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# QuCumber Documentation

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**PIQuIL**

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# CHAPTER 1

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## Installation

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QuCumber only supports Python 3, not Python 2. If you are using Python 2, please update! You will also want to install the following packages, if you have not already.

1. Pytorch v0.4.1 (<https://pytorch.org/>)
2. tqdm (<https://github.com/tqdm/tqdm>)

## 1.1 Github

Navigate to the qucumber page on github (<https://github.com/PIQuIL/QuCumber>) and clone the repository by typing:

```
git clone https://github.com/PIQuIL/QuCumber.git
```

Navigate to the main directory and type:

```
python setup.py install
```

## 1.2 Windows

Navigate to the directory (through command prompt) where pip.exe is installed (usually C:\Python\Scripts\pip.exe) and type:

```
pip.exe install qucumber
```

## 1.3 Linux / MacOS

Open up a terminal, then type:

```
pip install qucumber
```

## CHAPTER 2

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### Theory

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For a basic introduction to Restricted Boltzmann Machines, click [here](#).





## CHAPTER 3

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### Download the tutorials


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Once you have installed QuCumber, we recommend going through our tutorial that is divided into two parts.

1. Training a wave function to reconstruct a positive-real wave function (i.e. no phase) from a transverse-field Ising model (TFIM) and then generating new data.
2. Training an wave function to reconstruct a complex wave function (i.e. with a phase) from a simple two qubit random state and then generating new data.

We have made interactive python notebooks that can be downloaded (along with the data required) [here](https://qucumber.readthedocs.io/en/stable/). Note that the linked examples are from the most recent stable release (relative to the version of the docs you're currently viewing), and may not match the examples shown in the following pages. It is recommended that you refer to documentation for the latest stable release: <https://qucumber.readthedocs.io/en/stable/>.

If you wish to simply view the static, non-interactive notebooks, continue to the next page of the documentation.

Alternatively, you can view interactive notebooks online at: , though they may be slow.



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## Reconstruction of a positive-real wavefunction

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In this tutorial, a walkthrough of how to reconstruct a **positive-real** wavefunction via training a *Restricted Boltzmann Machine* (RBM), the neural network behind qucumber, will be presented. The data used for training will be  $\sigma^z$  measurements from a one-dimensional transverse-field Ising model (TFIM) with 10 sites at its critical point.

### 4.1 Transverse-field Ising model

The example dataset, located in `tfim1d_data.txt`, comprises of 10,000  $\sigma^z$  measurements from a one-dimensional transverse-field Ising model (TFIM) with 10 sites at its critical point. The Hamiltonian for the transverse-field Ising model (TFIM) is given by

$$\mathcal{H} = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x \quad (4.1)$$

where  $\sigma_i^z$  is the conventional spin-1/2 Pauli operator on site  $i$ . At the critical point,  $J = h = 1$ . As per convention, spins are represented in binary notation with zero and one denoting spin-down and spin-up, respectively.

### 4.2 Using qucumber to reconstruct the wavefunction

#### 4.2.1 Imports

To begin the tutorial, first import the required Python packages.

```
[1]: import numpy as np
import matplotlib.pyplot as plt

from qucumber.nn_states import PositiveWaveFunction
from qucumber.callbacks import MetricEvaluator

import qucumber.utils.training_statistics as ts
import qucumber.utils.data as data
```

The Python class *PositiveWaveFunction* contains generic properties of a RBM meant to reconstruct a positive-real wavefunction, the most notable one being the gradient function required for stochastic gradient descent.

To instantiate a *PositiveWaveFunction* object, one needs to specify the number of visible and hidden units in the RBM. The number of visible units, *num\_visible*, is given by the size of the physical system, i.e. the number of spins or qubits (10 in this case), while the number of hidden units, *num\_hidden*, can be varied to change the expressiveness of the neural network.

**Note:** The optimal *num\_hidden* : *num\_visible* ratio will depend on the system. For the TFIM, having this ratio be equal to 1 leads to good results with reasonable computational effort.

## 4.2.2 Training

To evaluate the training in real time, the fidelity between the true ground-state wavefunction of the system and the wavefunction that qucumber reconstructs,  $|\langle \psi | \psi_{RBM} \rangle|^2$ , will be calculated along with the Kullback-Leibler (KL) divergence (the RBM's cost function). It will also be shown that any custom function can be used to evaluate the training.

First, the training data and the true wavefunction of this system must be loaded using the *data* utility.

```
[2]: psi_path = "tfim1d_psi.txt"
    train_path = "tfim1d_data.txt"
    train_data, true_psi = data.load_data(train_path, psi_path)
```

As previously mentioned, to instantiate a *PositiveWaveFunction* object, one needs to specify the number of visible and hidden units in the RBM. These two quantities equal will be kept equal.

```
[3]: nv = train_data.shape[-1]
    nh = nv

    nn_state = PositiveWaveFunction(num_visible=nv, num_hidden=nh)
    # nn_state = PositiveWaveFunction(num_visible=nv, num_hidden=nh, gpu = False)
```

By default, qucumber will attempt to run on a GPU if one is available (if one is not available, qucumber will default to CPU). If one wishes to run qucumber on a CPU, add the flag “gpu = False” in the *PositiveWaveFunction* object instantiation (i.e. uncomment the line above).

Now the hyperparameters of the training process can be specified.

1. **epochs**: the total number of training cycles that will be performed (default = 100)
2. **pos\_batch\_size**: the number of data points used in the positive phase of the gradient (default = 100)
3. **neg\_batch\_size**: the number of data points used in the negative phase of the gradient (default = *pos\_batch\_size*)
4. **k**: the number of contrastive divergence steps (default = 1)
5. **lr**: the learning rate (default = 0.001)

**Note:** For more information on the hyperparameters above, it is strongly encouraged that the user to read through the brief, but thorough theory document on RBMs located in the qucumber documentation. One does not have to specify these hyperparameters, as their default values will be used without the user overwriting them. It is recommended to keep with the default values until the user has a stronger grasp on what these hyperparameters mean. The quality and the computational efficiency of the training will highly depend on the choice of hyperparameters. As such, playing around with the hyperparameters is almost always necessary.

For the TFIM with 10 sites, the following hyperparameters give excellent results.

```
[4]: epochs = 500
     pbs = 100 # pos_batch_size
     nbs = 200 # neg_batch_size
     lr = 0.01
     k = 10
```

For evaluating the training in real time, the *MetricEvaluator* will be called in order to calculate the training evaluators every 100 epochs. The *MetricEvaluator* requires the following arguments.

1. **log\_every**: the frequency of the training evaluators being calculated is controlled by the *log\_every* argument (e.g. *log\_every* = 200 means that the *MetricEvaluator* will update the user every 200 epochs)
2. A dictionary of functions you would like to reference to evaluate the training (arguments required for these functions are keyword arguments placed after the dictionary)

The following additional arguments are needed to calculate the fidelity and KL divergence in the *training\_statistics* utility.

- **target\_psi**: the true wavefunction of the system
- **space**: the hilbert space of the system

The training evaluators can be printed out via the *verbose=True* statement.

Although the fidelity and KL divergence are excellent training evaluators, they are not practical to calculate in most cases; the user may not have access to the target wavefunction of the system, nor may generating the hilbert space of the system be computationally feasible. However, evaluating the training in real time is extremely convenient.

Any custom function that the user would like to use to evaluate the training can be given to the *MetricEvaluator*, thus avoiding having to calculate fidelity and/or KL divergence. Any custom function given to *MetricEvaluator* must take the neural-network state (in this case, the *PositiveWaveFunction* object) and keyword arguments. As an example, the function to be passed to the *MetricEvaluator* will be the fifth coefficient of the reconstructed wavefunction multiplied by a parameter, *A*.

```
[5]: def psi_coefficient(nn_state, space, A, **kwargs):
     norm = nn_state.compute_normalization(space).sqrt_()
     return A * nn_state.psi(space)[0][4] / norm
```

Now the hilbert space of the system can be generated for the fidelity and KL divergence and the dictionary of functions the user would like to compute every “*log\_every*” epochs can be given to the *MetricEvaluator*.

```
[6]: log_every = 10
     space = nn_state.generate_hilbert_space(nv)
```

Now the training can begin. The *PositiveWaveFunction* object has a property called *fit* which takes care of this. *MetricEvaluator* must be passed to the *fit* function in a list (*callbacks*).

```
[7]: callbacks = [
     MetricEvaluator(
         log_every,
         {"Fidelity": ts.fidelity, "KL": ts.KL, "A_Ψrbm_5": psi_coefficient},
         target_psi=true_psi,
         verbose=True,
         space=space,
         A=3.,
     )
 ]

nn_state.fit(
```

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```

train_data,
epochs=epochs,
pos_batch_size=pbs,
neg_batch_size=nbs,
lr=lr,
k=k,
callbacks=callbacks,
)
# nn_state.fit(train_data, callbacks=callbacks)

```

Epoch: 10	Fidelity = 0.524441	KL = 1.311481	A_rbm_5 = 0.102333
Epoch: 20	Fidelity = 0.627167	KL = 0.887134	A_rbm_5 = 0.151670
Epoch: 30	Fidelity = 0.733927	KL = 0.582645	A_rbm_5 = 0.194329
Epoch: 40	Fidelity = 0.794879	KL = 0.445741	A_rbm_5 = 0.221883
Epoch: 50	Fidelity = 0.829248	KL = 0.363647	A_rbm_5 = 0.232239
Epoch: 60	Fidelity = 0.860589	KL = 0.287518	A_rbm_5 = 0.241004
Epoch: 70	Fidelity = 0.886160	KL = 0.231527	A_rbm_5 = 0.244122
Epoch: 80	Fidelity = 0.902777	KL = 0.196992	A_rbm_5 = 0.234641
Epoch: 90	Fidelity = 0.914448	KL = 0.174226	A_rbm_5 = 0.231594
Epoch: 100	Fidelity = 0.923648	KL = 0.156510	A_rbm_5 = 0.234137
Epoch: 110	Fidelity = 0.929855	KL = 0.142626	A_rbm_5 = 0.220506
Epoch: 120	Fidelity = 0.937082	KL = 0.127953	A_rbm_5 = 0.228048
Epoch: 130	Fidelity = 0.943320	KL = 0.114683	A_rbm_5 = 0.225533
Epoch: 140	Fidelity = 0.948913	KL = 0.102805	A_rbm_5 = 0.220003
Epoch: 150	Fidelity = 0.953720	KL = 0.092966	A_rbm_5 = 0.219529
Epoch: 160	Fidelity = 0.957696	KL = 0.085269	A_rbm_5 = 0.219721
Epoch: 170	Fidelity = 0.960716	KL = 0.079273	A_rbm_5 = 0.215919
Epoch: 180	Fidelity = 0.963032	KL = 0.075418	A_rbm_5 = 0.219223
Epoch: 190	Fidelity = 0.965285	KL = 0.071062	A_rbm_5 = 0.217072
Epoch: 200	Fidelity = 0.966294	KL = 0.069517	A_rbm_5 = 0.218791
Epoch: 210	Fidelity = 0.968279	KL = 0.065436	A_rbm_5 = 0.214237
Epoch: 220	Fidelity = 0.969002	KL = 0.063958	A_rbm_5 = 0.208316
Epoch: 230	Fidelity = 0.970735	KL = 0.060499	A_rbm_5 = 0.211827
Epoch: 240	Fidelity = 0.971954	KL = 0.058173	A_rbm_5 = 0.213458
Epoch: 250	Fidelity = 0.972797	KL = 0.056356	A_rbm_5 = 0.216414
Epoch: 260	Fidelity = 0.973940	KL = 0.054098	A_rbm_5 = 0.219072
Epoch: 270	Fidelity = 0.975173	KL = 0.051311	A_rbm_5 = 0.213439
Epoch: 280	Fidelity = 0.976146	KL = 0.049353	A_rbm_5 = 0.214791
Epoch: 290	Fidelity = 0.977626	KL = 0.046184	A_rbm_5 = 0.215294
Epoch: 300	Fidelity = 0.978880	KL = 0.043539	A_rbm_5 = 0.215247
Epoch: 310	Fidelity = 0.979931	KL = 0.041293	A_rbm_5 = 0.211467
Epoch: 320	Fidelity = 0.981140	KL = 0.038849	A_rbm_5 = 0.213601
Epoch: 330	Fidelity = 0.982012	KL = 0.036976	A_rbm_5 = 0.216033
Epoch: 340	Fidelity = 0.982764	KL = 0.035460	A_rbm_5 = 0.217036
Epoch: 350	Fidelity = 0.983499	KL = 0.033983	A_rbm_5 = 0.208566
Epoch: 360	Fidelity = 0.984789	KL = 0.031407	A_rbm_5 = 0.218186
Epoch: 370	Fidelity = 0.985142	KL = 0.030643	A_rbm_5 = 0.215245
Epoch: 380	Fidelity = 0.985985	KL = 0.028931	A_rbm_5 = 0.217562
Epoch: 390	Fidelity = 0.986345	KL = 0.028262	A_rbm_5 = 0.217989
Epoch: 400	Fidelity = 0.986798	KL = 0.027449	A_rbm_5 = 0.215068
Epoch: 410	Fidelity = 0.987459	KL = 0.026076	A_rbm_5 = 0.220650
Epoch: 420	Fidelity = 0.987785	KL = 0.025427	A_rbm_5 = 0.220902
Epoch: 430	Fidelity = 0.988085	KL = 0.024916	A_rbm_5 = 0.217657
Epoch: 440	Fidelity = 0.988270	KL = 0.024565	A_rbm_5 = 0.218701
Epoch: 450	Fidelity = 0.988164	KL = 0.024811	A_rbm_5 = 0.222711
Epoch: 460	Fidelity = 0.988564	KL = 0.024018	A_rbm_5 = 0.212042
Epoch: 470	Fidelity = 0.988859	KL = 0.023432	A_rbm_5 = 0.221610

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Epoch: 480	Fidelity = 0.989148	KL = 0.022804	A_rbm_5 = 0.224286
Epoch: 490	Fidelity = 0.989477	KL = 0.022194	A_rbm_5 = 0.223508
Epoch: 500	Fidelity = 0.989738	KL = 0.021626	A_rbm_5 = 0.223838

All of these training evaluators can be accessed after the training has completed, as well. The code below shows this, along with plots of each training evaluator versus the training cycle number (epoch).

```
[8]: fidelities = callbacks[0].Fidelity
     Kls = callbacks[0].KL
     coeffs = callbacks[0].A_Ψrbm_5
     # Please note that the key given to the *MetricEvaluator* must be what comes after_
     ↪callbacks[0].
     epoch = np.arange(log_every, epochs + 1, log_every)
```

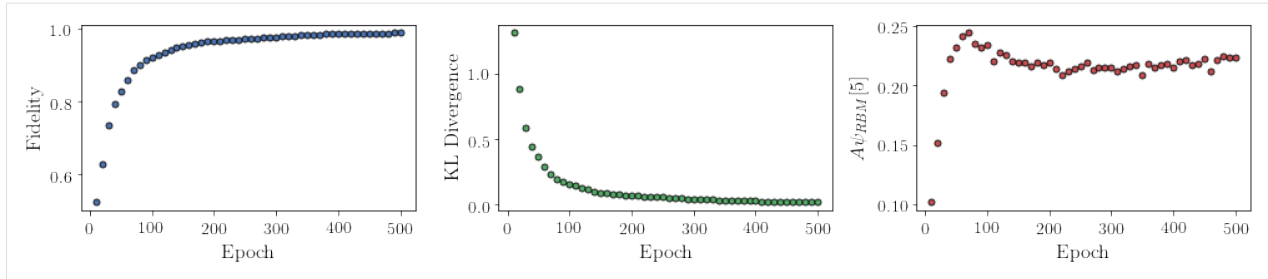
```
[9]: # Some parameters to make the plots look nice
     params = {'text.usetex': True,
               'font.family': 'serif',
               'legend.fontsize': 14,
               'figure.figsize': (10, 3),
               'axes.labelsize': 16,
               'xtick.labelsize': 14,
               'ytick.labelsize': 14,
               'lines.linewidth': 2,
               'lines.markeredgewidth': 0.8,
               'lines.markersize': 5,
               'lines.marker': "o",
               "patch.edgecolor": "black"
            }
     plt.rcParams.update(params)
     plt.style.use('seaborn-deep')
```

```
[10]: # Plotting
     fig, axs = plt.subplots(nrows=1, ncols=3, figsize=(14, 3))
     ax = axs[0]
     ax.plot(epoch, fidelities, "o", color = "C0", markeredgecolor="black")
     ax.set_ylabel(r'Fidelity')
     ax.set_xlabel(r'Epoch')

     ax = axs[1]
     ax.plot(epoch, Kls, "o", color = "C1", markeredgecolor="black")
     ax.set_ylabel(r'KL Divergence')
     ax.set_xlabel(r'Epoch')

     ax = axs[2]
     ax.plot(epoch, coeffs, "o", color = "C2", markeredgecolor="black")
     ax.set_ylabel(r'$A_{\psi_{RBM}}[5]$')
     ax.set_xlabel(r'Epoch')

     plt.tight_layout()
     plt.savefig("fid_KL.pdf")
     plt.show()
```



It should be noted that one could have just ran `nn_state.fit(train_samples)` and just used the default hyperparameters and no training evaluators.

To demonstrate how important it is to find the optimal hyperparameters for a certain system, restart this notebook and comment out the original `fit` statement and uncomment the one below. The default hyperparameters will be used instead. Using the non-default hyperparameters yielded a fidelity of approximately 0.994, while the default hyperparameters yielded a fidelity of approximately 0.523!

The RBM's parameters will also be saved for future use in other tutorials. They can be saved to a pickle file with the name "saved\_params.pt" with the code below.

```
[11]: nn_state.save("saved_params.pt")
```

This saves the weights, visible biases and hidden biases as torch tensors with the following keys: "weights", "visible\_bias", "hidden\_bias".



---

## Reconstruction of a complex wavefunction

---

In this tutorial, a walkthrough of how to reconstruct a **complex** wavefunction via training a *Restricted Boltzmann Machine* (RBM), the neural network behind qucumber, will be presented.

### 5.1 The wavefunction to be reconstructed

The simple wavefunction below describing two qubits (coefficients stored in *qubits\_psi.txt*) will be reconstructed.

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle \quad (5.1)$$

where the exact values of  $\alpha, \beta, \gamma$  and  $\delta$  used for this tutorial are

$$\alpha = 0.2861 + 0.0539i \quad (5.2)$$

$$\beta = 0.3687 - 0.3023i \quad (5.3)$$

$$\gamma = -0.1672 - 0.3529i \quad (5.4)$$

$$\delta = -0.5659 - 0.4639i. \quad (5.5)$$

The example dataset, *qubits\_train.txt*, comprises of 500  $\sigma$  measurements made in various bases (X, Y and Z). A corresponding file containing the bases for each data point in *qubits\_train.txt*, *qubits\_train\_bases.txt*, is also required. As per convention, spins are represented in binary notation with zero and one denoting spin-down and spin-up, respectively.

### 5.2 Using qucumber to reconstruct the wavefunction

#### 5.2.1 Imports

To begin the tutorial, first import the required Python packages.

```
[1]: import numpy as np
import torch
import matplotlib.pyplot as plt

from qucumber.nn_states import ComplexWaveFunction

from qucumber.callbacks import MetricEvaluator

import qucumber.utils.unitaries as unitaries
import qucumber.utils.cplx as cplx

import qucumber.utils.training_statistics as ts
import qucumber.utils.data as data
```

The Python class *ComplexWaveFunction* contains generic properties of a RBM meant to reconstruct a complex wavefunction, the most notable one being the gradient function required for stochastic gradient descent.

To instantiate a *ComplexWaveFunction* object, one needs to specify the number of visible and hidden units in the RBM. The number of visible units, *num\_visible*, is given by the size of the physical system, i.e. the number of spins or qubits (2 in this case), while the number of hidden units, *num\_hidden*, can be varied to change the expressiveness of the neural network.

**Note:** The optimal *num\_hidden* : *num\_visible* ratio will depend on the system. For the two-qubit wavefunction described above, good results are yielded when this ratio is 1.

On top of needing the number of visible and hidden units, a *ComplexWaveFunction* object requires the user to input a dictionary containing the unitary operators (2x2) that will be used to rotate the qubits in and out of the computational basis, Z, during the training process. The *unitaries* utility will take care of creating this dictionary.

The *MetricEvaluator* class and *training\_statistics* utility are built-in amenities that will allow the user to evaluate the training in real time.

Lastly, the *cplx* utility allows qucumber to be able to handle complex numbers. Currently, Pytorch does not support complex numbers.

## 5.2.2 Training

To evaluate the training in real time, the fidelity between the true wavefunction of the system and the wavefunction that qucumber reconstructs,  $|\langle \psi | \psi_{RBM} \rangle|^2$ , will be calculated along with the Kullback-Leibler (KL) divergence (the RBM's cost function). First, the training data and the true wavefunction of this system need to be loaded using the *data* utility.

```
[2]: train_path = "qubits_train.txt"
train_bases_path = "qubits_train_bases.txt"
psi_path = "qubits_psi.txt"
bases_path = "qubits_bases.txt"

train_samples, true_psi, train_bases, bases = data.load_data(
    train_path, psi_path, train_bases_path, bases_path
)
```

The file *qubits\_bases.txt* contains every unique basis in the *qubits\_train\_bases.txt* file. Calculation of the full KL divergence in every basis requires the user to specify each unique basis.

As previously mentioned, a *ComplexWaveFunction* object requires a dictionary that contains the unitary operators that will be used to rotate the qubits in and out of the computational basis, Z, during the training process. In the case of the provided dataset, the unitaries required are the well-known *H*, and *K* gates. The dictionary needed can be created with the following command.

```
[3]: unitary_dict = unitaries.create_dict()
# unitary_dict = unitaries.create_dict(unitary_name=torch.tensor([[real part],
#                                                                    [imaginary part]],
#                                                                    dtype=torch.double))
```

If the user wishes to add their own unitary operators from their experiment to *unitary\_dict*, uncomment the block above. When *unitaries.create\_dict()* is called, it will contain the identity and the *H* and *K* gates by default with the keys “Z”, “X” and “Y”, respectively.

The number of visible units in the RBM is equal to the number of qubits. The number of hidden units will also be taken to be the number of visible units.

```
[4]: nv = train_samples.shape[-1]
nh = nv

nn_state = ComplexWaveFunction(
    num_visible=nv, num_hidden=nh, unitary_dict=unitary_dict, gpu=False
)
# nn_state = ComplexWaveFunction(num_visible=nv, num_hidden=nh, unitary_dict=unitary_
↪dict)
```

By default, qucumber will attempt to run on a GPU if one is available (if one is not available, qucumber will default to CPU). If one wishes to run qucumber on a CPU, add the flag “gpu = False” in the *ComplexWaveFunction* object instantiation. Uncomment the line above to run this tutorial on a GPU.

Now the hyperparameters of the training process can be specified.

1. **epochs**: the total number of training cycles that will be performed (default = 100)
2. **pos\_batch\_size**: the number of data points used in the positive phase of the gradient (default = 100)
3. **neg\_batch\_size**: the number of data points used in the negative phase of the gradient (default = *pos\_batch\_size*)
4. **k**: the number of contrastive divergence steps (default = 1)
5. **lr**: the learning rate (default = 0.001)

**Note:** For more information on the hyperparameters above, it is strongly encouraged that the user to read through the brief, but thorough theory document on RBMs. One does not have to specify these hyperparameters, as their default values will be used without the user overwriting them. It is recommended to keep with the default values until the user has a stronger grasp on what these hyperparameters mean. The quality and the computational efficiency of the training will highly depend on the choice of hyperparameters. As such, playing around with the hyperparameters is almost always necessary.

The two-qubit example in this tutorial should be extremely easy to train, regardless of the choice of hyperparameters. However, the hyperparameters below will be used.

```
[5]: epochs = 100
pbs = 50 # pos_batch_size
nbs = 50 # neg_batch_size
lr = 0.1
k = 5
```

For evaluating the training in real time, the *MetricEvaluator* will be called to calculate the training evaluators every 10 epochs. The *MetricEvaluator* requires the following arguments.

1. **log\_every**: the frequency of the training evaluators being calculated is controlled by the *log\_every* argument (e.g. *log\_every* = 200 means that the *MetricEvaluator* will update the user every 200 epochs)
2. A dictionary of functions you would like to reference to evaluate the training (arguments required for these functions are keyword arguments placed after the dictionary)

The following additional arguments are needed to calculate the fidelity and KL divergence in the *training\_statistics* utility.

- **target\_psi** (the true wavefunction of the system)
- **space** (the hilbert space of the system)

The training evaluators can be printed out via the *verbose=True* statement.

Although the fidelity and KL divergence are excellent training evaluators, they are not practical to calculate in most cases; the user may not have access to the target wavefunction of the system, nor may generating the hilbert space of the system be computationally feasible. However, evaluating the training in real time is extremely convenient.

Any custom function that the user would like to use to evaluate the training can be given to the *MetricEvaluator*, thus avoiding having to calculate fidelity and/or KL divergence. As an example, functions that calculate the the norm of each of the reconstructed wavefunction's coefficients are presented. Any custom function given to *MetricEvaluator* must take the neural-network state (in this case, the *ComplexWaveFunction* object) and keyword arguments. Although the given example requires the hilbert space to be computed, the scope of the *MetricEvaluator*'s ability to be able to handle any function should still be evident.

```
[6]: def alpha(nn_state, space, **kwargs):
    rbm_psi = nn_state.psi(space)
    normalization = nn_state.compute_normalization(space).sqrt_()
    alpha_ = cplx.norm(
        torch.tensor([rbm_psi[0][0], rbm_psi[1][0]], device=nn_state.device)
        / normalization
    )

    return alpha_

def beta(nn_state, space, **kwargs):
    rbm_psi = nn_state.psi(space)
    normalization = nn_state.compute_normalization(space).sqrt_()
    beta_ = cplx.norm(
        torch.tensor([rbm_psi[0][1], rbm_psi[1][1]], device=nn_state.device)
        / normalization
    )

    return beta_

def gamma(nn_state, space, **kwargs):
    rbm_psi = nn_state.psi(space)
    normalization = nn_state.compute_normalization(space).sqrt_()
    gamma_ = cplx.norm(
        torch.tensor([rbm_psi[0][2], rbm_psi[1][2]], device=nn_state.device)
        / normalization
    )

    return gamma_

def delta(nn_state, space, **kwargs):
    rbm_psi = nn_state.psi(space)
    normalization = nn_state.compute_normalization(space).sqrt_()
    delta_ = cplx.norm(
        torch.tensor([rbm_psi[0][3], rbm_psi[1][3]], device=nn_state.device)
        / normalization
```

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```
)

return delta_
```

Now the hilbert space of the system must be generated for the fidelity and KL divergence and the dictionary of functions the user would like to compute every “*log\_every*” epochs must be given to the *MetricEvaluator*.

```
[7]: log_every = 2
space = nn_state.generate_hilbert_space(nv)

callbacks = [
    MetricEvaluator(
        log_every,
        {
            "Fidelity": ts.fidelity,
            "KL": ts.KL,
            "norm $\alpha$ ": alpha,
            "norm $\beta$ ": beta,
            "norm $\gamma$ ": gamma,
            "norm $\delta$ ": delta,
        },
        target_psi=true_psi,
        bases=bases,
        verbose=True,
        space=space,
    )
]
```

Now the training can begin. The *ComplexWaveFunction* object has a property called *fit* which takes care of this.

```
[8]: nn_state.fit(
    train_samples,
    epochs=epochs,
    pos_batch_size=pbs,
    neg_batch_size=nbs,
    lr=lr,
    k=k,
    input_bases=train_bases,
    callbacks=callbacks,
)
```

Epoch: 2	Fidelity = 0.609290	KL = 0.251365	norm = 0.328561
Epoch: 4	Fidelity = 0.761520	KL = 0.130756	norm = 0.268571
Epoch: 6	Fidelity = 0.838254	KL = 0.082158	norm = 0.253614
Epoch: 8	Fidelity = 0.882321	KL = 0.059876	norm = 0.251210
Epoch: 10	Fidelity = 0.909942	KL = 0.046754	norm = 0.259010
Epoch: 12	Fidelity = 0.929755	KL = 0.036943	norm = 0.258238
Epoch: 14	Fidelity = 0.942398	KL = 0.030965	norm = 0.262524
Epoch: 16	Fidelity = 0.951771	KL = 0.027162	norm = 0.250808
Epoch: 18	Fidelity = 0.958536	KL = 0.023913	norm = 0.257332
Epoch: 20	Fidelity = 0.963766	KL = 0.021570	norm = 0.259561
Epoch: 22	Fidelity = 0.968224	KL = 0.019610	norm = 0.263528
Epoch: 24	Fidelity = 0.970991	KL = 0.018523	norm = 0.256601
Epoch: 26	Fidelity = 0.974414	KL = 0.017127	norm = 0.256168
Epoch: 28	Fidelity = 0.976543	KL = 0.016030	norm = 0.261707
Epoch: 30	Fidelity = 0.977891	KL = 0.015551	norm = 0.254371
Epoch: 32	Fidelity = 0.978768	KL = 0.015847	norm = 0.242762

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Epoch: 34	Fidelity = 0.981126	KL = 0.013974	norm = 0.259100
Epoch: 36	Fidelity = 0.981330	KL = 0.013704	norm = 0.262152
Epoch: 38	Fidelity = 0.981989	KL = 0.013495	norm = 0.256111
Epoch: 40	Fidelity = 0.983230	KL = 0.012711	norm = 0.269000
Epoch: 42	Fidelity = 0.984230	KL = 0.012301	norm = 0.273091
Epoch: 44	Fidelity = 0.984190	KL = 0.012178	norm = 0.260481
Epoch: 46	Fidelity = 0.985494	KL = 0.011501	norm = 0.269168
Epoch: 48	Fidelity = 0.985192	KL = 0.011518	norm = 0.269217
Epoch: 50	Fidelity = 0.986754	KL = 0.010896	norm = 0.264035
Epoch: 52	Fidelity = 0.987266	KL = 0.011288	norm = 0.263792
Epoch: 54	Fidelity = 0.987998	KL = 0.010323	norm = 0.268859
Epoch: 56	Fidelity = 0.987993	KL = 0.009957	norm = 0.267215
Epoch: 58	Fidelity = 0.988191	KL = 0.009873	norm = 0.273412
Epoch: 60	Fidelity = 0.988129	KL = 0.009665	norm = 0.264751
Epoch: 62	Fidelity = 0.986891	KL = 0.010557	norm = 0.254349
Epoch: 64	Fidelity = 0.988134	KL = 0.009504	norm = 0.264387
Epoch: 66	Fidelity = 0.987419	KL = 0.009870	norm = 0.263105
Epoch: 68	Fidelity = 0.988299	KL = 0.009280	norm = 0.264269
Epoch: 70	Fidelity = 0.989128	KL = 0.008897	norm = 0.267263
Epoch: 72	Fidelity = 0.989572	KL = 0.008808	norm = 0.268239
Epoch: 74	Fidelity = 0.988996	KL = 0.008901	norm = 0.256966
Epoch: 76	Fidelity = 0.988131	KL = 0.009278	norm = 0.261540
Epoch: 78	Fidelity = 0.989458	KL = 0.008405	norm = 0.263894
Epoch: 80	Fidelity = 0.988967	KL = 0.008628	norm = 0.261319
Epoch: 82	Fidelity = 0.989337	KL = 0.008332	norm = 0.271008
Epoch: 84	Fidelity = 0.989170	KL = 0.008351	norm = 0.270172
Epoch: 86	Fidelity = 0.989256	KL = 0.008291	norm = 0.273329
Epoch: 88	Fidelity = 0.989592	KL = 0.008019	norm = 0.269137
Epoch: 90	Fidelity = 0.989677	KL = 0.007917	norm = 0.266120
Epoch: 92	Fidelity = 0.989260	KL = 0.008174	norm = 0.261290
Epoch: 94	Fidelity = 0.990006	KL = 0.007627	norm = 0.266389
Epoch: 96	Fidelity = 0.989957	KL = 0.007610	norm = 0.270035
Epoch: 98	Fidelity = 0.990623	KL = 0.007506	norm = 0.278505
Epoch: 100	Fidelity = 0.990754	KL = 0.007096	norm = 0.266719

All of these training evaluators can be accessed after the training has completed, as well. The code below shows this, along with plots of each training evaluator versus the training cycle number (epoch).

```
[9]: fidelities = callbacks[0].Fidelity
      Kls = callbacks[0].KL
      coeffs = callbacks[0].normα
      # Please note that the key given to the *MetricEvaluator* must be what comes after_
      ↪callbacks[0].
      epoch = np.arange(log_every, epochs + 1, log_every)
```

```
[10]: # Some parameters to make the plots look nice
      params = {'text.usetex': True,
                'font.family': 'serif',
                'legend.fontsize': 14,
                'figure.figsize': (10, 3),
                'axes.labelsize': 16,
                'xtick.labelsize': 14,
                'ytick.labelsize': 14,
                'lines.linewidth': 2,
                'lines.markeredgewidth': 0.8,
                'lines.markersize': 5,
```

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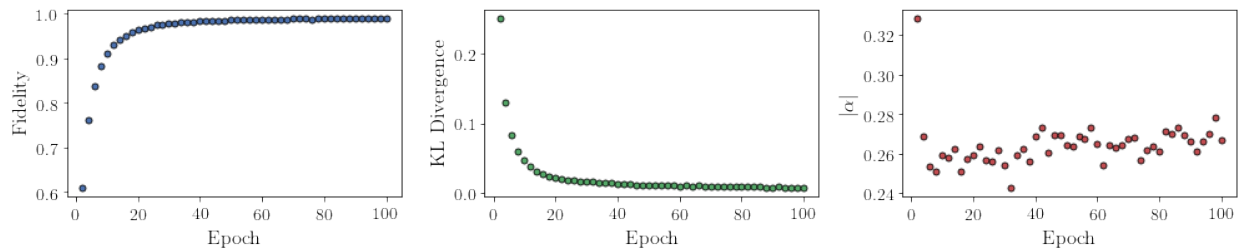
```
        'lines.marker': "o",
        "patch.edgecolor": "black"
    }
plt.rcParams.update(params)
plt.style.use('seaborn-deep')
```

```
[11]: fig, axs = plt.subplots(nrows=1, ncols=3, figsize=(14, 3))
ax = axs[0]
ax.plot(epoch, fidelities, "o", color = "C0", markeredgecolor="black")
ax.set_ylabel(r'Fidelity')
ax.set_xlabel(r'Epoch')

ax = axs[1]
ax.plot(epoch, KLs, "o", color = "C1", markeredgecolor="black")
ax.set_ylabel(r'KL Divergence')
ax.set_xlabel(r'Epoch')

ax = axs[2]
ax.plot(epoch, coeffs, "o", color = "C2", markeredgecolor="black")
ax.set_ylabel(r'$\alpha$')
ax.set_xlabel(r'Epoch')

plt.tight_layout()
plt.savefig("complex_fid_KL.pdf")
plt.show()
```



It should be noted that one could have just ran `nn_state.fit(train_samples)` and just used the default hyperparameters and no training evaluators.

At the end of the training process, the network parameters (the weights, visible biases and hidden biases) are stored in the `ComplexWaveFunction` object. One can save them to a pickle file, which will be called `saved_params.pt`, with the following command.

```
[12]: nn_state.save("saved_params.pt")
```

This saves the weights, visible biases and hidden biases as torch tensors with the following keys: “weights”, “visible\_bias”, “hidden\_bias”.





---

## Sampling and calculating observables

---

### 6.1 Generate new samples

Firstly, to generate meaningful data, an RBM needs to be trained. Please refer to the tutorials 1 and 2 on training an RBM if how to train an RBM using qucumber is unclear. An RBM with a positive-real wavefunction describing a transverse-field Ising model (TFIM) with 10 sites has already been trained in the first tutorial, with the parameters of the machine saved here as *saved\_params.pt*. The *autoload* function can be employed here to instantiate the corresponding *PositiveWaveFunction* object from the saved RBM parameters.

```
[1]: import numpy as np
import matplotlib.pyplot as plt

from qucumber.nn_states import PositiveWaveFunction

from qucumber.observables import ObservableBase

import quantum_ising_chain
from quantum_ising_chain import TFIMChainEnergy

nn_state = PositiveWaveFunction autoload("saved_params.pt")
```

A *PositiveWaveFunction* object has a property called *sample* that takes in the following arguments.

1. **k**: the number of Gibbs steps to perform to generate the new samples
2. **num\_samples**: the number of new data points to be generated

```
[2]: new_samples = nn_state.sample(k=100, num_samples=10000)
print(new_samples)

tensor([[1., 1., 1., ..., 1., 0., 0.],
        [1., 1., 1., ..., 1., 0., 0.],
        [0., 0., 0., ..., 0., 1., 1.],
        ...,
        [1., 1., 1., ..., 1., 1., 1.]])
```

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```
[0., 0., 1., ..., 0., 1., 1.],
[0., 0., 0., ..., 1., 1., 1.]], dtype=torch.float64)
```

With the newly generated samples, the user can now easily calculate observables that do not require any details associated with the RBM. A great example of this is the magnetization. To calculate the magnetization, the newly-generated samples must be converted to  $\pm 1$  from 1 and 0, respectively. The function below does the trick.

```
[3]: def to_pm1(samples):
      return samples.mul(2.).sub(1.)
```

Now, the magnetization is calculated as follows.

```
[4]: def Magnetization(samples):
      return to_pm1(samples).mean(1).abs().mean()

magnetization = Magnetization(new_samples).item()

print("Magnetization = %.5f" % magnetization)

Magnetization = 0.54968
```

The exact value for the magnetization is 0.5610.

The magnetization and the newly-generated samples can also be saved to a pickle file along with the RBM parameters in the *PositiveWaveFunction* object.

```
[5]: nn_state.save(
      "saved_params_and_new_data.pt",
      metadata={"samples": new_samples, "magnetization": magnetization},
      )
```

The *metadata* argument in the *save* function takes in a dictionary of data that you would like to save on top of the RBM parameters.

## 6.2 Calculate an observable using the *Observable* module

### 6.2.1 Custom observable

QuCumber has a built-in module called *Observable* which makes it easy for the user to compute any arbitrary observable from the RBM. To see the *Observable* module in action, an example observable called *PIQuIL*, which inherits properties from the *Observable* module, is shown below.

The *PIQuIL* observable takes an  $\sigma^z$  measurement at a site and multiplies it by the measurement two sites from it. There is also a parameter,  $P$ , that determines the strength of each of these interactions. For example, for the dataset  $(-1, 1, 1, -1)$ ,  $(1, 1, 1, 1)$  and  $(1, 1, -1, 1)$  with  $P = 2$ , the *PIQuIL* for each data point would be  $(2(-1 \times 1) + 2(1 \times -1) = -4)$ ,  $(2(1 \times 1) + 2(1 \times 1) = 4)$  and  $(2(1 \times -1) + 2(1 \times 1) = 0)$ , respectively.

```
[6]: class PIQuIL(ObservableBase):
      def __init__(self, P):
          super(PIQuIL, self).__init__()
          self.P = P

      # Required : function that calculates the PIQuIL. Must be named "apply"
```

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```
def apply(self, nn_state, samples):
    to_pml(samples)
    interaction_ = 0
    for i in range(samples.shape[-1]):
        if (i + 3) > samples.shape[-1]:
            continue
        else:
            interaction_ += self.P * samples[:, i] * samples[:, i + 2]

    return interaction_

P = 0.05
piquil = PIQuIL(P)
```

The *apply* function is contained in the *Observable* module, but is overwritten here. The *apply* function in *Observable* will compute the observable itself and must take in the RBM (*nn\_state*) and a batch of samples as arguments. Thus, any new class inheriting from *Observables* that the user would like to define must contain a function called *apply* that calculates this new observable.

Although the *PIQuIL* observable could technically be computed without the use of the *Observable* module since it does not ever use the RBM (*nn\_state*), it is still nonetheless a constructive example.

The real power in the *Observable* module is in the ability for the user to easily compute statistics of the observable from the generated sample. Since we have already generated new samples of data, the *PIQuIL* observable's mean, standard error and variance on the new data can be calculated with the *statistics\_from\_samples* function in the *Observable* module. The user must simply give the RBM and the samples as arguments.

```
[7]: piquil_stats1 = piquil.statistics_from_samples(nn_state, new_samples)
```

The *statistics\_from\_samples* function returns a dictionary containing the mean, standard error and the variance with the keys “mean”, “std\_error” and “variance”, respectively.

```
[8]: print(
    "Mean PIQuIL: %.4f" % piquil_stats1["mean"], "+/- %.4f" % piquil_stats1["std_error"]
)
print("Variance: %.4f" % piquil_stats1["variance"])

Mean PIQuIL: 0.1419 +/- 0.0014
Variance: 0.0188
```

However, if the user did not have samples generated already, that is no problem. The *statistics* function in the *Observable* module will generate new samples internally and compute the mean, standard error and variance on those samples. Since the samples are not an argument in the *statistics* function, the user must now give the following additional arguments to the *statistics* function to generate the new samples.

- **num\_samples**: the number of samples to generate internally
- **num\_chains**: the number of Markov chains to run in parallel (default = 0)
- **burn\_in**: the number of Gibbs steps to perform before recording any samples (default = 1000)
- **steps**: the number of Gibbs steps to perform between each sample (default = 1)

The *statistics* function will also return a dictionary containing the mean, standard error and the variance with the keys “mean”, “std\_error” and “variance”, respectively.

```
[9]: num_samples = 10000
    burn_in = 100
    steps = 100

    piqul_stats2 = piqul.statistics(nn_state, num_samples, burn_in=burn_in, steps=steps)
    print(
        "Mean PIQuIL: %.4f" % piqul_stats2["mean"], "+/- %.4f" % piqul_stats2["std_error"]
    )
    print("Variance: %.4f" % piqul_stats2["variance"])

Mean PIQuIL: 0.1409 +/- 0.0014
Variance: 0.0186
```

## 6.2.2 TFIM Energy

Some observables cannot be computed directly from samples, but instead depend on the RBM as previously mentioned. For example, the magnetization of the TFIM simply depends on the samples the user gives as input. Whereas the TFIM energy is much more complicated. An example for the computation of the energy is provided in the python file *quantum\_ising\_chain.py*, which takes advantage of qucumber's *Observable* module.

*quantum\_ising\_chain.py* comprises of a class that computes the energy of a TFIM (*TFIMChainEnergy*) that inherits properties from the *Observable* module. To instantiate a *TFIMChainEnergy* object, the  $\frac{h}{J}$  value must be specified. The trained RBM parameters are from the first tutorial, where the example data was from the TFIM with 10 sites at its critical point ( $\frac{h}{J} = 1$ ).

```
[10]: h = 1

    tfim_energy = TFIMChainEnergy(h)
```

To go ahead and calculate the mean energy and its standard error from the previously generated samples from this tutorial (*new\_samples*), the *statistics\_from\_samples* function in the *Observable* module is called upon.

```
[11]: energy_stats = tfim_energy.statistics_from_samples(nn_state, new_samples)
    print("Mean: %.4f" % energy_stats["mean"], "+/- %.4f" % energy_stats["std_error"])
    print("Variance: %.4f" % energy_stats["variance"])

Mean: -1.2362 +/- 0.0005
Variance: 0.0022
```

The exact value for the energy is -1.2381.

To illustrate how quickly the energy converges as a function of the sampling step (i.e. the number of Gibbs steps to perform to generate a new batch of samples), *steps*, the *Convergence* function in *quantum\_ising\_chain.py* will do the trick. *Convergence* creates a batch of random samples initially, which is then used to generate a new batch of samples from the RBM. The TFIM energy will be calculated at every Gibbs step. Please note that the samples generated previously (*new\_samples*) are not used here; different samples are generated.

```
[12]: steps = 200
    num_samples = 10000

    dict_observables = quantum_ising_chain.Convergence(
        nn_state, tfim_energy, num_samples, steps
    )

    energy = dict_observables["energies"]
```

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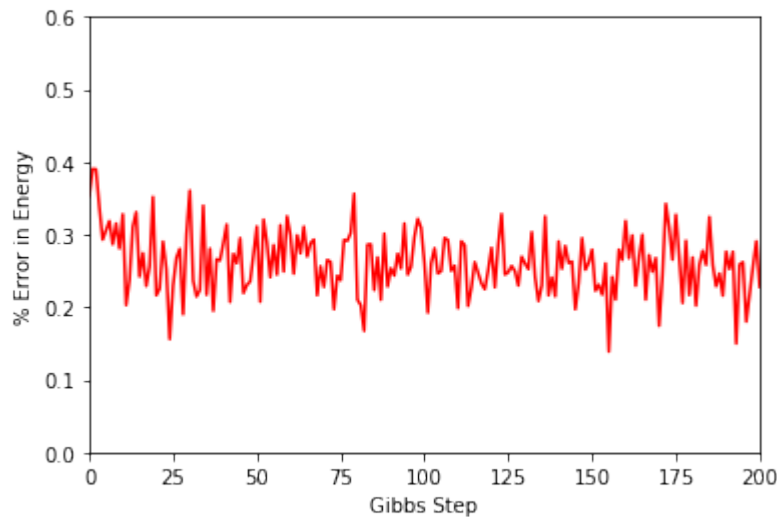
```
err_energy = dict_observables["error"]

step = np.arange(steps + 1)

E0 = -1.2381

ax = plt.axes()
ax.plot(step, abs((energy - E0) / E0) * 100, color="red")
ax.set_xlim(0, steps)
ax.set_ylim(0, 0.6)
ax.set_xlabel("Gibbs Step")
ax.set_ylabel("% Error in Energy")
```

```
[12]: Text(0,0.5,'% Error in Energy')
```



One can see a brief transient period in the magnetization observable, before the state of the machine “warms up” to equilibrium. After that, the values fluctuate around the calculated mean.

## 6.2.3 Adding observables

One may also add / subtract observables with the new observable also retaining the same properties in the *Observables* module. For instance, a new observable can be defined by adding the TFIM energy observable multiplied by an arbitrary constant to the PIQuIL observable.

```
[13]: new_obs = 0.01 * tfim_energy + piquil
```

The same statistics of this new observable can also be calculated.

```
[14]: new_obs_stats = new_obs.statistics_from_samples(nn_state, new_samples)
print("Mean: %.4f" % new_obs_stats["mean"], "+/- %.4f" % new_obs_stats["std_error"])
print("Variance: %.4f" % new_obs_stats["variance"])
```

```
Mean: 0.1295 +/- 0.0014
Variance: 0.0188
```

## 6.2.4 Template for your custom observable

Here is a generic template for you to try using the *Observable* module yourself.

```
[15]: import torch
      from qucumber.observables import ObservableBase

      class YourObservable(ObservableBase):
          def __init__(self, your_constants):
              super(YourObservable, self).__init__()
              self.your_constants = your_constants

          def apply(self, nn_state, samples):
              # arguments of "apply" must be in this order

              # calculate your observable for each data point
              obs = torch.tensor([42] * len(samples))

              # make sure the observables are on the same device and have the
              # same dtype as the samples
              obs = obs.to(samples)

              # return a torch tensor containing the observable values
              return obs
```

---

## Training while monitoring observables

---

As seen in the first tutorial that went through reconstructing the wavefunction describing the TFIM with 10 sites at its critical point, the user can evaluate the training in real time with the *MetricEvaluator* and custom functions. What is most likely more impactful in many cases is to calculate an observable, like the energy, during the training process. This is slightly more computationally involved than using the *MetricEvaluator* to evaluate functions because observables require that samples be drawn from the RBM.

Luckily, qucumber also has a module very similar to the *MetricEvaluator*, but for observables. This is called the *ObservableEvaluator*. The following implements the *ObservableEvaluator* to calculate the energy during the training on the TFIM data in the first tutorial. We will use the same hyperparameters as before.

It is assumed that the user has worked through tutorial 3 beforehand. Recall that *quantum\_ising\_chain.py* contains the *TFIMChainEnergy* class that inherits from the *Observable* module. The exact ground-state energy is -1.2381.

```
[1]: import os.path

import numpy as np
import matplotlib.pyplot as plt

from qucumber.nn_states import PositiveWaveFunction
from qucumber.callbacks import ObservableEvaluator

import qucumber.utils.data as data

from quantum_ising_chain import TFIMChainEnergy

[2]: train_data = data.load_data(
    os.path.join("../", "Tutorial1_TrainPosRealWaveFunction", "tfim1d_data.txt")
)[0]

nv = train_data.shape[-1]
nh = nv

nn_state = PositiveWaveFunction(num_visible=nv, num_hidden=nh)
```

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```
epochs = 1000
pbs = 100 # pos_batch_size
nbs = 200 # neg_batch_size
lr = 0.01
k = 10

log_every = 100

h = 1
num_samples = 10000
burn_in = 100
steps = 100

tfim_energy = TFIMChainEnergy(h)
```

Now, the *ObservableEvaluator* can be called. The *ObservableEvaluator* requires the following arguments.

1. **log\_every**: the frequency of the training evaluators being calculated is controlled by the *log\_every* argument (e.g. *log\_every* = 200 means that the *MetricEvaluator* will update the user every 200 epochs)
2. A list of *Observable* objects you would like to reference to evaluate the training (arguments required for generating samples to calculate the observables are keyword arguments placed after the list)

The following additional arguments are needed to calculate the statistics on the generated samples during training (these are the arguments of the *statistics* function in the *Observable* module, minus the *nn\_state* argument; this gets passed in as an argument to *fit*).

- **num\_samples**: the number of samples to generate internally
- **num\_chains**: the number of Markov chains to run in parallel (default = 0)
- **burn\_in**: the number of Gibbs steps to perform before recording any samples (default = 1000)
- **steps**: the number of Gibbs steps to perform between each sample (default = 1)

The training evaluators can be printed out via the *verbose=True* statement.

```
[3]: callbacks = [
    ObservableEvaluator(
        log_every,
        [tfim_energy],
        verbose=True,
        num_samples=num_samples,
        burn_in=burn_in,
        steps=steps,
    )
]

nn_state.fit(
    train_data,
    epochs=epochs,
    pos_batch_size=pbs,
    neg_batch_size=nbs,
    lr=lr,
    k=k,
    callbacks=callbacks,
)
```

Epoch: 100  
TFIMChainEnergy:

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mean: -1.197008	variance: 0.022882	std_error: 0.001513
Epoch: 200		
TFIMChainEnergy:		
mean: -1.216405	variance: 0.011845	std_error: 0.001088
Epoch: 300		
TFIMChainEnergy:		
mean: -1.224917	variance: 0.008271	std_error: 0.000909
Epoch: 400		
TFIMChainEnergy:		
mean: -1.228988	variance: 0.005977	std_error: 0.000773
Epoch: 500		
TFIMChainEnergy:		
mean: -1.230748	variance: 0.004908	std_error: 0.000701
Epoch: 600		
TFIMChainEnergy:		
mean: -1.232201	variance: 0.003850	std_error: 0.000620
Epoch: 700		
TFIMChainEnergy:		
mean: -1.233295	variance: 0.003404	std_error: 0.000583
Epoch: 800		
TFIMChainEnergy:		
mean: -1.233561	variance: 0.002842	std_error: 0.000533
Epoch: 900		
TFIMChainEnergy:		
mean: -1.235249	variance: 0.002480	std_error: 0.000498
Epoch: 1000		
TFIMChainEnergy:		
mean: -1.234220	variance: 0.002232	std_error: 0.000472

The `callbacks` list returns a list of dictionaries. The mean, standard error and the variance at each epoch can be accessed as follows.

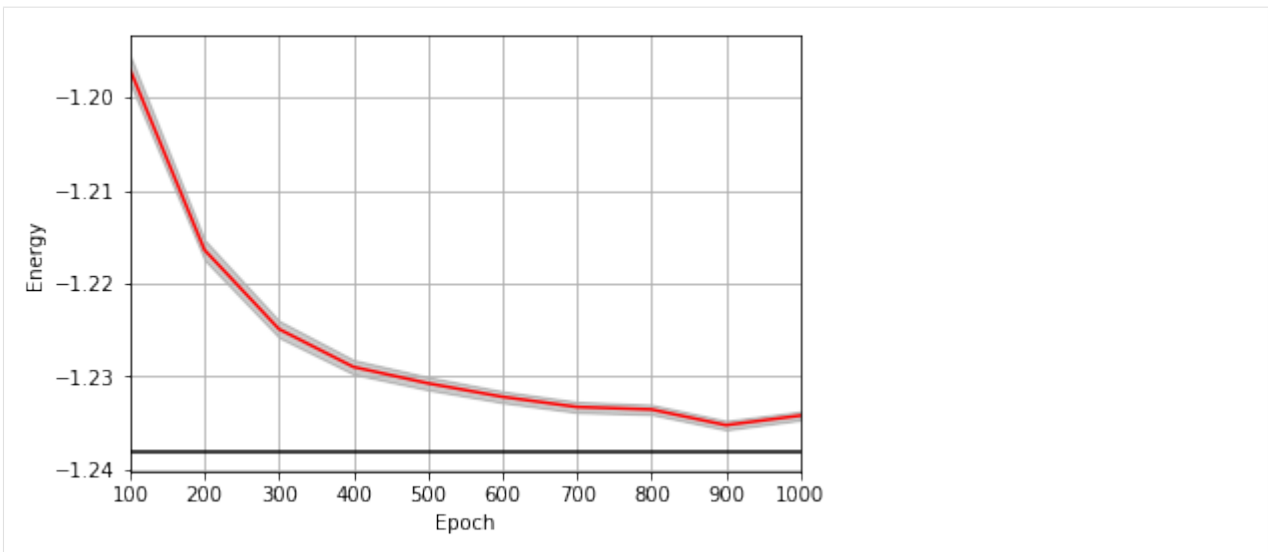
```
[4]: energies = callbacks[0].TFIMChainEnergy.mean
errors = callbacks[0].TFIMChainEnergy.std_error
variance = callbacks[0].TFIMChainEnergy.variance
# Please note that the name of the observable class that the user makes must be what_
↳ comes after callbacks[0].
```

A plot of the energy as a function of the training cycle is presented below.

```
[5]: epoch = np.arange(log_every, epochs + 1, log_every)

E0 = -1.2381

ax = plt.axes()
ax.plot(epoch, energies, color="red")
ax.set_xlim(log_every, epochs)
ax.axhline(E0, color="black")
ax.fill_between(epoch, energies - errors, energies + errors, alpha=0.2, color="black")
ax.set_xlabel("Epoch")
ax.set_ylabel("Energy")
ax.grid()
```



---

```
class qucumber.rbm.BinaryRBM(num_visible, num_hidden, zero_weights=False, gpu=True)
```

```
    Bases: torch.nn.modules.module.Module
```

```
    effective_energy(v)
```

The effective energies of the given visible states.

$$\mathcal{E}(v) = - \sum_j b_j v_j - \sum_i \log \left[ 1 + \exp \left( c_i + \sum_j W_{ij} v_j \right) \right]$$

**Parameters** **v** (*torch.Tensor*) – The visible states.

**Returns** The effective energies of the given visible states.

**Return type** *torch.Tensor*

```
    effective_energy_gradient(v)
```

The gradients of the effective energies for the given visible states.

**Parameters** **v** (*torch.Tensor*) – The visible states.

**Returns** 1d vector containing the gradients for all parameters (computed on the given visible states v).

**Return type** *torch.Tensor*

```
    gibbs_steps(k, initial_state, overwrite=False)
```

Performs k steps of Block Gibbs sampling. One step consists of sampling the hidden state  $h$  from the conditional distribution  $p(h | v)$ , and sampling the visible state  $v$  from the conditional distribution  $p(v | h)$ .

**Parameters**

- **k** (*int*) – Number of Block Gibbs steps.
- **initial\_state** (*torch.Tensor*) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (*bool*) – Whether to overwrite the initial\_state tensor, if it is provided.

**initialize\_parameters** (*zero\_weights=False*)

Randomize the parameters of the RBM

**partition** (*space*)

Compute the partition function of the RBM.

**Parameters** *space* (*torch.Tensor*) – A rank 2 tensor of the visible space.

**Returns** The value of the partition function evaluated at the current state of the RBM.

**Return type** *torch.Tensor*

**prob\_h\_given\_v** (*v, out=None*)

Given a visible unit configuration, compute the probability vector of the hidden units being on.

**Parameters**

- *h* (*torch.Tensor*) – The hidden unit.
- *out* (*torch.Tensor*) – The output tensor to write to.

**Returns** The probability of hidden units being active given the visible state.

**Return type** *torch.Tensor*

**prob\_v\_given\_h** (*h, out=None*)

Given a hidden unit configuration, compute the probability vector of the visible units being on.

**Parameters**

- *h* (*torch.Tensor*) – The hidden unit
- *out* (*torch.Tensor*) – The output tensor to write to.

**Returns** The probability of visible units being active given the hidden state.

**Return type** *torch.Tensor*

**sample\_h\_given\_v** (*v, out=None*)

Sample/generate a hidden state given a visible state.

**Parameters**

- *h* (*torch.Tensor*) – The visible state.
- *out* (*torch.Tensor*) – The output tensor to write to.

**Returns** Tuple containing *prob\_h\_given\_v(v)* and the sampled hidden state.

**Return type** *tuple(torch.Tensor, torch.Tensor)*

**sample\_v\_given\_h** (*h, out=None*)

Sample/generate a visible state given a hidden state.

**Parameters**

- *h* (*torch.Tensor*) – The hidden state.
- *out* (*torch.Tensor*) – The output tensor to write to.

**Returns** Tuple containing *prob\_v\_given\_h(h)* and the sampled visible state.

**Return type** *tuple(torch.Tensor, torch.Tensor)*

## 9.1 Positive WaveFunction

**class** `qucumber.nn_states.PositiveWaveFunction` (*num\_visible*, *num\_hidden=None*,  
*gpu=True*)

Bases: `qucumber.nn_states.WaveFunctionBase`

Class capable of learning wavefunctions with no phase.

### Parameters

- **num\_visible** (*int*) – The number of visible units, ie. the size of the system being learned.
- **num\_hidden** (*int*) – The number of hidden units in the internal RBM. Defaults to the number of visible units.
- **gpu** (*bool*) – Whether to perform computations on the default gpu.

**amplitude** (*v*)

Compute the (unnormalized) amplitude of a given vector/matrix of visible states.

$$\text{amplitude}(\sigma) = |\psi_{\lambda}(\sigma)| = e^{-\mathcal{E}_{\lambda}(\sigma)/2}$$

**Parameters** *v* (*torch.Tensor*) – visible states  $\sigma$

**Returns** Matrix/vector containing the amplitudes of *v*

**Return type** *torch.Tensor*

**static autoload** (*location*, *gpu=False*)

Initializes a WaveFunction from the parameters in the given location.

### Parameters

- **location** (*str or file*) – The location to load the model parameters from.
- **gpu** (*bool*) – Whether the returned model should be on the GPU.

**Returns** A new WaveFunction initialized from the given parameters. The returned WaveFunction will be of whichever type this function was called on.

**compute\_batch\_gradients** (*k*, *samples\_batch*, *neg\_batch*)

Compute the gradients of a batch of the training data (*samples\_batch*).

**Parameters**

- **k** (*int*) – Number of contrastive divergence steps in training.
- **samples\_batch** (*torch.Tensor*) – Batch of the input samples.
- **neg\_batch** (*torch.Tensor*) – Batch of the input samples for computing the negative phase.

**Returns** List containing the gradients of the parameters.

**Return type** *list*

**compute\_normalization** (*space*)

Compute the normalization constant of the wavefunction.

$$Z_{\lambda} = \sqrt{\sum_{\sigma} |\psi_{\lambda}|^2} = \sqrt{\sum_{\sigma} p_{\lambda}(\sigma)}$$

**Parameters** **space** (*torch.Tensor*) – A rank 2 tensor of the entire visible space.

**device**

The device that the model is on.

**fit** (*data*, *epochs=100*, *pos\_batch\_size=100*, *neg\_batch\_size=None*, *k=1*, *lr=0.001*, *progbar=False*, *starting\_epoch=1*, *time=False*, *callbacks=None*, *optimizer=<class 'torch.optim.sgd.SGD'>*, *\*\*kwargs*)

Train the WaveFunction.

**Parameters**

- **data** (*np.array*) – The training samples
- **epochs** (*int*) – The number of full training passes through the dataset. Technically, this specifies the index of the *last* training epoch, which is relevant if *starting\_epoch* is being set.
- **pos\_batch\_size** (*int*) – The size of batches for the positive phase taken from the data.
- **neg\_batch\_size** (*int*) – The size of batches for the negative phase taken from the data. Defaults to *pos\_batch\_size*.
- **k** (*int*) – The number of contrastive divergence steps.
- **lr** (*float*) – Learning rate
- **progbar** (*bool or str*) – Whether or not to display a progress bar. If “notebook” is passed, will use a Jupyter notebook compatible progress bar.
- **starting\_epoch** (*int*) – The epoch to start from. Useful if continuing training from a previous state.
- **callbacks** (*list [qucumber.callbacks.CallbackBase]*) – Callbacks to run while training.
- **optimizer** (*torch.optim.Optimizer*) – The constructor of a torch optimizer.
- **kwargs** – Keyword arguments to pass to the optimizer

**generate\_hilbert\_space** (*size=None, device=None*)

Generates Hilbert space of dimension  $2^{\text{size}}$ .

**Parameters**

- **size** (*int*) – The size of each element of the Hilbert space. Defaults to the number of visible units.
- **device** – The device to create the Hilbert space matrix on. Defaults to the device this model is on.

**Returns** A tensor with all the basis states of the Hilbert space.

**Return type** `torch.Tensor`

**gradient** (*v*)

Compute the gradient of the effective energy for a batch of states.

$\nabla_{\lambda} \mathcal{E}_{\lambda}(\sigma)$

**Parameters** **v** (*torch.Tensor*) – visible states  $\sigma$

**Returns** A single tensor containing all of the parameter gradients.

**Return type** `torch.Tensor`

**load** (*location*)

Loads the WaveFunction parameters from the given location ignoring any metadata stored in the file. Overwrites the WaveFunction's parameters.

---

**Note:** The WaveFunction object on which this function is called must have the same parameter shapes as the one who's parameters are being loaded.

---

**Parameters** **location** (*str or file*) – The location to load the WaveFunction parameters from.

**max\_size**

Maximum size of the Hilbert space for full enumeration

**networks**

A list of the names of the internal RBMs.

**phase** (*v*)

Compute the phase of a given vector/matrix of visible states.

In the case of a PositiveWaveFunction, the phase is just zero.

**Parameters** **v** (*torch.Tensor*) – visible states  $\sigma$

**Returns** Matrix/vector containing the phases of v

**Return type** `torch.Tensor`

**probability** (*v, Z*)

Evaluates the probability of the given vector(s) of visible states.

**Parameters**

- **v** (*torch.Tensor*) – The visible states.
- **Z** (*float*) – The partition function.

**Returns** The probability of the given vector(s) of visible units.

**Return type** `torch.Tensor`

**psi** (*v*)

Compute the (unnormalized) wavefunction of a given vector/matrix of visible states.

$$\psi_{\lambda}(\sigma) = e^{-\mathcal{E}_{\lambda}(\sigma)/2}$$

**Parameters** *v* (`torch.Tensor`) – visible states  $\sigma$

**Returns** Complex object containing the value of the wavefunction for each visible state

**Return type** `torch.Tensor`

**rbm\_am**

The RBM to be used to learn the wavefunction amplitude.

**reinitialize\_parameters** ()

Randomize the parameters of the internal RBMs.

**sample** (*k*, *num\_samples=1*, *initial\_state=None*, *overwrite=False*)

Performs *k* steps of Block Gibbs sampling. One step consists of sampling the hidden state *h* from the conditional distribution  $p_{\lambda}(h|v)$ , and sampling the visible state *v* from the conditional distribution  $p_{\lambda}(v|h)$ .

**Parameters**

- **k** (`int`) – Number of Block Gibbs steps.
- **num\_samples** (`int`) – The number of samples to generate.
- **initial\_state** (`torch.Tensor`) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (`bool`) – Whether to overwrite the *initial\_state* tensor, if it is provided.

**save** (*location*, *metadata=None*)

Saves the WaveFunction parameters to the given location along with any given metadata.

**Parameters**

- **location** (`str` or `file`) – The location to save the data.
- **metadata** (`dict`) – Any extra metadata to store alongside the WaveFunction parameters.

**stop\_training**

If *True*, will not train.

If this property is set to *True* during the training cycle, training will terminate once the current batch or epoch ends (depending on when *stop\_training* was set).

**subspace\_vector** (*num*, *size=None*, *device=None*)

Generates a single vector from the Hilbert space of dimension  $2^{\text{size}}$ .

**Parameters**

- **size** (`int`) – The size of each element of the Hilbert space.
- **num** (`int`) – The specific vector to return from the Hilbert space. Since the Hilbert space can be represented by the set of binary strings of length *size*, *num* is equivalent to the decimal representation of the returned vector.
- **device** – The device to create the vector on. Defaults to the device this model is on.

**Returns** A state from the Hilbert space.

**Return type** `torch.Tensor`



## 9.2 Complex WaveFunction

**class** qucumber.nn\_states.**ComplexWaveFunction** (*num\_visible*, *num\_hidden=None*, *unitary\_dict=None*, *gpu=True*)

Bases: *qucumber.nn\_states.WaveFunctionBase*

Class capable of learning wavefunctions with a non-zero phase.

### Parameters

- **num\_visible** (*int*) – The number of visible units, ie. the size of the system being learned.
- **num\_hidden** (*int*) – The number of hidden units in both internal RBMs. Defaults to the number of visible units.
- **unitary\_dict** (*dict[str, torch.Tensor]*) – A dictionary mapping unitary names to their matrix representations.
- **gpu** (*bool*) – Whether to perform computations on the default gpu.

**amplitude** (*v*)

Compute the (unnormalized) amplitude of a given vector/matrix of visible states.

$$\text{amplitude}(\sigma) = |\psi_{\lambda\mu}(\sigma)| = e^{-\mathcal{E}_{\lambda}(\sigma)/2}$$

**Parameters** *v* (*torch.Tensor*) – visible states  $\sigma$ .

**Returns** Vector containing the amplitudes of the given states.

**Return type** *torch.Tensor*

**static autoload** (*location*, *gpu=False*)

Initializes a WaveFunction from the parameters in the given location.

### Parameters

- **location** (*str or file*) – The location to load the model parameters from.
- **gpu** (*bool*) – Whether the returned model should be on the GPU.

**Returns** A new WaveFunction initialized from the given parameters. The returned WaveFunction will be of whichever type this function was called on.

**compute\_batch\_gradients** (*k*, *samples\_batch*, *neg\_batch*, *bases\_batch=None*)

Compute the gradients of a batch of the training data (*samples\_batch*).

If measurements are taken in bases other than the reference basis, a list of bases (*bases\_batch*) must also be provided.

### Parameters

- **k** (*int*) – Number of contrastive divergence steps in training.
- **samples\_batch** (*torch.Tensor*) – Batch of the input samples.
- **neg\_batch** (*torch.Tensor*) – Batch of the input samples for computing the negative phase.
- **bases\_batch** (*np.array*) – Batch of the input bases corresponding to the samples in *samples\_batch*.

**Returns** List containing the gradients of the parameters.

**Return type** *list*

**compute\_normalization** (*space*)

Compute the normalization constant of the wavefunction.

$$Z_{\lambda} = \sqrt{\sum_{\sigma} |\psi_{\lambda\mu}|^2} = \sqrt{\sum_{\sigma} p_{\lambda}(\sigma)}$$

**Parameters** **space** (*torch.Tensor*) – A rank 2 tensor of the entire visible space.

**device**

The device that the model is on.

**fit** (*data*, *epochs=100*, *pos\_batch\_size=100*, *neg\_batch\_size=None*, *k=1*, *lr=0.001*, *input\_bases=None*, *progbar=False*, *starting\_epoch=1*, *time=False*, *callbacks=None*, *optimizer=<class 'torch.optim.sgd.SGD'>*, *\*\*kwargs*)

Train the WaveFunction.

**Parameters**

- **data** (*np.array*) – The training samples
- **epochs** (*int*) – The number of full training passes through the dataset. Technically, this specifies the index of the *last* training epoch, which is relevant if *starting\_epoch* is being set.
- **pos\_batch\_size** (*int*) – The size of batches for the positive phase taken from the data.
- **neg\_batch\_size** (*int*) – The size of batches for the negative phase taken from the data. Defaults to *pos\_batch\_size*.
- **k** (*int*) – The number of contrastive divergence steps.
- **lr** (*float*) – Learning rate
- **input\_bases** (*np.array*) – The measurement bases for each sample. Must be provided if training a ComplexWaveFunction.
- **progbar** (*bool or str*) – Whether or not to display a progress bar. If “notebook” is passed, will use a Jupyter notebook compatible progress bar.
- **starting\_epoch** (*int*) – The epoch to start from. Useful if continuing training from a previous state.
- **callbacks** (*list [qucumber.callbacks.CallbackBase]*) – Callbacks to run while training.
- **optimizer** (*torch.optim.Optimizer*) – The constructor of a torch optimizer.
- **kwargs** – Keyword arguments to pass to the optimizer

**generate\_hilbert\_space** (*size=None*, *device=None*)

Generates Hilbert space of dimension  $2^{\text{size}}$ .

**Parameters**

- **size** (*int*) – The size of each element of the Hilbert space. Defaults to the number of visible units.
- **device** – The device to create the Hilbert space matrix on. Defaults to the device this model is on.

**Returns** A tensor with all the basis states of the Hilbert space.

**Return type** *torch.Tensor*

**gradient** (*basis, sample*)

Compute the gradient of a sample, measured in different bases.

**Parameters**

- **basis** (*np.array*) – A set of bases.
- **sample** (*np.array*) – A sample to compute the gradient of.

**Returns** A list of 2 tensors containing the parameters of each of the internal RBMs.

**Return type** `list[torch.Tensor]`

**load** (*location*)

Loads the WaveFunction parameters from the given location ignoring any metadata stored in the file. Overwrites the WaveFunction's parameters.

---

**Note:** The WaveFunction object on which this function is called must have the same parameter shapes as the one whose parameters are being loaded.

---

**Parameters** **location** (*str or file*) – The location to load the WaveFunction parameters from.

**max\_size**

Maximum size of the Hilbert space for full enumeration

**networks**

A list of the names of the internal RBMs.

**phase** (*v*)

Compute the phase of a given vector/matrix of visible states.

$$\text{phase}(\sigma) = -\mathcal{E}_{\mu}(\sigma)/2$$

**Parameters** **v** (*torch.Tensor*) – visible states  $\sigma$ .

**Returns** Vector containing the phases of the given states.

**Return type** `torch.Tensor`

**probability** (*v, Z*)

Evaluates the probability of the given vector(s) of visible states.

**Parameters**

- **v** (*torch.Tensor*) – The visible states.
- **Z** (*float*) – The partition function.

**Returns** The probability of the given vector(s) of visible units.

**Return type** `torch.Tensor`

**psi** (*v*)

Compute the (unnormalized) wavefunction of a given vector/matrix of visible states.

$$\psi_{\lambda\mu}(\sigma) = e^{-[\mathcal{E}_{\lambda}(\sigma) + i\mathcal{E}_{\mu}(\sigma)]/2}$$

**Parameters** **v** (*torch.Tensor*) – visible states  $\sigma$

**Returns** Complex object containing the value of the wavefunction for each visible state

**Return type** `torch.Tensor`

**rbm\_am**

The RBM to be used to learn the wavefunction amplitude.

**rbm\_ph**

RBM used to learn the wavefunction phase.

**reinitialize\_parameters** ()

Randomize the parameters of the internal RBMs.

**sample** (*k*, *num\_samples=1*, *initial\_state=None*, *overwrite=False*)

Performs *k* steps of Block Gibbs sampling. One step consists of sampling the hidden state  $h$  from the conditional distribution  $p_\lambda(h|v)$ , and sampling the visible state  $v$  from the conditional distribution  $p_\lambda(v|h)$ .

#### Parameters

- **k** (*int*) – Number of Block Gibbs steps.
- **num\_samples** (*int*) – The number of samples to generate.
- **initial\_state** (*torch.Tensor*) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (*bool*) – Whether to overwrite the *initial\_state* tensor, if it is provided.

**save** (*location*, *metadata=None*)

Saves the WaveFunction parameters to the given location along with any given metadata.

#### Parameters

- **location** (*str or file*) – The location to save the data.
- **metadata** (*dict*) – Any extra metadata to store alongside the WaveFunction parameters.

**stop\_training**

If *True*, will not train.

If this property is set to *True* during the training cycle, training will terminate once the current batch or epoch ends (depending on when *stop\_training* was set).

**subspace\_vector** (*num*, *size=None*, *device=None*)

Generates a single vector from the Hilbert space of dimension  $2^{\text{size}}$ .

#### Parameters

- **size** (*int*) – The size of each element of the Hilbert space.
- **num** (*int*) – The specific vector to return from the Hilbert space. Since the Hilbert space can be represented by the set of binary strings of length *size*, *num* is equivalent to the decimal representation of the returned vector.
- **device** – The device to create the vector on. Defaults to the device this model is on.

**Returns** A state from the Hilbert space.

**Return type** `torch.Tensor`

## 9.3 Abstract WaveFunction

---

**Note:** This is an Abstract Base Class, it is not meant to be used directly. The following API reference is mostly for developers.

---

**class** qucumber.nn\_states.WaveFunctionBase

Bases: `abc.ABC`

Abstract Base Class for WaveFunctions.

**amplitude** (*v*)

Compute the (unnormalized) amplitude of a given vector/matrix of visible states.

$$\text{amplitude}(\sigma) = |\psi(\sigma)|$$

**Parameters** *v* (`torch.Tensor`) – visible states  $\sigma$

**Returns** Matrix/vector containing the amplitudes of *v*

**Return type** `torch.Tensor`

**static autoload** (*location*, *gpu=False*)

Initializes a WaveFunction from the parameters in the given location.

**Parameters**

- **location** (*str or file*) – The location to load the model parameters from.
- **gpu** (*bool*) – Whether the returned model should be on the GPU.

**Returns** A new WaveFunction initialized from the given parameters. The returned WaveFunction will be of whichever type this function was called on.

**compute\_batch\_gradients** (*k*, *samples\_batch*, *neg\_batch*, *bases\_batch=None*)

Compute the gradients of a batch of the training data (*samples\_batch*).

If measurements are taken in bases other than the reference basis, a list of bases (*bases\_batch*) must also be provided.

**Parameters**

- **k** (*int*) – Number of contrastive divergence steps in training.
- **samples\_batch** (`torch.Tensor`) – Batch of the input samples.
- **neg\_batch** (`torch.Tensor`) – Batch of the input samples for computing the negative phase.
- **bases\_batch** (*np.array*) – Batch of the input bases corresponding to the samples in *samples\_batch*.

**Returns** List containing the gradients of the parameters.

**Return type** `list`

**compute\_normalization** (*space*)

Compute the normalization constant of the wavefunction.

$$Z_{\lambda} = \sqrt{\sum_{\sigma} |\psi_{\lambda\mu}|^2} = \sqrt{\sum_{\sigma} p_{\lambda}(\sigma)}$$

**Parameters** *space* (`torch.Tensor`) – A rank 2 tensor of the entire visible space.

**device**

The device that the model is on.

**fit** (*data*, *epochs*=100, *pos\_batch\_size*=100, *neg\_batch\_size*=None, *k*=1, *lr*=0.001, *input\_bases*=None, *progbar*=False, *starting\_epoch*=1, *time*=False, *callbacks*=None, *optimizer*=<class 'torch.optim.sgd.SGD'>, *\*\*kwargs*)  
 Train the WaveFunction.

#### Parameters

- **data** (*np.array*) – The training samples
- **epochs** (*int*) – The number of full training passes through the dataset. Technically, this specifies the index of the *last* training epoch, which is relevant if *starting\_epoch* is being set.
- **pos\_batch\_size** (*int*) – The size of batches for the positive phase taken from the data.
- **neg\_batch\_size** (*int*) – The size of batches for the negative phase taken from the data. Defaults to *pos\_batch\_size*.
- **k** (*int*) – The number of contrastive divergence steps.
- **lr** (*float*) – Learning rate
- **input\_bases** (*np.array*) – The measurement bases for each sample. Must be provided if training a ComplexWaveFunction.
- **progbar** (*bool* or *str*) – Whether or not to display a progress bar. If “notebook” is passed, will use a Jupyter notebook compatible progress bar.
- **starting\_epoch** (*int*) – The epoch to start from. Useful if continuing training from a previous state.
- **callbacks** (*list* [*qucumber.callbacks.CallbackBase*]) – Callbacks to run while training.
- **optimizer** (*torch.optim.Optimizer*) – The constructor of a torch optimizer.
- **kwargs** – Keyword arguments to pass to the optimizer

**generate\_hilbert\_space** (*size*=None, *device*=None)

Generates Hilbert space of dimension  $2^{\text{size}}$ .

#### Parameters

- **size** (*int*) – The size of each element of the Hilbert space. Defaults to the number of visible units.
- **device** – The device to create the Hilbert space matrix on. Defaults to the device this model is on.

**Returns** A tensor with all the basis states of the Hilbert space.

**Return type** *torch.Tensor*

**gradient** ()

Compute the gradient of a set of samples.

**load** (*location*)

Loads the WaveFunction parameters from the given location ignoring any metadata stored in the file. Overwrites the WaveFunction’s parameters.

---

**Note:** The WaveFunction object on which this function is called must have the same parameter shapes as the one who’s parameters are being loaded.

---

**Parameters** `location` (*str* or *file*) – The location to load the WaveFunction parameters from.

**max\_size**

Maximum size of the Hilbert space for full enumeration

**networks**

A list of the names of the internal RBMs.

**phase** (*v*)

Compute the phase of a given vector/matrix of visible states.

$\text{phase}(\sigma)$

**Parameters** `v` (*torch.Tensor*) – visible states  $\sigma$

**Returns** Matrix/vector containing the phases of `v`

**Return type** *torch.Tensor*

**probability** (*v*, *Z*)

Evaluates the probability of the given vector(s) of visible states.

**Parameters**

- `v` (*torch.Tensor*) – The visible states.
- `Z` (*float*) – The partition function.

**Returns** The probability of the given vector(s) of visible units.

**Return type** *torch.Tensor*

**psi** (*v*)

Compute the (unnormalized) wavefunction of a given vector/matrix of visible states.

$\psi(\sigma)$

**Parameters** `v` (*torch.Tensor*) – visible states  $\sigma$

**Returns** Complex object containing the value of the wavefunction for each visible state

**Return type** *torch.Tensor*

**rbm\_am**

The RBM to be used to learn the wavefunction amplitude.

**reinitialize\_parameters** ()

Randomize the parameters of the internal RBMs.

**sample** (*k*, *num\_samples=1*, *initial\_state=None*, *overwrite=False*)

Performs *k* steps of Block Gibbs sampling. One step consists of sampling the hidden state *h* from the conditional distribution  $p_{\lambda}(h|v)$ , and sampling the visible state *v* from the conditional distribution  $p_{\lambda}(v|h)$ .

**Parameters**

- `k` (*int*) – Number of Block Gibbs steps.
- `num_samples` (*int*) – The number of samples to generate.
- `initial_state` (*torch.Tensor*) – The initial state of the Markov Chain. If given, `num_samples` will be ignored.
- `overwrite` (*bool*) – Whether to overwrite the `initial_state` tensor, if it is provided.

**save** (*location*, *metadata=None*)

Saves the WaveFunction parameters to the given location along with any given metadata.

**Parameters**

- **location** (*str or file*) – The location to save the data.
- **metadata** (*dict*) – Any extra metadata to store alongside the WaveFunction parameters.

**stop\_training**

If *True*, will not train.

If this property is set to *True* during the training cycle, training will terminate once the current batch or epoch ends (depending on when *stop\_training* was set).

**subspace\_vector** (*num*, *size=None*, *device=None*)

Generates a single vector from the Hilbert space of dimension  $2^{\text{size}}$ .

**Parameters**

- **size** (*int*) – The size of each element of the Hilbert space.
- **num** (*int*) – The specific vector to return from the Hilbert space. Since the Hilbert space can be represented by the set of binary strings of length *size*, *num* is equivalent to the decimal representation of the returned vector.
- **device** – The device to create the vector on. Defaults to the device this model is on.

**Returns** A state from the Hilbert space.

**Return type** `torch.Tensor`



**class** `qucumber.callbacks.CallbackBase`

Base class for callbacks.

**on\_batch\_end** (*nn\_state*, *epoch*, *batch*)

Called at the end of each batch.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.
- **epoch** (*int*) – The current epoch.
- **batch** (*int*) – The current batch index.

**on\_batch\_start** (*nn\_state*, *epoch*, *batch*)

Called at the start of each batch.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.
- **epoch** (*int*) – The current epoch.
- **batch** (*int*) – The current batch index.

**on\_epoch\_end** (*nn\_state*, *epoch*)

Called at the end of each epoch.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.
- **epoch** (*int*) – The current epoch.

**on\_epoch\_start** (*nn\_state*, *epoch*)

Called at the start of each epoch.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.
- **epoch** (`int`) – The current epoch.

**on\_train\_end** (`nn_state`)

Called at the end of the training cycle.

**Parameters** **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.

**on\_train\_start** (`nn_state`)

Called at the start of the training cycle.

**Parameters** **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction being trained.

```
class qucumber.callbacks.LambdaCallback (on_train_start=None,      on_train_end=None,
                                         on_epoch_start=None,      on_epoch_end=None,
                                         on_batch_start=None, on_batch_end=None)
```

Class for creating simple callbacks.

This callback is constructed using the passed functions that will be called at the appropriate time.

#### Parameters

- **on\_train\_start** (*callable or None*) – A function to be called at the start of the training cycle. Must follow the same signature as `CallbackBase.on_train_start`.
- **on\_train\_end** (*callable or None*) – A function to be called at the end of the training cycle. Must follow the same signature as `CallbackBase.on_train_end`.
- **on\_epoch\_start** (*callable or None*) – A function to be called at the start of every epoch. Must follow the same signature as `CallbackBase.on_epoch_start`.
- **on\_epoch\_end** (*callable or None*) – A function to be called at the end of every epoch. Must follow the same signature as `CallbackBase.on_epoch_end`.
- **on\_batch\_start** (*callable or None*) – A function to be called at the start of every batch. Must follow the same signature as `CallbackBase.on_batch_start`.
- **on\_batch\_end** (*callable or None*) – A function to be called at the end of every batch. Must follow the same signature as `CallbackBase.on_batch_end`.

```
class qucumber.callbacks.ModelSaver (period, folder_path, file_name, save_initial=True, meta-
                                     data=None, metadata_only=False)
```

Callback which allows model parameters (along with some metadata) to be saved to disk at regular intervals.

This callback is called at the end of each epoch. If `save_initial` is `True`, will also be called at the start of the training cycle.

#### Parameters

- **period** (`int`) – Frequency of model saving (in epochs).
- **folder\_path** (`str`) – The directory in which to save the files
- **file\_name** (`str`) – The name of the output files. Should be a format string with one blank, which will be filled with either the epoch number or the word “initial”.
- **save\_initial** (`bool`) – Whether to save the initial parameters (and metadata).

- **metadata** (*callable or dict or None*) – The metadata to save to disk with the model parameters. Can be either a function or a dictionary. In the case of a function, it must take 2 arguments: the RBM being trained, and the current epoch number, and then return a dictionary containing the metadata to be saved.
- **metadata\_only** (*bool*) – Whether to save *only* the metadata to disk.

**class** qucumber.callbacks.Logger(*period*, *logger\_fn*=<built-in function print>, *msg\_gen*=None, *\*\*msg\_gen\_kwargs*)

Callback which logs output at regular intervals.

This callback is called at the end of each epoch.

#### Parameters

- **period** (*int*) – Logging frequency (in epochs).
- **logger\_fn** (*callable*) – The function used for logging. Must take 1 string as an argument. Defaults to the standard *print* function.
- **msg\_gen** (*callable*) – A callable which generates the string to be logged. Must take 2 positional arguments: the RBM being trained and the current epoch. It must also be able to take some keyword arguments.
- **\*\*kwargs** – Keyword arguments which will be passed to *msg\_gen*.

**class** qucumber.callbacks.EarlyStopping(*period*, *tolerance*, *patience*, *evaluator\_callback*, *quantity\_name*)

Stop training once the model stops improving. The specific criterion for stopping is:

$$\left| \frac{M_{t-p} - M_t}{M_{t-p}} \right| < \epsilon$$

where  $M_t$  is the metric value at the current evaluation (time  $t$ ),  $p$  is the “patience” parameter, and  $\epsilon$  is the tolerance.

This callback is called at the end of each epoch.

#### Parameters

- **period** (*int*) – Frequency with which the callback checks whether training has converged (in epochs).
- **tolerance** (*float*) – The maximum relative change required to consider training as having converged.
- **patience** (*int*) – How many intervals to wait before claiming the training has converged.
- **evaluator\_callback** (*MetricEvaluator or ObservableEvaluator*) – An instance of *MetricEvaluator* or *ObservableEvaluator* which computes the metric that we want to check for convergence.
- **quantity\_name** (*str*) – The name of the metric/observable stored in *evaluator\_callback*.

**class** qucumber.callbacks.VarianceBasedEarlyStopping(*period*, *tolerance*, *patience*, *evaluator\_callback*, *quantity\_name*, *variance\_name*)

Stop training once the model stops improving. This is a variation on the *EarlyStopping* class which takes the variance of the metric into account. The specific criterion for stopping is:

$$\left| \frac{M_{t-p} - M_t}{\sigma_{t-p}} \right| < \kappa$$

where  $M_t$  is the metric value at the current evaluation (time  $t$ ),  $p$  is the “patience” parameter,  $\sigma_t$  is the variance of the metric, and  $\kappa$  is the tolerance.

This callback is called at the end of each epoch.

#### Parameters

- **period** (*int*) – Frequency with which the callback checks whether training has converged (in epochs).
- **tolerance** (*float*) – The maximum (standardized) change required to consider training as having converged.
- **patience** (*int*) – How many intervals to wait before claiming the training has converged.
- **evaluator\_callback** (*MetricEvaluator* or *ObservableEvaluator*) – An instance of *MetricEvaluator* or *ObservableEvaluator* which computes the metric/observable that we want to check for convergence.
- **quantity\_name** (*str*) – The name of the metric/observable stored in *evaluator\_callback*.
- **variance\_name** (*str*) – The name of the variance stored in *evaluator\_callback*.

```
class qucumber.callbacks.MetricEvaluator(period, metrics, verbose=False, log=None,
                                         **metric_kwargs)
```

Evaluate and hold on to the results of the given metric(s).

This callback is called at the end of each epoch.

---

**Note:** Since callbacks are given to *fit* as a list, they will be called in a deterministic order. It is therefore recommended that instances of *MetricEvaluator* be among the first callbacks in the list passed to *fit*, as one would often use it in conjunction with other callbacks like *EarlyStopping* which may depend on *MetricEvaluator* having been called.

---

#### Parameters

- **period** (*int*) – Frequency with which the callback evaluates the given metric(s).
- **metrics** (*dict(str, callable)*) – A dictionary of callables where the keys are the names of the metrics and the callables take the WaveFunction being trained as their positional argument, along with some keyword arguments. The metrics are evaluated and put into an internal dictionary structure resembling the structure of *metrics*.
- **verbose** (*bool*) – Whether to print metrics to stdout.
- **log** (*str*) – A filepath to log metric values to in CSV format.
- **\*\*metric\_kwargs** – Keyword arguments to be passed to *metrics*.

```
__getattr__(metric)
```

Return an array of all recorded values of the given metric.

**Parameters** **metric** (*str*) – The metric to retrieve.

**Returns** The past values of the metric.

**Return type** *np.array*

```
__len__()
```

Return the number of timesteps that metrics have been evaluated for.

**Return type** *int*

**clear\_history()**

Delete all metric values the instance is currently storing.

**epochs**

Return a list of all epochs that have been recorded.

**Return type** np.array

**get\_value**(*name*, *index=None*)

Retrieve the value of the desired metric from the given timestep.

**Parameters**

- **name** (*str*) – The name of the metric to retrieve.
- **index** (*int* or *None*) – The index/timestep from which to retrieve the metric. Negative indices are supported. If None, will just get the most recent value.

**names**

The names of the tracked metrics.

**Return type** list[str]

**class** qucumber.callbacks.ObservableEvaluator(*period*, *observables*, *verbose=False*,  
*log=None*, *\*\*sampling\_kwargs*)

Evaluate and hold on to the results of the given observable(s).

This callback is called at the end of each epoch.

---

**Note:** Since callback are given to *fit* as a list, they will be called in a deterministic order. It is therefore recommended that instances of *ObservableEvaluator* be among the first callbacks in the list passed to *fit*, as one would often use it in conjunction with other callbacks like *EarlyStopping* which may depend on *ObservableEvaluator* having been called.

---

**Parameters**

- **period** (*int*) – Frequency with which the callback evaluates the given observables(s).
- **observables** (*list* (qucumber.observables.ObservableBase)) – A list of Observables. Observable statistics are evaluated by sampling the WaveFunction. Note that observables that have the same name will conflict, and precedence will be given to the right-most observable argument.
- **verbose** (*bool*) – Whether to print metrics to stdout.
- **log** (*str*) – A filepath to log metric values to in CSV format.
- **\*\*sampling\_kwargs** – Keyword arguments to be passed to *Observable.statistics*. Ex. *num\_samples*, *num\_chains*, *burn\_in*, *steps*.

**\_\_getattr\_\_**(*observable*)

Return an ObservableStatistics containing recorded statistics of the given observable.

**Parameters** **observable** (*str*) – The observable to retrieve.

**Returns** The past values of the observable.

**Return type** ObservableStatistics

**\_\_len\_\_**()

Return the number of timesteps that observables have been evaluated for.

**Return type** int

**clear\_history()**

Delete all statistics the instance is currently storing.

**epochs**

Return a list of all epochs that have been recorded.

**Return type** np.array

**get\_value**(*name*, *index=None*)

Retrieve the statistics of the desired observable from the given timestep.

**Parameters**

- **name** (*str*) – The name of the observable to retrieve.
- **index** (*int* or *None*) – The index/timestep from which to retrieve the observable. Negative indices are supported. If None, will just get the most recent value.

**names**

The names of the tracked observables.

**Return type** list[str]

**class** qucumber.callbacks.**LivePlotting**(*period*, *evaluator\_callback*, *quantity\_name*, *error\_name=None*, *total\_epochs=None*, *smooth=True*)

Plots metrics/observables.

This callback is called at the end of each epoch.

**Parameters**

- **period** (*int*) – Frequency with which the callback updates the plots (in epochs).
- **evaluator\_callback** (*MetricEvaluator* or *ObservableEvaluator*) – An instance of *MetricEvaluator* or *ObservableEvaluator* which computes the metric/observable that we want to plot.
- **quantity\_name** (*str*) – The name of the metric/observable stored in *evaluator\_callback*.
- **error\_name** (*str*) – The name of the error stored in *evaluator\_callback*.

**class** qucumber.callbacks.**Timer**(*verbose=True*)

Callback which records the training time.

This callback is always called at the start and end of training. It will run at the end of an epoch or batch if the given model's *stop\_training* property is set to True.

**Parameters** **verbose** (*bool*) – Whether to print the elapsed time at the end of training.

## 11.1 Pauli Operators

**class** `qucumber.observables.SigmaZ`

Bases: `qucumber.observables.ObservableBase`

The  $\sigma_z$  observable.

Computes the magnetization in the Z direction of a spin chain.

**apply** (*nn\_state*, *samples*)

Computes the magnetization of each sample given a batch of samples.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of samples to calculate the observable on. Must be using the  $\sigma_i = 0, 1$  convention.

**name**

The name of the Observable.

**sample** (*nn\_state*, *k*, *num\_samples=1*, *initial\_state=None*, *overwrite=False*)

Draws samples of the *observable* using the given WaveFunction.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **k** (`int`) – The number of Gibbs Steps to perform before drawing a sample.
- **num\_samples** (`int`) – The number of samples to draw.
- **initial\_state** (`torch.Tensor`) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.

- **overwrite** (*bool*) – Whether to overwrite the `initial_state` tensor, if it is provided, with the updated state of the Markov chain.

**statistics** (*nn\_state*, *num\_samples*, *num\_chains*=0, *burn\_in*=1000, *steps*=1)

Estimates the expected value, variance, and the standard error of the observable over the distribution defined by the WaveFunction.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **num\_samples** (*int*) – The number of samples to draw. The actual number of samples drawn may be slightly higher if `num_samples % num_chains != 0`.
- **num\_chains** (*int*) – The number of Markov chains to run in parallel; if 0, will use a number of chains equal to `num_samples`.
- **burn\_in** (*int*) – The number of Gibbs Steps to perform before recording any samples.
- **steps** (*int*) – The number of Gibbs Steps to take between each sample.

**Returns** A dictionary containing the (estimated) expected value (key: “mean”), variance (key: “variance”), and standard error (key: “std\_error”) of the observable.

**Return type** `dict(str, float)`

**statistics\_from\_samples** (*nn\_state*, *samples*)

Estimates the expected value, variance, and the standard error of the observable using the given samples.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of sample states to calculate the observable on.

**symbol**

The algebraic symbol representing the Observable.

**class** `qucumber.observables.SigmaX`

Bases: `qucumber.observables.ObservableBase`

The  $\sigma_x$  observable

Computes the magnetization in the X direction of a spin chain.

**apply** (*nn\_state*, *samples*)

Computes the magnetization along X of each sample in the given batch of samples.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of samples to calculate the observable on. Must be using the  $\sigma_i = 0, 1$  convention.

**name**

The name of the Observable.

**sample** (*nn\_state*, *k*, *num\_samples*=1, *initial\_state*=None, *overwrite*=False)

Draws samples of the *observable* using the given WaveFunction.

#### Parameters



- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **k** (`int`) – The number of Gibbs Steps to perform before drawing a sample.
- **num\_samples** (`int`) – The number of samples to draw.
- **initial\_state** (`torch.Tensor`) – The initial state of the Markov Chain. If given, `num_samples` will be ignored.
- **overwrite** (`bool`) – Whether to overwrite the initial\_state tensor, if it is provided, with the updated state of the Markov chain.

**statistics** (`nn_state, num_samples, num_chains=0, burn_in=1000, steps=1`)

Estimates the expected value, variance, and the standard error of the observable over the distribution defined by the WaveFunction.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **num\_samples** (`int`) – The number of samples to draw. The actual number of samples drawn may be slightly higher if `num_samples % num_chains != 0`.
- **num\_chains** (`int`) – The number of Markov chains to run in parallel; if 0, will use a number of chains equal to `num_samples`.
- **burn\_in** (`int`) – The number of Gibbs Steps to perform before recording any samples.
- **steps** (`int`) – The number of Gibbs Steps to take between each sample.

**Returns** A dictionary containing the (estimated) expected value (key: “mean”), variance (key: “variance”), and standard error (key: “std\_error”) of the observable.

**Return type** `dict(str, float)`

**statistics\_from\_samples** (`nn_state, samples`)

Estimates the expected value, variance, and the standard error of the observable using the given samples.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of sample states to calculate the observable on.

**symbol**

The algebraic symbol representing the Observable.

**class** `qucumber.observables.SigmaY`

Bases: `qucumber.observables.ObservableBase`

The  $\sigma_y$  observable

Computes the magnetization in the Y direction of a spin chain.

**apply** (`nn_state, samples`)

Computes the magnetization along Y of each sample in the given batch of samples.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.

- **samples** (*torch.Tensor*) – A batch of samples to calculate the observable on. Must be using the  $\sigma_i = 0, 1$  convention.

**name**

The name of the Observable.

**sample** (*nn\_state*, *k*, *num\_samples=1*, *initial\_state=None*, *overwrite=False*)

Draws samples of the *observable* using the given WaveFunction.

**Parameters**

- **nn\_state** (*qucumber.nn\_states.WaveFunctionBase*) – The WaveFunction to draw samples from.
- **k** (*int*) – The number of Gibbs Steps to perform before drawing a sample.
- **num\_samples** (*int*) – The number of samples to draw.
- **initial\_state** (*torch.Tensor*) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (*bool*) – Whether to overwrite the *initial\_state* tensor, if it is provided, with the updated state of the Markov chain.

**statistics** (*nn\_state*, *num\_samples*, *num\_chains=0*, *burn\_in=1000*, *steps=1*)

Estimates the expected value, variance, and the standard error of the observable over the distribution defined by the WaveFunction.

**Parameters**

- **nn\_state** (*qucumber.nn\_states.WaveFunctionBase*) – The WaveFunction to draw samples from.
- **num\_samples** (*int*) – The number of samples to draw. The actual number of samples drawn may be slightly higher if *num\_samples % num\_chains != 0*.
- **num\_chains** (*int*) – The number of Markov chains to run in parallel; if 0, will use a number of chains equal to *num\_samples*.
- **burn\_in** (*int*) – The number of Gibbs Steps to perform before recording any samples.
- **steps** (*int*) – The number of Gibbs Steps to take between each sample.

**Returns** A dictionary containing the (estimated) expected value (key: “mean”), variance (key: “variance”), and standard error (key: “std\_error”) of the observable.

**Return type** *dict(str, float)*

**statistics\_from\_samples** (*nn\_state*, *samples*)

Estimates the expected value, variance, and the standard error of the observable using the given samples.

**Parameters**

- **nn\_state** (*qucumber.nn\_states.WaveFunctionBase*) – The WaveFunction that drew the samples.
- **samples** (*torch.Tensor*) – A batch of sample states to calculate the observable on.

**symbol**

The algebraic symbol representing the Observable.

## 11.2 Neighbour Interactions

**class** qucumber.observables.NeighbourInteraction (*periodic\_bcs=False, c=1*)

Bases: `qucumber.observables.ObservableBase`

The  $\sigma_i^z \sigma_{i+c}^z$  observable

Computes the  $c$ -th nearest neighbour interaction for a spin chain with either open or periodic boundary conditions.

### Parameters

- **periodic\_bcs** (*bool*) – Specifies whether the system has periodic boundary conditions.
- **c** (*int*) – Interaction distance.

**apply** (*nn\_state, samples*)

Computes the energy of this neighbour interaction for each sample given a batch of samples.

### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of samples to calculate the observable on. Must be using the  $\sigma_i = 0, 1$  convention.

**name**

The name of the Observable.

**sample** (*nn\_state, k, num\_samples=1, initial\_state=None, overwrite=False*)

Draws samples of the *observable* using the given WaveFunction.

### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **k** (*int*) – The number of Gibbs Steps to perform before drawing a sample.
- **num\_samples** (*int*) – The number of samples to draw.
- **initial\_state** (`torch.Tensor`) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (*bool*) – Whether to overwrite the *initial\_state* tensor, if it is provided, with the updated state of the Markov chain.

**statistics** (*nn\_state, num\_samples, num\_chains=0, burn\_in=1000, steps=1*)

Estimates the expected value, variance, and the standard error of the observable over the distribution defined by the WaveFunction.

### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **num\_samples** (*int*) – The number of samples to draw. The actual number of samples drawn may be slightly higher if *num\_samples % num\_chains != 0*.
- **num\_chains** (*int*) – The number of Markov chains to run in parallel; if 0, will use a number of chains equal to *num\_samples*.
- **burn\_in** (*int*) – The number of Gibbs Steps to perform before recording any samples.

- **steps** (*int*) – The number of Gibbs Steps to take between each sample.

**Returns** A dictionary containing the (estimated) expected value (key: “mean”), variance (key: “variance”), and standard error (key: “std\_error”) of the observable.

**Return type** `dict(str, float)`

**statistics\_from\_samples** (*nn\_state, samples*)

Estimates the expected value, variance, and the standard error of the observable using the given samples.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of sample states to calculate the observable on.

**symbol**

The algebraic symbol representing the Observable.

## 11.3 Abstract Observable

---

**Note:** This is an Abstract Base Class, it is not meant to be used directly. The following API reference is mostly for developers.

---

**class** `qucumber.observables.ObservableBase`

Bases: `abc.ABC`

Base class for observables.

**apply** (*nn\_state, samples*)

Computes the value of the observable, row-wise, on a batch of samples. Must be implemented by any subclasses.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of sample states to calculate the observable on.

**name**

The name of the Observable.

**sample** (*nn\_state, k, num\_samples=1, initial\_state=None, overwrite=False*)

Draws samples of the *observable* using the given WaveFunction.

**Parameters**

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **k** (*int*) – The number of Gibbs Steps to perform before drawing a sample.
- **num\_samples** (*int*) – The number of samples to draw.
- **initial\_state** (`torch.Tensor`) – The initial state of the Markov Chain. If given, *num\_samples* will be ignored.
- **overwrite** (*bool*) – Whether to overwrite the *initial\_state* tensor, if it is provided, with the updated state of the Markov chain.

**statistics** (*nn\_state*, *num\_samples*, *num\_chains*=0, *burn\_in*=1000, *steps*=1)

Estimates the expected value, variance, and the standard error of the observable over the distribution defined by the WaveFunction.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction to draw samples from.
- **num\_samples** (*int*) – The number of samples to draw. The actual number of samples drawn may be slightly higher if *num\_samples % num\_chains != 0*.
- **num\_chains** (*int*) – The number of Markov chains to run in parallel; if 0, will use a number of chains equal to *num\_samples*.
- **burn\_in** (*int*) – The number of Gibbs Steps to perform before recording any samples.
- **steps** (*int*) – The number of Gibbs Steps to take between each sample.

**Returns** A dictionary containing the (estimated) expected value (key: “mean”), variance (key: “variance”), and standard error (key: “std\_error”) of the observable.

**Return type** `dict(str, float)`

**statistics\_from\_samples** (*nn\_state*, *samples*)

Estimates the expected value, variance, and the standard error of the observable using the given samples.

#### Parameters

- **nn\_state** (`qucumber.nn_states.WaveFunctionBase`) – The WaveFunction that drew the samples.
- **samples** (`torch.Tensor`) – A batch of sample states to calculate the observable on.

**symbol**

The algebraic symbol representing the Observable.



`qucumber.utils.cplx.absolute_value(x)`

Computes the complex absolute value elementwise.

**Parameters** `x` (*torch.Tensor*) – A complex tensor.

**Returns** A real tensor.

**Return type** *torch.Tensor*

`qucumber.utils.cplx.conjugate(x)`

A function that takes the conjugate transpose of the argument.

**Parameters** `x` (*torch.Tensor*) – A complex vector or matrix.

**Returns** The conjugate of `x`.

**Return type** *torch.Tensor*

`qucumber.utils.cplx.elementwise_division(x, y)`

Elementwise division of `x` by `y`.

**Parameters**

- `x` (*torch.Tensor*) – A complex tensor.
- `y` (*torch.Tensor*) – A complex tensor.

**Return type** *torch.Tensor*

`qucumber.utils.cplx.elementwise_mult(x, y)`

Alias for `scalar_mult()`.

`qucumber.utils.cplx.inner_prod(x, y)`

A function that returns the inner product of two complex vectors, `x` and `y` ( $\langle x|y \rangle$ ).

**Parameters**

- `x` (*torch.Tensor*) – A complex vector.
- `y` (*torch.Tensor*) – A complex vector.

**Raises** `ValueError` – If  $x$  and  $y$  are not complex vectors with their first dimensions being 2, then the function will not execute.

**Returns** The inner product,  $\langle x|y\rangle$ .

**Return type** `torch.Tensor`

`gucumber.utils.cplx.kronecker_prod(x, y)`

A function that returns the tensor / kronecker product of 2 complex tensors,  $x$  and  $y$ .

**Parameters**

- $\mathbf{x}$  (`torch.Tensor`) – A complex matrix.
- $\mathbf{y}$  (`torch.Tensor`) – A complex matrix.

**Raises** `ValueError` – If  $x$  and  $y$  do not have 3 dimensions or their first dimension is not 2, the function cannot execute.

**Returns** The tensorproduct of  $x$  and  $y$ ,  $x \otimes y$ .

**Return type** `torch.Tensor`

`gucumber.utils.cplx.make_complex(x, y=None)`

A function that combines the real ( $x$ ) and imaginary ( $y$ ) parts of a vector or a matrix.

---

**Note:**  $x$  and  $y$  must have the same shape. Also, this will not work for rank zero tensors.

---

**Parameters**

- $\mathbf{x}$  (`torch.Tensor`) – The real part
- $\mathbf{y}$  (`torch.Tensor`) – The imaginary part. Can be `None`, in which case, the resulting complex tensor will have imaginary part equal to zero.

**Returns** The tensor  $[x,y] = x + yi$ .

**Return type** `torch.Tensor`

`gucumber.utils.cplx.matmul(x, y)`

A function that computes complex matrix-matrix and matrix-vector products.

---

**Note:** If one wishes to do matrix-vector products, the vector must be the second argument ( $y$ ).

---

**Parameters**

- $\mathbf{x}$  (`torch.Tensor`) – A complex matrix.
- $\mathbf{y}$  (`torch.Tensor`) – A complex vector or matrix.

**Returns** The product between  $x$  and  $y$ .

**Return type** `torch.Tensor`

`gucumber.utils.cplx.norm(x)`

A function that returns the norm of the argument.

**Parameters**  $\mathbf{x}$  (`torch.Tensor`) – A complex scalar.

**Returns**  $|x|$ .



**Return type** `torch.Tensor`

`qucumber.utils.cplx.norm_sqr(x)`

A function that returns the squared norm of the argument.

**Parameters** `x` (`torch.Tensor`) – A complex scalar.

**Returns**  $|x|^2$ .

**Return type** `torch.Tensor`

`qucumber.utils.cplx.outer_prod(x, y)`

A function that returns the outer product of two complex vectors, x and y.

**Parameters**

- `x` (`torch.Tensor`) – A complex vector.
- `y` (`torch.Tensor`) – A complex vector.

**Raises** `ValueError` – If x and y are not complex vectors with their first dimensions being 2, then the function will not execute.

**Returns** The outer product between x and y,  $|x\rangle\langle y|$ .

**Return type** `torch.Tensor`

`qucumber.utils.cplx.scalar_divide(x, y)`

A function that computes the division of x by y.

**Parameters**

- `x` (`torch.Tensor`) – The numerator (a complex scalar, vector or matrix).
- `y` (`torch.Tensor`) – The denominator (a complex scalar).

**Returns**  $x / y$

**Return type** `torch.Tensor`

`qucumber.utils.cplx.scalar_mult(x, y, out=None)`

A function that computes the product between complex matrices and scalars, complex vectors and scalars or two complex scalars.

**Parameters**

- `x` (`torch.Tensor`) – A complex scalar, vector or matrix.
- `y` (`torch.Tensor`) – A complex scalar, vector or matrix.
- `z` (`torch.Tensor`) – The complex tensor to write the output to.
- `z` – A complex scalar, vector or matrix. Can be None, in which case, a new tensor is created and returned. Otherwise, the method overwrites z.

**Returns** The product between x and y. Either overwrites z, or returns a new tensor.

**Return type** `torch.Tensor`



`qucumber.utils.data.extract_refbasis_samples(train_samples, train_bases)`

Extract the reference basis samples from the data.

**Parameters**

- **train\_samples** (*numpy.array*) – The training samples.
- **train\_bases** (*numpy.array*) – The bases of the training samples.

**Returns** The samples in the data that are only in the reference basis.

**Return type** `torch.Tensor`

`qucumber.utils.data.load_data(tr_samples_path, tr_psi_path=None, tr_bases_path=None, bases_path=None)`

Load the data required for training.

**Parameters**

- **tr\_samples\_path** (*str*) – The path to the training data.
- **tr\_psi\_path** (*str*) – The path to the target/true wavefunction.
- **tr\_bases\_path** (*str*) – The path to the basis data.
- **bases\_path** (*str*) – The path to a file containing all possible bases used in the `tr_bases_path` file.

**Returns** A list of all input parameters.

**Return type** `list`



## CHAPTER 14

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