$0802-\text{sh}_1\text{qm}$

August 2, 2023

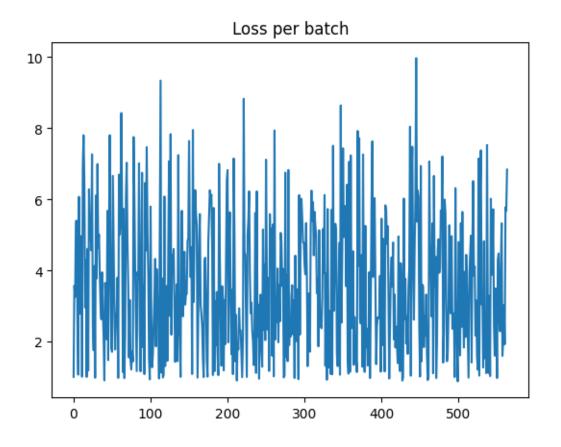
[]: initial_path = 'peptide-QML/'

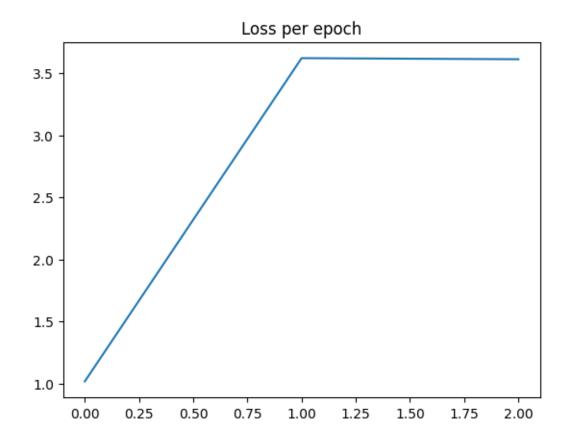
```
initial_path = '../'
[]: import numpy as np
[]: import sys
    sys.path.append(initial_path)
    from my_code import functions as f
    from my_code import pytorch_model as ptm
    from my_code import quantum_nodes as qn
    from my_code import pytorch_wrappers as pw
    1 Data
[]: file_path = initial_path + '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)
```

2 Quantum node

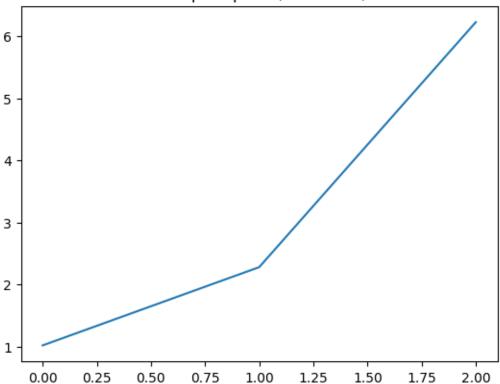
3 Hybrid model

```
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())
[]: tensor([-0.0065], grad_fn=<CatBackward0>)
[]: # train the model
    model.train(
        num_epochs=2,
        batch_size = 32,
    Epoch [0/2], Loss: 1.0165, Loss validation: 1.0164
                                            prediction: 0.2922,
                                                                   target: 0.1608,
             Validation string,
                                    i: 0;
    loss: 0.8172
             Validation string,
                                    i: 1;
                                            prediction: 0.2919,
                                                                   target: 0.1417,
    loss: 1.0595
             Validation string,
                               i: 2;
                                            prediction: 0.2922,
                                                                   target: 0.1656,
    loss: 0.7651
    Epoch [1/2], Loss: 3.6225, Loss validation: 2.2778, Time remaining: ~0.0h 2.0m
             Validation string,
                                    i: 0; prediction: 0.8043,
                                                                   target: 0.1608,
    loss: 4.0026
                                    i: 1;
                                            prediction: 0.8043,
                                                                   target: 0.1417,
             Validation string,
    loss: 4.6752
             Validation string,
                                    i: 2;
                                            prediction: 0.8043,
                                                                   target: 0.1656,
    loss: 3.8584
    Epoch [2/2], Loss: 3.6137, Loss validation: 6.2268, Time remaining: ~0.0h 0.0m
[]: # plot the losses of the training loop
    model.plot_losses()
```









```
[]: #save model
name_notebook = "0802-sh_1qm.ipynb"

version = model.save_state_dict(name_notebook=name_notebook,
initial_path=initial_path)
```

Model saved as ../Notebooks/models/0802/0802-sh_1qm_0.pth

```
[]: # push changes to git
!cd peptide-QML && git add . && git commit -m "data trained model" && git push
```

The system cannot find the path specified.

```
[]: #load model
model.load_state_dict(name_notebook=name_notebook, version=version,
→initial_path=initial_path)
```

Model loaded from ../Notebooks/models/0802/0802-sh_1qm_0.pth

```
[]:  # print validation model.print_validation()
```

i: 0, target: 0.161, output: 0.804, loss: 4.003

```
target: 0.138,
                                                            loss: 4.826
i: 1,
                                   output: 0.804,
i: 2,
         target: -0.071,
                                  output: 0.804,
                                                            loss: 12.318
i: 3,
                                  output: 0.804,
                                                            loss: 3.025
         target: 0.200,
i: 4,
         target: -0.031,
                                                            loss: 26.808
                                   output: 0.804,
i: 5.
         target: 0.196,
                                   output: 0.804,
                                                            loss: 3.096
i: 6,
         target: -0.076,
                                  output: 0.804,
                                                            loss: 11.602
i: 7,
         target: -0.033,
                                  output: 0.804,
                                                            loss: 25.254
i: 8.
         target: -0.088,
                                  output: 0.804,
                                                            loss: 10.092
i: 9,
         target: -0.058,
                                  output: 0.804,
                                                            loss: 14.826
i: 10,
         target: 0.142,
                                  output: 0.804,
                                                            loss: 4.675
         target: 0.029,
i: 11,
                                  output: 0.804,
                                                            loss: 26.669
i: 12,
         target: 0.017,
                                   output: 0.804,
                                                            loss: 46.614
i: 13,
         target: 0.193,
                                   output: 0.804,
                                                            loss: 3.176
i: 14,
         target: -0.076,
                                   output: 0.804,
                                                            loss: 11.603
                                   output: 0.804,
i: 15,
         target: 0.196,
                                                            loss: 3.096
i: 16,
         target: -0.080,
                                  output: 0.804,
                                                            loss: 11.096
i: 17,
         target: -0.075,
                                  output: 0.804,
                                                            loss: 11.656
                                                            loss: 10.069
i: 18,
         target: 0.073,
                                  output: 0.804,
i: 19,
         target: 0.020,
                                  output: 0.804,
                                                            loss: 38.928
i: 20,
         target: 0.166,
                                  output: 0.804,
                                                            loss: 3.858
i: 21,
         target: 0.048,
                                  output: 0.804,
                                                            loss: 15.741
i: 22,
         target: 0.187,
                                  output: 0.804,
                                                            loss: 3.296
i: 23,
         target: -0.084,
                                  output: 0.804,
                                                            loss: 10.627
i: 24,
         target: -0.067,
                                  output: 0.804,
                                                            loss: 12.998
i: 25,
         target: -0.073,
                                  output: 0.804,
                                                            loss: 11.956
i: 26,
         target: -0.070,
                                  output: 0.804,
                                                            loss: 12.450
i: 27,
         target: 0.146,
                                  output: 0.804,
                                                            loss: 4.521
i: 28,
         target: 0.120,
                                   output: 0.804,
                                                            loss: 5.676
i: 29,
         target: 0.001,
                                   output: 0.804,
                                                            loss: 618.677
                                  output: 0.804,
                                                            loss: 44.537
i: 30,
         target: -0.018,
i: 31,
         target: -0.094,
                                  output: 0.804,
                                                            loss: 9.560
i: 32,
         target: -0.082,
                                  output: 0.804,
                                                            loss: 10.756
i: 33,
         target: 0.299,
                                  output: 0.804,
                                                            loss: 1.686
i: 34,
         target: 0.127,
                                  output: 0.804,
                                                            loss: 5.341
i: 35,
         target: -0.112,
                                   output: 0.804,
                                                            loss: 8.165
i: 36,
         target: -0.063,
                                  output: 0.804,
                                                            loss: 13.822
i: 37,
         target: -0.066,
                                  output: 0.804,
                                                            loss: 13.223
         target: -0.041,
                                  output: 0.804,
                                                            loss: 20.558
i: 38,
i: 39,
         target: -0.082,
                                  output: 0.804,
                                                            loss: 10.805
i: 40,
         target: 0.127,
                                  output: 0.804,
                                                            loss: 5.355
                                                            loss: 18.520
i: 41,
         target: -0.046,
                                  output: 0.804,
i: 42,
         target: -0.073,
                                   output: 0.804,
                                                            loss: 11.948
                                                            loss: 32.832
i: 43,
         target: -0.025,
                                   output: 0.804,
i: 44,
         target: -0.087,
                                  output: 0.804,
                                                            loss: 10.281
i: 45,
                                  output: 0.804,
                                                            loss: 0.839
         target: 0.437,
                                                            loss: 47.539
i: 46,
         target: -0.017,
                                  output: 0.804,
i: 47,
         target: -0.082,
                                  output: 0.804,
                                                            loss: 10.847
i: 48,
         target: -0.071,
                                  output: 0.804,
                                                            loss: 12.307
```

```
target: 0.046,
                                                            loss: 16.305
i: 49,
                                   output: 0.804,
i: 50,
         target: -0.061,
                                   output: 0.804,
                                                            loss: 14.207
i: 51,
                                   output: 0.804,
                                                            loss: 2.269
         target: 0.246,
i: 52,
         target: 0.064,
                                   output: 0.804,
                                                            loss: 11.552
i: 53,
         target: -0.075,
                                   output: 0.804,
                                                            loss: 11.710
i: 54,
         target: -0.079,
                                   output: 0.804,
                                                            loss: 11.221
i: 55,
         target: -0.079,
                                   output: 0.804,
                                                            loss: 11.230
                                   output: 0.804,
i: 56,
         target: 0.001,
                                                            loss: 1143.156
i: 57,
         target: 0.081,
                                   output: 0.804,
                                                            loss: 8.924
i: 58,
         target: -0.101,
                                   output: 0.804,
                                                            loss: 8.990
         target: -0.048,
i: 59,
                                   output: 0.804,
                                                            loss: 17.749
i: 60,
         target: -0.070,
                                   output: 0.804,
                                                            loss: 12.557
                                                            loss: 11.237
i: 61,
         target: -0.079,
                                   output: 0.804,
i: 62,
         target: 0.139,
                                   output: 0.804,
                                                            loss: 4.773
                                   output: 0.804,
i: 63,
         target: 0.082,
                                                            loss: 8.789
i: 64,
         target: -0.031,
                                   output: 0.804,
                                                            loss: 26.621
i: 65,
         target: -0.088,
                                   output: 0.804,
                                                            loss: 10.177
                                                            loss: 18.086
i: 66,
         target: 0.042,
                                   output: 0.804,
i: 67,
         target: -0.087,
                                   output: 0.804,
                                                            loss: 10.220
         target: -0.064,
                                   output: 0.804,
                                                            loss: 13.478
i: 68.
i: 69,
         target: -0.071,
                                   output: 0.804,
                                                            loss: 12.260
i: 70,
         target: 0.021,
                                   output: 0.804,
                                                            loss: 38.057
i: 71,
         target: 0.096,
                                   output: 0.804,
                                                            loss: 7.417
i: 72,
         target: 0.049,
                                   output: 0.804,
                                                            loss: 15.577
i: 73,
         target: 0.195,
                                   output: 0.804,
                                                            loss: 3.126
i: 74,
         target: -0.072,
                                   output: 0.804,
                                                            loss: 12.210
i: 75,
         target: -0.051,
                                   output: 0.804,
                                                            loss: 16.753
i: 76,
         target: 0.124,
                                   output: 0.804,
                                                            loss: 5.509
i: 77,
         target: 0.189,
                                   output: 0.804,
                                                            loss: 3.247
i: 78,
         target: 0.213,
                                   output: 0.804,
                                                            loss: 2.769
i: 79,
                                                            loss: 18.270
         target: 0.042,
                                   output: 0.804,
i: 80,
         target: -0.038,
                                   output: 0.804,
                                                            loss: 22.172
i: 81,
         target: -0.080,
                                   output: 0.804,
                                                            loss: 11.010
i: 82,
                                                            loss: 10.338
         target: -0.086,
                                   output: 0.804,
i: 83,
         target: 0.141,
                                   output: 0.804,
                                                            loss: 4.721
i: 84,
         target: 0.199,
                                   output: 0.804,
                                                            loss: 3.050
i: 85,
         target: -0.076,
                                   output: 0.804,
                                                            loss: 11.563
         target: -0.065,
                                   output: 0.804,
                                                            loss: 13.434
i: 86,
i: 87,
         target: 0.178,
                                   output: 0.804,
                                                            loss: 3.520
i: 88,
         target: 0.092,
                                   output: 0.804,
                                                            loss: 7.762
                                                            loss: 21.647
i: 89,
         target: -0.039,
                                   output: 0.804,
i: 90,
         target: -0.083,
                                   output: 0.804,
                                                            loss: 10.633
                                                            loss: 3.874
i: 91,
         target: 0.165,
                                   output: 0.804,
i: 92,
         target: -0.059,
                                   output: 0.804,
                                                            loss: 14.659
i: 93,
         target: -0.054,
                                   output: 0.804,
                                                            loss: 16.033
i: 94,
         target: 0.157,
                                   output: 0.804,
                                                            loss: 4.130
i: 95,
         target: 0.164,
                                   output: 0.804,
                                                            loss: 3.913
i: 96,
         target: 0.218,
                                   output: 0.804,
                                                            loss: 2.685
```

```
target: 0.283,
                                   output: 0.804,
                                                            loss: 1.845
i: 97,
i: 98,
         target: -0.040,
                                   output: 0.804,
                                                            loss: 21.019
                                   output: 0.804,
                                                            loss: 4.569
i: 99,
         target: 0.144,
                  target: -0.073,
                                                                     loss: 12.041
i: 100,
                                           output: 0.804,
i: 101,
                  target: -0.083,
                                           output: 0.804,
                                                                     loss: 10.715
i: 102,
                  target: -0.075,
                                           output: 0.804,
                                                                     loss: 11.706
i: 103,
                  target: 0.032,
                                           output: 0.804,
                                                                     loss: 24.002
i: 104,
                  target: -0.067,
                                           output: 0.804,
                                                                     loss: 13.001
i: 105,
                  target: -0.049,
                                           output: 0.804,
                                                                     loss: 17.496
i: 106,
                  target: -0.079,
                                           output: 0.804,
                                                                     loss: 11.187
i: 107,
                                                                     loss: 3.288
                  target: 0.188,
                                           output: 0.804,
i: 108,
                  target: 0.025,
                                           output: 0.804,
                                                                     loss: 31.489
                                                                     loss: 21.723
i: 109,
                  target: 0.035,
                                           output: 0.804,
i: 110,
                  target: 0.025,
                                           output: 0.804,
                                                                     loss: 31.201
i: 111,
                  target: -0.053,
                                           output: 0.804,
                                                                     loss: 16.276
i: 112,
                  target: -0.059,
                                           output: 0.804,
                                                                     loss: 14.558
i: 113,
                  target: -0.060,
                                           output: 0.804,
                                                                     loss: 14.445
                                                                     loss: 16.644
i: 114,
                  target: -0.051,
                                           output: 0.804,
i: 115,
                  target: -0.068,
                                           output: 0.804,
                                                                     loss: 12.782
i: 116.
                                                                     loss: 11.697
                  target: -0.075,
                                           output: 0.804,
i: 117,
                  target: -0.075,
                                           output: 0.804,
                                                                     loss: 11.775
i: 118,
                  target: -0.064,
                                           output: 0.804,
                                                                     loss: 13.646
i: 119,
                  target: -0.039,
                                           output: 0.804,
                                                                     loss: 21.871
i: 120,
                  target: 0.156,
                                           output: 0.804,
                                                                     loss: 4.168
i: 121,
                  target: -0.074,
                                           output: 0.804,
                                                                     loss: 11.893
i: 122,
                                                                     loss: 10.209
                  target: -0.087,
                                           output: 0.804,
i: 123,
                  target: -0.074,
                                           output: 0.804,
                                                                     loss: 11.824
i: 124,
                  target: -0.056,
                                           output: 0.804,
                                                                     loss: 15.362
i: 125,
                  target: 0.146,
                                           output: 0.804,
                                                                     loss: 4.516
i: 126,
                                                                     loss: 10.588
                  target: 0.069,
                                           output: 0.804,
i: 127,
                  target: -0.053,
                                           output: 0.804,
                                                                     loss: 16.177
i: 128,
                  target: -0.074,
                                           output: 0.804,
                                                                     loss: 11.918
i: 129,
                  target: -0.031,
                                           output: 0.804,
                                                                     loss: 27.336
                                                                     loss: 21.225
i: 130,
                  target: -0.040,
                                           output: 0.804,
                                                                     loss: 32.567
i: 131,
                  target: 0.024,
                                           output: 0.804,
i: 132,
                  target: 0.029,
                                           output: 0.804,
                                                                     loss: 26.584
                                           output: 0.804,
i: 133,
                  target: 0.210,
                                                                     loss: 2.836
i: 134,
                  target: 0.200,
                                           output: 0.804,
                                                                     loss: 3.026
i: 135,
                  target: 0.315,
                                           output: 0.804,
                                                                     loss: 1.552
i: 136,
                                           output: 0.804,
                                                                     loss: 45.985
                  target: 0.017,
i: 137,
                  target: 0.220,
                                           output: 0.804,
                                                                     loss: 2.657
i: 138,
                  target: -0.102,
                                           output: 0.804,
                                                                     loss: 8.895
                                                                     loss: 7.653
i: 139,
                  target: 0.093,
                                           output: 0.804,
i: 140,
                  target: 0.051,
                                           output: 0.804,
                                                                     loss: 14.733
i: 141,
                                                                     loss: 14.498
                  target: -0.060,
                                           output: 0.804,
i: 142,
                  target: -0.018,
                                           output: 0.804,
                                                                     loss: 45.395
i: 143,
                  target: 0.045,
                                           output: 0.804,
                                                                     loss: 17.049
                  target: -0.075,
                                           output: 0.804,
                                                                     loss: 11.718
i: 144,
```

```
i: 146,
                 target: 0.298,
                                         output: 0.804,
                                                                 loss: 1.703
i: 147,
                 target: -0.067,
                                         output: 0.804,
                                                                 loss: 13.007
 KeyboardInterrupt
                                            Traceback (most recent call last)
 Cell In[21], line 2
       1 # print validation
 ---> 2 model.print_validation()
 File d:\Raul\OneDrive - Cornell University\Code\peptide-QML\Notebooks\..
  →\my_code\pytorch_model.py:177, in pytorch_model.print_validation(self)
     175 \text{ avg loss} = 0
     176 for x, (i, t) in enumerate(zip((self.data_X_validation), self.
  ⇔data Y validation)):
 --> 177
             outputs = self.model(i)
             loss = self.loss function(outputs, t)
     178
     179
             avg_loss += loss/len(self.data_Y_validation)
 File d:\Raul\Programs\envs\PennyLane\lib\site-packages\torch\nn\modules\module.
  ⇔py:1501, in Module._call_impl(self, *args, **kwargs)
    1496 # If we don't have any hooks, we want to skip the rest of the logic in
    1497 # this function, and just call forward.
    1498 if not (self._backward_hooks or self._backward_pre_hooks or self.
  →_forward_hooks or self._forward_pre_hooks
                 or _global_backward_pre_hooks or _global_backward_hooks
    1499
    1500
                 or _global_forward_hooks or _global_forward_pre_hooks):
             return forward_call(*args, **kwargs)
 -> 1501
    1502 # Do not call functions when jit is used
    1503 full_backward_hooks, non_full_backward_hooks = [], []
 File d:
  → \Raul\Programs\envs\PennyLane\lib\site-packages\torch\nn\modules\container.py
  →217, in Sequential.forward(self, input)
     215 def forward(self, input):
             for module in self:
     216
 --> 217
                 input = module(input)
     218
             return input
 File d:\Raul\Programs\envs\PennyLane\lib\site-packages\torch\nn\modules\module.

¬py:1501, in Module._call_impl(self, *args, **kwargs)
    1496 # If we don't have any hooks, we want to skip the rest of the logic in
    1497 # this function, and just call forward.
    1498 if not (self._backward_hooks or self._backward_pre_hooks or self.
  →_forward_hooks or self._forward_pre_hooks
    1499
                 or _global_backward_pre_hooks or _global_backward_hooks
                 or _global_forward_hooks or _global_forward_pre_hooks):
    1500
 -> 1501
           return forward_call(*args, **kwargs)
```

output: 0.804,

loss: 15.370

target: -0.056,

i: 145,

```
1502 # Do not call functions when jit is used
   1503 full_backward_hooks, non_full_backward_hooks = [], []
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\qnn\torch.py:
 →408, in TorchLayer.forward(self, inputs)
            results = torch.stack(reconstructor)
    405
    406 else:
    407
            # calculate the forward pass as usual
            results = self._evaluate_qnode(inputs)
    410 # reshape to the correct number of batch dims
    411 if has_batch_dim:
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\qnn\torch.py:
 417 """Evaluates the QNode for a single input datapoint.
   418
   419 Args:
   (...)
    423
            tensor: output datapoint
    424 """
    425 \text{ kwargs} = \{
            **{self.input arg: x},
    427
            **{arg: weight.to(x) for arg, weight in self.qnode_weights.items()}
    428 }
--> 429 res = self.qnode(**kwargs)
    431 if isinstance(res, torch.Tensor):
            return res.type(x.dtype)
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\qnode.py:950,_

→in QNode.__call__(self, *args, **kwargs)

            self.execute_kwargs.pop("mode")
    949 # pylint: disable=unexpected-keyword-arg
--> 950 res = qml.execute(
            [self.tape],
    951
            device=self.device,
    952
    953
            gradient fn=self.gradient fn,
            interface=self.interface,
    954
    955
            gradient_kwargs=self.gradient_kwargs,
            override_shots=override_shots,
    956
    957
            **self.execute_kwargs,
    958 )
    960 \text{ res} = \text{res}[0]
    962 # convert result to the interface in case the qfunc has no parameters
```

```
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\interfaces\executic \.
 →py:511, in execute(tapes, device, gradient_fn, interface, grad_on_execution, capradient_kwargs, cache, cachesize, max_diff, override_shots, expand_fn,
 →max_expansion, device_batch_transform)
    503
            # use qml.interfaces so that mocker can spy on it during testing
    504
            cached_execute_fn = qml.interfaces.cache_execute(
    505
                 batch execute,
    506
                 cache,
   (...)
    509
                 pass_kwargs=new_device_interface,
    510
--> 511
            results = cached_execute_fn(tapes, execution_config=config)
            return batch fn(results)
    512
    514 # the default execution function is batch execute
    515 # use qml.interfaces so that mocker can spy on it during testing
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\interfaces\executic \.
 py:287, in cache_execute.<locals>.wrapper(tapes, **kwargs)
                 return (res, []) if return_tuple else res
    284 else:
            # execute all unique tapes that do not exist in the cache
            # convert to list as new device interface returns a tuple
    286
--> 287
            res = list(fn(execution_tapes.values(), **kwargs))
    289 final res = []
    291 for i, tape in enumerate(tapes):
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\interfaces\executic ...
 →py:210, in cache_execute.<locals>.fn(tapes, **kwargs)
    208 def fn(tapes: Sequence[QuantumTape], **kwargs): # pylint:
 ⇔disable=function-redefined
    209
            tapes = [expand fn(tape) for tape in tapes]
--> 210
            return original_fn(tapes, **kwargs)
File d:\Raul\Programs\envs\PennyLane\lib\contextlib.py:79, in ContextDecorator.

    call .<locals>.inner(*args, **kwds)

     76 @wraps(func)
     77 def inner(*args, **kwds):
     78
            with self._recreate_cm():
---> 79
                 return func(*args, **kwds)
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\_qubit_device.
 ⇔py:603, in QubitDevice.batch execute(self, circuits)
    598 for circuit in circuits:
            # we need to reset the device here, else it will
    600
            # not start the next computation in the zero state
            self.reset()
    601
```

```
--> 603
            res = self.execute(circuit)
    604
            results.append(res)
    606 if self.tracker.active:
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\devices\default_qut_t_torch.
 →py:232, in DefaultQubitTorch.execute(self, circuit, **kwargs)
                if params_cuda_device != specified_device_cuda:
    224
    225
                    warnings.warn(
                        f"Torch device {self._torch_device} specified "
    226
    227
                        "upon PennyLane device creation does not match the "
    228
                        "Torch device of the gate parameters; "
                        f"{self._torch_device} will be used."
    229
    230
--> 232 return super().execute(circuit, **kwargs)
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\ qubit device.
 ⇒py:320, in QubitDevice.execute(self, circuit, **kwargs)
    317 self.check validity(circuit.operations, circuit.observables)
    319 # apply all circuit operations
--> 320 self.apply(circuit.operations, rotations=self.

    get_diagonalizing_gates(circuit), **kwargs)

    322 # generate computational basis samples
    323 if self.shots is not None or circuit.is_sampled:
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\devices\default qut t.
 apy:293, in DefaultQubit.apply(self, operations, rotations, **kwargs)
                self._state = self._apply_parametrized_evolution(self._state,__
 →operation)
    292
            else:
--> 293
                self._state = self._apply_operation(self._state, operation)
    295 # store the pre-rotated state
    296 self._pre_rotated_state = self._state
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\devices\default_qub.t.
 →py:333, in DefaultQubit._apply_operation(self, state, operation)
            axes = [ax + shift for ax in self.wires.indices(wires)]
            return self._apply_ops[operation.name](state, axes)
    331
--> 333 matrix = self._asarray(self._get_unitary_matrix(operation), dtype=self.
 →C DTYPE)
    335 if operation in diagonal_in_z_basis:
            return self._apply_diagonal_unitary(state, matrix, wires)
    336
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\devices\default_qub_t_torch.
 →py:304, in DefaultQubitTorch._get_unitary_matrix(self, unitary)
    302 if unitary in diagonal_in_z_basis:
```

```
return self._asarray(unitary.eigvals(), dtype=self.C_DTYPE)
--> 304 return self._asarray(unitary.matrix(), dtype=self.C_DTYPE)
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\operation.py:
 ⇔748, in Operator.matrix(self, wire order)
    728 def matrix(self, wire_order=None):
            r"""Representation of the operator as a matrix in the computational
 ⇔basis.
    730
    731
            If ``wire_order`` is provided, the numerical representation_
 ⇔considers the position of the
   (...)
    746
                tensor_like: matrix representation
    747
--> 748
            canonical_matrix = self.compute_matrix(*self.parameters, **self.
 →hyperparameters)
    750
            if wire_order is None or self.wires == Wires(wire_order):
    751
                return canonical_matrix
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\ops\qubit\parametri :_ops_single_
 →py:211, in RY.compute_matrix(theta)
    209 c = (1 + 0j) * c
    210 s = (1 + 0j) * s
--> 211 return qml.math.stack([stack_last([c, -s]), stack_last([s, c])], axis=-
File d:
 → \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\math\multi_dispatch
 →py:151, in multi_dispatch.<locals>.decorator.<locals>.wrapper(*args, **kwargs
    148 interface = interface or get_interface(*dispatch_args)
    149 kwargs["like"] = interface
--> 151 return fn(*args, **kwargs)
File d:
 \Raul\Programs\envs\PennyLane\lib\site-packages\pennylane\math\multi_dispatch
 →py:488, in stack(values, axis, like)
    459 """Stack a sequence of tensors along the specified axis.
    460
    461 .. warning::
   (...)
               [5.00e+00, 8.00e+00, 1.01e+02]], dtype=float32)>
    485
    486 """
    487 values = np.coerce(values, like=like)
--> 488 return np.stack(values, axis=axis, like=like)
File d:\Raul\Programs\envs\PennyLane\lib\site-packages\autoray\autoray.py:79, i:

do(fn, like, *args, **kwargs)
     30 """Do function named ``fn`` on ``(*args, **kwargs)``, peforming single
```