# 0810-mh_em_1qm

August 11, 2023

[ ]:
```
initial_path = 'peptide-QML/'
# initial_path = '../'
```

[ ]:
```
day = "0810"
name_notebook = day + "-mh_em_1qm.ipynb"

#ask the user if that is correct, if he says yes kkep going, otherwise stop
import sys
answer = input("{} is the name of the notebook | Is that correct? (y/n): ".
 ↪format(name_notebook))
if answer != "y":
    print("Please, change the name of the notebook")
    sys.exit()
```

[ ]:
```
import numpy as np
```

[ ]:
```
import sys
sys.path.append(initial_path)

%load_ext autoreload
%autoreload 2
from my_code import functions as f
from my_code import pytorch_model as ptm
from my_code import quantum_nodes as qn
from my_code import pytorch_wrappers as pw
```

## 1 Data

[ ]:
```
data_file_path = initial_path + 'data/Scores/PET/generated/
 ↪bb14_Strings_Energies_10_000_8_aa.txt'  # Replace with the actual path to␣
 ↪your 'data.txt' file
string_list, number_list = f.read_data_file(data_file_path)
score_list = np.array(number_list)/np.max(number_list)*10
vector_list = np.array([f.string_to_numbers(string) for string in string_list])␣
 ↪# one hot encoding
```

[ ]:
```
X, Y, X_validation, Y_validation = f.create_validating_set(vector_list,␣
↪score_list, percentage=0.1)
```

[ ]:
```
# Define the dataset
input_data = ptm.torch.tensor(X)
target_data = ptm.torch.tensor(Y).view(-1, 1)

# Define the validation set
input_validation = ptm.torch.tensor(X_validation)
target_validation = ptm.torch.tensor(Y_validation).view(-1, 1)
```

## 2 Quantum node

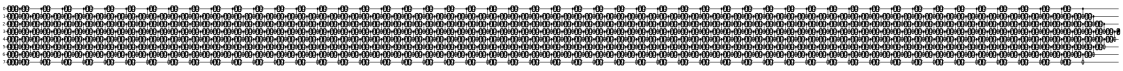
[ ]:
```
n_aminoacids = len(string_list[0])
```

[ ]:
```
quantum_layer = qn.circuit(
    n_qubits = n_aminoacids,
    device = "default.qubit.torch",
    device_options = {'shots': None},
    embedding = qn.parts.AngleEmbedding,
    # embedding_ansatz = qn.parts.Ansatz_11,
    block_ansatz = qn.parts.Ansatz_11,
    final_ansatz = qn.parts.Ansatz_final_11,
    measurement = qn.parts.Measurement('Z', (n_aminoacids-1)//2),
    # embedding_n_layers = 4,
    # different_inputs_per_layer = True,
    block_n_layers = 50,
    # wrapper_qlayer = pw.QLayer,
    wrapper_qlayer = None,
)
```

[ ]:
```
quantum_layer.draw(size=(50,3))
```

```
/usr/lib/python3.8/_collections_abc.py:832: MatplotlibDeprecationWarning:
The examples.directory rcparam was deprecated in Matplotlib 3.0 and will be
removed in 3.2. In the future, examples will be found relative to the 'datapath'
directory.
  self[key] = other[key]
/usr/lib/python3.8/_collections_abc.py:832: MatplotlibDeprecationWarning:
The savefig.frameon rcparam was deprecated in Matplotlib 3.1 and will be removed
in 3.3.
  self[key] = other[key]
/usr/lib/python3.8/_collections_abc.py:832: MatplotlibDeprecationWarning:
The text.latex.unicode rcparam was deprecated in Matplotlib 3.0 and will be
removed in 3.2.
  self[key] = other[key]
/usr/lib/python3.8/_collections_abc.py:832: MatplotlibDeprecationWarning:
```

```
The verbose.fileo rcparam was deprecated in Matplotlib 3.1 and will be removed
in 3.3.
  self[key] = other[key]
/usr/lib/python3.8/_collections_abc.py:832: MatplotlibDeprecationWarning:
The verbose.level rcparam was deprecated in Matplotlib 3.1 and will be removed
in 3.3.
  self[key] = other[key]
```



## 3 Hybrid model

[ ]:
```
import torch.nn as nn
import torch

class Reshape(nn.Module):
    def __init__(self):
        super(Reshape, self).__init__()

    def forward(self, x):
        dims = len(x.shape)
        return torch.transpose(x, dims-2, dims-1).reshape(x.shape[-3] if␣
 ↪dims==3 else 1, x.shape[-2]*x.shape[-1]).squeeze()
```

[ ]:
```
layers =  [ptm.nn.Embedding(num_embeddings=19, embedding_dim=quantum_layer.
 ↪input_shape[0]//n_aminoacids), Reshape()]
layers += [quantum_layer(), ptm.nn.Linear(1,1)]
```

[ ]:
```
# Create model and set data:
model = ptm.pytorch_model(
    layers,
    save_options = {'initial_path': initial_path, 'name_notebook':␣
 ↪name_notebook},
)
model.set_data(
    data_X=input_data,
    data_Y=target_data,
    data_X_validation=input_validation,
    data_Y_validation=target_validation
)
```

[ ]:
```
print(model(input_data[0:2]))
print(model(input_data[1]))
```

```
tensor([[-0.0537],
        [-0.1114]], grad_fn=<AddmmBackward>)
tensor([-0.1114], grad_fn=<AddBackward0>)
```

[ ]:
```
model.keep_track_params=False
```

[ ]:
```
import torch.optim as optim

# ask the user if he wants to start the training
out = input("Do you want to start the training? (y/n) ")
if out != 'y':
    sys.exit()

# train the model
model.train(
    optimizer= optim.Adam,
    optimizer_options={'lr': 0.2},
    num_epochs = 100,
    batch_size = 32,
    # initialization_options = [
    #     {
    #         'type': 'normal_',
    #         'layer': len(model.model)-1,
    #         'name': 'bias',
    #         'options': {'mean': 100, 'std': 10},
    #     },{
    #         'type': 'normal_',
    #         'layer': len(model.model)-1,
    #         'name': 'weight',
    #         'options': {'mean': 200, 'std': 10},
    #     },
    # ]
)
```

```
Epoch [0/100], Loss: 1.0173, Loss validation: 1.0185

/usr/lib/python3/dist-packages/torch/autograd/__init__.py:147: UserWarning: CUDA
initialization: Unexpected error from cudaGetDeviceCount(). Did you run some
cuda functions before calling NumCudaDevices() that might have already set an
error? Error 804: forward compatibility was attempted on non supported HW
(Triggered internally at  ../c10/cuda/CUDAFunctions.cpp:115.)
  Variable._execution_engine.run_backward(

        Validation string,      i: 0;   prediction: 3.5257,     target: 1.2085,
loss: 1.9174
        Validation string,      i: 1;   prediction: 3.4291,     target: 4.2057,
loss: 0.1847
        Validation string,      i: 2;   prediction: 3.4826,     target: 1.0491,
loss: 2.3196
```

```
Epoch [1/100], Loss: 0.5148, Loss validation: 0.4850, Time remaining: ~10.0h
55.0m 11s
        Validation string,      i: 0;   prediction: 3.4904,     target: 1.2085,
loss: 1.8882
        Validation string,      i: 1;   prediction: 3.5046,     target: 4.2057,
loss: 0.1667
        Validation string,      i: 2;   prediction: 3.1236,     target: 1.0491,
loss: 1.9773
Epoch [2/100], Loss: 0.5017, Loss validation: 0.4796, Time remaining: ~9.0h
55.0m 36s
        Validation string,      i: 0;   prediction: 3.4851,     target: 1.2085,
loss: 1.8838
        Validation string,      i: 1;   prediction: 3.5017,     target: 4.2057,
loss: 0.1674
        Validation string,      i: 2;   prediction: 3.5373,     target: 1.0491,
loss: 2.3717
Epoch [3/100], Loss: 0.5012, Loss validation: 0.4848, Time remaining: ~9.0h
34.0m 10s
        Validation string,      i: 0;   prediction: 3.2855,     target: 1.2085,
loss: 1.7187
        Validation string,      i: 1;   prediction: 3.0578,     target: 4.2057,
loss: 0.2729
        Validation string,      i: 2;   prediction: 3.2672,     target: 1.0491,
loss: 2.1142
Epoch [4/100], Loss: 0.5006, Loss validation: 0.4859, Time remaining: ~9.0h
21.0m 7s
        Validation string,      i: 0;   prediction: 3.3566,     target: 1.2085,
loss: 1.7775
        Validation string,      i: 1;   prediction: 3.3220,     target: 4.2057,
loss: 0.2101
        Validation string,      i: 2;   prediction: 3.2461,     target: 1.0491,
loss: 2.0941
Epoch [5/100], Loss: 0.5025, Loss validation: 0.4827, Time remaining: ~9.0h
10.0m 41s
        Validation string,      i: 0;   prediction: 3.5802,     target: 1.2085,
loss: 1.9625
        Validation string,      i: 1;   prediction: 3.6124,     target: 4.2057,
loss: 0.1411
        Validation string,      i: 2;   prediction: 3.5557,     target: 1.0491,
loss: 2.3892
Epoch [6/100], Loss: 0.4999, Loss validation: 0.4853, Time remaining: ~9.0h 2.0m
14s
        Validation string,      i: 0;   prediction: 3.3073,     target: 1.2085,
loss: 1.7366
        Validation string,      i: 1;   prediction: 3.2777,     target: 4.2057,
loss: 0.2207
        Validation string,      i: 2;   prediction: 3.2728,     target: 1.0491,
loss: 2.1196
```

```
Epoch [7/100], Loss: 0.5021, Loss validation: 0.4851, Time remaining: ~8.0h
54.0m 44s
        Validation string,      i: 0;   prediction: 3.2936,     target: 1.2085,
loss: 1.7253
        Validation string,      i: 1;   prediction: 3.2872,     target: 4.2057,
loss: 0.2184
        Validation string,      i: 2;   prediction: 3.2343,     target: 1.0491,
loss: 2.0828
Epoch [8/100], Loss: 0.5006, Loss validation: 0.4829, Time remaining: ~8.0h
47.0m 32s
        Validation string,      i: 0;   prediction: 3.2193,     target: 1.2085,
loss: 1.6639
        Validation string,      i: 1;   prediction: 3.1888,     target: 4.2057,
loss: 0.2418
        Validation string,      i: 2;   prediction: 3.1458,     target: 1.0491,
loss: 1.9985
Epoch [9/100], Loss: 0.5003, Loss validation: 0.4824, Time remaining: ~8.0h
40.0m 38s
        Validation string,      i: 0;   prediction: 3.3463,     target: 1.2085,
loss: 1.7689
        Validation string,      i: 1;   prediction: 3.3175,     target: 4.2057,
loss: 0.2112
        Validation string,      i: 2;   prediction: 3.3403,     target: 1.0491,
loss: 2.1839
Epoch [10/100], Loss: 0.5002, Loss validation: 0.4826, Time remaining: ~8.0h
34.0m 4s
        Validation string,      i: 0;   prediction: 3.4279,     target: 1.2085,
loss: 1.8364
        Validation string,      i: 1;   prediction: 3.4457,     target: 4.2057,
loss: 0.1807
        Validation string,      i: 2;   prediction: 3.4249,     target: 1.0491,
loss: 2.2646
Epoch [11/100], Loss: 0.5007, Loss validation: 0.4837, Time remaining: ~8.0h
27.0m 43s
        Validation string,      i: 0;   prediction: 3.1073,     target: 1.2085,
loss: 1.5711
        Validation string,      i: 1;   prediction: 3.2449,     target: 4.2057,
loss: 0.2284
        Validation string,      i: 2;   prediction: 3.1171,     target: 1.0491,
loss: 1.9711
Epoch [12/100], Loss: 0.5021, Loss validation: 0.4884, Time remaining: ~8.0h
21.0m 28s
        Validation string,      i: 0;   prediction: 2.9549,     target: 1.2085,
loss: 1.4450
        Validation string,      i: 1;   prediction: 2.9390,     target: 4.2057,
loss: 0.3012
        Validation string,      i: 2;   prediction: 3.0617,     target: 1.0491,
loss: 1.9184
```

```
Epoch [13/100], Loss: 0.4997, Loss validation: 0.4984, Time remaining: ~8.0h
15.0m 17s
        Validation string,      i: 0;   prediction: 3.3534,     target: 1.2085,
loss: 1.7748
        Validation string,      i: 1;   prediction: 3.1919,     target: 4.2057,
loss: 0.2410
        Validation string,      i: 2;   prediction: 3.4281,     target: 1.0491,
loss: 2.2676
Epoch [14/100], Loss: 0.5004, Loss validation: 0.4802, Time remaining: ~8.0h
9.0m 7s
        Validation string,      i: 0;   prediction: 3.3892,     target: 1.2085,
loss: 1.8045
        Validation string,      i: 1;   prediction: 3.5412,     target: 4.2057,
loss: 0.1580
        Validation string,      i: 2;   prediction: 3.5280,     target: 1.0491,
loss: 2.3628
Epoch [15/100], Loss: 0.4992, Loss validation: 0.4855, Time remaining: ~8.0h
3.0m 9s
        Validation string,      i: 0;   prediction: 3.3134,     target: 1.2085,
loss: 1.7417
        Validation string,      i: 1;   prediction: 3.3986,     target: 4.2057,
loss: 0.1919
        Validation string,      i: 2;   prediction: 3.4142,     target: 1.0491,
loss: 2.2543
Epoch [16/100], Loss: 0.4996, Loss validation: 0.4818, Time remaining: ~7.0h
57.0m 11s
        Validation string,      i: 0;   prediction: 3.4149,     target: 1.2085,
loss: 1.8257
        Validation string,      i: 1;   prediction: 3.4209,     target: 4.2057,
loss: 0.1866
        Validation string,      i: 2;   prediction: 3.4416,     target: 1.0491,
loss: 2.2805
Epoch [17/100], Loss: 0.5014, Loss validation: 0.4829, Time remaining: ~7.0h
51.0m 15s
        Validation string,      i: 0;   prediction: 3.6358,     target: 1.2085,
loss: 2.0085
        Validation string,      i: 1;   prediction: 3.6554,     target: 4.2057,
loss: 0.1309
        Validation string,      i: 2;   prediction: 3.6219,     target: 1.0491,
loss: 2.4523
Epoch [18/100], Loss: 0.4996, Loss validation: 0.4859, Time remaining: ~7.0h
45.0m 23s
        Validation string,      i: 0;   prediction: 3.5150,     target: 1.2085,
loss: 1.9085
        Validation string,      i: 1;   prediction: 3.4082,     target: 4.2057,
loss: 0.1896
        Validation string,      i: 2;   prediction: 3.4317,     target: 1.0491,
loss: 2.2710
```

```
Epoch [19/100], Loss: 0.5007, Loss validation: 0.4836, Time remaining: ~7.0h
39.0m 29s
        Validation string,      i: 0;   prediction: 3.6488,     target: 1.2085,
loss: 2.0192
        Validation string,      i: 1;   prediction: 3.6172,     target: 4.2057,
loss: 0.1399
        Validation string,      i: 2;   prediction: 3.6289,     target: 1.0491,
loss: 2.4590
Epoch [20/100], Loss: 0.4994, Loss validation: 0.4872, Time remaining: ~7.0h
33.0m 38s
        Validation string,      i: 0;   prediction: 3.5638,     target: 1.2085,
loss: 1.9489
        Validation string,      i: 1;   prediction: 3.4477,     target: 4.2057,
loss: 0.1802
        Validation string,      i: 2;   prediction: 3.6051,     target: 1.0491,
loss: 2.4363
Epoch [21/100], Loss: 0.5002, Loss validation: 0.4832, Time remaining: ~7.0h
27.0m 50s
        Validation string,      i: 0;   prediction: 3.1327,     target: 1.2085,
loss: 1.5922
        Validation string,      i: 1;   prediction: 3.2302,     target: 4.2057,
loss: 0.2319
        Validation string,      i: 2;   prediction: 3.1056,     target: 1.0491,
loss: 1.9602
Epoch [22/100], Loss: 0.5022, Loss validation: 0.4857, Time remaining: ~7.0h
22.0m 2s
        Validation string,      i: 0;   prediction: 2.8669,     target: 1.2085,
loss: 1.3722
        Validation string,      i: 1;   prediction: 2.9348,     target: 4.2057,
loss: 0.3022
        Validation string,      i: 2;   prediction: 2.8759,     target: 1.0491,
loss: 1.7413
Epoch [23/100], Loss: 0.5006, Loss validation: 0.4948, Time remaining: ~7.0h
16.0m 14s
        Validation string,      i: 0;   prediction: 3.1217,     target: 1.2085,
loss: 1.5831
        Validation string,      i: 1;   prediction: 3.0377,     target: 4.2057,
loss: 0.2777
        Validation string,      i: 2;   prediction: 3.1807,     target: 1.0491,
loss: 2.0318
Epoch [24/100], Loss: 0.5017, Loss validation: 0.4861, Time remaining: ~7.0h
10.0m 27s
        Validation string,      i: 0;   prediction: 3.4998,     target: 1.2085,
loss: 1.8960
        Validation string,      i: 1;   prediction: 3.4674,     target: 4.2057,
loss: 0.1756
        Validation string,      i: 2;   prediction: 3.4975,     target: 1.0491,
loss: 2.3338
```

```
Epoch [25/100], Loss: 0.5009, Loss validation: 0.4823, Time remaining: ~7.0h
4.0m 39s
         Validation string,      i: 0;   prediction: 3.2450,     target: 1.2085,
loss: 1.6851
         Validation string,      i: 1;   prediction: 3.2700,     target: 4.2057,
loss: 0.2225
         Validation string,      i: 2;   prediction: 3.2224,     target: 1.0491,
loss: 2.0715
Epoch [26/100], Loss: 0.5014, Loss validation: 0.4824, Time remaining: ~6.0h
58.0m 52s
         Validation string,      i: 0;   prediction: 3.4131,     target: 1.2085,
loss: 1.8242
         Validation string,      i: 1;   prediction: 3.3701,     target: 4.2057,
loss: 0.1987
         Validation string,      i: 2;   prediction: 3.3670,     target: 1.0491,
loss: 2.2094
Epoch [27/100], Loss: 0.5014, Loss validation: 0.4826, Time remaining: ~6.0h
53.0m 5s
         Validation string,      i: 0;   prediction: 3.5514,     target: 1.2085,
loss: 1.9386
         Validation string,      i: 1;   prediction: 3.5333,     target: 4.2057,
loss: 0.1599
         Validation string,      i: 2;   prediction: 3.5680,     target: 1.0491,
loss: 2.4010
Epoch [28/100], Loss: 0.5003, Loss validation: 0.4852, Time remaining: ~6.0h
47.0m 19s
         Validation string,      i: 0;   prediction: 3.1707,     target: 1.2085,
loss: 1.6236
         Validation string,      i: 1;   prediction: 3.1007,     target: 4.2057,
loss: 0.2628
         Validation string,      i: 2;   prediction: 3.0718,     target: 1.0491,
loss: 1.9280
Epoch [29/100], Loss: 0.4996, Loss validation: 0.4859, Time remaining: ~6.0h
41.0m 35s
         Validation string,      i: 0;   prediction: 3.0082,     target: 1.2085,
loss: 1.4892
         Validation string,      i: 1;   prediction: 3.0033,     target: 4.2057,
loss: 0.2859
         Validation string,      i: 2;   prediction: 3.0336,     target: 1.0491,
loss: 1.8916
Epoch [30/100], Loss: 0.5008, Loss validation: 0.4907, Time remaining: ~6.0h
35.0m 52s
         Validation string,      i: 0;   prediction: 3.4744,     target: 1.2085,
loss: 1.8750
         Validation string,      i: 1;   prediction: 3.4792,     target: 4.2057,
loss: 0.1728
         Validation string,      i: 2;   prediction: 3.4320,     target: 1.0491,
loss: 2.2713
```

```
Epoch [31/100], Loss: 0.4994, Loss validation: 0.4823, Time remaining: ~6.0h
30.0m 7s
        Validation string,      i: 0;   prediction: 3.5596,     target: 1.2085,
loss: 1.9454
        Validation string,      i: 1;   prediction: 3.5342,     target: 4.2057,
loss: 0.1597
        Validation string,      i: 2;   prediction: 3.5771,     target: 1.0491,
loss: 2.4096
Epoch [32/100], Loss: 0.5013, Loss validation: 0.4847, Time remaining: ~6.0h
24.0m 23s
        Validation string,      i: 0;   prediction: 3.6657,     target: 1.2085,
loss: 2.0332
        Validation string,      i: 1;   prediction: 3.6591,     target: 4.2057,
loss: 0.1300
        Validation string,      i: 2;   prediction: 3.6106,     target: 1.0491,
loss: 2.4416
Epoch [33/100], Loss: 0.5004, Loss validation: 0.4860, Time remaining: ~6.0h
18.0m 39s
        Validation string,      i: 0;   prediction: 3.5948,     target: 1.2085,
loss: 1.9745
        Validation string,      i: 1;   prediction: 3.5777,     target: 4.2057,
loss: 0.1493
        Validation string,      i: 2;   prediction: 3.5605,     target: 1.0491,
loss: 2.3938
Epoch [34/100], Loss: 0.5014, Loss validation: 0.4840, Time remaining: ~6.0h
12.0m 57s
        Validation string,      i: 0;   prediction: 3.1393,     target: 1.2085,
loss: 1.5977
        Validation string,      i: 1;   prediction: 3.3391,     target: 4.2057,
loss: 0.2060
        Validation string,      i: 2;   prediction: 3.1451,     target: 1.0491,
loss: 1.9978
Epoch [35/100], Loss: 0.4999, Loss validation: 0.4844, Time remaining: ~6.0h
7.0m 15s
        Validation string,      i: 0;   prediction: 3.2356,     target: 1.2085,
loss: 1.6773
        Validation string,      i: 1;   prediction: 3.1758,     target: 4.2057,
loss: 0.2449
        Validation string,      i: 2;   prediction: 3.1517,     target: 1.0491,
loss: 2.0041
Epoch [36/100], Loss: 0.4999, Loss validation: 0.4869, Time remaining: ~6.0h
1.0m 33s
        Validation string,      i: 0;   prediction: 3.4005,     target: 1.2085,
loss: 1.8138
        Validation string,      i: 1;   prediction: 3.1856,     target: 4.2057,
loss: 0.2425
        Validation string,      i: 2;   prediction: 3.2320,     target: 1.0491,
loss: 2.0807
```

```
Epoch [37/100], Loss: 0.4997, Loss validation: 0.4864, Time remaining: ~5.0h
55.0m 50s
        Validation string,      i: 0;   prediction: 3.7750,     target: 1.2085,
loss: 2.1237
        Validation string,      i: 1;   prediction: 3.7691,     target: 4.2057,
loss: 0.1038
        Validation string,      i: 2;   prediction: 3.7162,     target: 1.0491,
loss: 2.5422
Epoch [38/100], Loss: 0.5006, Loss validation: 0.4987, Time remaining: ~5.0h
50.0m 7s
        Validation string,      i: 0;   prediction: 3.2161,     target: 1.2085,
loss: 1.6612
        Validation string,      i: 1;   prediction: 3.1852,     target: 4.2057,
loss: 0.2426
        Validation string,      i: 2;   prediction: 3.2184,     target: 1.0491,
loss: 2.0677
Epoch [39/100], Loss: 0.5012, Loss validation: 0.4838, Time remaining: ~5.0h
44.0m 26s
        Validation string,      i: 0;   prediction: 3.3417,     target: 1.2085,
loss: 1.7651
        Validation string,      i: 1;   prediction: 3.4480,     target: 4.2057,
loss: 0.1802
        Validation string,      i: 2;   prediction: 3.4422,     target: 1.0491,
loss: 2.2811
Epoch [40/100], Loss: 0.5009, Loss validation: 0.4870, Time remaining: ~5.0h
38.0m 44s
        Validation string,      i: 0;   prediction: 3.5324,     target: 1.2085,
loss: 1.9229
        Validation string,      i: 1;   prediction: 3.4835,     target: 4.2057,
loss: 0.1717
        Validation string,      i: 2;   prediction: 3.5534,     target: 1.0491,
loss: 2.3870
Epoch [41/100], Loss: 0.5009, Loss validation: 0.4844, Time remaining: ~5.0h
33.0m 3s
        Validation string,      i: 0;   prediction: 3.3865,     target: 1.2085,
loss: 1.8022
        Validation string,      i: 1;   prediction: 3.3809,     target: 4.2057,
loss: 0.1961
        Validation string,      i: 2;   prediction: 3.3721,     target: 1.0491,
loss: 2.2142
Epoch [42/100], Loss: 0.5011, Loss validation: 0.4826, Time remaining: ~5.0h
27.0m 23s
        Validation string,      i: 0;   prediction: 3.3004,     target: 1.2085,
loss: 1.7310
        Validation string,      i: 1;   prediction: 3.2424,     target: 4.2057,
loss: 0.2290
        Validation string,      i: 2;   prediction: 3.3283,     target: 1.0491,
loss: 2.1724
```

```
Epoch [43/100], Loss: 0.5004, Loss validation: 0.4840, Time remaining: ~5.0h
21.0m 42s
        Validation string,      i: 0;   prediction: 3.5606,     target: 1.2085,
loss: 1.9463
        Validation string,      i: 1;   prediction: 3.5642,     target: 4.2057,
loss: 0.1525
        Validation string,      i: 2;   prediction: 3.5681,     target: 1.0491,
loss: 2.4011
Epoch [44/100], Loss: 0.5014, Loss validation: 0.4853, Time remaining: ~5.0h
16.0m 1s
        Validation string,      i: 0;   prediction: 3.5158,     target: 1.2085,
loss: 1.9092
        Validation string,      i: 1;   prediction: 3.4824,     target: 4.2057,
loss: 0.1720
        Validation string,      i: 2;   prediction: 3.4259,     target: 1.0491,
loss: 2.2655
Epoch [45/100], Loss: 0.4999, Loss validation: 0.4840, Time remaining: ~5.0h
10.0m 21s
        Validation string,      i: 0;   prediction: 3.1879,     target: 1.2085,
loss: 1.6379
        Validation string,      i: 1;   prediction: 3.3007,     target: 4.2057,
loss: 0.2152
        Validation string,      i: 2;   prediction: 3.0815,     target: 1.0491,
loss: 1.9372
Epoch [46/100], Loss: 0.5003, Loss validation: 0.4840, Time remaining: ~5.0h
4.0m 41s
        Validation string,      i: 0;   prediction: 3.7233,     target: 1.2085,
loss: 2.0809
        Validation string,      i: 1;   prediction: 3.7984,     target: 4.2057,
loss: 0.0969
        Validation string,      i: 2;   prediction: 3.8431,     target: 1.0491,
loss: 2.6632
Epoch [47/100], Loss: 0.5008, Loss validation: 0.4918, Time remaining: ~4.0h
59.0m 1s
        Validation string,      i: 0;   prediction: 3.1530,     target: 1.2085,
loss: 1.6090
        Validation string,      i: 1;   prediction: 3.2181,     target: 4.2057,
loss: 0.2348
        Validation string,      i: 2;   prediction: 3.1384,     target: 1.0491,
loss: 1.9914
Epoch [48/100], Loss: 0.4996, Loss validation: 0.4867, Time remaining: ~4.0h
53.0m 20s
        Validation string,      i: 0;   prediction: 3.4134,     target: 1.2085,
loss: 1.8245
        Validation string,      i: 1;   prediction: 3.4687,     target: 4.2057,
loss: 0.1752
        Validation string,      i: 2;   prediction: 3.3417,     target: 1.0491,
loss: 2.1852
```

```
Epoch [49/100], Loss: 0.5019, Loss validation: 0.4910, Time remaining: ~4.0h
47.0m 40s
        Validation string,      i: 0;   prediction: 3.1217,     target: 1.2085,
loss: 1.5831
        Validation string,      i: 1;   prediction: 3.1114,     target: 4.2057,
loss: 0.2602
        Validation string,      i: 2;   prediction: 3.1541,     target: 1.0491,
loss: 2.0064
Epoch [50/100], Loss: 0.4992, Loss validation: 0.4846, Time remaining: ~4.0h
41.0m 60s
        Validation string,      i: 0;   prediction: 3.1299,     target: 1.2085,
loss: 1.5899
        Validation string,      i: 1;   prediction: 3.1731,     target: 4.2057,
loss: 0.2455
        Validation string,      i: 2;   prediction: 3.1202,     target: 1.0491,
loss: 1.9741
Epoch [51/100], Loss: 0.5000, Loss validation: 0.4836, Time remaining: ~4.0h
36.0m 20s
        Validation string,      i: 0;   prediction: 3.4870,     target: 1.2085,
loss: 1.8854
        Validation string,      i: 1;   prediction: 3.3507,     target: 4.2057,
loss: 0.2033
        Validation string,      i: 2;   prediction: 3.4922,     target: 1.0491,
loss: 2.3287
Epoch [52/100], Loss: 0.5006, Loss validation: 0.4844, Time remaining: ~4.0h
30.0m 40s
        Validation string,      i: 0;   prediction: 3.2202,     target: 1.2085,
loss: 1.6646
        Validation string,      i: 1;   prediction: 3.2887,     target: 4.2057,
loss: 0.2180
        Validation string,      i: 2;   prediction: 3.2042,     target: 1.0491,
loss: 2.0541
Epoch [53/100], Loss: 0.4995, Loss validation: 0.4829, Time remaining: ~4.0h
25.0m 0s
        Validation string,      i: 0;   prediction: 3.1458,     target: 1.2085,
loss: 1.6031
        Validation string,      i: 1;   prediction: 3.2481,     target: 4.2057,
loss: 0.2277
        Validation string,      i: 2;   prediction: 3.1232,     target: 1.0491,
loss: 1.9770
Epoch [54/100], Loss: 0.5003, Loss validation: 0.4863, Time remaining: ~4.0h
19.0m 20s
        Validation string,      i: 0;   prediction: 3.0812,     target: 1.2085,
loss: 1.5496
        Validation string,      i: 1;   prediction: 3.0742,     target: 4.2057,
loss: 0.2690
        Validation string,      i: 2;   prediction: 3.1601,     target: 1.0491,
loss: 2.0122
```

```
Epoch [55/100], Loss: 0.5026, Loss validation: 0.4873, Time remaining: ~4.0h
13.0m 41s
        Validation string,      i: 0;   prediction: 3.1675,     target: 1.2085,
loss: 1.6210
        Validation string,      i: 1;   prediction: 3.0632,     target: 4.2057,
loss: 0.2716
        Validation string,      i: 2;   prediction: 3.1444,     target: 1.0491,
loss: 1.9972
Epoch [56/100], Loss: 0.5013, Loss validation: 0.4844, Time remaining: ~4.0h
8.0m 1s
        Validation string,      i: 0;   prediction: 3.6940,     target: 1.2085,
loss: 2.0567
        Validation string,      i: 1;   prediction: 3.7914,     target: 4.2057,
loss: 0.0985
        Validation string,      i: 2;   prediction: 3.5255,     target: 1.0491,
loss: 2.3604
Epoch [57/100], Loss: 0.5013, Loss validation: 0.4919, Time remaining: ~4.0h
2.0m 22s
        Validation string,      i: 0;   prediction: 3.6646,     target: 1.2085,
loss: 2.0323
        Validation string,      i: 1;   prediction: 3.3531,     target: 4.2057,
loss: 0.2027
        Validation string,      i: 2;   prediction: 3.3916,     target: 1.0491,
loss: 2.2328
Epoch [58/100], Loss: 0.5009, Loss validation: 0.4859, Time remaining: ~3.0h
56.0m 44s
        Validation string,      i: 0;   prediction: 3.2674,     target: 1.2085,
loss: 1.7037
        Validation string,      i: 1;   prediction: 3.2365,     target: 4.2057,
loss: 0.2305
        Validation string,      i: 2;   prediction: 3.2123,     target: 1.0491,
loss: 2.0619
Epoch [59/100], Loss: 0.5012, Loss validation: 0.4828, Time remaining: ~3.0h
51.0m 5s
        Validation string,      i: 0;   prediction: 3.1540,     target: 1.2085,
loss: 1.6098
        Validation string,      i: 1;   prediction: 3.4100,     target: 4.2057,
loss: 0.1892
        Validation string,      i: 2;   prediction: 2.9864,     target: 1.0491,
loss: 1.8465
Epoch [60/100], Loss: 0.5024, Loss validation: 0.4806, Time remaining: ~3.0h
45.0m 26s
        Validation string,      i: 0;   prediction: 3.6070,     target: 1.2085,
loss: 1.9846
        Validation string,      i: 1;   prediction: 3.5779,     target: 4.2057,
loss: 0.1493
        Validation string,      i: 2;   prediction: 3.5409,     target: 1.0491,
loss: 2.3751
```

```
Epoch [61/100], Loss: 0.5016, Loss validation: 0.4867, Time remaining: ~3.0h
39.0m 48s
        Validation string,      i: 0;   prediction: 3.1433,     target: 1.2085,
loss: 1.6009
        Validation string,      i: 1;   prediction: 3.3016,     target: 4.2057,
loss: 0.2150
        Validation string,      i: 2;   prediction: 3.3721,     target: 1.0491,
loss: 2.2142
Epoch [62/100], Loss: 0.5002, Loss validation: 0.4853, Time remaining: ~3.0h
34.0m 9s
        Validation string,      i: 0;   prediction: 3.3529,     target: 1.2085,
loss: 1.7744
        Validation string,      i: 1;   prediction: 3.3187,     target: 4.2057,
loss: 0.2109
        Validation string,      i: 2;   prediction: 3.4665,     target: 1.0491,
loss: 2.3042
Epoch [63/100], Loss: 0.5007, Loss validation: 0.4822, Time remaining: ~3.0h
28.0m 30s
        Validation string,      i: 0;   prediction: 3.3505,     target: 1.2085,
loss: 1.7724
        Validation string,      i: 1;   prediction: 3.3208,     target: 4.2057,
loss: 0.2104
        Validation string,      i: 2;   prediction: 3.3489,     target: 1.0491,
loss: 2.1921
Epoch [64/100], Loss: 0.5019, Loss validation: 0.4837, Time remaining: ~3.0h
22.0m 52s
        Validation string,      i: 0;   prediction: 3.1614,     target: 1.2085,
loss: 1.6160
        Validation string,      i: 1;   prediction: 3.3542,     target: 4.2057,
loss: 0.2025
        Validation string,      i: 2;   prediction: 3.1152,     target: 1.0491,
loss: 1.9693
Epoch [65/100], Loss: 0.5000, Loss validation: 0.4863, Time remaining: ~3.0h
17.0m 13s
        Validation string,      i: 0;   prediction: 3.2191,     target: 1.2085,
loss: 1.6637
        Validation string,      i: 1;   prediction: 3.3102,     target: 4.2057,
loss: 0.2129
        Validation string,      i: 2;   prediction: 3.1833,     target: 1.0491,
loss: 2.0343
Epoch [66/100], Loss: 0.4996, Loss validation: 0.4852, Time remaining: ~3.0h
11.0m 34s
        Validation string,      i: 0;   prediction: 3.0365,     target: 1.2085,
loss: 1.5126
        Validation string,      i: 1;   prediction: 3.0626,     target: 4.2057,
loss: 0.2718
        Validation string,      i: 2;   prediction: 3.0888,     target: 1.0491,
loss: 1.9441
```

```
Epoch [67/100], Loss: 0.5019, Loss validation: 0.4897, Time remaining: ~3.0h
5.0m 55s
         Validation string,      i: 0;   prediction: 3.4629,     target: 1.2085,
loss: 1.8654
         Validation string,      i: 1;   prediction: 3.5723,     target: 4.2057,
loss: 0.1506
         Validation string,      i: 2;   prediction: 3.4941,     target: 1.0491,
loss: 2.3305
Epoch [68/100], Loss: 0.4999, Loss validation: 0.4819, Time remaining: ~3.0h
0.0m 17s
         Validation string,      i: 0;   prediction: 3.2051,     target: 1.2085,
loss: 1.6521
         Validation string,      i: 1;   prediction: 3.0656,     target: 4.2057,
loss: 0.2711
         Validation string,      i: 2;   prediction: 3.2150,     target: 1.0491,
loss: 2.0645
Epoch [69/100], Loss: 0.5001, Loss validation: 0.4896, Time remaining: ~2.0h
54.0m 39s
         Validation string,      i: 0;   prediction: 3.6265,     target: 1.2085,
loss: 2.0008
         Validation string,      i: 1;   prediction: 3.5940,     target: 4.2057,
loss: 0.1455
         Validation string,      i: 2;   prediction: 3.5412,     target: 1.0491,
loss: 2.3754
Epoch [70/100], Loss: 0.5000, Loss validation: 0.4860, Time remaining: ~2.0h
49.0m 0s
         Validation string,      i: 0;   prediction: 3.1793,     target: 1.2085,
loss: 1.6308
         Validation string,      i: 1;   prediction: 3.1698,     target: 4.2057,
loss: 0.2463
         Validation string,      i: 2;   prediction: 3.1804,     target: 1.0491,
loss: 2.0315
Epoch [71/100], Loss: 0.5022, Loss validation: 0.4848, Time remaining: ~2.0h
43.0m 22s
         Validation string,      i: 0;   prediction: 3.2396,     target: 1.2085,
loss: 1.6807
         Validation string,      i: 1;   prediction: 3.4584,     target: 4.2057,
loss: 0.1777
         Validation string,      i: 2;   prediction: 3.3625,     target: 1.0491,
loss: 2.2050
Epoch [72/100], Loss: 0.4998, Loss validation: 0.4831, Time remaining: ~2.0h
37.0m 44s
         Validation string,      i: 0;   prediction: 3.2079,     target: 1.2085,
loss: 1.6544
         Validation string,      i: 1;   prediction: 3.2211,     target: 4.2057,
loss: 0.2341
         Validation string,      i: 2;   prediction: 3.2120,     target: 1.0491,
loss: 2.0616
```

```
Epoch [73/100], Loss: 0.5010, Loss validation: 0.4832, Time remaining: ~2.0h
32.0m 5s
        Validation string,      i: 0;   prediction: 3.0176,     target: 1.2085,
loss: 1.4970
        Validation string,      i: 1;   prediction: 2.9316,     target: 4.2057,
loss: 0.3029
        Validation string,      i: 2;   prediction: 2.9121,     target: 1.0491,
loss: 1.7758
Epoch [74/100], Loss: 0.5028, Loss validation: 0.4936, Time remaining: ~2.0h
26.0m 27s
        Validation string,      i: 0;   prediction: 3.1579,     target: 1.2085,
loss: 1.6131
        Validation string,      i: 1;   prediction: 3.1392,     target: 4.2057,
loss: 0.2536
        Validation string,      i: 2;   prediction: 3.1361,     target: 1.0491,
loss: 1.9893
Epoch [75/100], Loss: 0.5009, Loss validation: 0.4851, Time remaining: ~2.0h
20.0m 49s
        Validation string,      i: 0;   prediction: 3.3009,     target: 1.2085,
loss: 1.7314
        Validation string,      i: 1;   prediction: 3.2649,     target: 4.2057,
loss: 0.2237
        Validation string,      i: 2;   prediction: 3.2955,     target: 1.0491,
loss: 2.1412
Epoch [76/100], Loss: 0.5008, Loss validation: 0.4826, Time remaining: ~2.0h
15.0m 10s
        Validation string,      i: 0;   prediction: 3.2685,     target: 1.2085,
loss: 1.7046
        Validation string,      i: 1;   prediction: 3.3003,     target: 4.2057,
loss: 0.2153
        Validation string,      i: 2;   prediction: 3.1643,     target: 1.0491,
loss: 2.0162
Epoch [77/100], Loss: 0.5004, Loss validation: 0.4884, Time remaining: ~2.0h
9.0m 32s
        Validation string,      i: 0;   prediction: 3.2468,     target: 1.2085,
loss: 1.6866
        Validation string,      i: 1;   prediction: 3.2493,     target: 4.2057,
loss: 0.2274
        Validation string,      i: 2;   prediction: 3.2506,     target: 1.0491,
loss: 2.0984
Epoch [78/100], Loss: 0.5003, Loss validation: 0.4834, Time remaining: ~2.0h
3.0m 54s
        Validation string,      i: 0;   prediction: 3.6769,     target: 1.2085,
loss: 2.0425
        Validation string,      i: 1;   prediction: 3.4967,     target: 4.2057,
loss: 0.1686
        Validation string,      i: 2;   prediction: 3.6913,     target: 1.0491,
loss: 2.5185
```

```
Epoch [79/100], Loss: 0.5014, Loss validation: 0.4893, Time remaining: ~1.0h
58.0m 16s
        Validation string,      i: 0;   prediction: 3.3463,     target: 1.2085,
loss: 1.7689
        Validation string,      i: 1;   prediction: 3.4074,     target: 4.2057,
loss: 0.1898
        Validation string,      i: 2;   prediction: 3.3219,     target: 1.0491,
loss: 2.1664
Epoch [80/100], Loss: 0.5014, Loss validation: 0.4804, Time remaining: ~1.0h
52.0m 38s
        Validation string,      i: 0;   prediction: 3.3534,     target: 1.2085,
loss: 1.7748
        Validation string,      i: 1;   prediction: 3.2171,     target: 4.2057,
loss: 0.2351
        Validation string,      i: 2;   prediction: 3.4056,     target: 1.0491,
loss: 2.2462
Epoch [81/100], Loss: 0.5017, Loss validation: 0.4837, Time remaining: ~1.0h
46.0m 60s
        Validation string,      i: 0;   prediction: 3.2840,     target: 1.2085,
loss: 1.7174
        Validation string,      i: 1;   prediction: 3.2939,     target: 4.2057,
loss: 0.2168
        Validation string,      i: 2;   prediction: 3.2730,     target: 1.0491,
loss: 2.1198
Epoch [82/100], Loss: 0.5016, Loss validation: 0.4824, Time remaining: ~1.0h
41.0m 22s
        Validation string,      i: 0;   prediction: 3.3270,     target: 1.2085,
loss: 1.7529
        Validation string,      i: 1;   prediction: 3.3305,     target: 4.2057,
loss: 0.2081
        Validation string,      i: 2;   prediction: 3.3629,     target: 1.0491,
loss: 2.2054
Epoch [83/100], Loss: 0.4998, Loss validation: 0.4835, Time remaining: ~1.0h
35.0m 44s
        Validation string,      i: 0;   prediction: 3.4733,     target: 1.2085,
loss: 1.8740
        Validation string,      i: 1;   prediction: 3.5046,     target: 4.2057,
loss: 0.1667
        Validation string,      i: 2;   prediction: 3.4057,     target: 1.0491,
loss: 2.2463
Epoch [84/100], Loss: 0.5003, Loss validation: 0.4833, Time remaining: ~1.0h
30.0m 6s
        Validation string,      i: 0;   prediction: 3.3058,     target: 1.2085,
loss: 1.7355
        Validation string,      i: 1;   prediction: 3.3308,     target: 4.2057,
loss: 0.2080
        Validation string,      i: 2;   prediction: 3.2983,     target: 1.0491,
loss: 2.1438
```

```
Epoch [85/100], Loss: 0.5019, Loss validation: 0.4830, Time remaining: ~1.0h
24.0m 28s
        Validation string,      i: 0;   prediction: 3.3320,     target: 1.2085,
loss: 1.7571
        Validation string,      i: 1;   prediction: 3.5060,     target: 4.2057,
loss: 0.1664
        Validation string,      i: 2;   prediction: 3.4095,     target: 1.0491,
loss: 2.2499
Epoch [86/100], Loss: 0.5010, Loss validation: 0.4822, Time remaining: ~1.0h
18.0m 50s
        Validation string,      i: 0;   prediction: 3.2978,     target: 1.2085,
loss: 1.7288
        Validation string,      i: 1;   prediction: 3.2438,     target: 4.2057,
loss: 0.2287
        Validation string,      i: 2;   prediction: 3.2401,     target: 1.0491,
loss: 2.0884
Epoch [87/100], Loss: 0.5009, Loss validation: 0.4837, Time remaining: ~1.0h
13.0m 12s
        Validation string,      i: 0;   prediction: 3.6487,     target: 1.2085,
loss: 2.0192
        Validation string,      i: 1;   prediction: 3.5160,     target: 4.2057,
loss: 0.1640
        Validation string,      i: 2;   prediction: 3.6256,     target: 1.0491,
loss: 2.4559
Epoch [88/100], Loss: 0.5007, Loss validation: 0.4870, Time remaining: ~1.0h
7.0m 34s
        Validation string,      i: 0;   prediction: 3.4559,     target: 1.2085,
loss: 1.8596
        Validation string,      i: 1;   prediction: 3.4808,     target: 4.2057,
loss: 0.1724
        Validation string,      i: 2;   prediction: 3.3905,     target: 1.0491,
loss: 2.2317
Epoch [89/100], Loss: 0.4999, Loss validation: 0.4828, Time remaining: ~1.0h
1.0m 56s
        Validation string,      i: 0;   prediction: 3.0915,     target: 1.2085,
loss: 1.5581
        Validation string,      i: 1;   prediction: 3.0920,     target: 4.2057,
loss: 0.2648
        Validation string,      i: 2;   prediction: 3.1112,     target: 1.0491,
loss: 1.9656
Epoch [90/100], Loss: 0.5013, Loss validation: 0.4865, Time remaining: ~0.0h
56.0m 18s
        Validation string,      i: 0;   prediction: 3.2678,     target: 1.2085,
loss: 1.7040
        Validation string,      i: 1;   prediction: 3.3023,     target: 4.2057,
loss: 0.2148
        Validation string,      i: 2;   prediction: 3.2075,     target: 1.0491,
loss: 2.0573
```

```
Epoch [91/100], Loss: 0.5001, Loss validation: 0.4815, Time remaining: ~0.0h
50.0m 40s
        Validation string,      i: 0;   prediction: 3.4230,     target: 1.2085,
loss: 1.8324
        Validation string,      i: 1;   prediction: 3.2731,     target: 4.2057,
loss: 0.2217
        Validation string,      i: 2;   prediction: 3.3529,     target: 1.0491,
loss: 2.1959
Epoch [92/100], Loss: 0.4996, Loss validation: 0.4827, Time remaining: ~0.0h
45.0m 2s
        Validation string,      i: 0;   prediction: 3.1871,     target: 1.2085,
loss: 1.6372
        Validation string,      i: 1;   prediction: 3.0466,     target: 4.2057,
loss: 0.2756
        Validation string,      i: 2;   prediction: 3.0095,     target: 1.0491,
loss: 1.8686
Epoch [93/100], Loss: 0.5003, Loss validation: 0.4906, Time remaining: ~0.0h
39.0m 25s
        Validation string,      i: 0;   prediction: 3.2509,     target: 1.2085,
loss: 1.6900
        Validation string,      i: 1;   prediction: 3.2564,     target: 4.2057,
loss: 0.2257
        Validation string,      i: 2;   prediction: 3.3583,     target: 1.0491,
loss: 2.2010
Epoch [94/100], Loss: 0.5005, Loss validation: 0.4799, Time remaining: ~0.0h
33.0m 47s
        Validation string,      i: 0;   prediction: 3.5699,     target: 1.2085,
loss: 1.9539
        Validation string,      i: 1;   prediction: 3.5836,     target: 4.2057,
loss: 0.1479
        Validation string,      i: 2;   prediction: 3.5807,     target: 1.0491,
loss: 2.4130
Epoch [95/100], Loss: 0.5028, Loss validation: 0.4859, Time remaining: ~0.0h
28.0m 9s
        Validation string,      i: 0;   prediction: 3.3013,     target: 1.2085,
loss: 1.7317
        Validation string,      i: 1;   prediction: 3.3325,     target: 4.2057,
loss: 0.2076
        Validation string,      i: 2;   prediction: 3.2574,     target: 1.0491,
loss: 2.1049
Epoch [96/100], Loss: 0.5024, Loss validation: 0.4820, Time remaining: ~0.0h
22.0m 31s
        Validation string,      i: 0;   prediction: 3.5215,     target: 1.2085,
loss: 1.9139
        Validation string,      i: 1;   prediction: 3.5308,     target: 4.2057,
loss: 0.1605
        Validation string,      i: 2;   prediction: 3.5237,     target: 1.0491,
loss: 2.3587
```

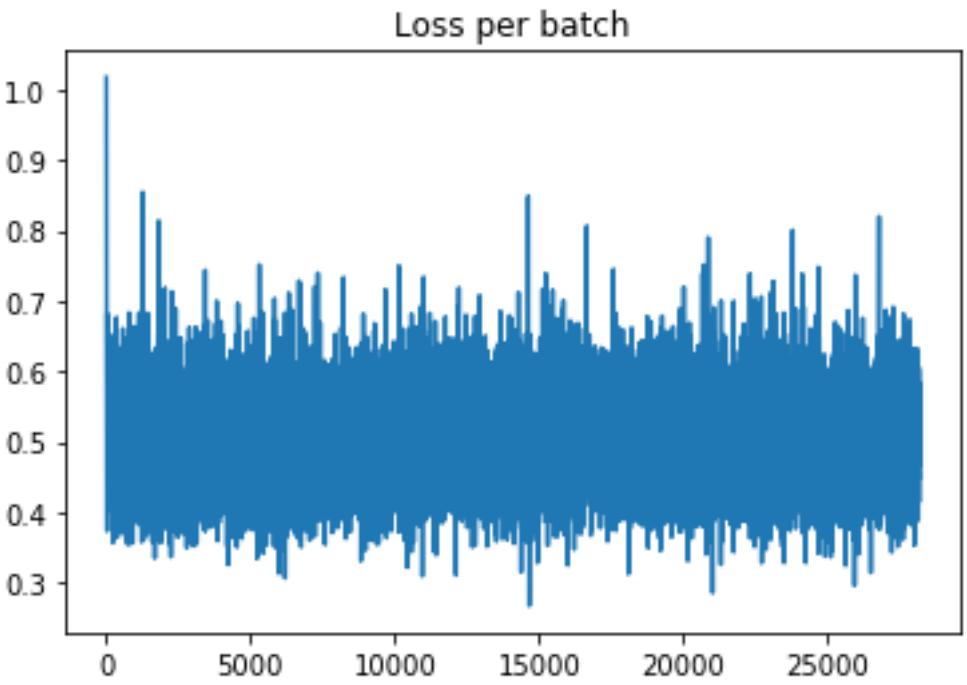
```
Epoch [97/100], Loss: 0.5006, Loss validation: 0.4841, Time remaining: ~0.0h
16.0m 53s
        Validation string,      i: 0;   prediction: 3.7159,     target: 1.2085,
loss: 2.0748
        Validation string,      i: 1;   prediction: 3.7541,     target: 4.2057,
loss: 0.1074
        Validation string,      i: 2;   prediction: 3.7292,     target: 1.0491,
loss: 2.5546
Epoch [98/100], Loss: 0.5011, Loss validation: 0.4912, Time remaining: ~0.0h
11.0m 16s
        Validation string,      i: 0;   prediction: 3.4776,     target: 1.2085,
loss: 1.8776
        Validation string,      i: 1;   prediction: 3.5846,     target: 4.2057,
loss: 0.1477
        Validation string,      i: 2;   prediction: 3.4941,     target: 1.0491,
loss: 2.3305
Epoch [99/100], Loss: 0.5006, Loss validation: 0.4885, Time remaining: ~0.0h
5.0m 38s
        Validation string,      i: 0;   prediction: 3.2481,     target: 1.2085,
loss: 1.6876
        Validation string,      i: 1;   prediction: 3.1836,     target: 4.2057,
loss: 0.2430
        Validation string,      i: 2;   prediction: 3.1727,     target: 1.0491,
loss: 2.0242
Epoch [100/100], Loss: 0.5015, Loss validation: 0.4834, Time remaining: ~0.0h
0.0m 0s
```

[ ]:
```python
# save string of the model
model.save_str(
    metadata={
        "data_file_path": data_file_path,
    }
)
```

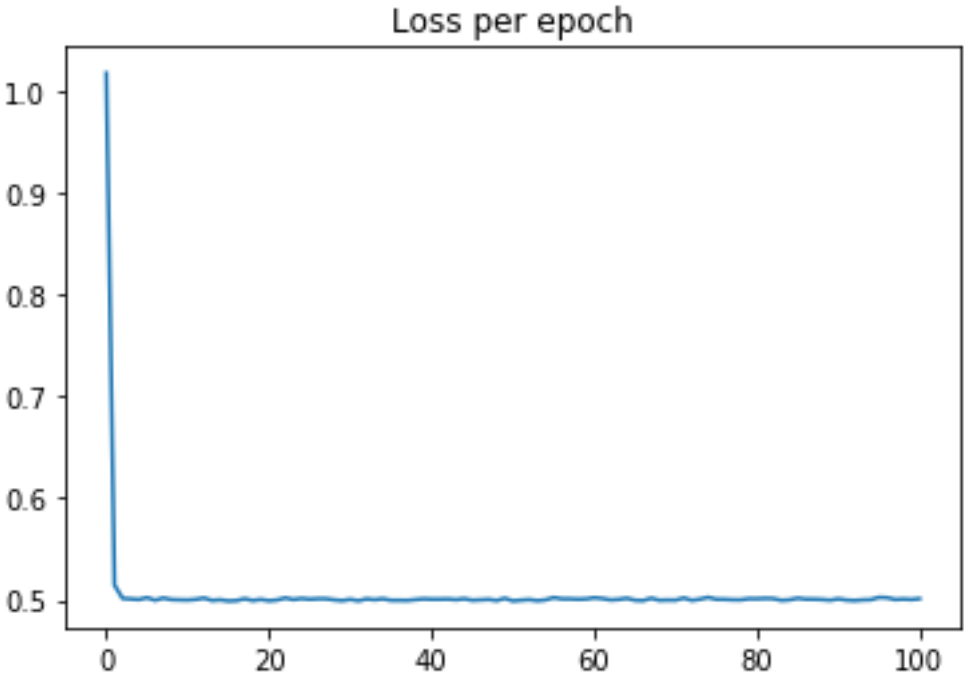
```
Saved in:  peptide-QML/checkpoints/0810/txts/0810-mh_em_1qm_model_str_5.txt
```

[ ]:
```python
# plot the losses of the trainig loop and save the figures
model.plot_losses(save=True)
```

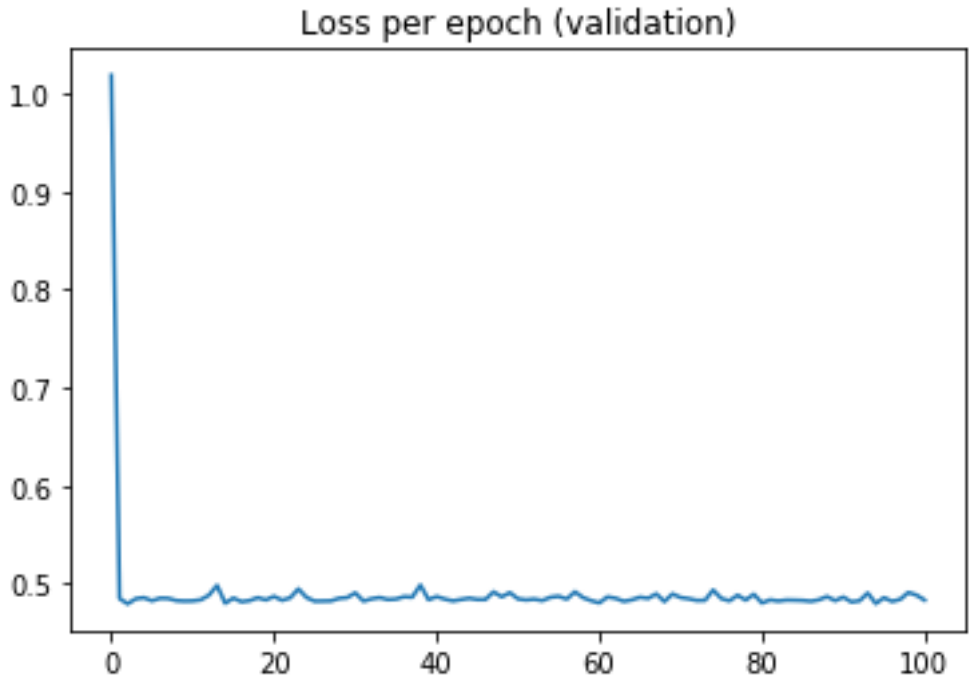
```
Saved in:  peptide-
QML/checkpoints/0810/plots/0810-mh_em_1qm_losses_batches_5.png
```




Saved in: peptide-QML/checkpoints/0810/plots/0810-mh_em_1qm_losses_epoch_5.png



```
Saved in:  peptide-
QML/checkpoints/0810/plots/0810-mh_em_1qm_losses_epoch_validation_5.png
```




[ ]:
```
# plot how the average of the parameters in each layer changes over time, and␣
 ↪save that
for layer in model.model.state_dict().keys():
    model.plot_parameter(layer=layer, save=True)
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-23-cb7518267280> in <module>
      1 # plot how the average of the parameters in each layer changes over␣
 ↪time, and save that
      2 for layer in model.model.state_dict().keys():
----> 3     model.plot_parameter(layer=layer, save=True)

~/peptide-QML/my_code/pytorch_model.py in plot_parameter(self, layer, index,␣
 ↪save)
    221
    222         if index is None:
--> 223             for i in range(len(self.parameters)):
    224                 parameter_evolution.append(torch.mean(self.
 ↪parameters[i][layer]).item())
    225         else:
```

```
TypeError: object of type 'NoneType' has no len()
```

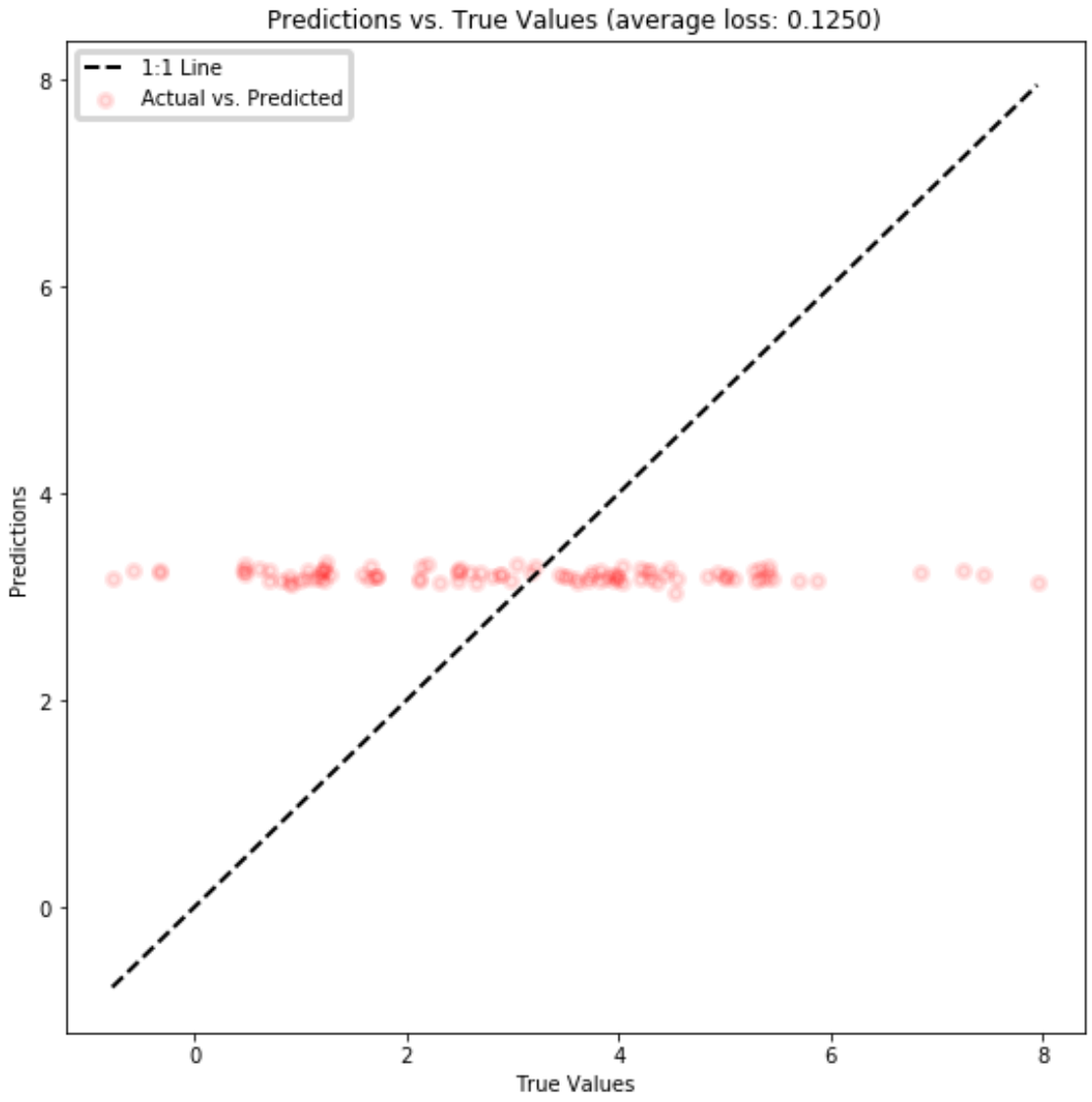
[ ]:
```
# model.plot_parameter(layer='7.weights', index=50)
```

[ ]:
```
#save all the parameters of the model and the intermediate parameters of the␣
↪model
model.save_state_dict(intermediate=False)
```

```
Model saved as peptide-QML/checkpoints/0810/models/0810-mh_em_1qm_5.pth
```

[ ]:
```
model.plot_validation(save=True, fig_size=(9,9), percentatge=0.1)
```

```
The file peptide-QML/checkpoints/0810/plots/0810-mh_em_1qm_validation_5.png
already exists, it will be replaced
Saved in:  peptide-QML/checkpoints/0810/plots/0810-mh_em_1qm_validation_5.png
```




[ ]:
```
# print validation and save it
model.print_validation(save=True, precision=4, percentatge=0.1)
```

```
i: 0,           target: 1.2085,         prediction: 3.2481,     loss: 1.6876
i: 1,           target: 2.1149,         prediction: 3.1530,     loss: 0.4909
i: 2,           target: 4.2601,         prediction: 3.2624,     loss: 0.2342
i: 3,           target: 5.4525,         prediction: 3.1863,     loss: 0.4156
i: 4,           target: 0.4727,         prediction: 3.2479,     loss: 5.8703
i: 5,           target: 5.3038,         prediction: 3.1513,     loss: 0.4058
i: 6,           target: 7.2482,         prediction: 3.2579,     loss: 0.5505
i: 7,           target: 1.7112,         prediction: 3.1877,     loss: 0.8628
i: 8,           target: 2.1105,         prediction: 3.1802,     loss: 0.5069
i: 9,           target: 3.5118,         prediction: 3.1966,     loss: 0.0898
```

```
i: 10,          target: 4.2057,         prediction: 3.1836,     loss: 0.2430
i: 11,          target: 7.9475,         prediction: 3.1417,     loss: 0.6047
i: 12,          target: 3.7404,         prediction: 3.2270,     loss: 0.1373
i: 13,          target: 3.9884,         prediction: 3.1729,     loss: 0.2045
i: 14,          target: 0.7019,         prediction: 3.2603,     loss: 3.6448
i: 15,          target: 4.2942,         prediction: 3.1818,     loss: 0.2590
i: 16,          target: 4.9275,         prediction: 3.2364,     loss: 0.3432
i: 17,          target: 4.3633,         prediction: 3.1365,     loss: 0.2812
i: 18,          target: 1.2119,         prediction: 3.1645,     loss: 1.6113
i: 19,          target: 1.7022,         prediction: 3.1937,     loss: 0.8763
i: 20,          target: 1.0491,         prediction: 3.1727,     loss: 2.0242
i: 21,          target: 3.0441,         prediction: 3.3186,     loss: 0.0902
i: 22,          target: 3.2082,         prediction: 3.3036,     loss: 0.0297
i: 23,          target: 3.9221,         prediction: 3.2222,     loss: 0.1785
i: 24,          target: 3.4724,         prediction: 3.1874,     loss: 0.0821
i: 25,          target: 6.8442,         prediction: 3.2374,     loss: 0.5270
i: 26,          target: 5.3831,         prediction: 3.1777,     loss: 0.4097
i: 27,          target: 4.8266,         prediction: 3.1908,     loss: 0.3389
i: 28,          target: 0.9925,         prediction: 3.1551,     loss: 2.1790
i: 29,          target: 2.8893,         prediction: 3.2199,     loss: 0.1144
i: 30,          target: 1.6492,         prediction: 3.3031,     loss: 1.0028
i: 31,          target: 1.5728,         prediction: 3.2200,     loss: 1.0472
i: 32,          target: 1.6326,         prediction: 3.1790,     loss: 0.9472
i: 33,          target: 5.8696,         prediction: 3.1497,     loss: 0.4634
i: 34,          target: 2.9738,         prediction: 3.1606,     loss: 0.0628
i: 35,          target: 4.4263,         prediction: 3.2074,     loss: 0.2754
i: 36,          target: 4.5223,         prediction: 3.0377,     loss: 0.3283
i: 37,          target: 2.6630,         prediction: 3.1432,     loss: 0.1803
i: 38,          target: 3.8160,         prediction: 3.1556,     loss: 0.1730
i: 39,          target: 1.1251,         prediction: 3.1821,     loss: 1.8284
i: 40,          target: 5.4176,         prediction: 3.2389,     loss: 0.4022
i: 41,          target: 0.4447,         prediction: 3.2590,     loss: 6.3280
i: 42,          target: 4.0349,         prediction: 3.1281,     loss: 0.2247
i: 43,          target: 2.2002,         prediction: 3.3183,     loss: 0.5082
i: 44,          target: 2.1458,         prediction: 3.2990,     loss: 0.5375
i: 45,          target: -0.7770,        prediction: 3.1802,     loss: 5.0928
i: 46,          target: 4.4673,         prediction: 3.2674,     loss: 0.2686
i: 47,          target: 3.6137,         prediction: 3.1297,     loss: 0.1339
i: 48,          target: 2.3090,         prediction: 3.1299,     loss: 0.3555
i: 49,          target: 4.9907,         prediction: 3.2032,     loss: 0.3582
i: 50,          target: 2.8753,         prediction: 3.2063,     loss: 0.1151
i: 51,          target: 1.2186,         prediction: 3.2812,     loss: 1.6926
i: 52,          target: 3.9634,         prediction: 3.1520,     loss: 0.2047
i: 53,          target: 0.9172,         prediction: 3.1106,     loss: 2.3915
i: 54,          target: 5.7036,         prediction: 3.1607,     loss: 0.4459
i: 55,          target: 2.4951,         prediction: 3.2792,     loss: 0.3143
i: 56,          target: -0.3259,        prediction: 3.2510,     loss: 10.9757
i: 57,          target: 4.3077,         prediction: 3.2490,     loss: 0.2458
```

```
i: 58,          target: 3.8818,         prediction: 3.1723,     loss: 0.1828
i: 59,          target: 0.4731,         prediction: 3.2200,     loss: 5.8068
i: 60,          target: 5.0085,         prediction: 3.1801,     loss: 0.3651
i: 61,          target: 2.4797,         prediction: 3.1653,     loss: 0.2765
i: 62,          target: 3.8152,         prediction: 3.2476,     loss: 0.1488
i: 63,          target: 4.5573,         prediction: 3.1812,     loss: 0.3019
i: 64,          target: 5.3347,         prediction: 3.1770,     loss: 0.4045
i: 65,          target: 3.4399,         prediction: 3.2108,     loss: 0.0666
i: 66,          target: 2.4752,         prediction: 3.2420,     loss: 0.3098
i: 67,          target: 3.5888,         prediction: 3.1728,     loss: 0.1159
i: 68,          target: 0.8220,         prediction: 3.1610,     loss: 2.8453
i: 69,          target: 1.1807,         prediction: 3.1766,     loss: 1.6903
i: 70,          target: 5.0771,         prediction: 3.1774,     loss: 0.3742
i: 71,          target: -0.3308,        prediction: 3.2374,     loss: 10.7868
i: 72,          target: 4.2039,         prediction: 3.2705,     loss: 0.2220
i: 73,          target: 3.9716,         prediction: 3.2215,     loss: 0.1889
i: 74,          target: 1.1815,         prediction: 3.2114,     loss: 1.7180
i: 75,          target: 0.8840,         prediction: 3.2051,     loss: 2.6257
i: 76,          target: 3.1676,         prediction: 3.2276,     loss: 0.0189
i: 77,          target: -0.5823,        prediction: 3.2473,     loss: 6.5762
i: 78,          target: 2.8107,         prediction: 3.2016,     loss: 0.1391
i: 79,          target: 5.0323,         prediction: 3.2169,     loss: 0.3607
i: 80,          target: 0.6020,         prediction: 3.2654,     loss: 4.4238
i: 81,          target: 3.6985,         prediction: 3.1617,     loss: 0.1451
i: 82,          target: 1.7253,         prediction: 3.2051,     loss: 0.8577
i: 83,          target: 0.7078,         prediction: 3.1629,     loss: 3.4687
i: 84,          target: 5.3377,         prediction: 3.2785,     loss: 0.3858
i: 85,          target: 1.2440,         prediction: 3.3285,     loss: 1.6757
i: 86,          target: 4.0394,         prediction: 3.2975,     loss: 0.1837
i: 87,          target: 1.0727,         prediction: 3.2506,     loss: 2.0303
i: 88,          target: 0.8952,         prediction: 3.1425,     loss: 2.5103
i: 89,          target: 0.4779,         prediction: 3.3077,     loss: 5.9207
i: 90,          target: 1.2700,         prediction: 3.2064,     loss: 1.5248
i: 91,          target: 1.2195,         prediction: 3.2465,     loss: 1.6622
i: 92,          target: 3.7290,         prediction: 3.1934,     loss: 0.1436
i: 93,          target: 5.4170,         prediction: 3.2873,     loss: 0.3932
i: 94,          target: 2.6034,         prediction: 3.2384,     loss: 0.2439
i: 95,          target: 3.9816,         prediction: 3.1965,     loss: 0.1972
i: 96,          target: 2.6859,         prediction: 3.2398,     loss: 0.2062
i: 97,          target: 5.2708,         prediction: 3.2466,     loss: 0.3840
i: 98,          target: 2.4895,         prediction: 3.2559,     loss: 0.3078
i: 99,          target: 7.4392,         prediction: 3.2077,     loss: 0.5688
Average loss: 0.1250
The file peptide-QML/checkpoints/0810/txts/0810-mh_em_1qm_validation_5.txt
already exists, it will be replaced
Saved in:  peptide-QML/checkpoints/0810/txts/0810-mh_em_1qm_validation_5.txt
```

[ ]:
```
# push changes to git
if initial_path != '../':
    !cd peptide-QML && git add . && git commit -m "data trained model" && git␣
 ↪push
```

```
[main d295cd4f] data trained model
 7 files changed, 142 insertions(+)
 create mode 100644 checkpoints/0810/models/0810-mh_em_1qm_5.pth
 create mode 100644 checkpoints/0810/plots/0810-mh_em_1qm_losses_batches_5.png
 create mode 100644 checkpoints/0810/plots/0810-mh_em_1qm_losses_epoch_5.png
 create mode 100644
checkpoints/0810/plots/0810-mh_em_1qm_losses_epoch_validation_5.png
 create mode 100644 checkpoints/0810/plots/0810-mh_em_1qm_validation_5.png
 create mode 100644 checkpoints/0810/txts/0810-mh_em_1qm_model_str_5.txt
 create mode 100644 checkpoints/0810/txts/0810-mh_em_1qm_validation_5.txt
Enumerating objects: 20, done.
Counting objects: 100% (20/20), done.
Delta compression using up to 24 threads
Compressing objects: 100% (14/14), done.
Writing objects: 100% (14/14), 74.44 KiB | 8.27 MiB/s, done.
Total 14 (delta 5), reused 0 (delta 0)
remote: Resolving deltas: 100% (5/5), completed with 5 local objects.
To github.com:raulconchello/peptide-QML.git
   a3aaaaa7..d295cd4f  main -> main
```

[ ]:
```

```