52862  | Test Loss 0.65885
Ep 18    | Loss 0.47017  | Test Loss 0.63821
Ep 19    | Loss 0.48479  | Test Loss 0.57926
Ep 20    | Loss 0.46618  | Test Loss 0.61937
Ep 21    | Loss 0.4734   | Test Loss 0.69924
Ep 22    | Loss 0.45781  | Test Loss 0.53125
Ep 23    | Loss 0.45508  | Test Loss 0.60449
Ep 24    | Loss 0.48375  | Test Loss 0.65486
Ep 25    | Loss 0.42713  | Test Loss 0.63316
Ep 26    | Loss 0.43215  | Test Loss 0.60139
Ep 27    | Loss 0.43976  | Test Loss 0.6247
Ep 28    | Loss 0.41966  | Test Loss 0.62488
Ep 29    | Loss 0.40448  | Test Loss 0.62369
Ep 30    | Loss 0.42499  | Test Loss 0.60963
```

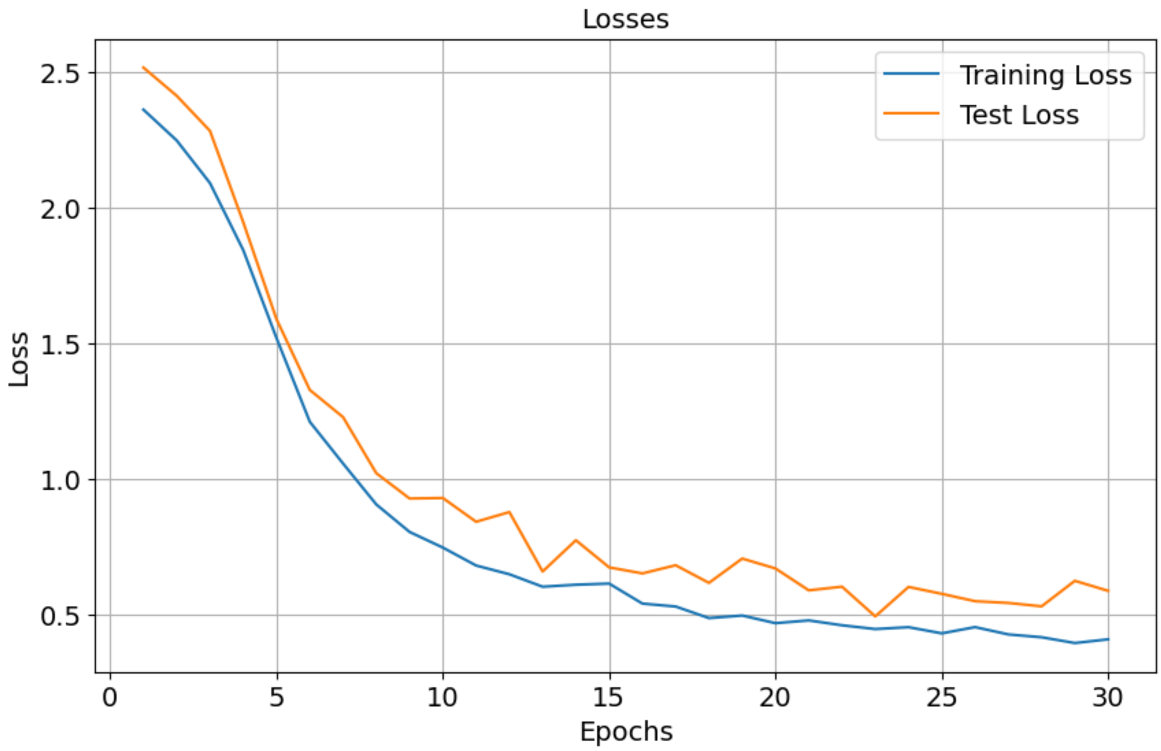


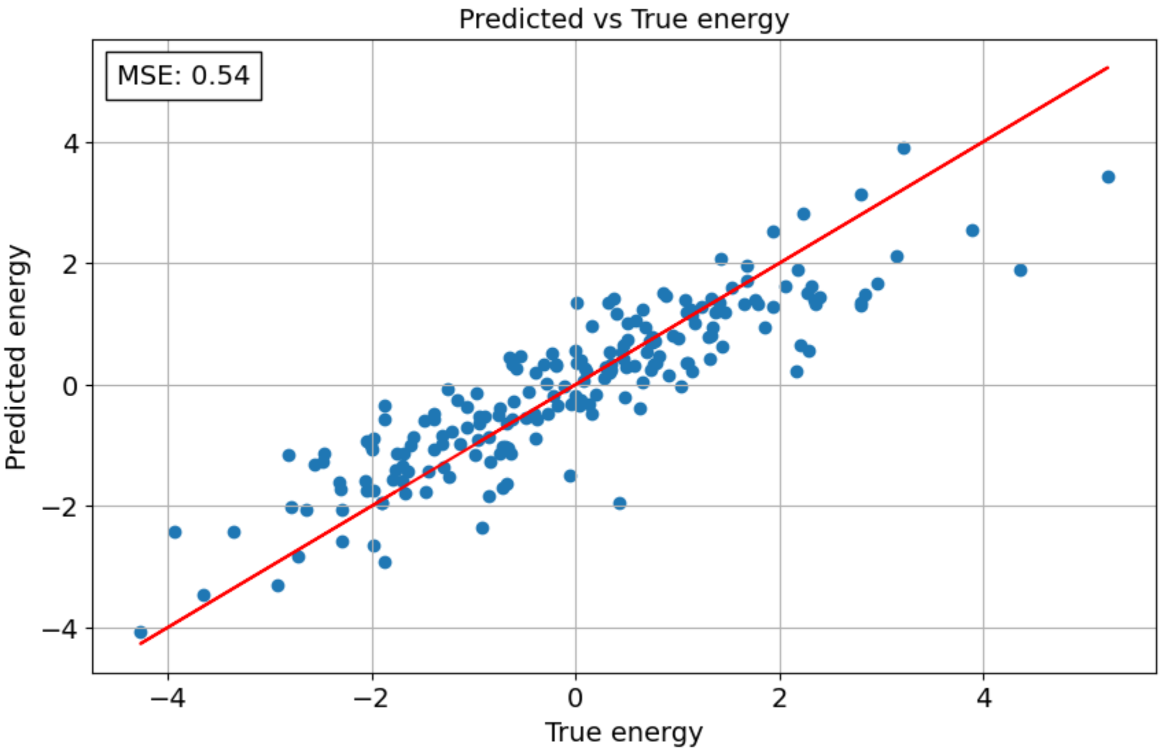


```
n_dimensions: 4, periodic: False, number of connections: 30
```



```
Training ...
Ep 1     | Loss 2.36042  | Test Loss 2.5152
Ep 2     | Loss 2.2469   | Test Loss 2.41139
Ep 3     | Loss 2.09015  | Test Loss 2.28221
Ep 4     | Loss 1.8434   | Test Loss 1.94607
Ep 5     | Loss 1.51956  | Test Loss 1.58907
Ep 6     | Loss 1.21173  | Test Loss 1.32881
Ep 7     | Loss 1.05792  | Test Loss 1.22864
Ep 8     | Loss 0.90725  | Test Loss 1.02228
Ep 9     | Loss 0.80605  | Test Loss 0.92919
Ep 10    | Loss 0.74857  | Test Loss 0.93106
Ep 11    | Loss 0.68249  | Test Loss 0.84351
Ep 12    | Loss 0.6503   | Test Loss 0.87928
Ep 13    | Loss 0.60444  | Test Loss 0.66041
Ep 14    | Loss 0.61183  | Test Loss 0.77557
Ep 15    | Loss 0.61601  | Test Loss 0.67562
Ep 16    | Loss 0.54235  | Test Loss 0.65348
Ep 17    | Loss 0.5316   | Test Loss 0.68347
Ep 18    | Loss 0.48902  | Test Loss 0.6186
Ep 19    | Loss 0.49841  | Test Loss 0.70811
Ep 20    | Loss 0.47028  | Test Loss 0.67164
Ep 21    | Loss 0.48044  | Test Loss 0.59116
Ep 22    | Loss 0.46252  | Test Loss 0.6046
Ep 23    | Loss 0.44866  | Test Loss 0.49531
Ep 24    | Loss 0.45551  | Test Loss 0.60377
Ep 25    | Loss 0.43278  | Test Loss 0.57828
Ep 26    | Loss 0.45579  | Test Loss 0.55121
Ep 27    | Loss 0.42887  | Test Loss 0.54476
Ep 28    | Loss 0.41849  | Test Loss 0.53231
Ep 29    | Loss 0.3972   | Test Loss 0.62619
Ep 30    | Loss 0.4108   | Test Loss 0.58932
```






```
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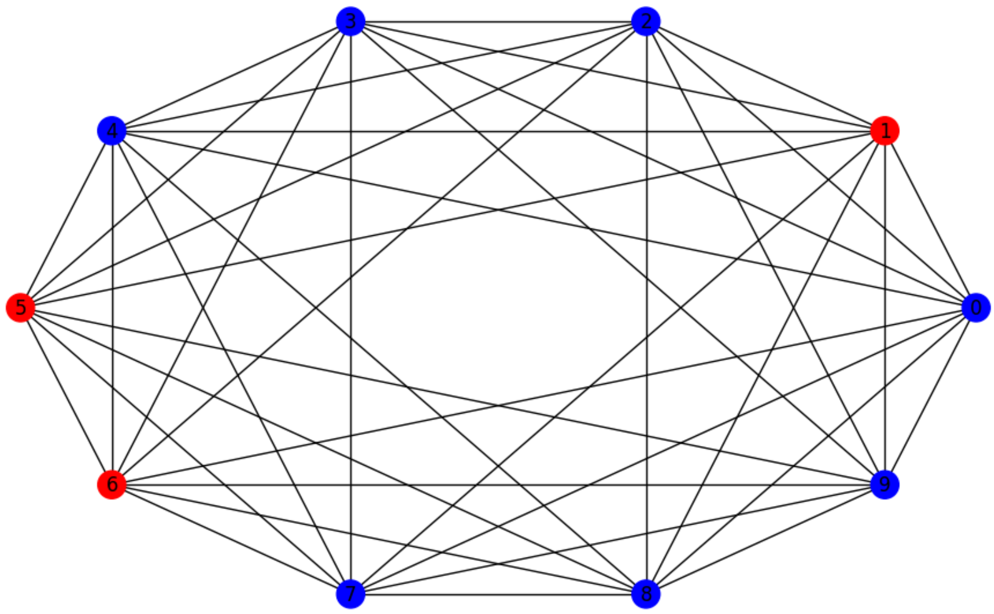
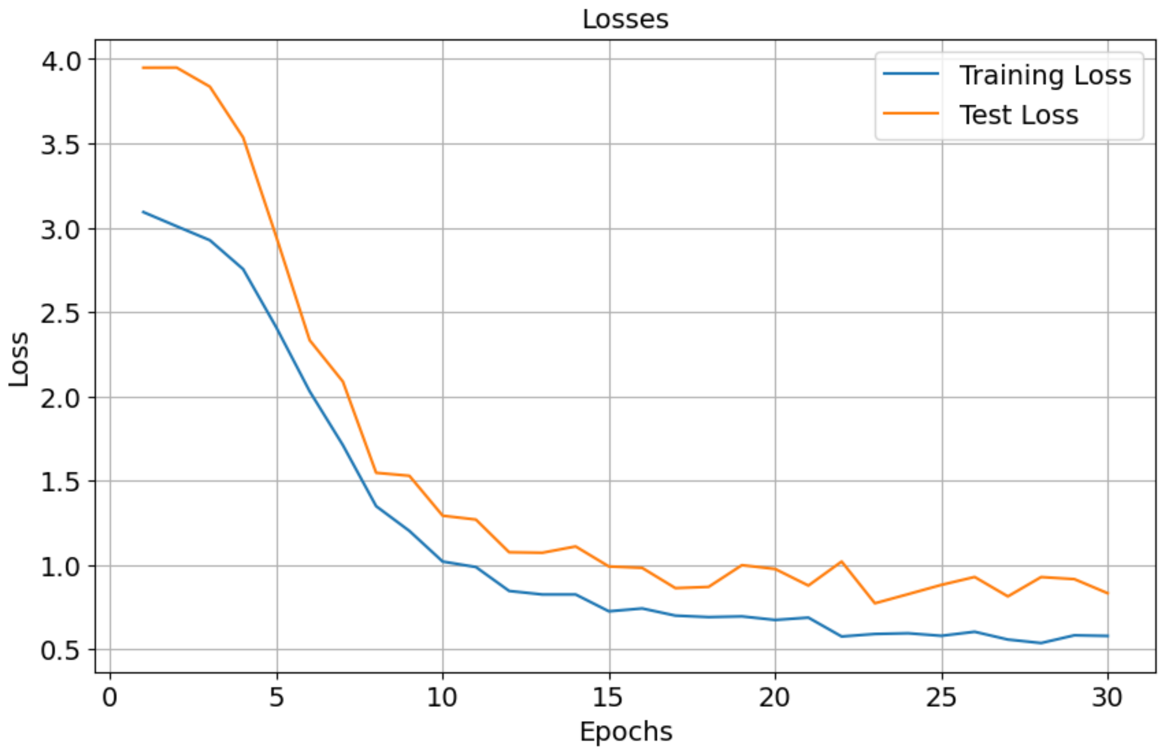
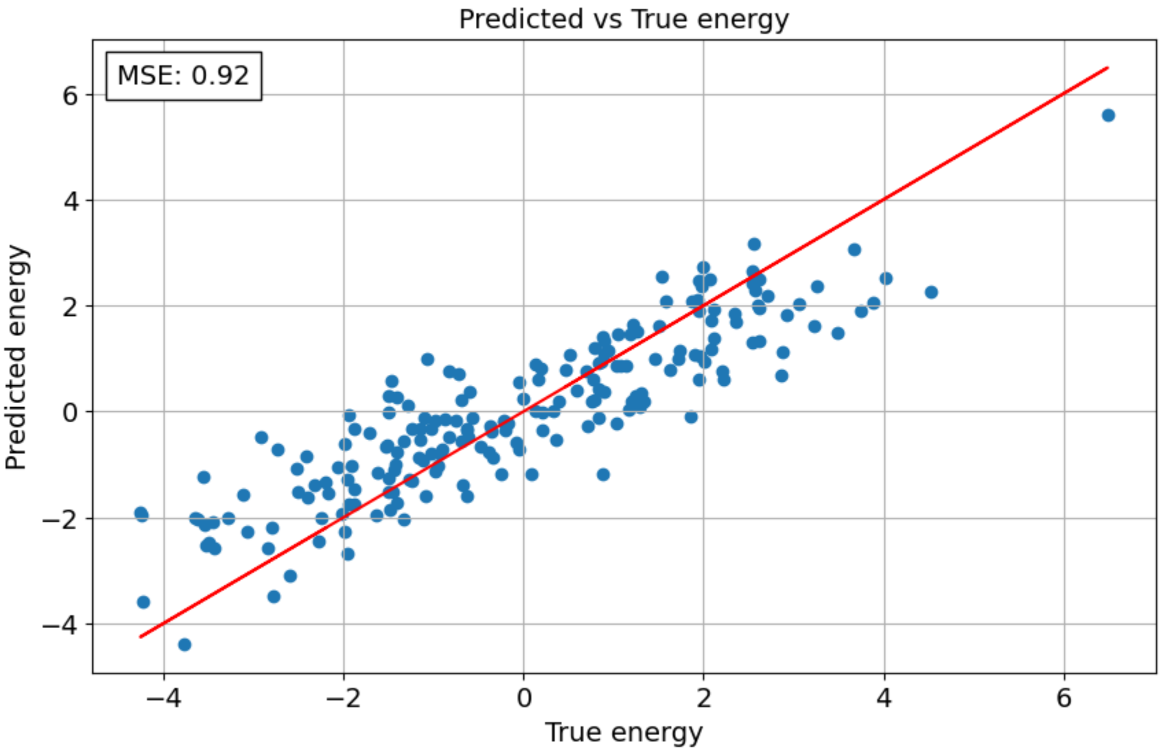
n_dimensions: 4, periodic: True, number of connections: 40
```



```
Training ...
Ep 1     | Loss 3.09263  | Test Loss 3.94882
Ep 2     | Loss 3.00851  | Test Loss 3.94941
Ep 3     | Loss 2.92569  | Test Loss 3.8362
Ep 4     | Loss 2.75429  | Test Loss 3.53524
Ep 5     | Loss 2.40774  | Test Loss 2.94444
Ep 6     | Loss 2.03013  | Test Loss 2.33322
Ep 7     | Loss 1.7107   | Test Loss 2.08753
Ep 8     | Loss 1.34894  | Test Loss 1.54682
Ep 9     | Loss 1.20217  | Test Loss 1.52907
Ep 10    | Loss 1.02057  | Test Loss 1.29253
Ep 11    | Loss 0.98804  | Test Loss 1.26953
Ep 12    | Loss 0.84622  | Test Loss 1.07569
Ep 13    | Loss 0.82532  | Test Loss 1.07274
Ep 14    | Loss 0.82536  | Test Loss 1.11009
Ep 15    | Loss 0.72548  | Test Loss 0.99135
Ep 16    | Loss 0.74263  | Test Loss 0.98305
Ep 17    | Loss 0.70004  | Test Loss 0.86308
Ep 18    | Loss 0.69128  | Test Loss 0.87042
Ep 19    | Loss 0.6954   | Test Loss 0.99916
Ep 20    | Loss 0.67432  | Test Loss 0.97654
Ep 21    | Loss 0.68811  | Test Loss 0.87822
Ep 22    | Loss 0.57625  | Test Loss 1.02061
Ep 23    | Loss 0.59111  | Test Loss 0.77305
Ep 24    | Loss 0.59531  | Test Loss 0.82718
Ep 25    | Loss 0.58033  | Test Loss 0.88221
Ep 26    | Loss 0.60419  | Test Loss 0.92905
Ep 27    | Loss 0.5581   | Test Loss 0.81388
Ep 28    | Loss 0.53745  | Test Loss 0.92857
Ep 29    | Loss 0.58327  | Test Loss 0.91637
Ep 30    | Loss 0.57958  | Test Loss 0.8328
```



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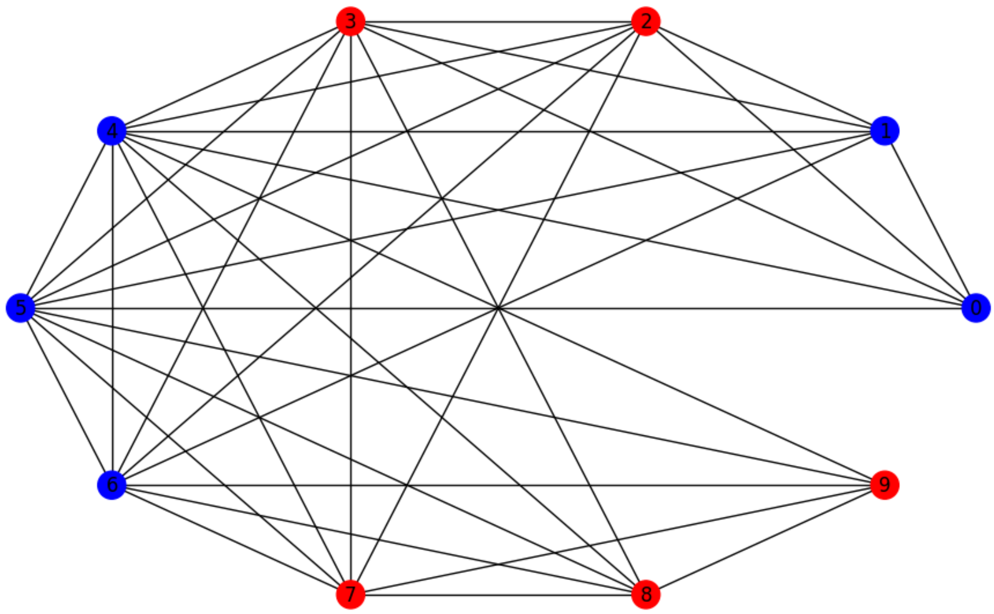
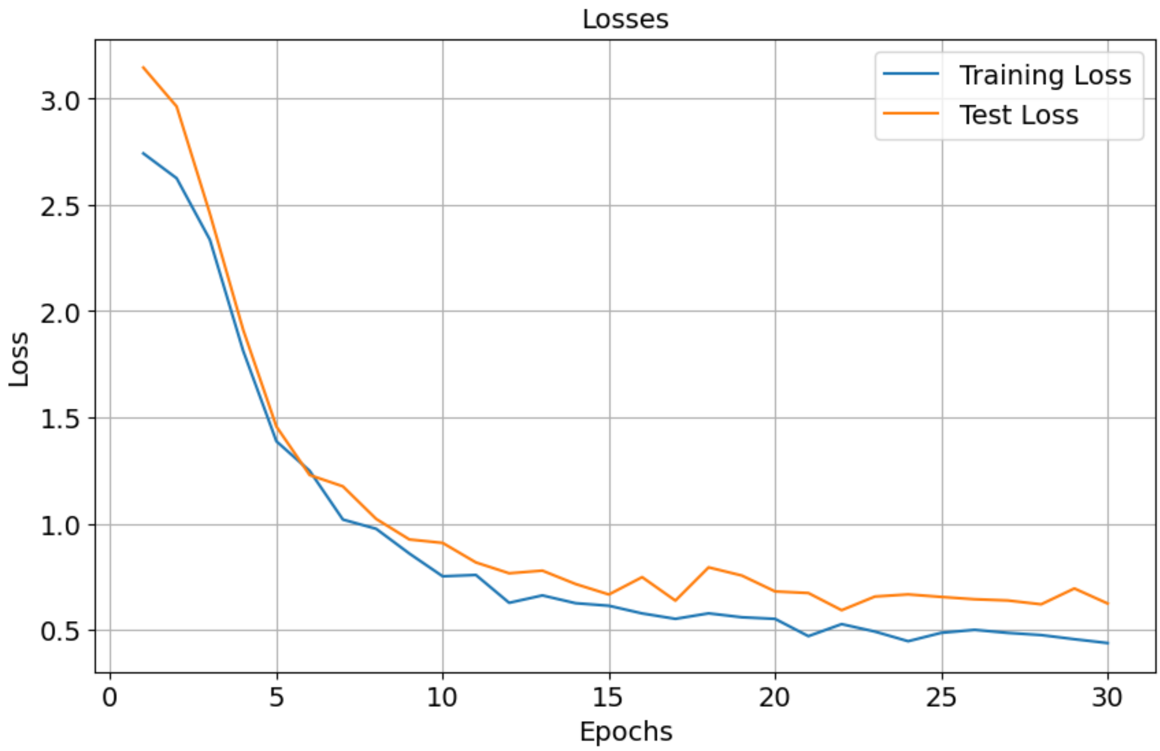
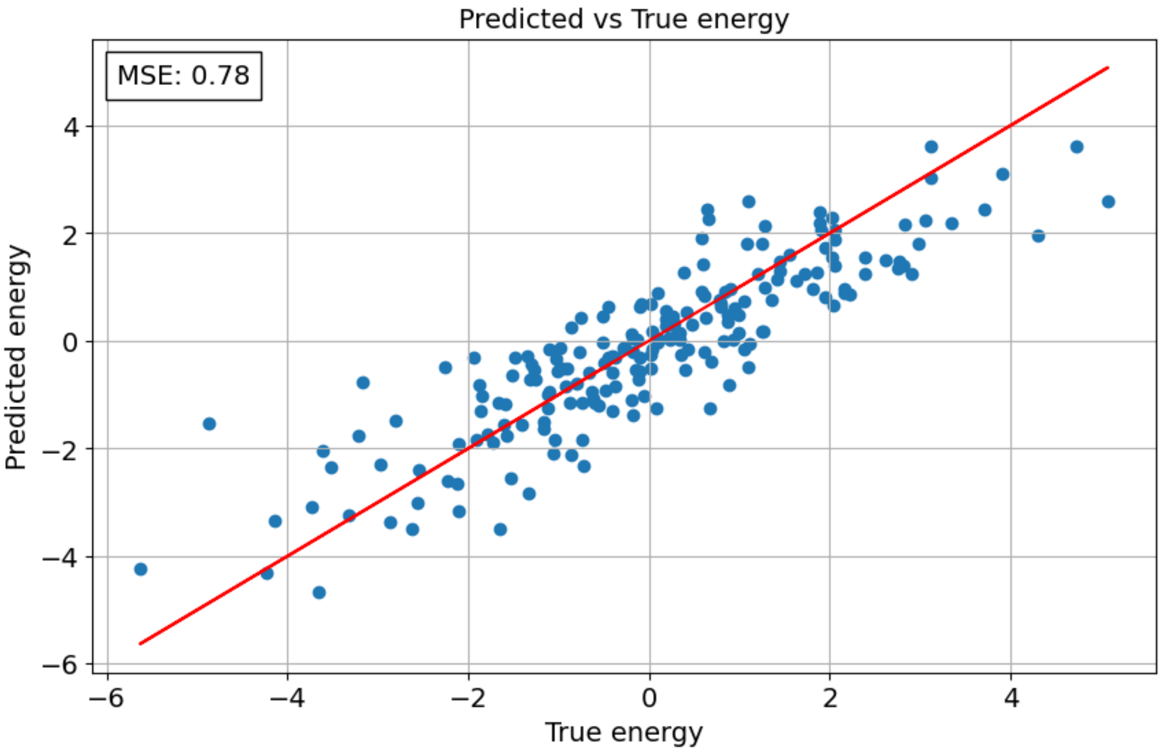
n_dimensions: 5, periodic: False, number of connections: 35
```



```
Training ...
Ep 1     | Loss 2.74246  | Test Loss 3.14667
Ep 2     | Loss 2.62571  | Test Loss 2.96347
Ep 3     | Loss 2.33604  | Test Loss 2.45879
Ep 4     | Loss 1.81337  | Test Loss 1.91244
Ep 5     | Loss 1.38734  | Test Loss 1.45674
Ep 6     | Loss 1.24818  | Test Loss 1.22835
Ep 7     | Loss 1.01881  | Test Loss 1.17502
Ep 8     | Loss 0.97516  | Test Loss 1.02185
Ep 9     | Loss 0.85864  | Test Loss 0.92499
Ep 10    | Loss 0.7516   | Test Loss 0.9088
Ep 11    | Loss 0.75785  | Test Loss 0.81685
Ep 12    | Loss 0.62678  | Test Loss 0.76581
Ep 13    | Loss 0.66154  | Test Loss 0.77821
Ep 14    | Loss 0.62491  | Test Loss 0.71515
Ep 15    | Loss 0.61293  | Test Loss 0.66595
Ep 16    | Loss 0.57683  | Test Loss 0.74757
Ep 17    | Loss 0.55124  | Test Loss 0.63706
Ep 18    | Loss 0.57713  | Test Loss 0.79369
Ep 19    | Loss 0.5587   | Test Loss 0.75504
Ep 20    | Loss 0.55104  | Test Loss 0.68028
Ep 21    | Loss 0.46971  | Test Loss 0.67276
Ep 22    | Loss 0.52642  | Test Loss 0.59197
Ep 23    | Loss 0.49139  | Test Loss 0.65619
Ep 24    | Loss 0.44591  | Test Loss 0.66638
Ep 25    | Loss 0.48553  | Test Loss 0.65435
Ep 26    | Loss 0.49955  | Test Loss 0.64354
Ep 27    | Loss 0.48506  | Test Loss 0.63766
Ep 28    | Loss 0.47493  | Test Loss 0.61961
Ep 29    | Loss 0.45545  | Test Loss 0.69426
Ep 30    | Loss 0.4374   | Test Loss 0.62358
```






```
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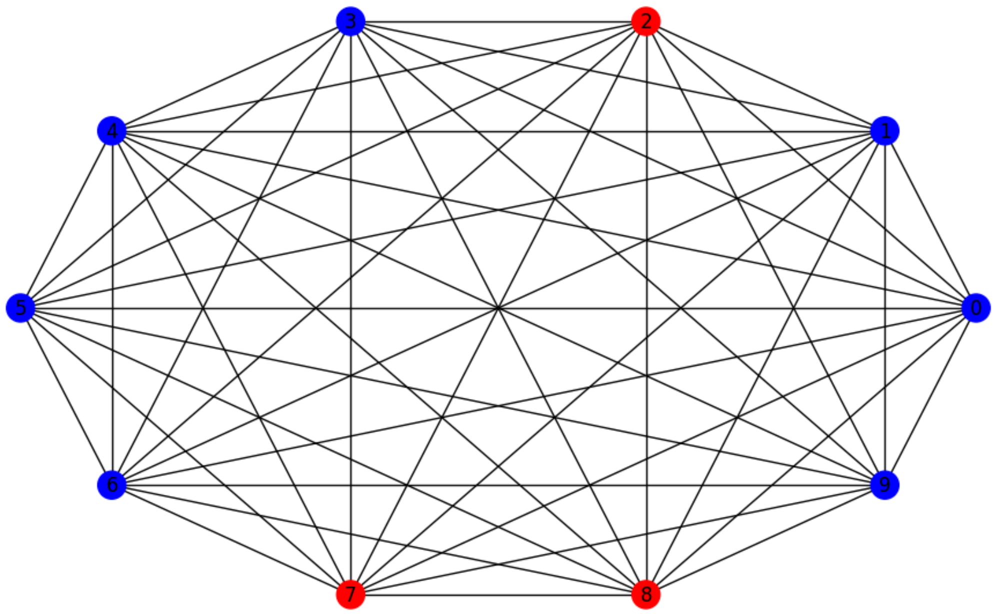
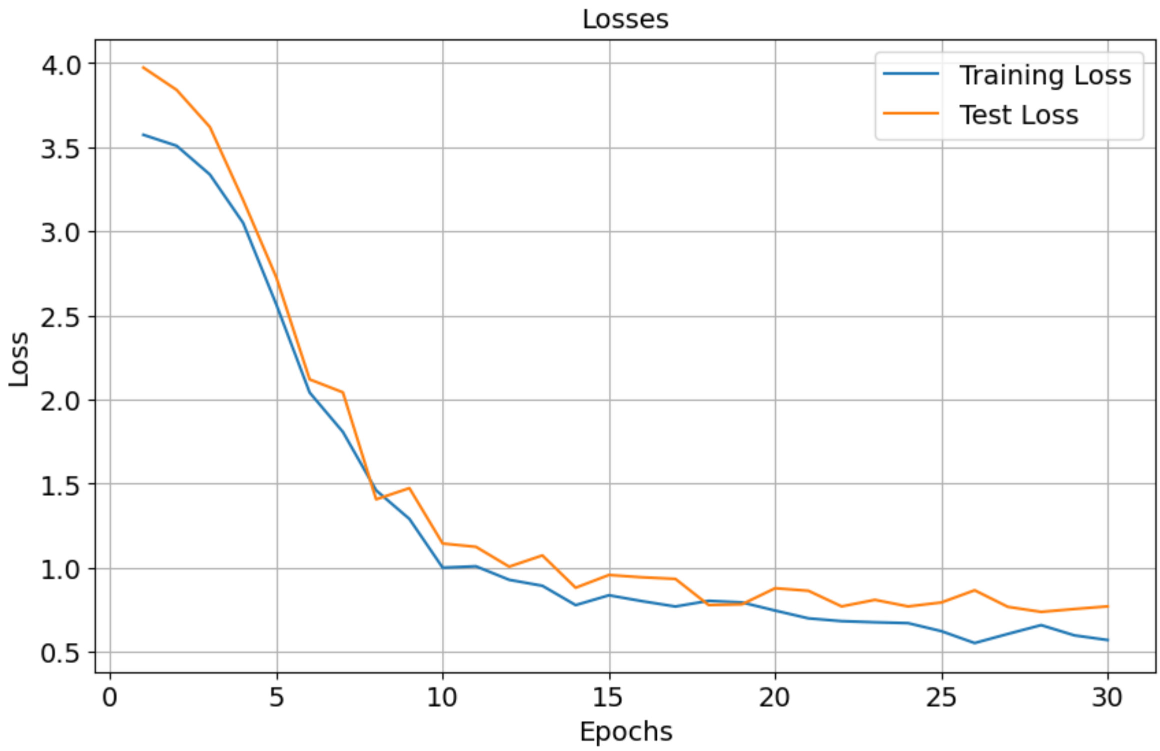
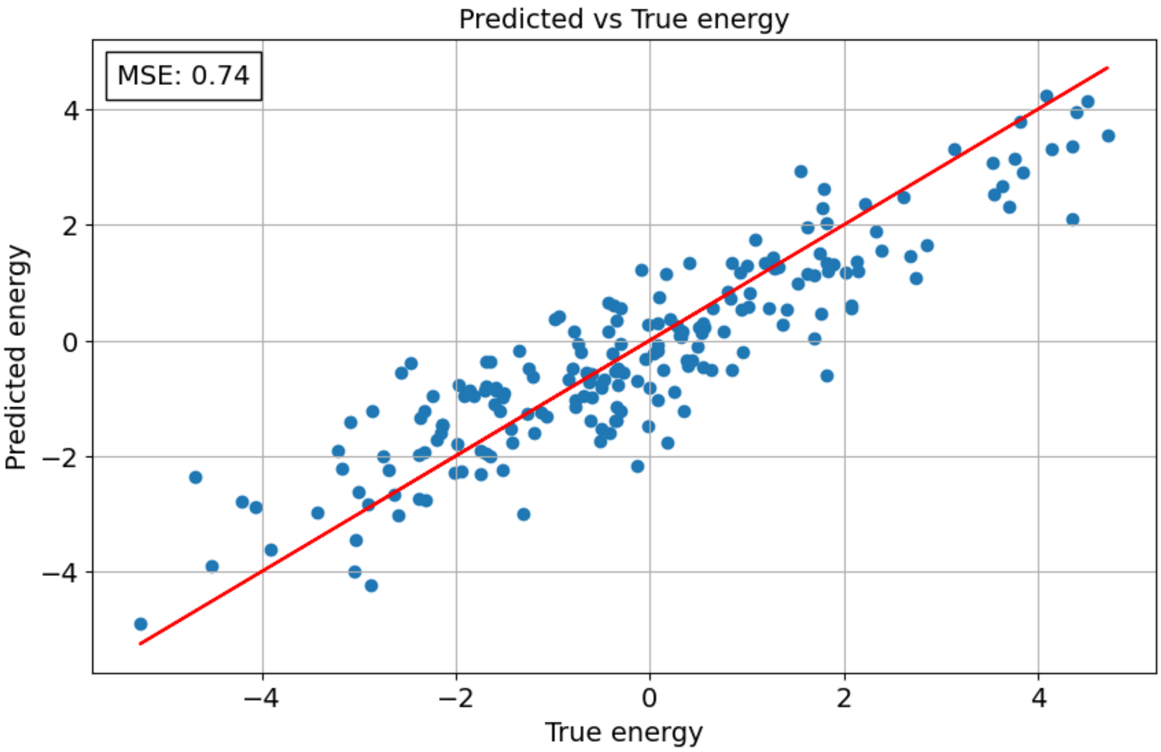
n_dimensions: 5, periodic: True, number of connections: 45
```



```
Training ...
Ep 1     | Loss 3.57358  | Test Loss 3.9731
Ep 2     | Loss 3.5083   | Test Loss 3.84035
Ep 3     | Loss 3.33753  | Test Loss 3.61988
Ep 4     | Loss 3.04992  | Test Loss 3.18603
Ep 5     | Loss 2.56408  | Test Loss 2.72533
Ep 6     | Loss 2.04185  | Test Loss 2.12009
Ep 7     | Loss 1.80806  | Test Loss 2.04305
Ep 8     | Loss 1.46041  | Test Loss 1.40719
Ep 9     | Loss 1.29091  | Test Loss 1.47371
Ep 10    | Loss 1.00111  | Test Loss 1.14458
Ep 11    | Loss 1.00936  | Test Loss 1.12514
Ep 12    | Loss 0.92904  | Test Loss 1.00716
Ep 13    | Loss 0.89346  | Test Loss 1.07383
Ep 14    | Loss 0.77868  | Test Loss 0.8819
Ep 15    | Loss 0.837    | Test Loss 0.95769
Ep 16    | Loss 0.80203  | Test Loss 0.94385
Ep 17    | Loss 0.77035  | Test Loss 0.93437
Ep 18    | Loss 0.80408  | Test Loss 0.77915
Ep 19    | Loss 0.79472  | Test Loss 0.78334
Ep 20    | Loss 0.74625  | Test Loss 0.87889
Ep 21    | Loss 0.6999   | Test Loss 0.86378
Ep 22    | Loss 0.68335  | Test Loss 0.77096
Ep 23    | Loss 0.67659  | Test Loss 0.80989
Ep 24    | Loss 0.67142  | Test Loss 0.77086
Ep 25    | Loss 0.62379  | Test Loss 0.7943
Ep 26    | Loss 0.55328  | Test Loss 0.86685
Ep 27    | Loss 0.60735  | Test Loss 0.76826
Ep 28    | Loss 0.65966  | Test Loss 0.73832
Ep 29    | Loss 0.59875  | Test Loss 0.75551
Ep 30    | Loss 0.57116  | Test Loss 0.77101
```




Predicted vs True energy
MSE: 0.74
Predicted energy
True energy
4
2
0
−2
−4
−4
−2
0
2
4

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