0802-sh_1qm_1

August 3, 2023

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

[ ]:
```
day = "0802"
name_notebook = day + "-sh_1qm.ipynb"
```

[ ]:
```
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

[ ]:
```
file_path = initial_path + 'data/energies/PET/generated/
 ↪bb14_Strings_Energies_10_000_4_aa.txt'  # Replace with the actual path to␣
 ↪your 'data.txt' file
string_list, number_list = f.read_data_file(file_path)
score_list = np.array(number_list)/1000
vector_list = np.array([f.string_to_vector(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)

X = X.reshape(X.shape[0], X.shape[1]*X.shape[2]) # flatten
X_validation = X_validation.reshape(X_validation.shape[0], X_validation.
 ↪shape[1]*X_validation.shape[2]) # flatten
```

[ ]:
```
# Define the dataset
input_data = ptm.torch.tensor(X, dtype=ptm.torch.float64)
```

```
target_data = ptm.torch.tensor(Y, dtype=ptm.torch.float64).view(-1, 1)

# Define the validation set
input_validation = ptm.torch.tensor(X_validation, dtype=ptm.torch.float64)
target_validation = ptm.torch.tensor(Y_validation, dtype=ptm.torch.float64).
 ↪view(-1, 1)
```

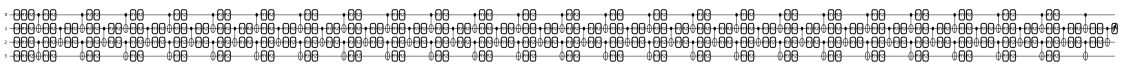
2 Quantum node

[ ]:
```
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,
    ansatz = qn.parts.Ansatz_11,
    measurement = qn.parts.exp_Z(1),
    n_layers = 25,
    # 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

[ ]:
```
input_dim = input_data.size(1)

n_pre_classical_layers = 4
layers_dim = np.linspace(n_aminoacids, input_dim, 4).astype(int)
```

[ ]:
```
layers = []
for i in range(1, len(layers_dim)):
    layers += [ptm.nn.Linear(layers_dim[-1*i], layers_dim[-1*(i+1)]), ptm.nn.
 ↪ReLU()]
layers += [ptm.nn.Linear(layers_dim[0], layers_dim[0])]
layers += [quantum_layer()]
# layers += [nn.Linear(1, 1)]
# layers += [nn.Linear(2, 4), nn.ReLU()]
# layers += [nn.Linear(4, 1)]
```

[ ]:
```
# Create model and set data:
model = ptm.pytorch_model(
    layers,
    save_options = {'initial_path': initial_path, 'name_notebook':␣
 ↪name_notebook},
    keep_track_params=True,
)
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]).item())
print(model(input_data[1]).item())
```

```
0.4397516791058914
0.4397447280566661
```

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

# train the model
model.train(
```

```
    optimizer= optim.Adam,
    optimizer_options={'lr': 0.5},
    num_epochs = 25,
    batch_size = 32,
)
```

```
Epoch [0/25], Loss: 3.3016, Loss validation: 3.3231
- Epoch [1/25], i: [0/9000], Loss: 4.4792

/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: -0.0602,    target:
-0.0662,        loss: 0.0897
        Validation string,      i: 1;   prediction: -0.0602,    target: 0.2078,
loss: 1.2898
        Validation string,      i: 2;   prediction: -0.0602,    target:
-0.0342,        loss: 0.7619
Epoch [1/25], Loss: 2.0729, Loss validation: 1.1877, Time remaining: ~0.0h 20.0m
29s
        Validation string,      i: 0;   prediction: 0.3950,     target:
-0.0662,        loss: 6.9699
        Validation string,      i: 1;   prediction: 0.3950,     target: 0.2078,
loss: 0.9003
        Validation string,      i: 2;   prediction: 0.3950,     target:
-0.0342,        loss: 12.5549
Epoch [2/25], Loss: 2.0238, Loss validation: 2.9915, Time remaining: ~0.0h 18.0m
34s
        Validation string,      i: 0;   prediction: -0.0395,    target:
-0.0662,        loss: 0.4024
        Validation string,      i: 1;   prediction: -0.0395,    target: 0.2078,
loss: 1.1902
        Validation string,      i: 2;   prediction: -0.0395,    target:
-0.0342,        loss: 0.1567
Epoch [3/25], Loss: 1.9761, Loss validation: 1.1051, Time remaining: ~0.0h 17.0m
29s
        Validation string,      i: 0;   prediction: -0.0353,    target:
-0.0662,        loss: 0.4661
        Validation string,      i: 1;   prediction: -0.0353,    target: 0.2078,
loss: 1.1700
        Validation string,      i: 2;   prediction: -0.0353,    target:
-0.0342,        loss: 0.0334
Epoch [4/25], Loss: 2.0789, Loss validation: 1.0903, Time remaining: ~0.0h 16.0m
37s
        Validation string,      i: 0;   prediction: 0.2259,     target:
```

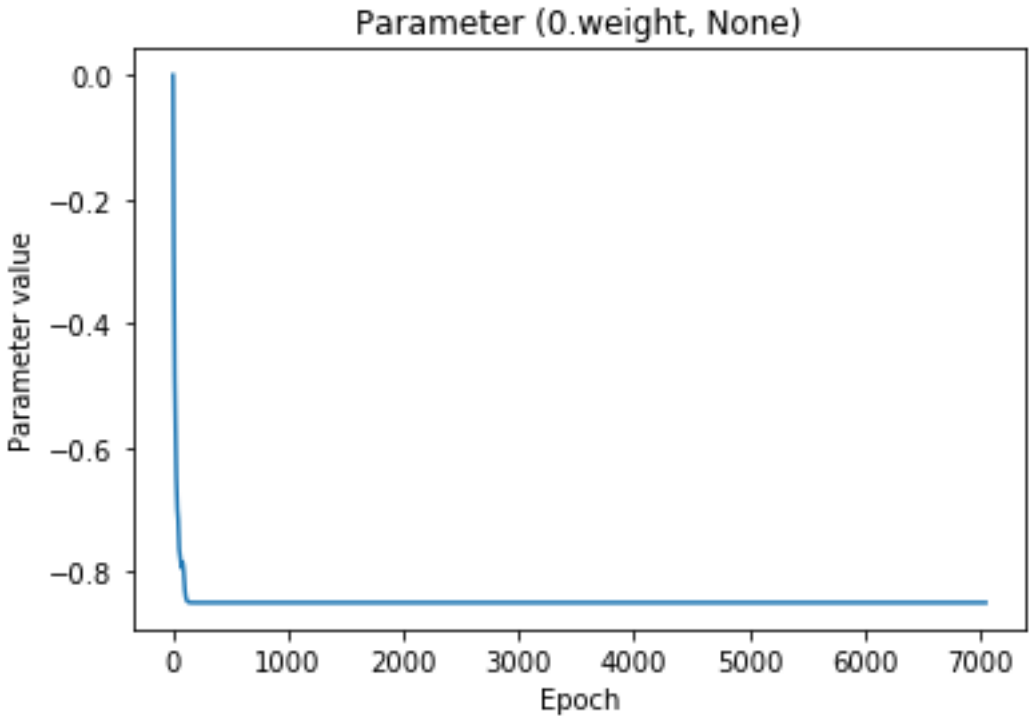
```
-0.0662,        loss: 4.4139
         Validation string,      i: 1;   prediction: 0.2259,     target: 0.2078,
loss: 0.0867
         Validation string,      i: 2;   prediction: 0.2259,     target:
-0.0342,        loss: 7.6076
Epoch [5/25], Loss: 2.0009, Loss validation: 1.8124, Time remaining: ~0.0h 15.0m
47s
         Validation string,      i: 0;   prediction: 0.1962,     target:
-0.0662,        loss: 3.9662
         Validation string,      i: 1;   prediction: 0.1962,     target: 0.2078,
loss: 0.0558
         Validation string,      i: 2;   prediction: 0.1962,     target:
-0.0342,        loss: 6.7411
Epoch [6/25], Loss: 2.0727, Loss validation: 1.6252, Time remaining: ~0.0h 14.0m
58s
         Validation string,      i: 0;   prediction: 0.2072,     target:
-0.0662,        loss: 4.1313
         Validation string,      i: 1;   prediction: 0.2072,     target: 0.2078,
loss: 0.0033
         Validation string,      i: 2;   prediction: 0.2072,     target:
-0.0342,        loss: 7.0607
Epoch [7/25], Loss: 2.0895, Loss validation: 1.6931, Time remaining: ~0.0h 14.0m
9s
         Validation string,      i: 0;   prediction: -0.1175,    target:
-0.0662,        loss: 0.7753
         Validation string,      i: 1;   prediction: -0.1175,    target: 0.2078,
loss: 1.5651
         Validation string,      i: 2;   prediction: -0.1175,    target:
-0.0342,        loss: 2.4361
Epoch [8/25], Loss: 2.1258, Loss validation: 1.4828, Time remaining: ~0.0h 13.0m
21s
         Validation string,      i: 0;   prediction: -0.2003,    target:
-0.0662,        loss: 2.0273
         Validation string,      i: 1;   prediction: -0.2003,    target: 0.2078,
loss: 1.9636
         Validation string,      i: 2;   prediction: -0.2003,    target:
-0.0342,        loss: 4.8595
Epoch [9/25], Loss: 1.9507, Loss validation: 2.0065, Time remaining: ~0.0h 12.0m
34s
         Validation string,      i: 0;   prediction: -0.2234,    target:
-0.0662,        loss: 2.3767
         Validation string,      i: 1;   prediction: -0.2234,    target: 0.2078,
loss: 2.0748
         Validation string,      i: 2;   prediction: -0.2234,    target:
-0.0342,        loss: 5.5356
Epoch [10/25], Loss: 2.0871, Loss validation: 2.1636, Time remaining: ~0.0h
11.0m 47s
         Validation string,      i: 0;   prediction: 0.0078,     target:
```

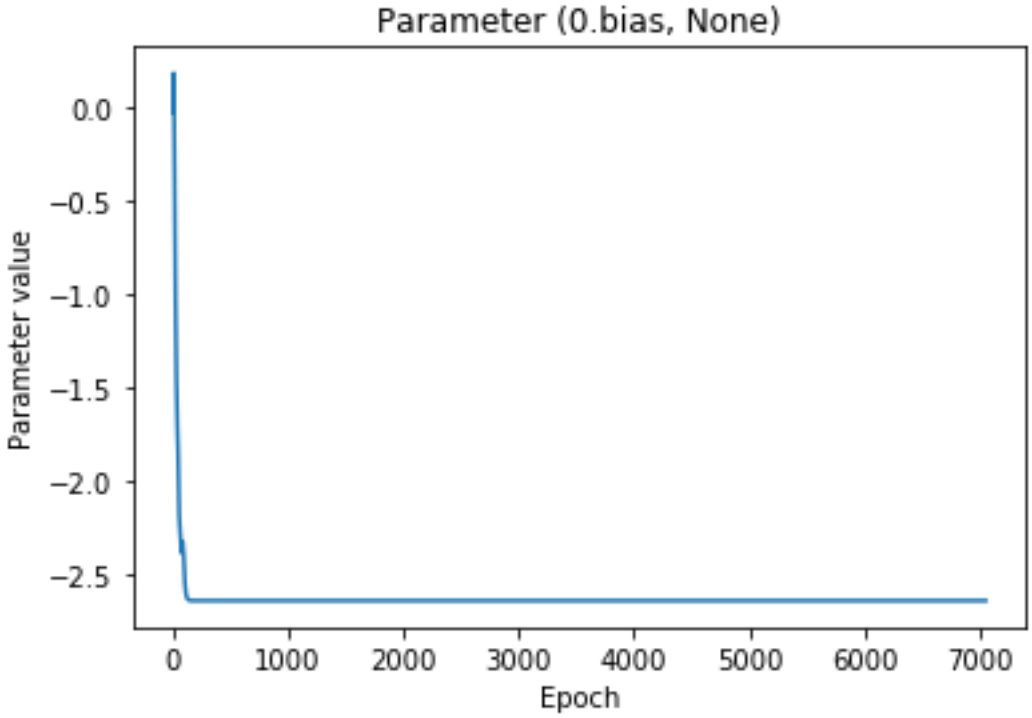
```
-0.0662,        loss: 1.1185
         Validation string,      i: 1;   prediction: 0.0078,     target: 0.2078,
loss: 0.9623
         Validation string,      i: 2;   prediction: 0.0078,     target:
-0.0342,        loss: 1.2293
Epoch [11/25], Loss: 2.1810, Loss validation: 0.9890, Time remaining: ~0.0h
11.0m 0s
         Validation string,      i: 0;   prediction: 0.4253,     target:
-0.0662,        loss: 7.4291
         Validation string,      i: 1;   prediction: 0.4253,     target: 0.2078,
loss: 1.0465
         Validation string,      i: 2;   prediction: 0.4253,     target:
-0.0342,        loss: 13.4437
Epoch [12/25], Loss: 2.0754, Loss validation: 3.2133, Time remaining: ~0.0h
10.0m 14s
         Validation string,      i: 0;   prediction: 0.3977,     target:
-0.0662,        loss: 7.0116
         Validation string,      i: 1;   prediction: 0.3977,     target: 0.2078,
loss: 0.9136
         Validation string,      i: 2;   prediction: 0.3977,     target:
-0.0342,        loss: 12.6355
Epoch [13/25], Loss: 2.0241, Loss validation: 3.0116, Time remaining: ~0.0h 9.0m
27s
         Validation string,      i: 0;   prediction: 0.0102,     target:
-0.0662,        loss: 1.1549
         Validation string,      i: 1;   prediction: 0.0102,     target: 0.2078,
loss: 0.9507
         Validation string,      i: 2;   prediction: 0.0102,     target:
-0.0342,        loss: 1.2997
Epoch [14/25], Loss: 2.1457, Loss validation: 0.9863, Time remaining: ~0.0h 8.0m
40s
         Validation string,      i: 0;   prediction: -0.1676,    target:
-0.0662,        loss: 1.5334
         Validation string,      i: 1;   prediction: -0.1676,    target: 0.2078,
loss: 1.8064
         Validation string,      i: 2;   prediction: -0.1676,    target:
-0.0342,        loss: 3.9034
Epoch [15/25], Loss: 2.0592, Loss validation: 1.7911, Time remaining: ~0.0h 7.0m
53s
         Validation string,      i: 0;   prediction: 0.0647,     target:
-0.0662,        loss: 1.9785
         Validation string,      i: 1;   prediction: 0.0647,     target: 0.2078,
loss: 0.6885
         Validation string,      i: 2;   prediction: 0.0647,     target:
-0.0342,        loss: 2.8939
Epoch [16/25], Loss: 2.0060, Loss validation: 1.0186, Time remaining: ~0.0h 7.0m
6s
         Validation string,      i: 0;   prediction: -0.0899,    target:
```

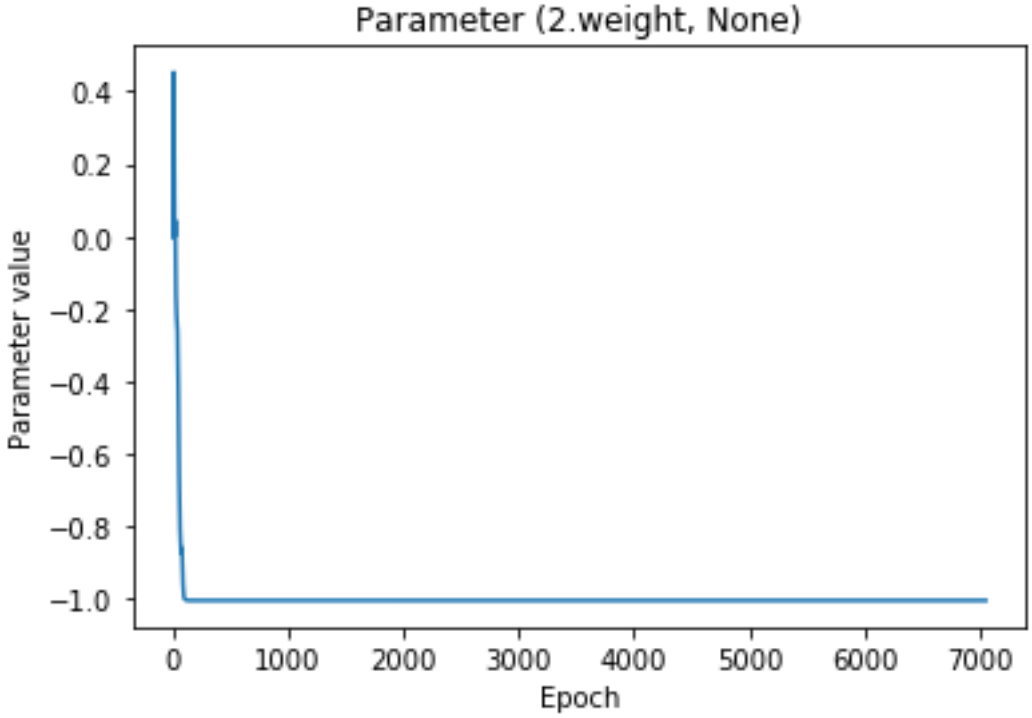
```
-0.0662,        loss: 0.3581
         Validation string,      i: 1;   prediction: -0.0899,    target: 0.2078,
loss: 1.4323
         Validation string,      i: 2;   prediction: -0.0899,    target:
-0.0342,        loss: 1.6286
Epoch [17/25], Loss: 2.1112, Loss validation: 1.3305, Time remaining: ~0.0h 6.0m
19s
         Validation string,      i: 0;   prediction: -0.2626,    target:
-0.0662,        loss: 2.9699
         Validation string,      i: 1;   prediction: -0.2626,    target: 0.2078,
loss: 2.2637
         Validation string,      i: 2;   prediction: -0.2626,    target:
-0.0342,        loss: 6.6838
Epoch [18/25], Loss: 2.0810, Loss validation: 2.4368, Time remaining: ~0.0h 5.0m
32s
         Validation string,      i: 0;   prediction: 0.2428,     target:
-0.0662,        loss: 4.6699
         Validation string,      i: 1;   prediction: 0.2428,     target: 0.2078,
loss: 0.1682
         Validation string,      i: 2;   prediction: 0.2428,     target:
-0.0342,        loss: 8.1032
Epoch [19/25], Loss: 1.9664, Loss validation: 1.9235, Time remaining: ~0.0h 4.0m
45s
         Validation string,      i: 0;   prediction: 0.1165,     target:
-0.0662,        loss: 2.7610
         Validation string,      i: 1;   prediction: 0.1165,     target: 0.2078,
loss: 0.4395
         Validation string,      i: 2;   prediction: 0.1165,     target:
-0.0342,        loss: 4.4084
Epoch [20/25], Loss: 2.1668, Loss validation: 1.1935, Time remaining: ~0.0h 3.0m
58s
         Validation string,      i: 0;   prediction: 0.1096,     target:
-0.0662,        loss: 2.6559
         Validation string,      i: 1;   prediction: 0.1096,     target: 0.2078,
loss: 0.4729
         Validation string,      i: 2;   prediction: 0.1096,     target:
-0.0342,        loss: 4.2050
Epoch [21/25], Loss: 2.0400, Loss validation: 1.1636, Time remaining: ~0.0h 3.0m
10s
         Validation string,      i: 0;   prediction: -0.4862,    target:
-0.0662,        loss: 6.3487
         Validation string,      i: 1;   prediction: -0.4862,    target: 0.2078,
loss: 3.3392
         Validation string,      i: 2;   prediction: -0.4862,    target:
-0.0342,        loss: 13.2235
Epoch [22/25], Loss: 2.0316, Loss validation: 4.0711, Time remaining: ~0.0h 2.0m
23s
         Validation string,      i: 0;   prediction: 0.0956,     target:
```

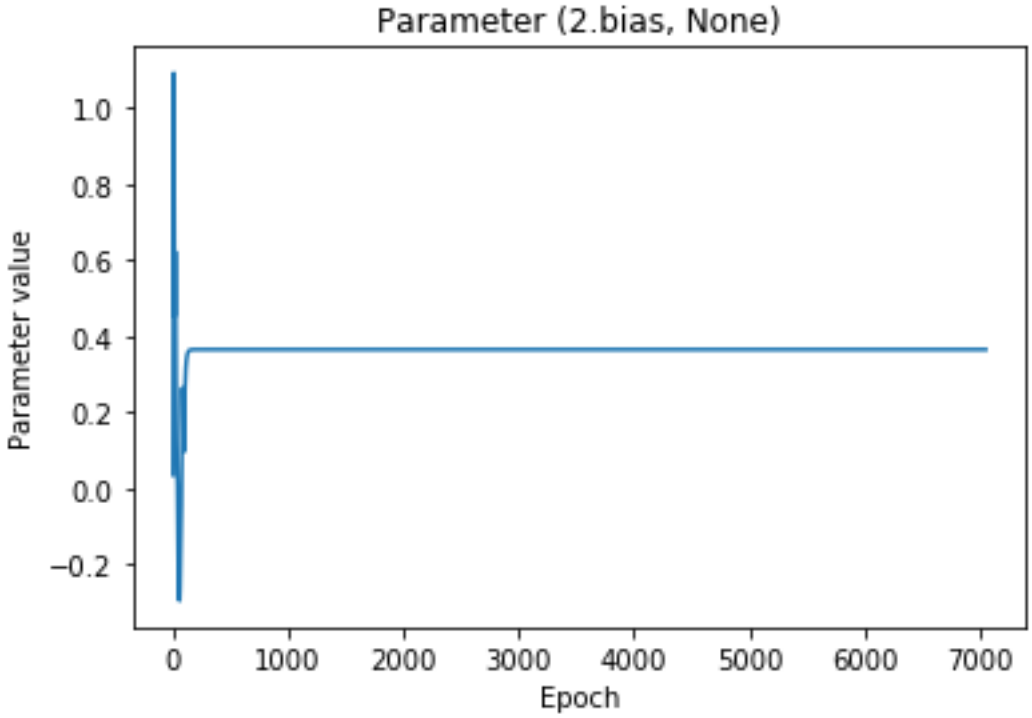
```
-0.0662,        loss: 2.4454
         Validation string,      i: 1;   prediction: 0.0956,     target: 0.2078,
loss: 0.5399
         Validation string,      i: 2;   prediction: 0.0956,     target:
-0.0342,        loss: 3.7976
Epoch [23/25], Loss: 2.1422, Loss validation: 1.1091, Time remaining: ~0.0h 1.0m
35s
         Validation string,      i: 0;   prediction: -0.5706,    target:
-0.0662,        loss: 7.6250
         Validation string,      i: 1;   prediction: -0.5706,    target: 0.2078,
loss: 3.7454
         Validation string,      i: 2;   prediction: -0.5706,    target:
-0.0342,        loss: 15.6939
Epoch [24/25], Loss: 2.0592, Loss validation: 4.7044, Time remaining: ~0.0h 0.0m
48s
         Validation string,      i: 0;   prediction: 0.1418,     target:
-0.0662,        loss: 3.1427
         Validation string,      i: 1;   prediction: 0.1418,     target: 0.2078,
loss: 0.3180
         Validation string,      i: 2;   prediction: 0.1418,     target:
-0.0342,        loss: 5.1472
Epoch [25/25], Loss: 2.0286, Loss validation: 1.3146, Time remaining: ~0.0h 0.0m
0s
```

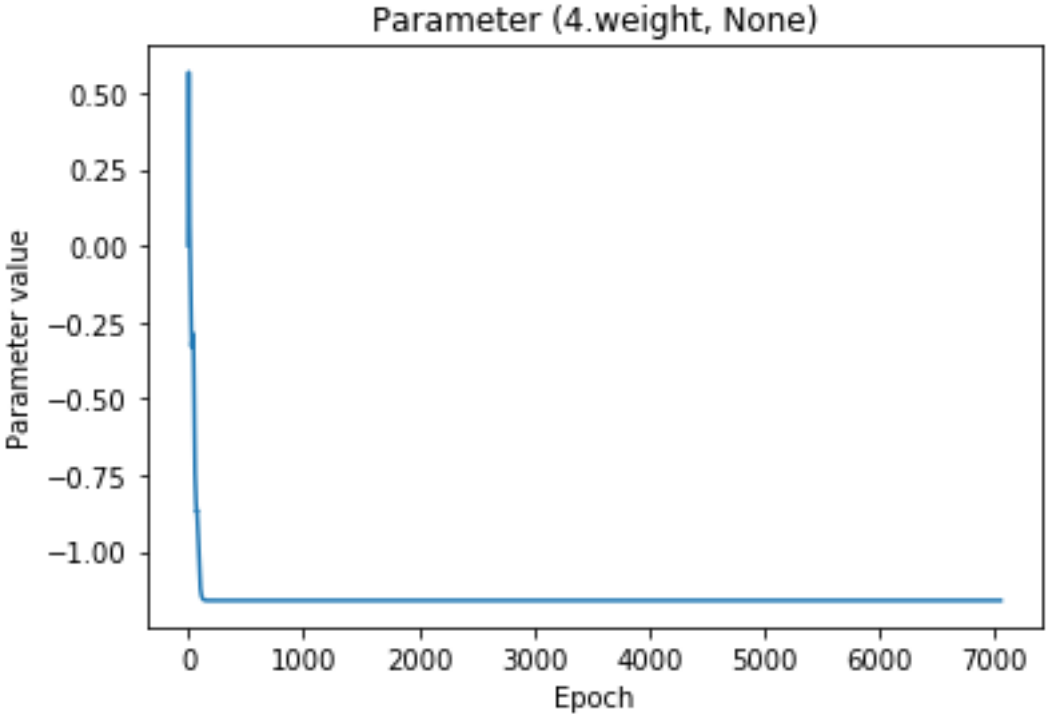
[ ]:
```
for layer in model.model.state_dict().keys():
    model.plot_parameter(layer=layer)
```

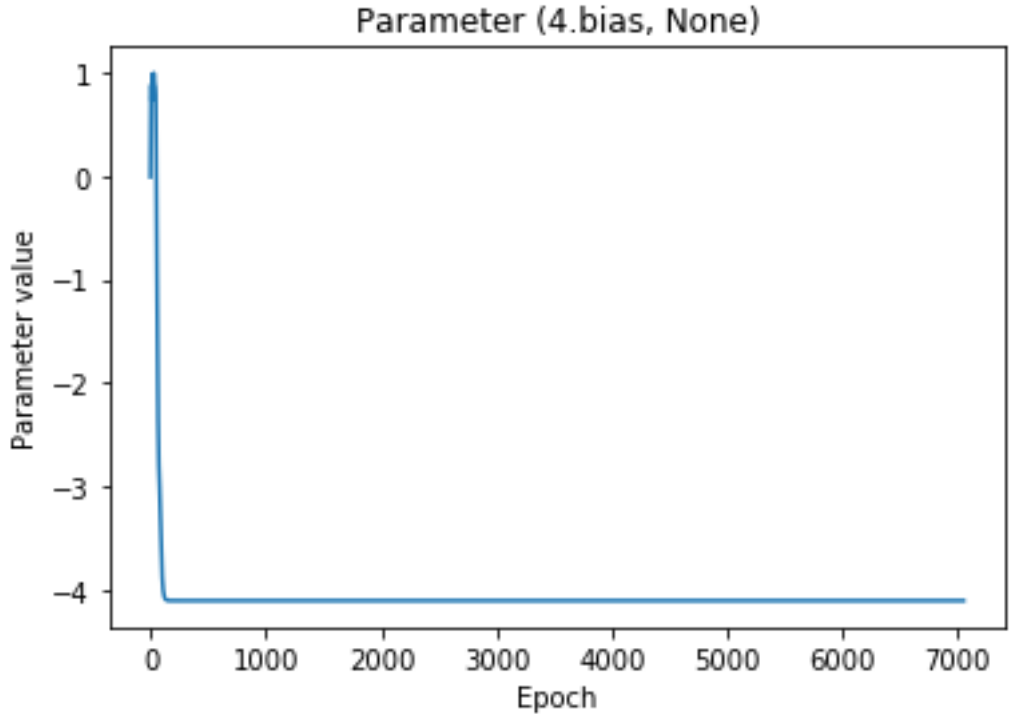


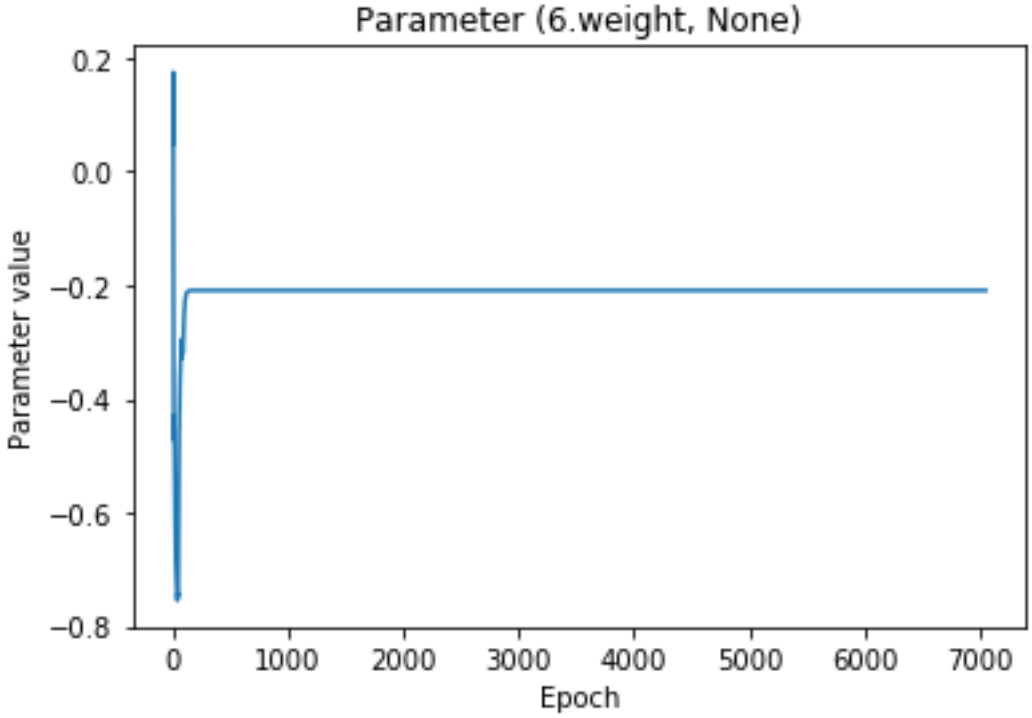

Parameter (0.bias, None)
Parameter value
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
1000
2000
3000
4000
5000
6000
7000
Epoch

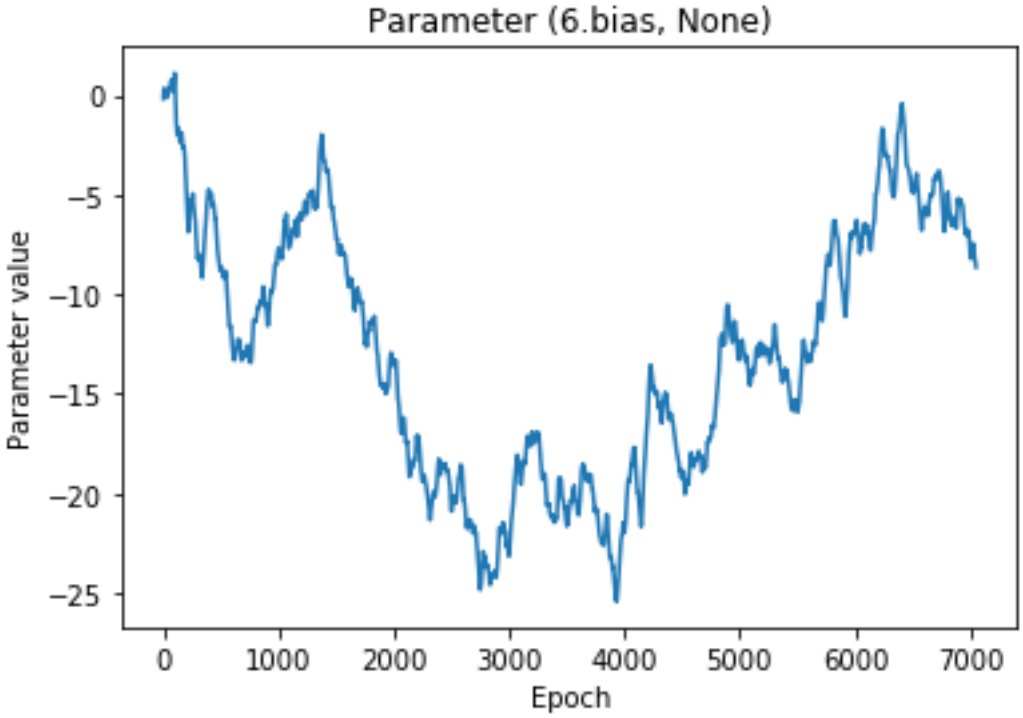

Parameter (2.weight, None)
Parameter value
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
0
1000
2000
3000
4000
5000
6000
7000
Epoch

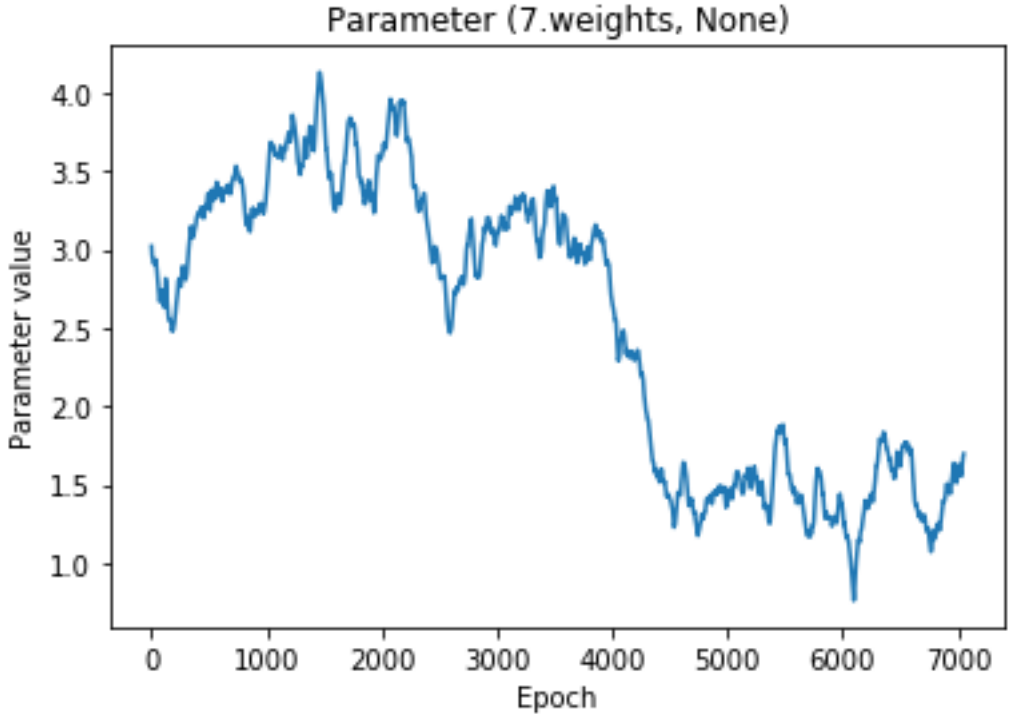

Parameter (2.bias, None)
Parameter value
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0
1000
2000
3000
4000
5000
6000
7000
Epoch


Parameter (4.weight, None)
Parameter value
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
1000
2000
3000
4000
5000
6000
7000
Epoch

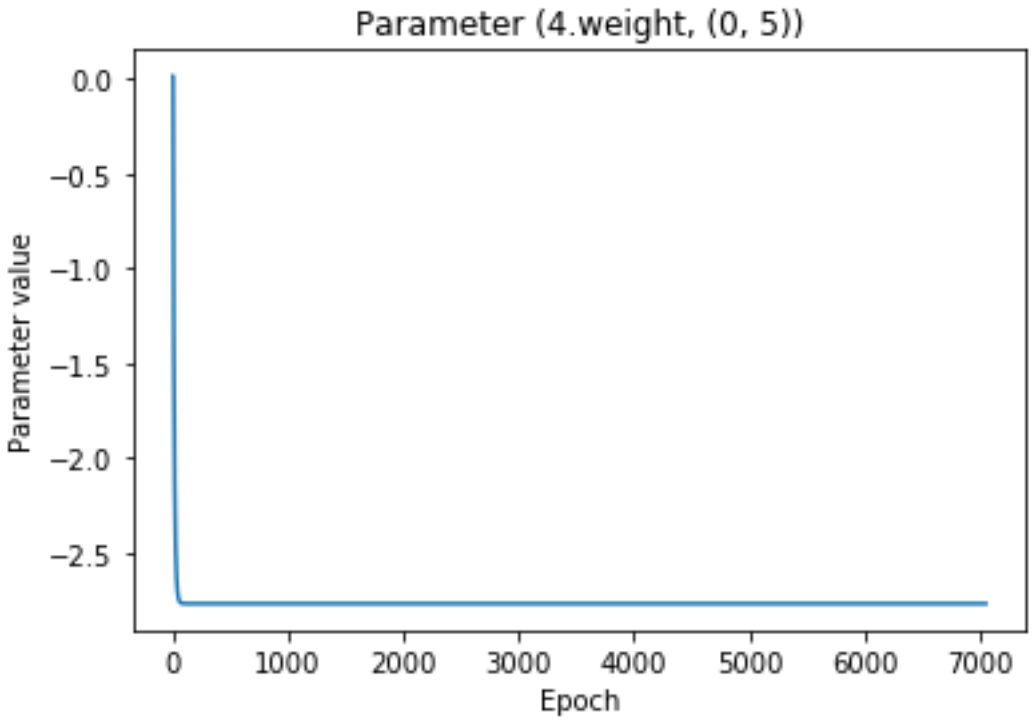

Parameter (4.bias, None)
Parameter value
1
0
−1
−2
−3
−4
0
1000
2000
3000
4000
5000
6000
7000
Epoch


Parameter (6.weight, None)
Parameter value
0.2
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000
5000
6000
7000
Epoch


Parameter (6.bias, None)
Parameter value
0
−5
−10
−15
−20
−25
0
1000
2000
3000
4000
5000
6000
7000
Epoch


Parameter (7.weights, None)
Parameter value
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
1000
2000
3000
4000
5000
6000
7000
Epoch

[ ]:
```
model.plot_parameter(layer='4.weight', index=(0,5))
```

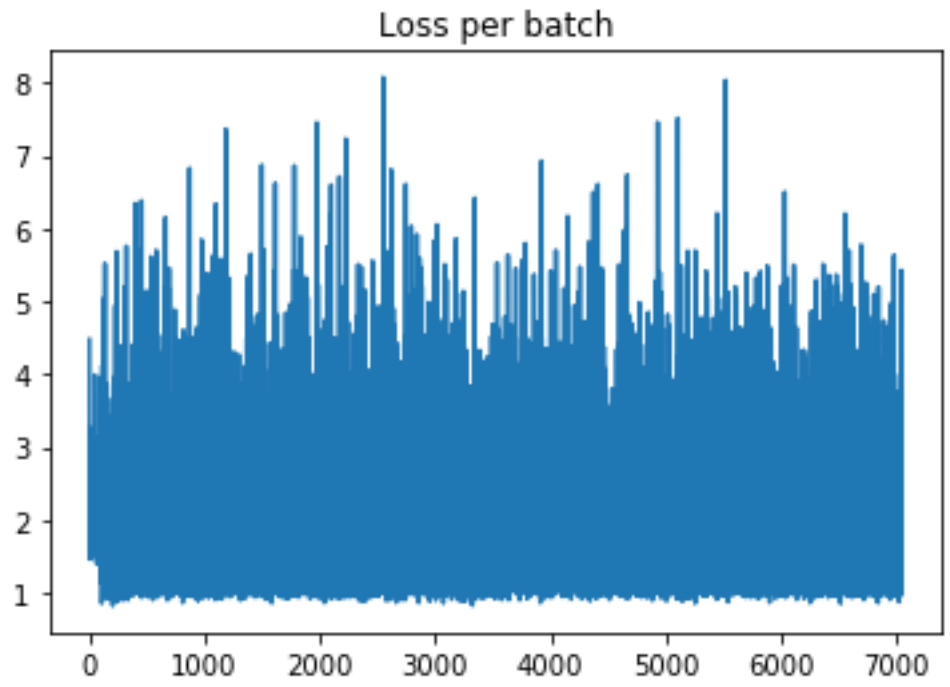


[ ]:
```
model
```

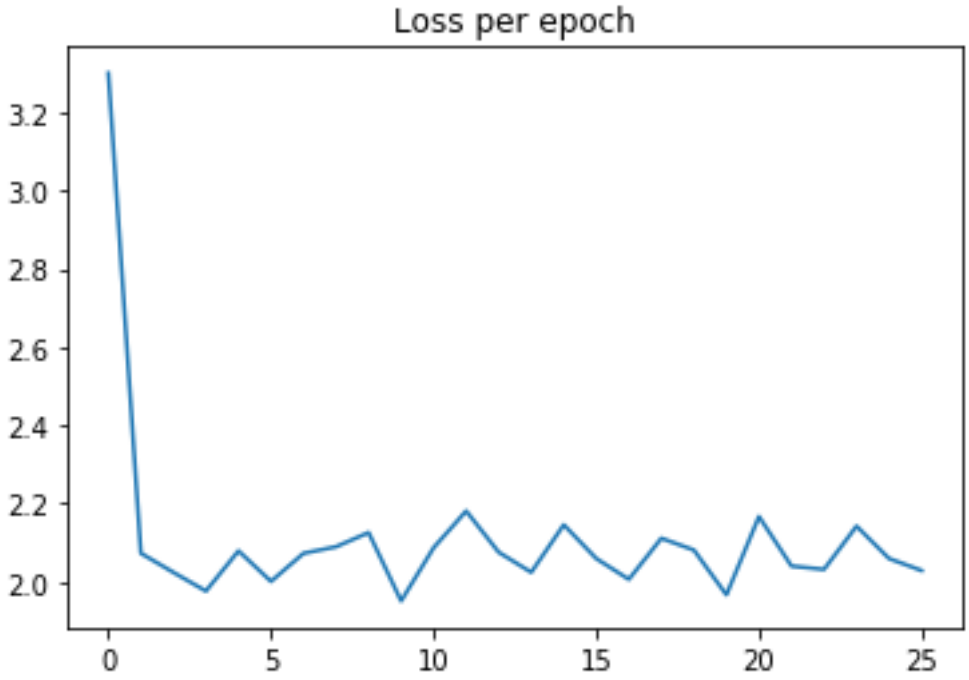
[ ]:
```
Sequential(
  (0): Linear(in_features=76, out_features=52, bias=True)
  (1): ReLU()
  (2): Linear(in_features=52, out_features=28, bias=True)
  (3): ReLU()
  (4): Linear(in_features=28, out_features=4, bias=True)
  (5): ReLU()
  (6): Linear(in_features=4, out_features=4, bias=True)
  (7): <Quantum Torch Layer: func=circuit>
)
```

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

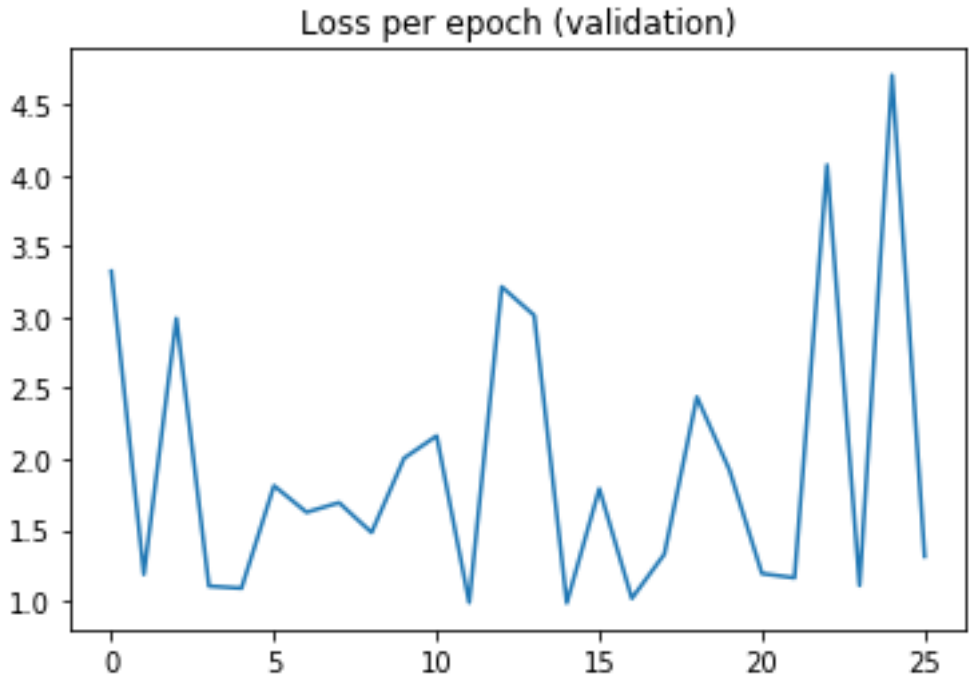
```
The file peptide-QML/checkpoints/0802/plots/0802-sh_1qm_losses_batches_1.png
already exists, it will be replaced
Saved in:  peptide-QML/checkpoints/0802/plots/0802-sh_1qm_losses_batches_1.png
```




```
The file peptide-QML/checkpoints/0802/plots/0802-sh_1qm_losses_epoch_1.png
already exists, it will be replaced
Saved in:  peptide-QML/checkpoints/0802/plots/0802-sh_1qm_losses_epoch_1.png
```



```
The file peptide-
QML/checkpoints/0802/plots/0802-sh_1qm_losses_epoch_validation_1.png already
exists, it will be replaced
Saved in:  peptide-
QML/checkpoints/0802/plots/0802-sh_1qm_losses_epoch_validation_1.png
```



[ ]:
```
model.save_state_dict()
```

```
The file peptide-QML/checkpoints/0802/models/0802-sh_1qm_1.pth already exists,
it will be replaced
Model saved as peptide-QML/checkpoints/0802/models/0802-sh_1qm_1.pth
```

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

```
[main 083ab78] data trained model
 4 files changed, 0 insertions(+), 0 deletions(-)
 rewrite checkpoints/0802/models/0802-sh_1qm_1.pth (97%)
 rewrite checkpoints/0802/plots/0802-sh_1qm_losses_batches_1.png (99%)
 rewrite checkpoints/0802/plots/0802-sh_1qm_losses_epoch_1.png (99%)
 rewrite checkpoints/0802/plots/0802-sh_1qm_losses_epoch_validation_1.png (99%)
Enumerating objects: 19, done.
```

```
Counting objects: 100% (19/19), done.
Delta compression using up to 24 threads
Compressing objects: 100% (10/10), done.
Writing objects: 100% (10/10), 92.32 KiB | 8.39 MiB/s, done.
Total 10 (delta 3), reused 0 (delta 0)
remote: Resolving deltas: 100% (3/3), completed with 3 local objects.
To github.com:raulconchello/peptide-QML.git
   399e5f6..083ab78  main -> main
```

[ ]:
```python
#load model
model.load_state_dict()
```

```
Model loaded from peptide-QML/checkpoints/0802/models/0802-sh_1qm_1.pth
```

[ ]:
```python
# print validation
model.print_validation(save=True, precision=4, percentatge=0.02)
```

```
i: 0,           target: -0.0662,        output: 0.1418,         loss: 3.1427
i: 1,           target: 0.1805,         output: 0.1418,         loss: 0.2145
i: 2,           target: -0.0357,        output: 0.1418,         loss: 4.9707
i: 3,           target: 0.0385,         output: 0.1418,         loss: 2.6820
i: 4,           target: -0.0717,        output: 0.1418,         loss: 2.9777
i: 5,           target: -0.0594,        output: 0.1418,         loss: 3.3850
i: 6,           target: -0.0711,        output: 0.1418,         loss: 2.9929
i: 7,           target: -0.0688,        output: 0.1418,         loss: 3.0590
i: 8,           target: 0.3044,         output: 0.1418,         loss: 0.5344
i: 9,           target: 0.0461,         output: 0.1418,         loss: 2.0780
i: 10,          target: 0.2078,         output: 0.1418,         loss: 0.3180
i: 11,          target: 0.0697,         output: 0.1418,         loss: 1.0333
i: 12,          target: -0.0814,        output: 0.1418,         loss: 2.7407
i: 13,          target: 0.1593,         output: 0.1418,         loss: 0.1103
i: 14,          target: -0.0499,        output: 0.1418,         loss: 3.8418
i: 15,          target: -0.0617,        output: 0.1418,         loss: 3.2992
i: 16,          target: -0.0773,        output: 0.1418,         loss: 2.8329
i: 17,          target: 0.2600,         output: 0.1418,         loss: 0.4548
i: 18,          target: -0.0994,        output: 0.1418,         loss: 2.4254
i: 19,          target: -0.0748,        output: 0.1418,         loss: 2.8956
Average loss: 0.0460
The file peptide-QML/checkpoints/0802/txts/0802-sh_1qm_validation_1.txt already
exists, it will be replaced
Saved in:  peptide-QML/checkpoints/0802/txts/0802-sh_1qm_validation_1.txt
```