

```
[]: from google.colab import drive
drive.mount('mnt')

Mounted at mnt

[]: cd 'mnt/My Drive/DL_SDRG'

/content/mnt/My Drive/DL_SDRG

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

```
import tensorflow as tf
from matplotlib import pyplot
```

Background

The quantum Ising model is described by the following Hamiltonian:

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^x \sigma_j^x - \sum_i h_i \sigma_i^z, \quad (1)$$

A Hamiltonian, in general, measures the total energy of the system, serving as a concise description of the model. Here, the Ising model Hamiltonian describes the interaction of entangled particles on a hypercubic lattice (e.g., a grid in two dimensions). The indices i, j indicate two neighboring particles, and $\sigma_{i,j}^{x,z}$, indicates the spin along the x or z direction of the i th or j th particle. Further, $J_{ij} > 0$ is known as the coupling between particles i and j , aligning the spins, and h_i measures the strength of an external field applied to each particle. The solutions to this problem, namely the ways to optimize the particles arrangements to minimize the total energy, is highly nontrivial and falls under a broader class of optimization problems known as non-deterministic polynomial-time hard (NP-hard) problems.

The ground state of the RIM is conveniently determined by an efficient Strong Disorder Renormalization Group (SDRG) algorithm. During the SDRG method the largest local terms in the Hamiltonian are successively eliminated and new Hamiltonians are generated through perturbation calculation. The critical properties of the RIM are governed by an infinite disorder fixed point, in which the strength of disorder grows without limit during renormalization. Therefore, the SDRG results are %universal, i.e. independent of the original disorder distributions, as well as asymptotically exact in the vicinity of the critical point, which is indeed demonstrated both analytically and numerically. After decimating all degrees of freedom, the ground state of the RIM is found as a collection of independent ferromagnetic clusters of various sizes, each cluster being in a GHZ state $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\dots\uparrow\rangle + |\downarrow\downarrow\dots\downarrow\rangle)$.

The figure below visualizes the SDRG with each iteration.

The diagram illustrates the SDRG process in two iterations. In the first iteration, a pair of spins i and j with coupling J_{ij} is renormalized into a single effective spin with field $h'_i = h_i h_j / J_{ij}$. In the second iteration, a chain of three spins i , j , and k with couplings J_{ij} and J_{ik} is renormalized, with the J_{ik} bond crossed out, indicating it has been integrated out.

This project aims to explore and demonstrate the capability of machine learning applications for quantum mechanical treatments, namely the SDRG. Specifically, by training neural networks to learn the SDRG, it can not only demonstrate the ability of NNs to learn exotic physics, but since the SDRG is well understood, this can give insight toward the dynamics of NNs, and provide potential theoretical guarantees.

Generating Clusters

Below is the cluster-forming algorithm that was used for the SDRG:

```
In [ ]: def pbc(arr,i): # Gives the system periodic boundary conditions (PBC)
```

```
    id=np.arange(1,10)
    for index in range(1,10):
        id[index]=index
    return id
```

```
    chain=np.vstack((chain, np.array([[1/np.e,
return np.delete(chain, (0),axis=0)
```

```
clust_length): # Checks to see whether a cluster has a larger size  
# than the so-called 'largest_size'  
:  
:
```

```

largest_size = 0
largest_cluster = np.array([])
j=np.copy(coupling)
h=np.copy(field)
a=np.array([])
for i in range(np.size(j)):
    h[i,0]=np.log(h[i,0])
j=np.log(j)
size_j=np.size(j)
while size_j>2:
    for i in range(np.size(j)): # We cycle through each site in the system
        if i>np.size(j):
            break
        elif j[i]>h[i,0] and j[i]>pbc(h[:,0],i+1): # There are various conditions on h given the site i
            # and the coupling j. When the condition of each of
            # the proceeding if statements is satisfied, we make
            # a new cluster, join the site to an existing
            # cluster, or put an "empty" label (0) on the site
            # (so it is not in a cluster). When a cluster fully
            # forms, we check whether it is larger than the
            # variable 'largest_size' (initialized at 0), and
            # if so, then that cluster replaces the largest
            # cluster. In this way, we can output the final
            # result of 'largest_cluster.'
            max_index=i
            next_index=np.mod(i+1, np.size(j))
            h[next_index, 0] = h[max_index, 0]+h[next_index, 0]-j[max_index]
            h[next_index, 1] = np.sort(np.append(h[max_index, 1], h[next_index, 1]))
            h=np.delete(h, max_index, 0)
            j=np.delete(j, max_index)
        elif h[i,0]>j[i] and h[i,0]>pbc(j, i-1):
            max_index=i
            prev_index=np.mod(i-1, np.size(j))
            if np.size(h[max_index, 1])>1:
                clust_len = len(site_id(h[max_index, 1]))
                if clust_length_larger(largest_size, clust_len):
                    largest_cluster = site_id(h[max_index, 1])
                    largest_size = clust_len
                j[prev_index] = j[prev_index]+j[max_index]-h[max_index, 0]
            h=np.delete(h, max_index, 0)
            j=np.delete(j, max_index)
    size_j=np.size(j)
    if size_j==2:
        break

```

```

break

if np.max(h[:,0])>np.max(j):
    if np.size(h[np.argmax(h[:,0]),1])>1:
        clust_len = len(site_id(h[np.argmax(h[:,0]),1]))
        if clust_length_larger(largest_size, clust_len):
            largest_cluster = site_id(h[np.argmax(h[:,0]),1])
            largest_size = clust_len
h=np.delete(h, np.argmax(h[:,0]), 0)
if np.size(h[np.argmax(h[:,0]),1])>1:
    clust_len = len(site_id(h[np.argmax(h[:,0]),1]))
    if clust_length_larger(largest_size, clust_len):
        largest_cluster = site_id(h[np.argmax(h[:,0]),1])
        largest_size = clust_len

else:
    cluster_1=h[np.argmax(h[:,0]),1]
    h=np.delete(h, np.argmax(h[:,0]), 0)
    if np.size(np.sort(np.append(h[np.argmax(h[:,0]),1], cluster_1)))>1:
        clust_len = len(site_id(np.sort(np.append(h[np.argmax(h[:,0]),1], cluster_1))))
        if clust_length_larger(largest_size, clust_len):
            largest_cluster = site_id(np.sort(np.append(h[np.argmax(h[:,0]),1], cluster_1)))
            largest_size = clust_len
return largest_cluster

def site_id_to_array(site_ids, size): # Changes output from a condensed format to a readable array
arr = np.zeros((size))
for index in np.arange(1, len(site_ids)):
    site_ids[index] += site_ids[index - 1]
for site_id in site_ids:
    arr[site_id] = 1
return arr

```

Below is an example of a coupling and field at L=32 that generates a system called 'largest_clust_test.' Note that only the largest cluster is shown -- not every cluster.

```
    j_test, h_test=gen_chain(size_test)
j_test

]: array([0.10894029, 0.76193948, 0.26892573, 0
       0.37620774, 0.73348718, 0.92004969, 0
       0.97301634, 0.07612448, 0.48421457, 0
       0.27731709, 0.67146939, 0.80777123, 0
       0.2711859, 0.75858082, 0.70211352, 0
```



```
hist_csv_file = 'history64.csv'
with open(hist_csv_file, mode='w') as f:
    hist_df.to_csv(f)
!mkdir -p saved_model
model.save('saved_model/model64')

]:
```

```
j = np.loadtxt('data/128_j')
clust = np.loadtxt('data/128_arr')
X = np.array(j).reshape(j.shape[0], j.shape[1])
Y = np.array(clust).reshape(clust.shape[0], clust.shape[1])
model = Sequential()
model.add(Dense(8*2*2*2*2, activation='relu'))
model.add(Dense(16*2*2*2*2, activation='relu'))
model.add(Dense(64*2*2*2*2, activation='relu'))
model.add(Dense(256*2*2*2*2, activation='relu'))
model.add(Dense(32*2*2*2*2, activation='relu'))
model.add(Dense(8*2*2*2*2, activation='sigmoid'))
```

```
history = model.fit(X,
hist_df = pd.DataFrame()
hist_csv_file = 'histo'
with open(hist_csv_file, 'w') as f:
    hist_df.to_csv(f)
!mkdir -p saved_model
model.save('saved_model')
```

```
[]:  
j = np.loadtxt('data/128_j')  
clust = np.loadtxt('data/128_arr')  
X = np.array(j).reshape(j.shape[0], j.shape[1])  
Y = np.array(clust).reshape(clust.shape[0], clust.shape[1])  
model = Sequential()  
model.add(Dense(256, activation='relu'))  
model.add(Dense(512, activation='relu'))
```

```

model.add(Dense(512, activation='relu'))
model.add(Dense(256, activation='sigmoid'))
model.compile(loss='BinaryCrossentropy', optimizer='adam', metrics='MSE')
history = model.fit(X, Y, validation_split=0.2, epochs=50, batch_size=30, verbose=0)
hist_df = pd.DataFrame(history.history)
hist_csv_file = 'history128.csv'
with open(hist_csv_file, mode='w') as f:
    hist_df.to_csv(f)
!mkdir -p saved_model
model.save('saved_model/model128')

```

In [6]:

```

history = pd.read_csv('history8.csv')
training_loss_8 = history['loss'].to_numpy()
training_acc_8 = history['MSE'].to_numpy()
testing_loss_8 = history['val_loss'].to_numpy()
testing_acc_8 = history['val_MSE'].to_numpy()
history = pd.read_csv('history16.csv')
training_loss_16 = history['loss'].to_numpy()
training_acc_16 = history['MSE'].to_numpy()
testing_loss_16 = history['val_loss'].to_numpy()
testing_acc_16 = history['val_MSE'].to_numpy()
history = pd.read_csv('history32.csv')
training_loss_32 = history['loss'].to_numpy()
training_acc_32 = history['MSE'].to_numpy()
testing_loss_32 = history['val_loss'].to_numpy()
testing_acc_32 = history['val_MSE'].to_numpy()
history = pd.read_csv('history64.csv')
training_loss_64 = history['loss'].to_numpy()
training_acc_64 = history['MSE'].to_numpy()
testing_loss_64 = history['val_loss'].to_numpy()
testing_acc_64 = history['val_MSE'].to_numpy()
history = pd.read_csv('history128.csv')
training_loss_128 = history['loss'].to_numpy()
training_acc_128 = history['MSE'].to_numpy()
testing_loss_128 = history['val_loss'].to_numpy()
testing_acc_128 = history['val_MSE'].to_numpy()
history = pd.read_csv('history256.csv')
training_loss_256 = history['loss'].to_numpy()
training_acc_256 = history['MSE'].to_numpy()
testing_loss_256 = history['val_loss'].to_numpy()
testing_acc_256 = history['val_MSE'].to_numpy()

```

In [7]:

```

fig, axs = plt.subplots(nrows=1, ncols=2, figsize=(15, 5))

axs[0].set_title(f'Training Cost History')
axs[0].plot(np.array(range(50)), training_loss_8, 'b', marker = 'o', label='size 8')
axs[0].plot(np.array(range(50)), training_loss_16, 'g', marker = 'o', label='size 16')
axs[0].plot(np.array(range(50)), training_loss_32, 'r', marker = 'o', label='size 32')
axs[0].plot(np.array(range(50)), training_loss_64, 'c', marker = 'o', label='size 64')
axs[0].plot(np.array(range(50)), training_loss_128, 'm', marker = 'o', label='size 128')
axs[0].plot(np.array(range(50)), training_loss_256, 'y', marker = 'o', label='size 256')
axs[0].set_xlabel('Epoch')
axs[0].set_ylabel('BinaryCrossEntropy Loss')
axs[0].legend()

axs[1].set_title(f'Testing Cost History')
axs[1].plot(np.array(range(50)), testing_loss_8, 'b', marker = 'x', label='size 8')
axs[1].plot(np.array(range(50)), testing_loss_16, 'g', marker = 'x', label='size 16')
axs[1].plot(np.array(range(50)), testing_loss_32, 'r', marker = 'x', label='size 32')
axs[1].plot(np.array(range(50)), testing_loss_64, 'c', marker = 'x', label='size 64')
axs[1].plot(np.array(range(50)), testing_loss_128, 'm', marker = 'x', label='size 128')
axs[1].plot(np.array(range(50)), testing_loss_256, 'y', marker = 'x', label='size 256')
axs[1].set_xlabel('Epoch')
axs[1].set_ylabel('BinaryCrossEntropy Loss')
axs[1].legend()

```

Out[7]:

The figure consists of two side-by-side line plots. The left plot, titled 'Training Cost History', shows the training loss (BinaryCrossEntropy Loss) on the y-axis (ranging from 0.1 to 0.6) against the epoch number on the x-axis (ranging from 0 to 50). Six data series are plotted for different model sizes: size 8 (blue circles), size 16 (green crosses), size 32 (red diamonds), size 64 (cyan squares), size 128 (purple stars), and size 256 (yellow diamonds). All series show a downward trend, indicating that the loss is decreasing over time. The size 8 series starts at approximately 0.35 and ends at 0.12. The size 256 series starts highest at approximately 0.62 and ends at 0.40. The right plot, titled 'Testing Cost History', shows the testing loss (BinaryCrossEntropy Loss) on the y-axis (ranging from 0.2 to 1.0) against the epoch number on the x-axis (ranging from 0 to 50). The same six data series are plotted. All series show an upward trend, indicating that the loss is increasing over time. The size 8 series starts at approximately 0.28 and ends at 0.10. The size 256 series starts at approximately 0.65 and ends at 0.65.

In [8]:

```

fig, axs = plt.subplots(nrows=1, ncols=2, figsize=(15, 5))

axs[0].set_title(f'Training Metric History')
axs[0].plot(np.array(range(50)), training_acc_8, 'b', marker = 'o', label='size 8')
axs[0].plot(np.array(range(50)), training_acc_16, 'g', marker = 'o', label='size 16')
axs[0].plot(np.array(range(50)), training_acc_32, 'r', marker = 'o', label='size 32')
axs[0].plot(np.array(range(50)), training_acc_64, 'c', marker = 'o', label='size 64')
axs[0].plot(np.array(range(50)), training_acc_128, 'm', marker = 'o', label='size 128')
axs[0].plot(np.array(range(50)), training_acc_256, 'y', marker = 'o', label='size 256')
axs[0].set_xlabel('Epoch')
axs[0].set_ylabel('MSE')
axs[0].legend()

axs[1].set_title(f'Testing Metric History')
axs[1].plot(np.array(range(50)), testing_acc_8, 'b', marker = 'x', label='size 8')
axs[1].plot(np.array(range(50)), testing_acc_16, 'g', marker = 'x', label='size 16')
axs[1].plot(np.array(range(50)), testing_acc_32, 'r', marker = 'x', label='size 32')
axs[1].plot(np.array(range(50)), testing_acc_64, 'c', marker = 'x', label='size 64')
axs[1].plot(np.array(range(50)), testing_acc_128, 'm', marker = 'x', label='size 128')
axs[1].plot(np.array(range(50)), testing_acc_256, 'y', marker = 'x', label='size 256')
axs[1].set_xlabel('Epoch')
axs[1].set_ylabel('MSE')
axs[1].legend()

```

The figure consists of two side-by-side line plots. The left plot is titled "Training Metric History" and the right plot is titled "Testing Metric History". Both plots show the Mean Squared Error (MSE) on the y-axis against the number of epochs on the x-axis (ranging from 0 to 50). Six data series are plotted for different model sizes: size 8 (blue circles), size 16 (green squares), size 32 (red triangles), size 64 (cyan diamonds), size 128 (magenta crosses), and size 256 (yellow stars). In the training metric history plot, all sizes show a downward trend in MSE over time, with size 8 reaching the lowest error (~0.04) and size 256 reaching the highest (~0.19). In the testing metric history plot, the error plateaus after epoch 10. Size 8 has the lowest error (~0.05), while size 256 has the highest (~0.20).

Results

In *Table 1* and *Figure 1*, we show the average accuracy (accuracy = $1 - \frac{\text{number of misclassifications}}{\text{number of sites}}$) for 10,000 samples of the training set and 9,000 samples of the testing set (the entire testing set):

Table 1a: Average accuracy for the training and testing sets. As size increases, we see that the training and testing accuracies decrease. Also notice that the accuracies are very similar for L=256.

Table 1b: Average number of misclassifications per sample. Again we see a general increase with size, with the number of misclassifications being approximately equal between training and testing samples at L=256.

Average Accuracy

	Training Set (10000 samples)	Testing Set (9000 samples)
8	0.9683	0.9621
16	0.9598	0.9202
32	0.9621	0.8319
64	0.9668	0.7667
128	0.8102	0.7550
256	0.7145	0.7111

Average Number of Misclassifications / Sample

	Training Set (10000 samples)	Testing Set (9000 samples)
8	0.2540	0.3031
16	0.6436	1.2763
32	1.2135	5.3808
64	2.1230	14.9301
128	24.2969	31.3609
256	73.0961	73.9461

Figure 1a-f: Number of misclassifications for various sizes among the testing/training sets. Across all, the number of misclassifications is roughly uniform across all sites, indicating that **our models learned periodic boundary conditions** (i.e., we don't see a greater number of misclassifications near the ends of the systems). Additionally, the number of false negatives is approximately equal to the number of false positives.

The figure consists of four subplots arranged in a 2x2 grid. The top row shows stacked bar charts for testing data, and the bottom row shows stacked bar charts for training data. Each chart has 'Total Misclassifications' in dark purple at the bottom and 'False Negatives' in light purple at the top. The x-axis for all charts represents sites from 0 to 7. The y-axis for the top row ranges from 0 to 100, and for the bottom row from 0 to 400.

The figure consists of four subplots arranged in a 2x2 grid. The top row shows histograms of misclassification counts for testing and training sets. The bottom row shows stacked bar charts of misclassifications by site for testing and training sets.

- Top Left:** Histogram of misclassification counts for the testing set. The x-axis ranges from 0 to 60, and the y-axis ranges from 0 to 500. The distribution is highly skewed towards zero, with most sites having 0 or 1 misclassification.
- Top Right:** Histogram of misclassification counts for the training set. The x-axis ranges from 0 to 60, and the y-axis ranges from 0 to 100. Similar to the testing set, it shows a high frequency of 0 misclassifications.
- Bottom Left:** Stacked bar chart titled "L=256: Misclassifications by Site (Testing)". The x-axis lists sites from 0 to 60. The y-axis ranges from 0 to 2500. The total misclassification count (dark purple) fluctuates between approximately 2000 and 3000 across sites. The false negative count (light purple) is consistently around 1400-1500.
- Bottom Right:** Stacked bar chart titled "L=256: Misclassifications by Site (Training)". The x-axis lists sites from 0 to 60. The y-axis ranges from 0 to 3000. The total misclassification count (dark purple) fluctuates between approximately 2500 and 3000 across sites. The false negative count (light purple) is consistently around 1500-1600.

The figure consists of four subplots arranged in a 2x2 grid, each showing a comparison between 'Sample' (blue bars) and 'Predicted Output' (red bars). The top row corresponds to $L=32$ and the bottom row to $L=64$. The left column shows the distribution for indices 0 to 6, while the right column shows it for indices 0.0 to 15.0. In all cases, the red bars closely match the blue bars, indicating high model accuracy. The y-axis for the top row ranges from 0.0 to 0.6, and for the bottom row from 0.0 to 1.0.

Figure 5a-b: Misclassification analysis on a training set sample at L=64. We see general agreement between model and system except for an obvious incorrect prediction of a cluster around site 60. Accuracy: 84.4%

The misclassification analysis of *Figure 5b* demonstrates that the predicted output can be interpreted as the probability that a 1 exists at a particular site. Below we perform this analysis for several training and testing samples at $L=128$ and $L=256$ (where the accuracy of the prediction is expected to be much lower than for smaller sizes, see *Table 1a-b*).

Figure 6a-b: A training sample at size $L=128$. Notice that the predicted output can be interpreted as a smooth approximation of the actual system. Also, we see that the most disagreement tends to occur near the boundaries of clusters (this is generally found to be the case). Accuracy: 76.6%

L=128: Sample vs. Predicted Output

L=128: Correct and Incorrect Predictions

The figure consists of two side-by-side bar charts. The left chart has a y-axis from 0.0 to 0.6 and an x-axis from 0 to 120. It contains two series: 'Sample' (blue bars) and 'Predicted Output' (red bars). The right chart has a y-axis from 0.0 to 0.4 and an x-axis from 0 to 120. It contains two series: 'Correct' (light blue bars) and 'Misclassification' (red bars).

Figure 7a-b: A testing sample at size $L=128$. Notice that the spikes in the predicted output around sites 60-80 and 120 do not meet the 0.5 threshold to be considered misclassifications (i.e., they are rounded down to 0). Accuracy: 93.0%

L=128: Sample vs. Predicted Output

A zoomed-in plot of the Sample vs. Predicted Output for $L=128$. The x-axis is labeled 'Site' and ranges from 55 to 75. The y-axis ranges from 0.0 to 1.0. Blue bars represent the Sample, and red bars represent the Predicted Output. There are several sharp peaks in both series, notably around site 60 where the predicted output reaches nearly 1.0.

L=128: Correct and Incorrect Predictions

A zoomed-in plot of the Correct and Incorrect Predictions for $L=128$. The x-axis is labeled 'Site' and ranges from 55 to 75. The y-axis ranges from 0.0 to 1.0. Light blue bars represent 'Correct' predictions, and red bars represent 'Misclassification'. A prominent peak in the light blue bars occurs around site 60, reaching a value slightly above 1.0.

The figure consists of two side-by-side bar charts. The left chart, titled 'L=256: Sample vs. Predicted Output', compares 'Sample' (blue bars) and 'Predicted Output' (red bars) across 256 samples. The y-axis ranges from 0.0 to 1.0. Both series show high accuracy, with most values near 1.0. The right chart, titled 'L=256: Correct and Incorrect Predictions', compares 'Correct' (blue bars) and 'Misclassification' (red bars). A horizontal line at y=0.5 indicates chance level. The 'Correct' series shows high accuracy, peaking around 0.85, while the 'Misclassification' series shows lower accuracy, peaking around 0.8.

Figure 10a-b consists of two side-by-side bar charts. Both charts have an x-axis ranging from 0 to 250. A horizontal line is drawn across both charts at y=0.5.

- Chart 10a: Sample vs. Predicted Output (Testing)**
- Chart 10b: Correct and Incorrect Predictions (Testing)**

The figure consists of two side-by-side bar charts. Both charts have a y-axis ranging from 0.0 to 0.2 and an x-axis labeled with numerical ticks at 0, 50, 100, 150, 200, and 250. The left chart features red bars. It has a very low baseline, followed by a small peak at bin 100 (~0.25), a larger peak at bin 150 (~0.2), and a final smaller peak at bin 250 (~0.15). The right chart features blue bars. It also has a very low baseline, but shows three distinct peaks: one at bin 100 (~0.2), another at bin 150 (~0.2), and a third at bin 200 (~0.2).

Conclusions and Next Steps

We demonstrated the ability to use deep learning to gain meaningful results about SDRG systems. In fact, even naive architectures (FCNNs) are able to demonstrate good results. Next steps would include allocating more computational resources toward larger sizes, such as increasing the number of layers, neurons, and epochs. We expect better convergence for training and testing costs and metrics.

Also, we tend to see misclassifications around the edges of clusters, so using different activation functions, such as the hard-sigmoid would be a logical next step in improving our current models.

Additional analytic work should be studied. Specifically, since the SDRG is well studied, comparing the weights of each neuron to that of the SDRG will give insight on the dynamics of FCNNs. An intuitive place to start is to have the same number of layers and neurons as the number of SDRG steps and remaining sites, and see if the two algorithms behave similarly.

More exotic neural networks should also be explored. Specifically, there is a natural connection between neural networks and

