# Machine Learning Applied to Multi-Electron Events in Scintillator

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This repository contains much more documentation and source code files related to this project.

### 1 Introduction

This *Jupyter* notebook serves as an interactive document and compilation of all the successful work that has gone into this machine learning project provided to Morten's theory group by the experimentalist, Sean Liddick. I provide a quick introduction to the problem for context, however for more material on this please go here.

The classical picture of spherical nuclei is far from the reality of the true nuclear structure. Shape coexistence is a nuclear phenomenon, where the nucleus exists in two stable shapes at the same excitation energy [1]. Nuclear properties provide unique information on the impetuses that foster changes to the nuclear structure of rare isotopes. In some neutron-rich nuclei,  $0^+$  states are predicted to exhibit shape coexistence. Therefore they are compelling to study, but experimentally challenging [2]. At low energies, where the only energetically allowed decay mode is  $0^+ \rightarrow 0^+$ , conversion electron spectroscopy is the only viable technique to probe their properties.

Sean Liddick's group employs conversion electron spectroscopy to study these transition rates. When a neutron-rich nucleus beta decays, a neutron transforms into a proton and emits an electron ( $\beta$ ). The excited nucleus can then interact electromagnetically with the surrounding orbital electrons. This can result in the ejection of an internal conversion electron ( $e^-$ ) from the atom [3]. Because this process is essentially simultaneous in time, it is pivotal to differentiate between the electron ( $\beta$ ) emitted from the nucleus and the internal conversion electron ( $e^-$ ) emitted from the atom.

This project attempts to use supervised machine learning algorithms as a means to distinguish between one and two electron events and predict the electron(s) corresponding initial position(s) in a scintillator.

**Note**: This notebook has the following dependencies: needs electron data ('BetaScint2DEnergy.csv' and 'BetaScint2DEnergyElectron.csv') and ProcessingData.py, which contains functions used throughout this notebook. The ProcessingData library can be found here.

### 2 Electron Events

We want to (i.) distinguish between one and two electron events and (ii.) predict the origin(s) of the electron(s) from within the scintillator. Let us begin by noticing the difference between a one and two electron event to further understand the problem at hand.

```
In [2]: # Load electorn data files
    import sys
    sys.path.append('/Users/harrisonlabollita/Library/Mobile Documents/com~apple~CloudDocs/Mimport ProcessingData as data
    filename_1 = '/Users/harrisonlabollita/Library/Mobile Documents/com~apple~CloudDocs/MSU
    filename_2 = '/Users/harrisonlabollita/Library/Mobile Documents/com~apple~CloudDocs/MSU
    grid_1, outputs_1 = data.get_data(filename_1)
    grid_2, outputs_2 = data.get_data(filename_2)
    print('Finished loading data!')
```

Finished loading data!

### 2.1 One and Two Electron events

Below are the different kinds of events that we would like to use supervised machine learning to distinguish between. We also need to train our algorithms to predict where the electron(s) started from within the scintillator. This is denoted by a red circle(s) on the plots.

```
In [14]: import matplotlib.pyplot as plt
         fig, ax = plt.subplots(2,3, figsize = (15,15))
         ax[0,0].imshow(grid_1[0], cmap='BuGn', origin = 'lower')
         ax[0,0].scatter((outputs_1[0][1])/3 + 8, (outputs_1[0][2])/3 + 8, c = 'r', s=100, marketer((outputs_1[0][1])/3 + 8)
         ax[0,0].axes.get_xaxis().set_visible(False)
         ax[0,0].axes.get_yaxis().set_visible(False)
         ax[0,1].set_title('ONE ELECTRON EVENTS', fontsize = 20)
         ax[0,1].imshow(grid_1[8500], cmap='BuGn', origin = 'lower')
         ax[0,1].scatter((outputs_1[8500][1])/3 + 8, (outputs_1[8500][2])/3 + 8, c = 'r', s=100,
         ax[0,1].axes.get_xaxis().set_visible(False)
         ax[0,1].axes.get_yaxis().set_visible(False)
         ax[0,2].imshow(grid_1[290118], cmap='BuGn', origin = 'lower')
         ax[0,2].scatter((outputs_1[290118][1])/3 + 8, (outputs_1[290118][2])/3 + 8, c = 'r', s=
         ax[0,2].axes.get_xaxis().set_visible(False)
         ax[0,2].axes.get_yaxis().set_visible(False)
         ax[1,0].imshow(grid_2[0], cmap='BuGn', origin = 'lower')
         ax[1,0].scatter((outputs_2[0][1])/3 + 8, (outputs_2[0][2])/3 + 8, c = 'r', s=100, marketer((outputs_2[0][1])/3 + 8)
         ax[1,0].scatter((outputs_2[0][4])/3 + 8, (outputs_2[0][5])/3 + 8, c = 'r', s=100, marketer((outputs_2[0][4])/3 + 8)
         ax[1,0].axes.get_xaxis().set_visible(False)
         ax[1,0].axes.get_yaxis().set_visible(False)
```

```
ax[1,1].set_title('TWO ELECTRON EVENTS', fontsize = 20)
ax[1,1].imshow(grid_2[15], cmap='BuGn', origin = 'lower')
ax[1,1].scatter((outputs_2[15][1])/3 + 8, (outputs_2[15][2])/3 + 8, c = 'r', s=100, max_{scatter}((outputs_2[15][1])/3 + 8)
ax[1,1].scatter((outputs_2[15][4])/3 + 8, (outputs_2[15][5])/3 + 8, c = 'r', s=100, max_{scatter}((outputs_2[15][4])/3 + 8)
ax[1,1].axes.get_xaxis().set_visible(False)
ax[1,1].axes.get_yaxis().set_visible(False)
ax[1,2].imshow(grid_2[75], cmap='BuGn', origin = 'lower')
ax[1,2].scatter((outputs_2[75][1])/3 + 8, (outputs_2[75][2])/3 + 8, c = 'r', s=100, max_{scatter}((outputs_2[75][1])/3 + 8)
ax[1,2].scatter((outputs_2[75][4])/3 + 8, (outputs_2[75][5])/3 + 8, c = 'r', s=100, max
ax[1,2].axes.get_xaxis().set_visible(False)
ax[1,2].axes.get_yaxis().set_visible(False)
plt.show()
                         ONE ELECTRON EVENTS
                         TWO ELECTRON EVENTS
```

After performing extensive data analyses, we gained valuable insight into the problem at hand. The first piece of information is that 70% of the electrons in the one-electorn case start in the pixel with the highest energy. It was also found that 100% of the time if the electron does not start in

the pixel with the highest energy deposited, it started in a neighboring pixel to the one with the highest energy. For the two electron cases, we decided that an event that looked like the one on the far left would be an "easy" two electron event, because it is trivial. We deemed events that looked like the remaining two electron events as "hard". We found that only 15% of the entire two electron data set was made of "hard" cases. This gave us a good idea of how well our machine learning algorithms should perform.

The Python scripts that produce these metrics can be found in the GitHub repository linked here. The files are labeled *electron\_densities.py* and *sort\_hard\_and\_easy.py* 

## 3 Convolutional Neural Networks

We chose to use convolutional neural networks to combat our problem. Convolutional neural networks (CNN) are a class of deep neural networks optimized for analyzing images. CNNs provide the computer with the ability to see. This will allow us to treat each scintillator event as a visual image, so the computer can see where the electron by looking at all of the non-zero pixels. For more information on convoluational neural networks, see here. We developed our CNN architectures in Keras, which is a Python deep learning library.

### 3.1 Single - Electron Model

The first CNN architecture is designed to predict where the electron started from in the one-electron case. Our input data is the entire scintillator, which is a  $16 \times 16$  matrix, where non-zero matrix elements correspond to the amount of energy that was deposited into that pixel on the scintillator.

We begin by creating two mutually exclusive datasets. Our training set will be one-third of the  $10^6$  single electron events we have avaliable. Our testing set or validation set is of size 20000.

Training set size: 333333 Testing set size: 20000

### 3.1.1 Build Network

Here we define a function that will contain our CNN. Its inputs will be the training and testing datasets, as well as, the number of epochs.

```
In [19]: # BUILD NETWORK
         import keras
         from keras.models import Sequential
         from keras.layers import Dense, Dropout, Flatten
         from keras.layers import Conv2D, MaxPooling2D
         def Model(x_train, y_train, x_test, y_test, epochs):
             batch_size = 128
             epochs = epochs
             model = Sequential()
             model.add(Conv2D(32, kernel_size=(3,3), activation = 'relu', input_shape= (16,16,1)
             model.add(Flatten())
             model.add(Dense(512, input_dim = 100, activation = 'relu'))
             model.add(Dense(2, activation='linear'))
             model.compile(loss= 'mse', optimizer='adam', metrics = ['accuracy'])
             history = model.fit(x_train, y_train,
                     batch_size= batch_size,
                     epochs = epochs,
                     verbose = 1, validation_data = (x_test, y_test))
             model.summary()
             return model, history
```

/anaconda3/lib/python3.6/site-packages/h5py/\_\_init\_\_.py:36: FutureWarning: Conversion of the sec from .\_conv import register\_converters as \_register\_converters Using TensorFlow backend.

### 3.1.2 Train Network

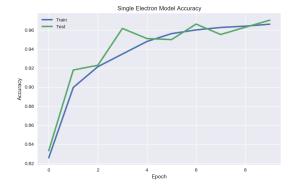
```
Epoch 4/10
Epoch 5/10
Epoch 6/10
Epoch 7/10
Epoch 8/10
Epoch 9/10
Epoch 10/10
Layer (type) Output Shape
              Param #
______
conv2d_1 (Conv2D)
       (None, 14, 14, 32)
              320
_____
flatten_1 (Flatten) (None, 6272)
_____
dense_1 (Dense)
       (None, 512)
              3211776
_____
dense_2 (Dense) (None, 2)
              1026
Total params: 3,213,122
Trainable params: 3,213,122
Non-trainable params: 0
```

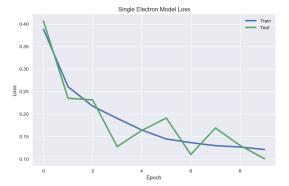
### 3.1.3 Performance History

Plot the accuracy and loss during training and testing over the ten epochs

```
In [92]: plt.style.use('seaborn')
    fig, ax = plt.subplots(1,2)
    ax[0].plot(history.history['acc'], linewidth = 3, label = 'Train')
    ax[0].plot(history.history['val_acc'], linewidth = 3, label = 'Test')
    ax[0].set_title('Single Electron Model Accuracy')
    ax[0].set_xlabel('Epoch')
    ax[0].set_ylabel('Accuracy')
    ax[0].legend(loc = 'best')
    ax[1].plot(history.history['loss'], linewidth = 3, label = 'Train')
    ax[1].plot(history.history['val_loss'], linewidth = 3, label = 'Test')
    ax[1].set_title('Single Electron Model Loss')
    ax[1].set_xlabel('Epoch')
    ax[1].set_ylabel('Loss')
```

```
ax[1].legend(loc = 'best')
fig.subplots_adjust(right = 2)
plt.show()
```





### 3.1.4 Predictions

We use our model to make predictions on the testing set. The model is predicting  $(x_0, y_0)$  of the electron for a given event.

```
In [23]: prediction = model.predict(x_test)
```

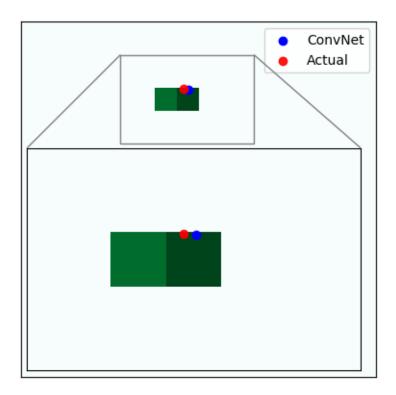
### 3.1.5 Example

Below is an example of our model's predictive capabilites. The blue dot is our model's prediction and the red dot is the actual prediction of the electron.

```
In [29]: plt.style.use('default')
                                               from mpl_toolkits.axes_grid1.inset_locator import zoomed_inset_axes
                                               fig, ax = plt.subplots()
                                               axins = zoomed_inset_axes(ax, 2.5, loc=3)
                                               ax.imshow(grid_1[500001], cmap='BuGn', origin = 'lower')
                                               ax.scatter((prediction[1][0])/3 + 8, (prediction[1][1])/3 + 8, c = 'blue', label = 'Converge or converge or conv
                                               ax.scatter((y_test[1][0])/3 + 8, (y_test[1][1])/3 + 8, c = 'r', alpha = 0.9, label = 'According to the state of the stat
                                               axins.imshow(grid_1[500001], cmap='BuGn', origin = 'lower')
                                               axins.scatter((prediction[1][0])/3 + 8, (prediction[1][1])/3 + 8, c = \frac{blue}{a}, label = \frac{c}{a}
                                               axins.scatter((y_test[1][0])/3 + 8, (y_test[1][1])/3 + 8, c = 'r', alpha =0.9, label =
                                               ax.axes.get_xaxis().set_visible(False)
                                               ax.axes.get_yaxis().set_visible(False)
                                               ax.legend(loc = 'best')
                                               x1, x2, y1, y2 = 4,10,10,14
                                               axins.set_xlim(x1, x2)
                                               axins.set_ylim(y1, y2)
                                               from mpl_toolkits.axes_grid1.inset_locator import mark_inset
                                               mark_inset(ax, axins, loc1=2, loc2=1, fc="none", ec="0.5")
```

axins.axes.get\_xaxis().set\_visible(False)

```
axins.axes.get_yaxis().set_visible(False)
#plt.savefig('ConvNet_prediction.png')
plt.show()
print('For this example, our prediction was %f mm away from the actual origin ' %(data.
```



For this example, our prediction was 0.640723 mm away from the actual origin

### 3.1.6 Single-Electron Model vs. Random Guessing

It is imperative to determine if our model is actually learning something during training. So to test this we have developed a random guesser that randomly guesses a point in the pixel with the highest energy. We have chosen this assumption, because we have shown that the electron starts in the pixel with the highest energy 70% of the time. Therefore without machine learning, a person could randomly guess a point inside of this pixel and be relatively close to the starting location of the electron most of the time.

We begin by finding the error, i.e. the distances between the predicted points/random guesses and the actual points.

```
In [32]: sys.path.append('/Users/harrisonlabollita/Library/Mobile Documents/com~apple~CloudDocs/
    import setup_electron_densities as setup
    # MODEL ERRORS
    errors = []
```

```
for i in range(len(prediction)):
    error = data.distance_formula(prediction[i][0], prediction[i][1], y_test[i][0], y_t
    errors.append(error)
# RANDOM GUESS
random_answers = outputs_1[:20000]
starting_pixels = setup.starting_pixels()
ranges = setup.ranges()
pixels = data.find_starting_pixel(random_answers)
x_predictions = []
y_predictions = []
for i in range(len(pixels)):
    n = int(pixels[i])
   pixel = starting_pixels[n]
    xmin = ranges[n][0][0]
    xmax = ranges[n][0][1]
    ymin = ranges[n][1][0]
    ymax = ranges[n][1][1]
    x_predict = np.random.randint(xmin, xmax) + np.random.rand()
    y_predict = np.random.randint(ymin, ymax) + np.random.rand()
    while xmax < x_predict < xmin and ymax < ypredict < ymin:
        x_predict = np.random.randint(xmin, xmax) + np.random.rand()
        y_predict = np.random.randint(ymin, ymax) + np.random.rand()
    x_predictions.append(x_predict)
    y_predictions.append(y_predict)
random_errors = []
for i in range(len(random_answers)):
    error = data.distance_formula(x_predictions[i], y_predictions[i], random_answers[i]
    random_errors.append(error)
```

### 3.1.7 Error Plots

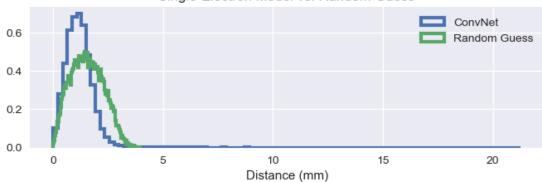
The following plots were generated:

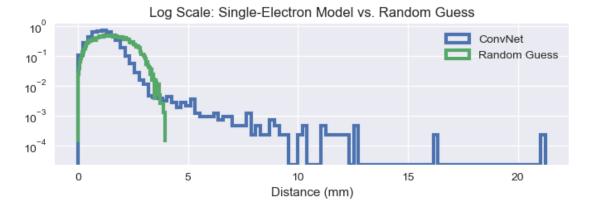
- 1. Histogram plot of the error between the predicted/random guess value and the actual value.
- 2. Log-y histrogram plot showing the our model's "bad" predictions
- 3. A zoomed histrogram plot restricting the x-axis is 0 to 3mm

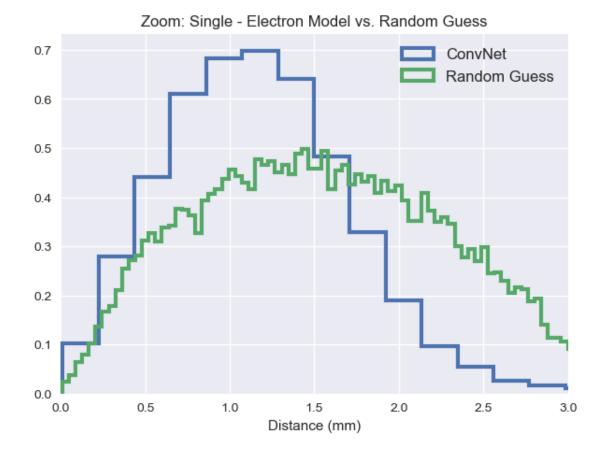
```
In [33]: plt.style.use('seaborn')
    fig, (ax1,ax3) = plt.subplots(2, 1)
    ax1.set_title('Single-Electron Model vs. Random Guess')
    ax1.hist(errors, bins = 100, histtype = 'step', normed = True, linewidth = 3, label = '
    ax1.hist(random_errors, bins = 100, histtype = 'step', normed = True, linewidth = 3, la
    ax1.legend(loc = 'best', fontsize = 10)
    ax1.set_xlabel('Distance (mm)')
```

```
ax3.set_title('Log Scale: Single-Electron Model vs. Random Guess')
ax3.hist(errors, bins = 100, histtype = 'step', log =True, normed = True, linewidth = 3
ax3.hist(random_errors, bins = 100, histtype = 'step', log = True, normed = True, linew
ax3.legend(loc = 'best', fontsize = 10)
ax3.set_xlabel('Distance (mm)')
plt.subplots_adjust(hspace = 0.5)
#plt.savefig('Norm and Log Single-Electron Model vs Random Guess.png')
plt.show()
fig, ax = plt.subplots(figsize = (7,5))
ax.set_title('Zoom: Single - Electron Model vs. Random Guess')
ax.hist(errors, bins = 100, histtype = 'step', normed = True, linewidth = 3, label = 'C
ax.hist(random_errors, bins = 100, histtype = 'step', normed = True, linewidth = 3, lab
ax.set_xlim([0,3])
ax.legend(fontsize = 12)
ax.set_xlabel('Distance (mm)')
#plt.savefig('Zoom: Single-Electron Model vs Random Guess.png',bbox_inches = 'tight')
plt.show()
```

### Single-Electron Model vs. Random Guess







Our model's error was less than the mean of the random guessing algorithm 77% of the time. This metric was calculated below.

76.385000 percent of ConvNet is to the left of the mean 1.555133 of our random guess.

### 3.1.8 Metrics

This is a table providing some metrics for our model. We have the average distance between the actual value and predicted, as well, as the minimum and maximum differences. We are also showing the  $90^{th}$ ,  $95^{th}$ , and  $99^{th}$  percentiles. *Note*: All metrics are in millimeters (mm).

Method	Average	Min	Max	90%	95%	99%
Single Electron Model	1.2117	0.011	21.253	1.900	2.165	3.293

Method	Average	Min	Max	90%	95%	99%
Random Guessing	1.555	0.008	3.944	2.574	2.805	3.218

### 3.2 Multi - Event Model

The second CNN architecture that we developed is to solve the catergorization problem. For a given event we would like to train our model to correctly identify whether the event was a one or two electron event.

We begin by creating a new dataset that contains both one and two electron events. We do this by randomly picking an event from each individual dataset depending if the random number generated is greater than 0.5. We have labeled the dataset such that a single electron event has label 0 and a one electron event has label 1. (The inconvenience is due to a subtlety in the Keras packages, so we will just have to deal with it.) Our total dataset will contain 200000 events. We will then separate this into mutually exclusive sets for training and testing.

```
In [43]: # CREATE DATASET FROM ONE AND TWO ELECTRON DATA SIZE: 200000 EVENTS
    data = []
    answers = []
    i = 0
    while len(data) < 2000000:
        num = np.random.rand()
        if num > 0.5:
            data.append(grid_1[i])
            answers.append(0)
        else:
            data.append(grid_2[i])
            answers.append(1)
        i +=1

    data = np.array(data)/3060. # Normalize the dataset
```

### 3.2.1 Build Network

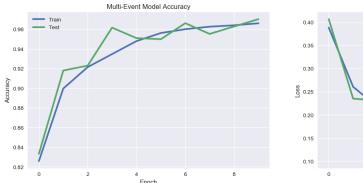
```
y_train = keras.utils.to_categorical(y_train, num_classes)
         y_test = keras.utils.to_categorical(y_test, num_classes)
         # DEFINE CNN MODEL
         def Model(x_train, y_train, x_test, y_test, epochs):
             batch_size = 128
             epochs = epochs
             num_classes = 2 # 0 for one electron event, 1 for two electron event
             model = Sequential()
             model.add(Conv2D(32, kernel_size=(3,3), activation = 'relu', input_shape= (16,16,1)
             model.add(Conv2D(64, (3,3), activation = 'relu'))
             model.add(MaxPooling2D(pool_size=(2,2)))
             model.add(Dropout(0.25))
             model.add(Dense(128, activation = 'relu'))
             model.add(Dropout(0.5))
             model.add(Flatten())
             model.add(Dense(num_classes, activation = 'softmax'))
             model.compile(loss= keras.losses.categorical_crossentropy,
                             optimizer = keras.optimizers.Adadelta(),
                             metrics = ['accuracy'])
             history = model.fit(x_train, y_train,
                         batch_size= batch_size,
                         epochs = epochs,
                         verbose = 1, validation_data = (x_test, y_test))
             return model, history
3.2.2 Train Network
In [45]: model, history = Model(x_train, y_train, x_test, y_test, 10)
```

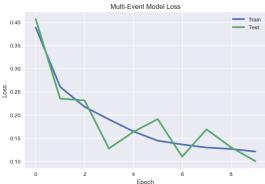
```
Train on 150000 samples, validate on 50000 samples
Epoch 1/10
Epoch 2/10
Epoch 3/10
Epoch 4/10
Epoch 5/10
Epoch 6/10
Epoch 7/10
Epoch 8/10
```

### 3.2.3 Evaluate Model

### 3.2.4 Performance History

```
In [49]: plt.style.use('seaborn')
         fig, ax = plt.subplots(1,2, figsize = (7,5))
         ax[0].set_aspect('auto')
         ax[0].plot(history.history['acc'], linewidth = 3, label = 'Train')
         ax[0].plot(history.history['val_acc'],linewidth = 3, label = 'Test')
         ax[0].set_title('Multi-Event Model Accuracy')
         ax[0].set_xlabel('Epoch')
         ax[0].set_ylabel('Accuracy')
         ax[0].legend(loc = 'best')
         ax[1].set_aspect('auto')
         ax[1].plot(history.history['loss'], linewidth = 3, label = 'Train')
         ax[1].plot(history.history['val_loss'],linewidth = 3, label = 'Test')
         ax[1].set_title('Multi-Event Model Loss')
         ax[1].set_xlabel('Epoch')
         ax[1].set_ylabel('Loss')
         ax[1].legend(loc = 'best')
         fig.subplots_adjust(right = 2)
         #plt.savefig('Multi-Event Model.png', bbox_inches = 'tight')
         plt.show()
```

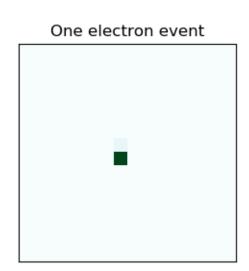




### 3.2.5 Example

```
In [50]: prediction = model.predict(x_test)
In [84]: plt.style.use('default')
    fig, ax = plt.subplots(1,2)
    ax[0].set_title('Two electron event')
    ax[0].imshow(data[9], cmap='BuGn', origin = 'lower')
    ax[0].axes.get_xaxis().set_visible(False)
    ax[0].axes.get_yaxis().set_visible(False)
    ax[1].set_title('One electron event')
    ax[1].imshow(data[11], cmap = 'BuGn', origin = 'lower')
    ax[1].axes.get_xaxis().set_visible(False)
    ax[1].axes.get_yaxis().set_visible(False)
    plt.show()
```

# Two electron event



Event 9 in data is a 2 electron event. Our model predicted the probability to be [0.01227101 0.9 Event 11 in data is a 1 electron event. Our model predicted the probability to be [0.9826361 0.

So we can see that our model correctly identified event 9 in our testing set as a two electron event with 0.99% certainty, and for event 11 our model predicted it to be a one electron event with 0.98% certainity. As shown above in the **Evaluate** section, our model achieved a total accuracy score of 97%.

## 4 Conclusion

With the implementation of machine learning techniques, we were able to successfully train a convolutional neural network (CNN) to distinguish between a one and two electron event. Furthermore, we successfully trained a CNN to predict the origin of the electron for one electron events. However, our model's performance was only marginally better than the random guessing. Therefore, a proper uncertainty quantification needs to be explored. This technique will be generalized to predict the origins of the electrons in the multi-event case and their respective initial energies. These models were trained and tested on simulated data provided by Sean Liddick, so they will need to be tested with a noisy dataset. Once these models are completely generalized, they can then be applied to real experimental data. If they perform well on the experimental data, then machine learning will be a viable data analysis technique for the Sean Liddick group and conversion electron spectroscopy in general.