Neural Network Classification of Top Quark Production at the Large Hadron Collider

Raveel Tejani

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1 Introduction

At the Large Hadron Collider (LHC), where protons are collided at a staggering rate of 40 MHz across various points within the LHC ring, the ATLAS experiment plays a pivotal role as a general-purpose detector at one of these collision sites. It precisely tracks particles emitted from these collisions, an essential task for understanding fundamental physics. The integration of machine learning, specifically neural networks, is instrumental in distinguishing between different physics processes: "signals" and the more prevalent "background" events. Achieving accurate discrimination between these is crucial due to the relatively rare occurrence of signal events. The focus of this project was to explore several key objectives within the context of high-energy physics:

1. Training a Classifier: Develop a neural network classifier to accurately distinguish between ttZ (the production of a pair of top quarks associated with a Z boson) and WZ (the production of a W and a Z boson) events. This distinction is critical as both ttZ and WZ can produce similar detector-level features, yet represent different underlying physics processes.

2. Feature Selection: Experiment with the addition and removal of various detector-level features to evaluate how each alteration affects the classifier's performance. This analysis helps in understanding which features are most predictive and thus critical for accurate event classification.

3. Optimization of Neural Network: Enhance the architecture and training parameters of the neural network to maximize its performance in classifying ttZ and WZ events. This includes adjustments in network structure, learning rates, and other hyperparameters to refine the model efficacy.

4. Feature Ranking: Determine and rank the importance of these features in the neural network to prioritize data collection and processing strategies at the detector level.

To accomplish these goals, simulated data samples of ttZ and WZ events, produced using Monte Carlo simulations, were utilized to train the neural network. This training enables the classifier to learn the distinctive patterns of each event type. Once optimized, the classifier is then applied to actual recorded data from the LHC, using its outputs for further statistical analysis and insights. This project not only advances the accuracy and efficiency of particle identification at the ATLAS experiment but also contributes significantly to the broader field of particle physics, enhancing our understanding of particle interactions and the fundamental forces of nature.

2 Methods

Describe briefly the ML algorithms that will be used in the project

We will mainly be using a Neural Network for classification.

We are given a base model with recommended feature selection.

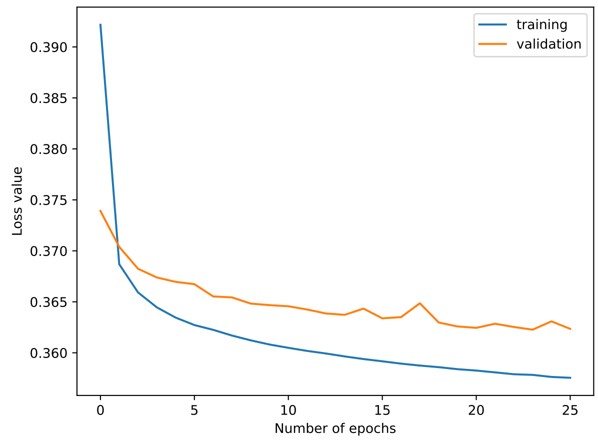
For the context

First we will start by using SRS for feature selection. Perform Base model on all features.

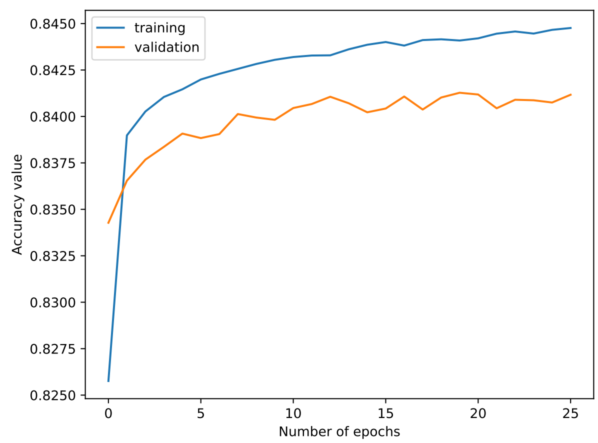
Then we will use gridSearch CV for model selection

We start with the base model provided with the project.

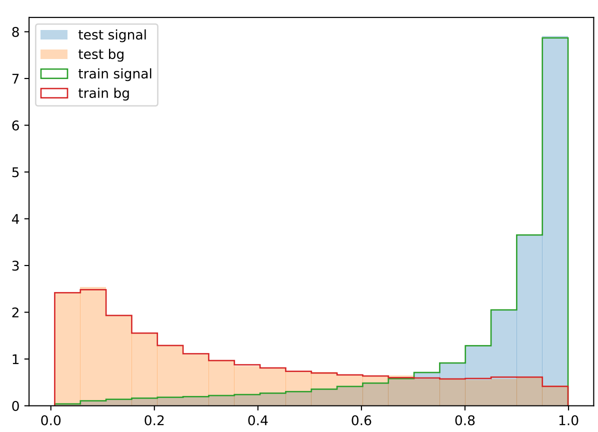
We can see the various plots generated



(a) Loss reduction as a function of epochs



(b) Accuracy performance as a function of epochs

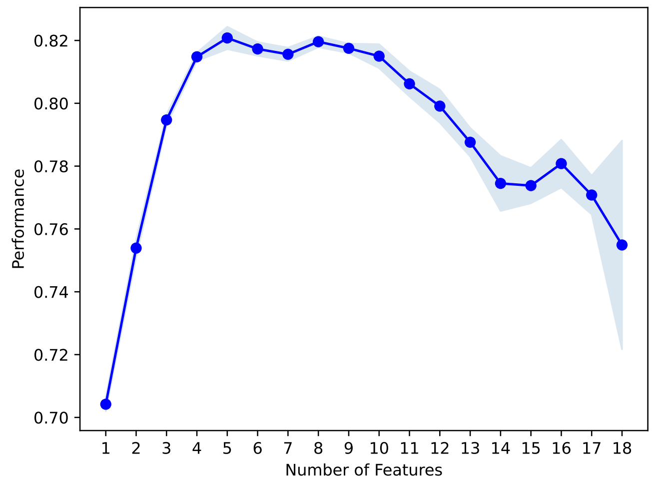


(c) Probability distribution of test and train cases, based on trained Neural network

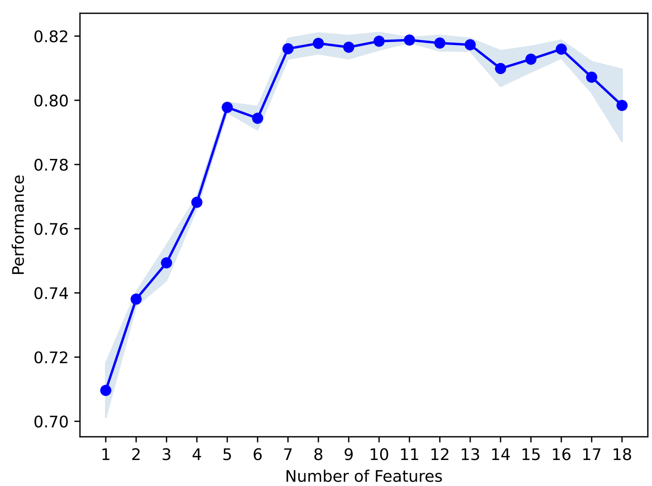
Figure 1: The base Neural Netwoek model provided with model.

3 Results

Address all project questions and support your findings with appropriate graphs. Present clearly defined figures with good layout. Make sure data interpretation is easy to infer from figures and tables. Throughout the results, employ good practices of ML such as cross-validation and hyperparameter optimization.



(a) 10 000 samples



(b) 30 000 samples

Figure 2: The accuracy performance of Sequential Feature Selector with two subsets of the data.

Average CV Score	Feature Names
70.96%	('bjet_1_pt',)
73.81%	('bjet_1_pt', 'n_jets')
74.94%	('bjet_1_pt', 'n_jets', 'n_bjets')
76.82%	('jet_1_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
79.78%	('jet_1_twb', 'jet_2_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
79.44%	('jet_3_pt', 'jet_1_twb', 'jet_2_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
81.61%	('jet_3_pt', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
81.77%	('jet_3_pt', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
81.65%	('jet_3_pt', 'jet_1_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'n_jets', 'n_bjets')
81.84%	('jet_3_pt', 'jet_1_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'n_jets', 'n_bjets', 'n_leptons')
81.88%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'n_jets', 'n_bjets', 'n_leptons')
81.78%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'n_jets', 'n_bjets', 'n_leptons')
81.73%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'n_jets', 'n_bjets', 'n_leptons')
80.99%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'n_jets', 'n_bjets', 'n_leptons', 'H_T')
81.28%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'n_jets', 'n_bjets', 'n_leptons', 'met_met', 'H_T')
81.59%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'lep_2_pt', 'n_jets', 'n_bjets', 'n_leptons', 'met_met', 'H_T')
80.72%	('jet_1_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'lep_2_pt', 'lep_3_pt', 'n_jets', 'n_bjets', 'n_leptons', 'met_met', 'H_T')
79.84%	('jet_1_pt', 'jet_2_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta', 'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt', 'lep_1_pt', 'lep_2_pt', 'lep_3_pt', 'n_jets', 'n_bjets', 'n_leptons', 'met_met', 'H_T')

Table 1: Results of the Secqquential Feature Selector. We can gather Feature Importances from these tables. The ones highlighed in green is what we use to continue our analysis

Parameter	Trial 1	Trial 2	Trial 3
Nodes: Dense Layer 1	25	50	100
Nodes: Dense Layer 2	12	25	50
Nodes: Dense Layer 3	5	10	15
Batch Size	100	150	300
Adam Learning Rate	0.002	0.0002	0.00002
Best Score	82.96%	83.39%	82.7%

Table 2: Parameters we will swift through in gridsearchCV.

Model Selection:

Parameters	Base List	SRS: Best List	SRS: Best Small List
Nodes: Dense Layer 1	50	25	50
Nodes: Dense Layer 2	12	25	50
Nodes: Dense Layer 3	10	15	5
Batch Size	300	100	150
Adam Learning Rate	0.002	0.002	0.0002
Best Score	82.96%	83.39%	82.7%

Table 3: Best Parameters for the 3 Feature Lists.

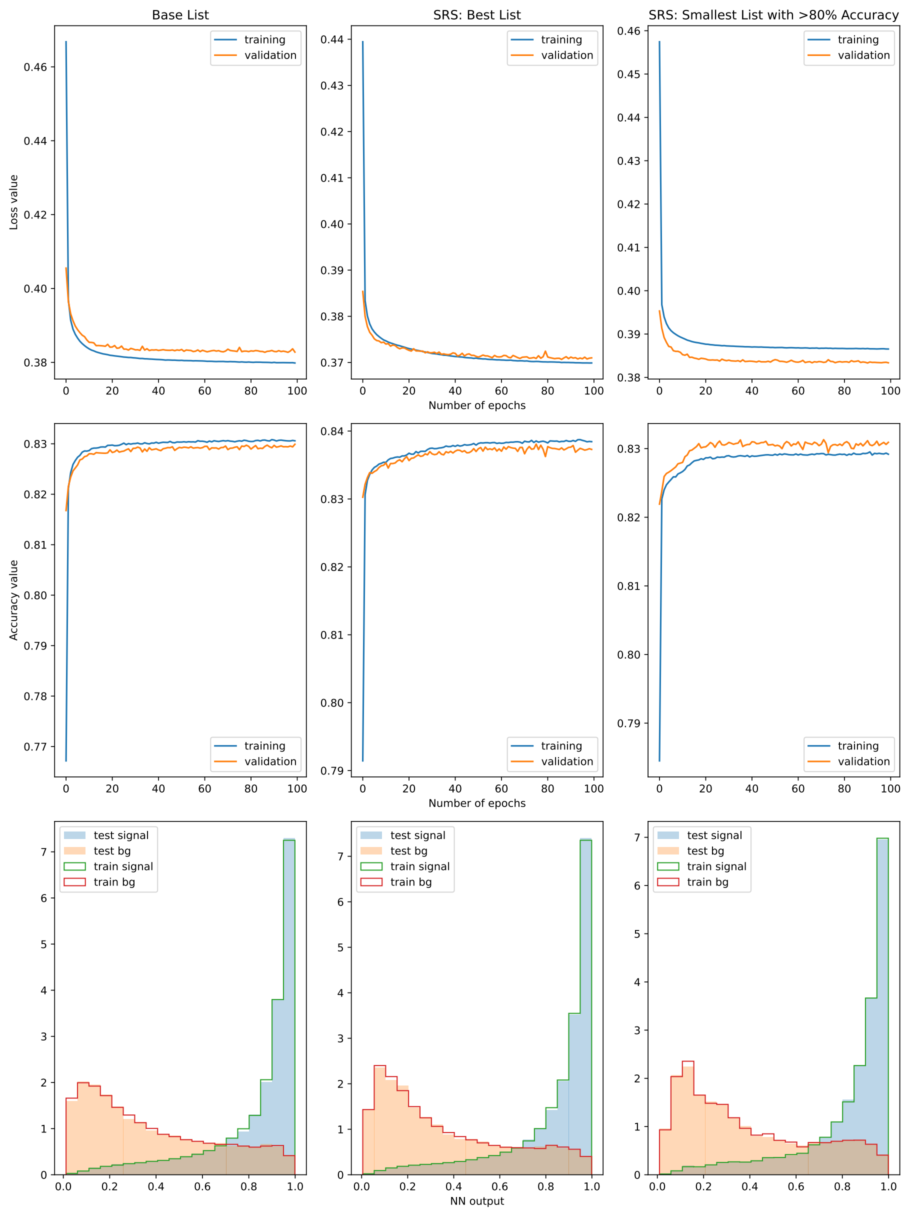


Figure 3: Performance plots of all 3 feature lists based on the base model provided

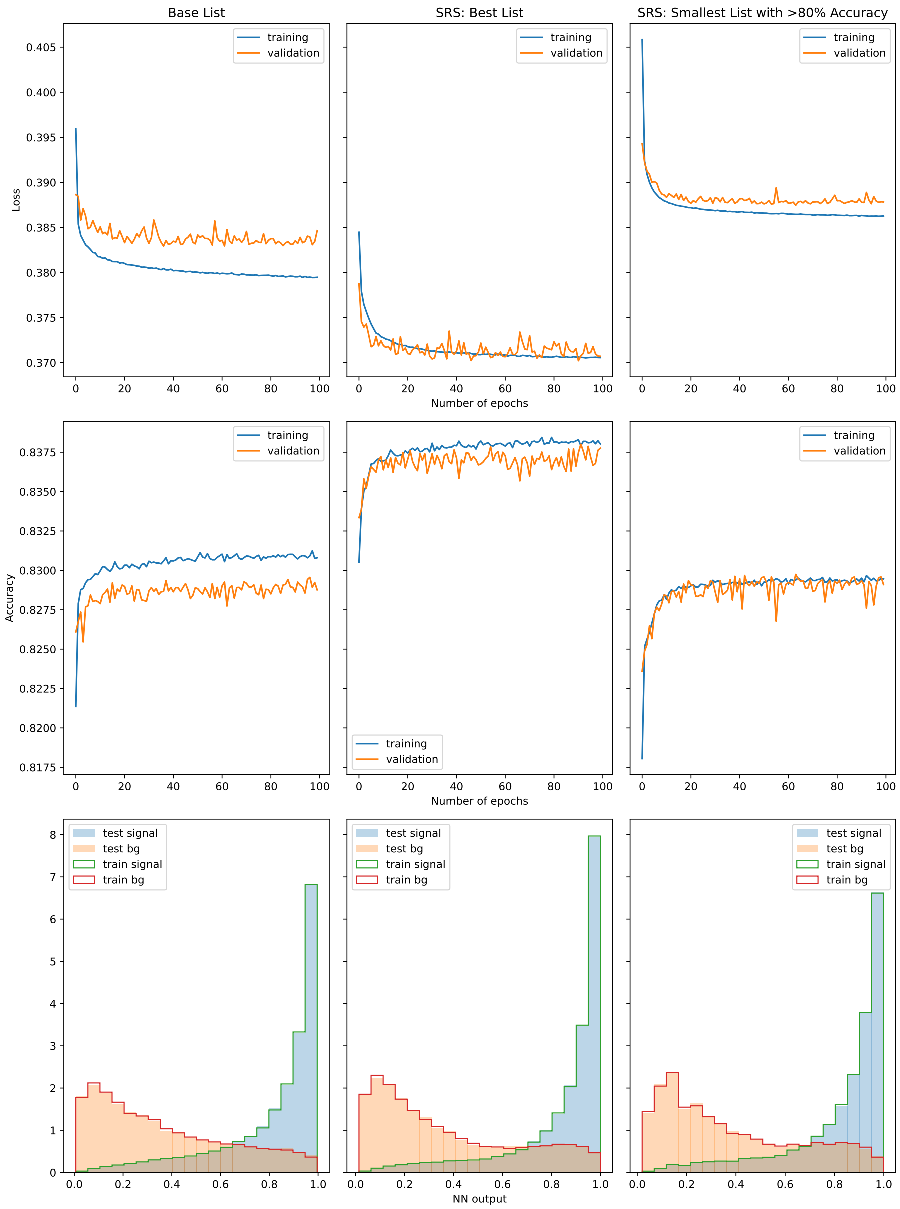


Figure 4: Performance plots of all 3 feature lists based on best parameters found for each.

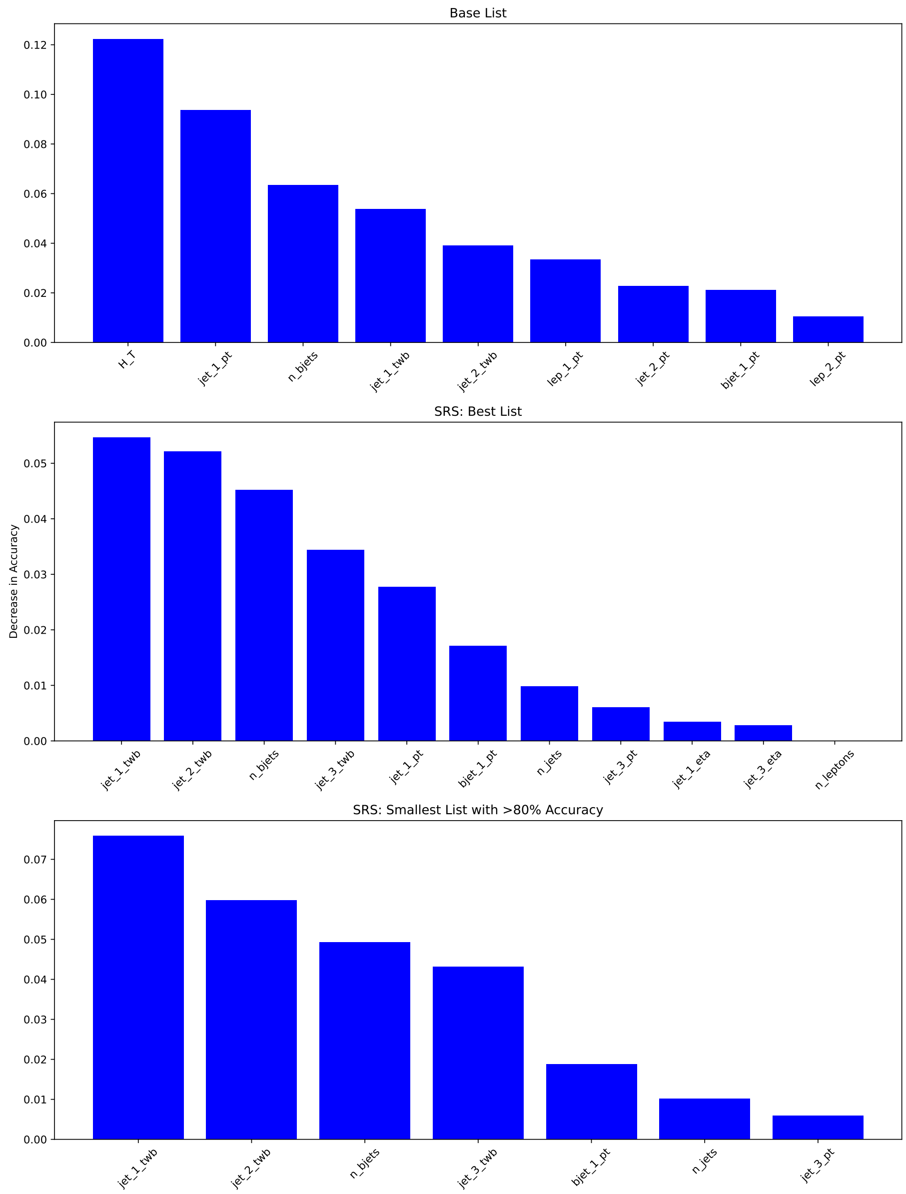


Figure 5: Performance plots of all 3 feature lists based on best parameters found for each.

4 Discussion and Summary

– Discussion and Summary: We were not able to improve accuracy significantly, but we we were able to show that we can reduce the dimensionality of our feature space and still maintain similiar accuracy.

Provide a concise summary of findings, successes and failures, as well as outlook for the study.

A Code: Base Model

In this section we can find the code associated with the base model provided at the begining of this project. This code was used to generate the plots in Fig. 1

[1]:
```
import h5py
import matplotlib.pyplot as plt
import numpy as np
import tensorflow.keras as K
from numpy.lib.recfunctions import structured_to_unstructured
from sklearn.model_selection import train_test_split
import pandas as pd
```

```
2024-04-16 16:46:04.583009: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: SSE4.1 SSE4.2, in other operations,
rebuild TensorFlow with the appropriate compiler flags.
```

1 Loading The Data

[2]:
```
with h5py.File("info/data/output_signal.h5", "r") as file:
    signal_data = file["events"][:]

with h5py.File("info/data/output_bg.h5", "r") as file:
    bg_data = file["events"][:]
```

2 'Unstructuring' Data

[4]:
```
signal_data = structured_to_unstructured(signal_data)
bg_data = structured_to_unstructured(bg_data)
```

3 Train - Validation - Test Splits

[5]:
```
X = np.concatenate([signal_data, bg_data])
y = np.concatenate([np.ones(signal_data.shape[0], dtype=int), np.zeros(bg_data.
 ↪shape[0], dtype=int)])

x_train, x_rem, y_train, y_rem = train_test_split(X, y, train_size=0.8)
x_val, x_test, y_val, y_test = train_test_split(x_rem, y_rem, train_size=0.5)
```

4 Data Preprocessing

[6]:
```
preprocessing_layer = K.layers.Normalization()
preprocessing_layer.adapt(x_train)
```

5 Model training

[7]:
```
model = K.Sequential(
    [
        preprocessing_layer,
        K.layers.Dense(50, activation="relu", name="hidden1"),
        K.layers.Dense(25, activation="relu", name="hidden2"),
        K.layers.Dense(10, activation="relu", name="hidden3"),
        K.layers.Dense(1, activation="sigmoid", name="output"),
    ]
)

model.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 18)               37
 n)

 hidden1 (Dense)             (None, 50)                950

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,533
Trainable params: 2,496
Non-trainable params: 37
_________________________________________________________________
```

[8]:
```
model.compile(
    optimizer=K.optimizers.Adam(learning_rate=0.0002),
    loss=K.losses.BinaryCrossentropy(),
    metrics=[K.metrics.BinaryAccuracy()],
)
```

[9]:
```
early_stopping_callback = K.callbacks.EarlyStopping(
    monitor='val_loss',
    patience=10,
    min_delta=0.002,
    restore_best_weights=True,
    verbose=1,)
```

[10]:
```python
fit_history = model.fit(
        x_train,
        y_train,
        batch_size=100,
        epochs=100,
        validation_data=(x_val, y_val),
        callbacks=[early_stopping_callback],
    )

print("Printing summary of the trained model:")
print(model.summary())
```

```
Epoch 1/100
1159/1159 [==============================] - 2s 1ms/step - loss: 0.4256 -
binary_accuracy: 0.8084 - val_loss: 0.3800 - val_binary_accuracy: 0.8312
        ⋮
Epoch 29/100
1159/1159 [==============================] - 1s 1ms/step - loss: 0.3594 -
binary_accuracy: 0.8435 - val_loss: 0.3579 - val_binary_accuracy: 0.8433
Epoch 30/100
1127/1159 [============================>.] - ETA: 0s - loss: 0.3591 -
binary_accuracy: 0.8439Restoring model weights from the end of the best epoch:
20.
1159/1159 [==============================] - 2s 1ms/step - loss: 0.3592 -
binary_accuracy: 0.8438 - val_loss: 0.3577 - val_binary_accuracy: 0.8437
Epoch 30: early stopping
Printing summary of the trained model:
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 18)               37
 n)

 hidden1 (Dense)             (None, 50)                950

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,533
Trainable params: 2,496
Non-trainable params: 37
_________________________________________________________________
```

```
None
```

[11]:
```
save_name = "my_model"
print(f'Storing model with name "{save_name}" now. You can convert '
        'this to ONNX format with the "tf2onnx" command-line utility.')
model.save(save_name)
```

```
Storing model with name "my_model" now. You can convert this to ONNX format with
the "tf2onnx" command-line utility.
```

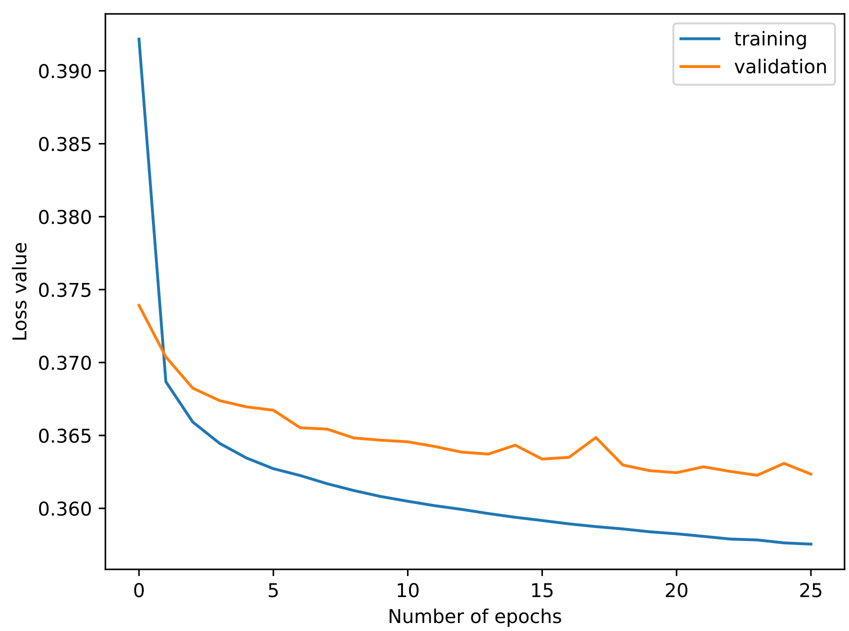
```
WARNING:absl:Found untraced functions such as _update_step_xla while saving
(showing 1 of 1). These functions will not be directly callable after loading.
```

```
INFO:tensorflow:Assets written to: my_model/assets
```

```
INFO:tensorflow:Assets written to: my_model/assets
```

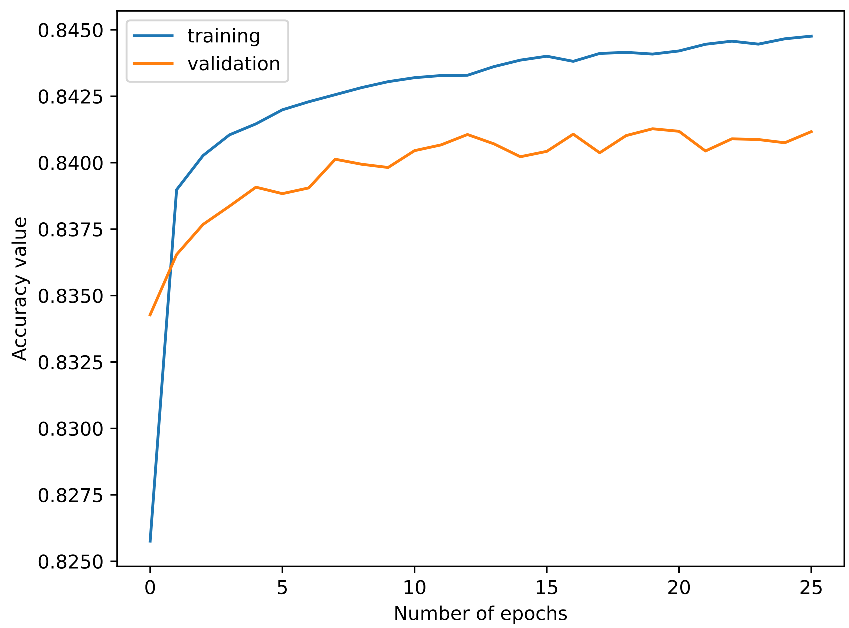
The following code produces a plot of the loss evolution for training and validation:

[12]:
```
plt.plot(fit_history.history["loss"], label="training")
plt.plot(fit_history.history["val_loss"], label="validation")
plt.xlabel("Number of epochs")
plt.ylabel("Loss value")
plt.legend()
plt.tight_layout()
plt.show()
```



The following code produces a plot of the accuracy evolution per epoch for training and validation:

[13]:
```
plt.figure()
plt.plot(fit_history.history["binary_accuracy"], label="training")
plt.plot(fit_history.history["val_binary_accuracy"], label="validation")
plt.xlabel("Number of epochs")
plt.ylabel("Accuracy value")
plt.legend()
plt.tight_layout()
#plt.savefig(output_file)
```

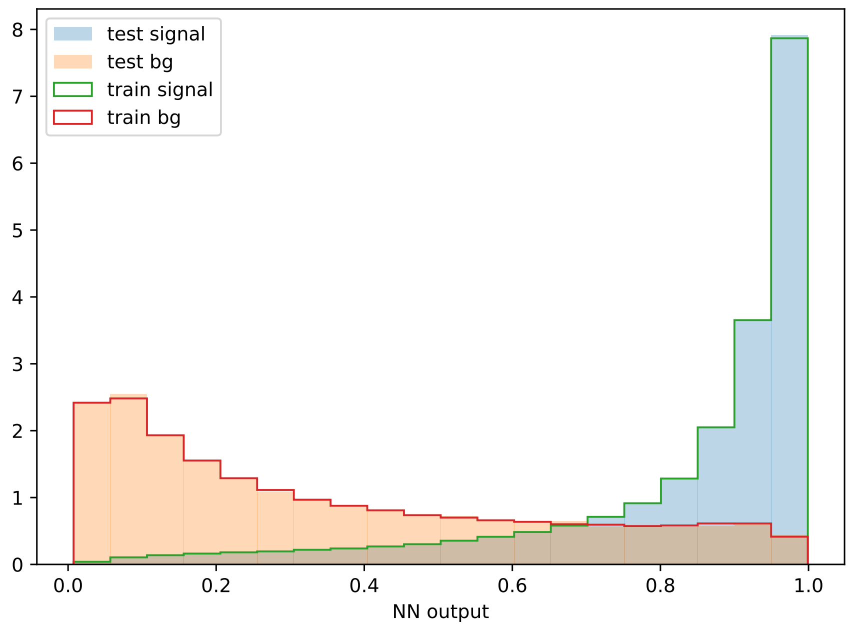


The following code plots the distribution of the neural-network output node for both training and test data to check for possible differences between the two. The datasets are sliced according to their truth labels (i.e. the two classes).

[14]:
```
 """Creates a plot of the NN output for training and test data.

    The function slices both training and test data according to the truth
    labels, so that the displayed spectra can be split into "background" and
    "signal" events (i.e. the two classes the model was trained on).

    """

_, bins, _ = plt.hist(model.predict(x_test[y_test.astype(bool)]), bins=20,␣
 ↪alpha=0.3, density=True, label="test signal")
plt.hist(model.predict(x_test[~y_test.astype(bool)]), bins=bins, alpha=0.3,␣
 ↪density=True, label="test bg")
```

```
plt.hist(model.predict(x_train[y_train.astype(bool)]), bins=bins, density=True,␣
↪histtype="step", label="train signal")
plt.hist(model.predict(x_train[~y_train.astype(bool)]), bins=bins, density=True,␣
↪histtype="step", label="train bg")
plt.xlabel("NN output")
plt.legend()
plt.tight_layout()
plt.show()
#plt.savefig(output_file)
print("Created plots of loss, accuracy, and NN output.")
```

```
1595/1595 [==============================] - 1s 422us/step
723/723 [==============================] - 0s 420us/step
12717/12717 [==============================] - 5s 429us/step
5823/5823 [==============================] - 3s 446us/step
```




```
Created plots of loss, accuracy, and NN output.
```

B Code: Feature Selection

In this section we can find the code associated with using the Sequential Feature Selector. This code was used to generate the plots in Fig. 2 and Table 1.

[1]:
```
import h5py
import matplotlib.pyplot as plt
import numpy as np
import tensorflow.keras as K
import pandas as pd
from tensorflow.keras.wrappers.scikit_learn import KerasClassifier
from mlxtend.feature_selection import SequentialFeatureSelector as SFS
from mlxtend.plotting import plot_sequential_feature_selection as plot_sfs
import pandas as pd
```

```
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.

2024-04-14 01:18:28.522266: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: SSE4.1 SSE4.2, in other operations,
rebuild TensorFlow with the appropriate compiler flags.
```

1 Loading The Data

[2]:
```
with h5py.File("info/data/output_signal.h5", "r") as file:
    signal_data = file["events"][:]

with h5py.File("info/data/output_bg.h5", "r") as file:
    bg_data = file["events"][:]
```

2 Subset of the Data

[3]:
```
# storing signal and background data in panda DataFrame
signal = pd.DataFrame(signal_data)
background = pd.DataFrame(bg_data)

# concatenating the data frames to be part of one big set
df = pd.concat([signal, background])

# reseting the indicies
df = df.reset_index()

# creating the labels for the data sets i.e; signal = 1, background = 0 for␣
↪classification
labels = np.concatenate([np.ones(signal.shape[0]), np.zeros(background.shape[0])])
labels = pd.DataFrame({'ttZ': labels})

# adding labels as a column at the end of the DataFrame
df = df.join(labels)
```

```
# shuffling the DataFrame
df_shuffled = df.sample(frac=1, random_state=42)  # 'random_state' for reproducibility
df_shuffled.head()
```

[3]:

```
         index    jet_1_pt    jet_2_pt    jet_3_pt  jet_1_eta  jet_2_eta  \
469349  469349  110.017174   89.244843   42.692078  -1.638234  -1.114363
8248      8248  183.934067  125.170509   93.043922   0.185653  -1.264277
699594  190559  195.334396  155.822617   39.977455  -0.860027   1.231296
149760  149760  165.566879  136.009689  124.258598   0.903266  -0.343321
72006    72006  128.334076   54.510422   45.616039  -0.975434  -2.489865

        jet_3_eta  jet_1_twb  jet_2_twb  jet_3_twb   bjet_1_pt    lep_1_pt  \
469349   0.334825          3          1          1  110.017174  165.685593
8248     1.190622          1          4          1  125.170509   68.110207
699594   2.197089          1          1          1   35.366051  184.187210
149760   0.041760          5          5          1  165.566879  113.711166
72006   -1.147104          1          1          1   32.256153  109.551361

          lep_2_pt   lep_3_pt  n_jets  n_bjets  n_leptons     met_met  \
469349   81.492973  32.393501       3        1          3   64.430573
8248     35.741417  12.237628       4        1          3  104.903961
699594   82.709946  36.546856       5        1          3   48.988052
149760  112.550560  34.406342       6        2          3  172.116821
72006   100.125435  48.681091       6        2          3   29.693062

                H_T  ttZ
469349   585.956726  1.0
8248     654.210388  1.0
699594   807.437683  0.0
149760  1007.604309  1.0
72006    606.260437  1.0
```

[4]:

```
# taking the first 30 000 rows from the shuffled DataFrame
subset_df = df_shuffled.iloc[:30000]

# splitting the labels from the rest of the dataset
X_sub = subset_df[['jet_1_pt', 'jet_2_pt', 'jet_3_pt', 'jet_1_eta', 'jet_2_eta',
       'jet_3_eta', 'jet_1_twb', 'jet_2_twb', 'jet_3_twb', 'bjet_1_pt',
       'lep_1_pt', 'lep_2_pt', 'lep_3_pt', 'n_jets', 'n_bjets', 'n_leptons',
       'met_met', 'H_T']]
y_sub = subset_df['ttZ']

# we can check the class distribution in the subset
print('ttZ events: {:.2f}%'.format(np.sum(y_sub)/len(y_sub) * 100))
print('WZ events: {:.2f}%'.format((1 - np.sum(y_sub)/len(y_sub)) * 100))
```

```
ttZ events: 68.69%
WZ events: 31.31%
```

3 Sequential Feature Selector

https://rasbt.github.io/mlxtend/user_guide/feature_selection/SequentialFeatureSelector/#example-9-selecting-the-best-feature-combination-in-a-k-range

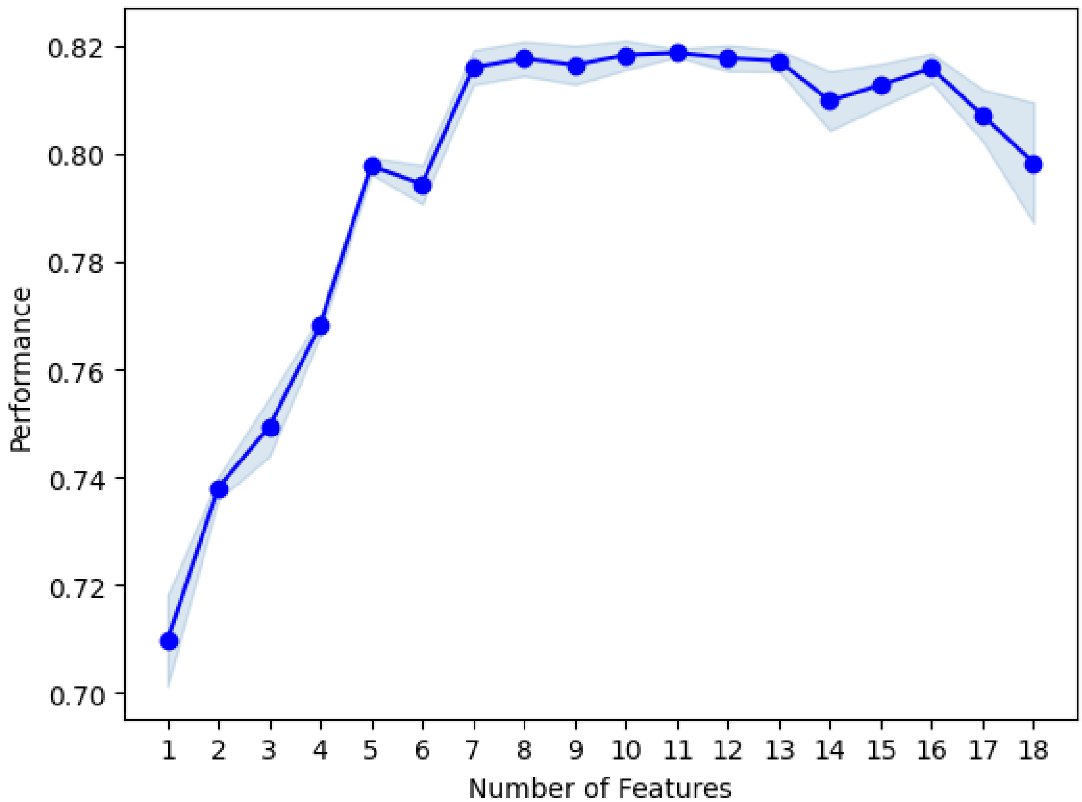
[5]:
```
# model for classification
def build_model(input_dim=None):
    model = K.Sequential([
        K.layers.Normalization(),
        K.layers.Dense(50, activation="relu", input_dim=input_dim),
        K.layers.Dense(25, activation="relu"),
        K.layers.Dense(10, activation="relu"),
        K.layers.Dense(1, activation="sigmoid")
    ])
    model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])
    return model

# wrapper function
model = KerasClassifier(build_fn=lambda: build_model(input_dim=X_sub.shape[1]),␣
 ↪epochs=10, batch_size=32, verbose=0)
```

```
/var/folders/3x/lv7sddxn2gg8mq0dwdcn1wg40000gn/T/ipykernel_29259/2265007354.py:1
3: DeprecationWarning: KerasClassifier is deprecated, use Sci-Keras
(https://github.com/adriangb/scikeras) instead. See
https://www.adriangb.com/scikeras/stable/migration.html for help migrating.
  model = KerasClassifier(build_fn=lambda:
build_model(input_dim=X_sub.shape[1]), epochs=10, batch_size=32, verbose=0)
```

[6]:
```
# SFS model, will check performance from 1 feature to all 18
sfs = SFS(model,
          k_features = (1,18),
          forward=True,
          floating=False,
          scoring='accuracy',
          cv=5,
          verbose=0)

sfs = sfs.fit(X_sub, y_sub)
```

[7]:
```
# plotting performance improvement with each additional feature

print('best combination (ACC: %.3f): %s\n' % (sfs.k_score_, sfs.k_feature_idx_))
plot_sfs(sfs.get_metric_dict(), kind='std_err');
plt.savefig('feature_num_performance_30k.pdf')
```

```
best combination (ACC: 0.819): (0, 2, 3, 5, 6, 7, 8, 9, 13, 14, 15)
```



[8]:
```python
# saving performance of all feature sets

feature_performance_df = pd.DataFrame.from_dict(sfs.get_metric_dict()).T
feature_performance_df.to_csv('performance_30k.csv', index=False)
feature_performance_df
```

[8]:
```
                                           feature_idx  \
1                                                 (9,)
2                                              (9, 13)
3                                          (9, 13, 14)
4                                       (6, 9, 13, 14)
5                                    (6, 7, 9, 13, 14)
6                                 (2, 6, 7, 9, 13, 14)
7                              (2, 6, 7, 8, 9, 13, 14)
8                           (2, 5, 6, 7, 8, 9, 13, 14)
9                        (2, 3, 5, 6, 7, 8, 9, 13, 14)
10                   (2, 3, 5, 6, 7, 8, 9, 13, 14, 15)
11                (0, 2, 3, 5, 6, 7, 8, 9, 13, 14, 15)
12            (0, 2, 3, 5, 6, 7, 8, 9, 10, 13, 14, 15)
13         (0, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15)
14     (0, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 17)
15   (0, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 16...
16   (0, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15...
17   (0, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...
```

```
18  (0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13,...

                                            cv_scores avg_score  \
1   [0.7248333333333333, 0.6886666666666666, 0.721...  0.709633
2   [0.7351666666666666, 0.7353333333333333, 0.735...  0.738067
3   [0.7548333333333334, 0.765, 0.7485, 0.747, 0.7...  0.749367
4   [0.765, 0.7721666666666667, 0.7733333333333333...  0.768233
5   [0.7918333333333333, 0.8003333333333333, 0.8, ...    0.7978
6   [0.7828333333333334, 0.8046666666666666, 0.794...    0.7944
7   [0.8116666666666666, 0.8283333333333334, 0.810...  0.816067
8   [0.8115, 0.8275, 0.8211666666666667, 0.81, 0.8...  0.817733
9   [0.815, 0.8263333333333334, 0.812, 0.8065, 0.8...  0.816533
10  [0.8146666666666667, 0.8246666666666667, 0.811...    0.8184
11  [0.8196666666666667, 0.8185, 0.817, 0.8175, 0...  0.818767
12  [0.8168333333333333, 0.8203333333333334, 0.816...  0.817833
13  [0.8201666666666667, 0.8226666666666667, 0.811...    0.8173
14  [0.8206666666666667, 0.8223333333333334, 0.810...    0.8099
15            [0.8215, 0.82, 0.8055, 0.8155, 0.8015]    0.8128
16  [0.817, 0.8243333333333334, 0.811, 0.808666666...  0.815933
17  [0.8131666666666667, 0.789, 0.806, 0.815333333...    0.8072
18  [0.7715, 0.8163333333333334, 0.8115, 0.8218333...    0.7984

                                        feature_names  ci_bound   std_dev  \
1                                         (bjet_1_pt,)  0.021713  0.016894
2                                  (bjet_1_pt, n_jets)  0.005534  0.004306
3                        (bjet_1_pt, n_jets, n_bjets)  0.014078  0.010953
4             (jet_1_twb, bjet_1_pt, n_jets, n_bjets)  0.004797  0.003732
5   (jet_1_twb, jet_2_twb, bjet_1_pt, n_jets, n_bj...  0.003981  0.003097
6   (jet_3_pt, jet_1_twb, jet_2_twb, bjet_1_pt, n_...  0.009342  0.007268
7   (jet_3_pt, jet_1_twb, jet_2_twb, jet_3_twb, bj...  0.008231  0.006404
8   (jet_3_pt, jet_3_eta, jet_1_twb, jet_2_twb, je...  0.008258  0.006425
9   (jet_3_pt, jet_1_eta, jet_3_eta, jet_1_twb, je...  0.009256  0.007201
10  (jet_3_pt, jet_1_eta, jet_3_eta, jet_1_twb, je...  0.006957  0.005413
11  (jet_1_pt, jet_3_pt, jet_1_eta, jet_3_eta, jet...  0.001938  0.001508
12  (jet_1_pt, jet_3_pt, jet_1_eta, jet_3_eta, jet...  0.006169  0.004799
13  (jet_1_pt, jet_3_pt, jet_1_eta, jet_2_eta, jet...  0.005066  0.003942
14  (jet_1_pt, jet_3_pt, jet_1_eta, jet_2_eta, jet...  0.014196  0.011045
15  (jet_1_pt, jet_3_pt, jet_1_eta, jet_2_eta, jet...  0.010215  0.007947
16  (jet_1_pt, jet_3_pt, jet_1_eta, jet_2_eta, jet...  0.007186  0.005591
17  (jet_1_pt, jet_3_pt, jet_1_eta, jet_2_eta, jet...  0.012362  0.009618
18  (jet_1_pt, jet_2_pt, jet_3_pt, jet_1_eta, jet_...  0.028888  0.022476

     std_err
1   0.008447
2   0.002153
3   0.005477
4   0.001866
5   0.001549
6   0.003634
7   0.003202
8   0.003213
9   0.003601
10  0.002706
```

11	0.000754
12	0.0024
13	0.001971
14	0.005523
15	0.003974
16	0.002796
17	0.004809
18	0.011238

C Code: Feature Comparison

This code was used to generate the plots in Fig. 3

[1]:
```python
import h5py
import matplotlib.pyplot as plt
import numpy as np
import tensorflow.keras as K
from sklearn.model_selection import train_test_split
import pandas as pd
```

```
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.

2024-04-17 15:29:47.130479: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: SSE4.1 SSE4.2, in other operations,
rebuild TensorFlow with the appropriate compiler flags.
```

[2]:
```python
with h5py.File("info/data/output_signal.h5", "r") as file:
    signal_data = file["events"][:]

with h5py.File("info/data/output_bg.h5", "r") as file:
    bg_data = file["events"][:]
```

1 Loading the Data

[3]:
```python
# storing signal and background data in panda DataFrame
signal = pd.DataFrame(signal_data)
background = pd.DataFrame(bg_data)

# concatenating the data frames to be part of one big set
df = pd.concat([signal, background])

# reseting the indicies
df = df.reset_index()

# creating the labels for the data sets i.e; signal = 1, background = 0 for␣
 ↪classification
labels = np.concatenate([np.ones(signal.shape[0]), np.zeros(background.
 ↪shape[0])])
labels = pd.DataFrame({'ttZ': labels})

# adding labels as a column at the end of the DataFrame
```

```
df = df.join(labels)

# shuffling the DataFrame
df_shuffled = df.sample(frac=1, random_state=42)  # 'random_state' for␣
↪reproducibility
df_shuffled.head()

# splitting the labels from the rest of the dataset
y = df_shuffled['ttZ']

# we can check the class distribution in the subset
print('ttZ events: {:.2f}%'.format(np.sum(y)/len(y) * 100))
print('WZ events: {:.2f}%'.format((1 - np.sum(y)/len(y)) * 100))
```

```
ttZ events: 68.65%
WZ events: 31.35%
```

2 Various Feature Lists

[4]:
```
# base input list suggested by the project
input_list = [ "H_T",
              "jet_1_pt",
              "jet_2_pt",
              "lep_1_pt",
              "lep_2_pt",
              "n_bjets",
              "jet_1_twb",
              "jet_2_twb",
              "bjet_1_pt"]

# best input list suggested by SRS
input_list_2 = ['jet_1_pt',
                'jet_3_pt',
                'jet_1_eta',
                'jet_3_eta',
                'jet_1_twb',
                'jet_2_twb',
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets',
                'n_leptons']

# smallest input list that still has an accuracy >80%, suggested by SRS
input_list_3 = ['jet_3_pt',
                'jet_1_twb',
                'jet_2_twb',
```

```
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets']

input_lists = [input_list, input_list_2, input_list_3]
```

3 Running Base Model for all Feature Lists

[5]:
```
fig, axs = plt.subplots(3, 3, figsize=(12, 16))

for i, feature_list in enumerate(input_lists):
    names = ['base list', 'SRS: best list', 'SRS: best smallest list']
    X = df_shuffled[feature_list]
    x_train, x_rem, y_train, y_rem = train_test_split(X, y, train_size=0.8)
    x_val, x_test, y_val, y_test = train_test_split(x_rem, y_rem, train_size=0.5)

    preprocessing_layer = K.layers.Normalization()
    preprocessing_layer.adapt(x_train)

    model = K.Sequential(
    [
        preprocessing_layer,
        K.layers.Dense(50, activation="relu", name="hidden1"),
        K.layers.Dense(25, activation="relu", name="hidden2"),
        K.layers.Dense(10, activation="relu", name="hidden3"),
        K.layers.Dense(1, activation="sigmoid", name="output"),
    ]
    )

    model.summary()

    model.compile(optimizer=K.optimizers.Adam(learning_rate=0.0002),
                  loss=K.losses.BinaryCrossentropy(),
                  metrics=[K.metrics.BinaryAccuracy()])

    fit_history = model.fit(
        x_train,
        y_train,
        batch_size=512,
        epochs=100,
        validation_data=(x_val, y_val),
        verbose = 0)


    print("Printing summary of the trained model:")
```

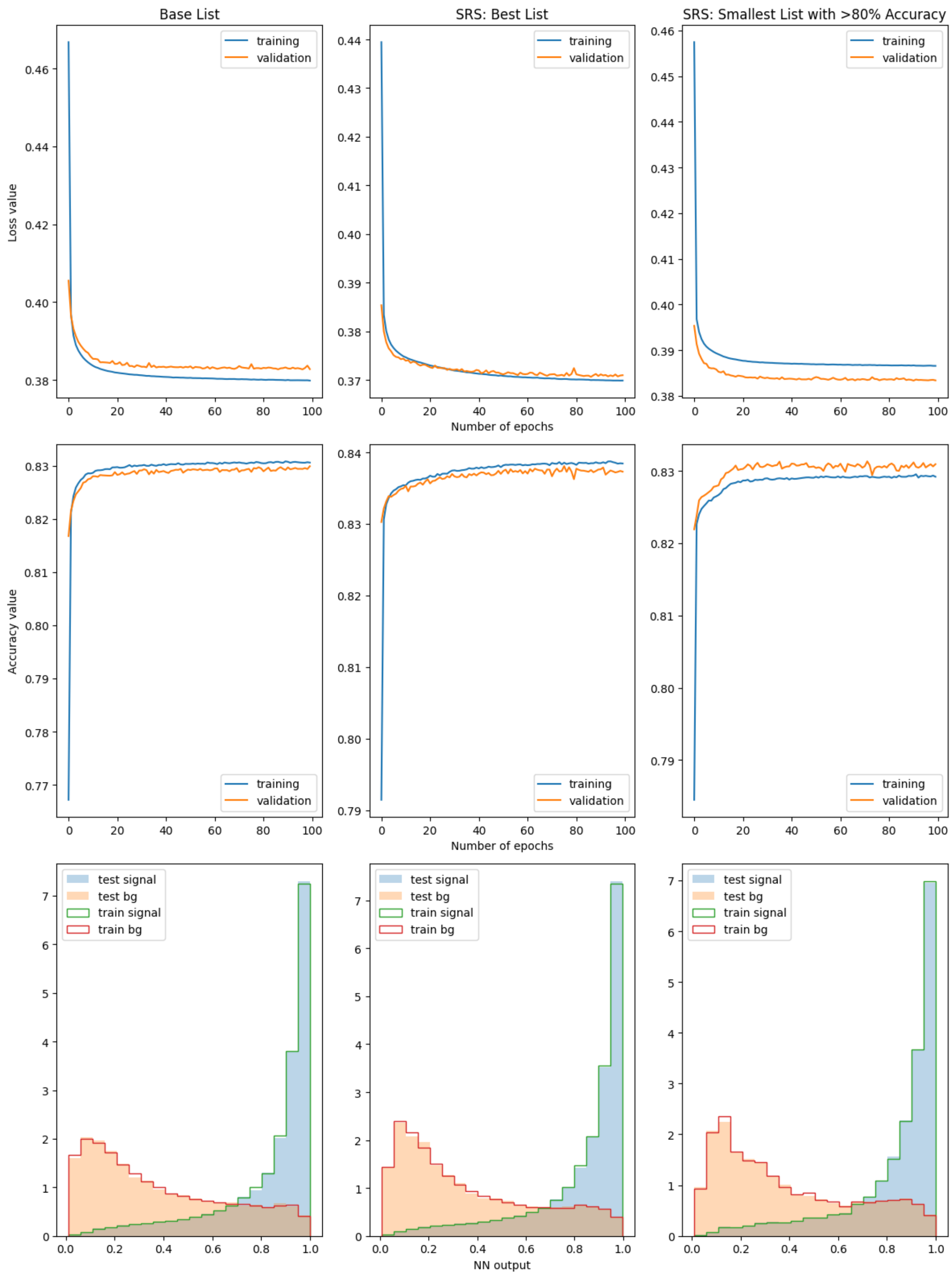
```
    print(model.summary())

    titles = ['Base List', 'SRS: Best List', 'SRS: Smallest List with >80%␣
↪Accuracy']

    axs[0, i].plot(fit_history.history["loss"], label="training")
    axs[0, i].plot(fit_history.history["val_loss"], label="validation")
    axs[0, i].legend()
    axs[0, i].set_title(titles[i])

    axs[1, i].plot(fit_history.history["binary_accuracy"], label="training")
    axs[1, i].plot(fit_history.history["val_binary_accuracy"],␣
↪label="validation")
    axs[1, i].legend()

    _, bins, _ = axs[2, i].hist(model.predict(x_test[y_test.astype(bool)]),␣
↪bins=20, alpha=0.3, density=True, label="test signal")
    axs[2, i].hist(model.predict(x_test[~y_test.astype(bool)]), bins=bins,␣
↪alpha=0.3, density=True, label="test bg")
    axs[2, i].hist(model.predict(x_train[y_train.astype(bool)]), bins=bins,␣
↪density=True, histtype="step", label="train signal")
    axs[2, i].hist(model.predict(x_train[~y_train.astype(bool)]), bins=bins,␣
↪density=True, histtype="step", label="train bg")
    axs[2, i].legend()

    if i == 0:
            axs[0, i].set_ylabel("Loss value")
            axs[1, i].set_ylabel("Accuracy value")

    elif i == 1:
        axs[0, i].set_xlabel("Number of epochs")
        axs[1, i].set_xlabel("Number of epochs")
        axs[2, i].set_xlabel("NN output")

fig.tight_layout()
plt.savefig("feat-comparison.pdf")
plt.show()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 9)                19
 n)

 hidden1 (Dense)             (None, 50)                500
```

```
 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,065
Trainable params: 2,046
Non-trainable params: 19
_________________________________________________________________
Printing summary of the trained model:
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 9)                19
 n)

 hidden1 (Dense)             (None, 50)                500

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,065
Trainable params: 2,046
Non-trainable params: 19
_________________________________________________________________
None
1595/1595 [==============================] - 1s 375us/step
723/723 [==============================] - 0s 375us/step
12723/12723 [==============================] - 5s 388us/step
5817/5817 [==============================] - 2s 380us/step
Model: "sequential_1"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_1 (Normalizat  (None, 11)               23
 ion)

 hidden1 (Dense)             (None, 50)                600

 hidden2 (Dense)             (None, 25)                1275
```

```
 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,169
Trainable params: 2,146
Non-trainable params: 23
_________________________________________________________________
Printing summary of the trained model:
Model: "sequential_1"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_1 (Normalizat  (None, 11)               23
 ion)

 hidden1 (Dense)             (None, 50)                600

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 2,169
Trainable params: 2,146
Non-trainable params: 23
_________________________________________________________________
None
1587/1587 [==============================] - 1s 440us/step
731/731 [==============================] - 0s 397us/step
12725/12725 [==============================] - 5s 398us/step
5815/5815 [==============================] - 2s 383us/step
Model: "sequential_2"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_2 (Normalizat  (None, 7)                15
 ion)

 hidden1 (Dense)             (None, 50)                400

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260
```

```
 output (Dense)              (None, 1)                 11

=================================================================
Total params: 1,961
Trainable params: 1,946
Non-trainable params: 15
_________________________________________________________________
Printing summary of the trained model:
Model: "sequential_2"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_2 (Normalizat  (None, 7)                15
 ion)

 hidden1 (Dense)             (None, 50)                400

 hidden2 (Dense)             (None, 25)                1275

 hidden3 (Dense)             (None, 10)                260

 output (Dense)              (None, 1)                 11

=================================================================
Total params: 1,961
Trainable params: 1,946
Non-trainable params: 15
_________________________________________________________________
None
1589/1589 [==============================] - 1s 385us/step
729/729 [==============================] - 0s 382us/step
12724/12724 [==============================] - 6s 469us/step
5815/5815 [==============================] - 2s 384us/step
```


Base List
SRS: Best List
SRS: Smallest List with >80% Accuracy
Loss value
Accuracy value
Number of epochs
NN output
training
validation
test signal
test bg
train signal
train bg

D Code: Model Selection

In this section we can find the code associated with using gridSearchCV for model selection. This code was used to generate the plots in Tables 2 and 3.

[1]:
```python
import h5py
import matplotlib.pyplot as plt
import numpy as np
import tensorflow.keras as K
import pandas as pd
from scikeras.wrappers import KerasClassifier
from sklearn.model_selection import GridSearchCV
```

```
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.
Intel MKL WARNING: Support of Intel(R) Streaming SIMD Extensions 4.2 (Intel(R)
SSE4.2) enabled only processors has been deprecated. Intel oneAPI Math Kernel
Library 2025.0 will require Intel(R) Advanced Vector Extensions (Intel(R) AVX)
instructions.
```

```
2024-04-16 23:38:19.943206: I tensorflow/core/platform/cpu_feature_guard.cc:182]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: SSE4.1 SSE4.2, in other operations,
rebuild TensorFlow with the appropriate compiler flags.
```

1 Loading the Data

[2]:
```python
with h5py.File("info/data/output_signal.h5", "r") as file:
    signal_data = file["events"][:]

with h5py.File("info/data/output_bg.h5", "r") as file:
    bg_data = file["events"][:]
```

[3]:
```python
# storing signal and background data in panda DataFrame
signal = pd.DataFrame(signal_data)
background = pd.DataFrame(bg_data)

# concatenating the data frames to be part of one big set
df = pd.concat([signal, background])

# reseting the indicies
df = df.reset_index()

# creating the labels for the data sets i.e; signal = 1, background = 0 for␣
↪classification
labels = np.concatenate([np.ones(signal.shape[0]), np.zeros(background.
↪shape[0])])
labels = pd.DataFrame({'ttZ': labels})
```

```
# adding labels as a column at the end of the DataFrame
df = df.join(labels)

# shuffling the DataFrame
df_shuffled = df.sample(frac=1, random_state=42)  # 'random_state' for␣
↪reproducibility
df_shuffled.head()


# taking the first 30 000 rows from the shuffled DataFrame
subset_df = df_shuffled.iloc[:30000]

# splitting the labels from the rest of the dataset
y = subset_df['ttZ']

# we can check the class distribution in the subset
print('ttZ events: {:.2f}%'.format(np.sum(y)/len(y) * 100))
print('WZ events: {:.2f}%'.format((1 - np.sum(y)/len(y)) * 100))
```

```
ttZ events: 68.69%
WZ events: 31.31%
```

2 Various Feature Lists

[4]:

```
# base input list suggested by the project
input_list = [ "H_T",
              "jet_1_pt",
              "jet_2_pt",
              "lep_1_pt",
              "lep_2_pt",
              "n_bjets",
              "jet_1_twb",
              "jet_2_twb",
              "bjet_1_pt"]

# best input list suggested by SRS
input_list_2 = ['jet_1_pt',
                'jet_3_pt',
                'jet_1_eta',
                'jet_3_eta',
                'jet_1_twb',
                'jet_2_twb',
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets',
                'n_leptons']
```

```
# smallest input list that still has an accuracy >80%, suggested by SRS
input_list_3 = ['jet_3_pt',
                'jet_1_twb',
                'jet_2_twb',
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets']

input_lists = [input_list, input_list_2, input_list_3]
```

3 Grid Search through Various Parameters

[5]:
```
# model for classification
def build_model(lr=0.002, layer1=25, layer2=12, layer3=5):
    model = K.Sequential([
        preprocessing_layer,
        K.layers.Dense(layer1, activation="relu"),
        K.layers.Dense(layer2, activation="relu"),
        K.layers.Dense(layer3, activation="relu"),
        K.layers.Dense(1, activation="sigmoid")
    ])
    model.compile(optimizer=K.optimizers.Adam(learning_rate=lr),␣
 ↪loss='binary_crossentropy', metrics=['accuracy'])
    return model

# wrapper function
model = KerasClassifier(model=build_model, verbose=0, epochs = 30)

# Parameters to search through
param_grid = {'model__optimizer__lr': [0.002, 0.0002, 0.00002],
              'model__layer1': [25, 50, 100],
              'model__layer2': [12, 25, 50],
              'model__layer3': [5, 10, 15],
              'batch_size': [100, 150, 300]}

# Create GridSearchCV
gridCV = GridSearchCV(estimator=model, param_grid=param_grid, n_jobs=1, cv=3,␣
 ↪verbose = 1)

# GridSearch through all parameters and all suggested feature lists
names = ['base list', 'SRS: best list', 'SRS: best smallest list']
for i, feature_list in enumerate(input_lists):
    X = subset_df[feature_list]
    preprocessing_layer = K.layers.Normalization()
```

```
    preprocessing_layer.adapt(X)
    grid_result = gridCV.fit(X, y)

# saving results into a DataFrame
    if i == 0:
        df = pd.DataFrame.from_dict(grid_result.best_params_, orient='index')
        df.loc['best score'] = grid_result.best_score_
        df = df.rename(columns={0: names[i]})
    else:
        df2 = pd.DataFrame.from_dict(grid_result.best_params_, orient='index')
        df2.loc['best score'] = grid_result.best_score_
        df2 = df2.rename(columns={0: names[i]})
        df = pd.concat([df, df2], axis=1)

df.to_csv('model_selection.csv', index=True)
df
```

```
Fitting 3 folds for each of 243 candidates, totalling 729 fits
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```

[5]:

	base list	SRS: best list	SRS: best smallest list
batch_size	300.0000	100.0000	150.0000
model__layer1	50.0000	25.0000	50.0000
model__layer2	12.0000	25.0000	50.0000
model__layer3	10.0000	15.0000	5.0000
model__optimizer__lr	0.0020	0.0020	0.0002
best score	0.8296	0.8339	0.8270

E Code: Best Models

This code was used to generate the plots in Fig. 4 and Fig. 5

[1]:
```python
import h5py
import matplotlib.pyplot as plt
import numpy as np
import tensorflow.keras as K
from sklearn.model_selection import train_test_split
import pandas as pd
from sklearn.metrics import accuracy_score
from sklearn.utils import shuffle
```

1 Loading the Data

[2]:
```python
with h5py.File("info/data/output_signal.h5", "r") as file:
    signal_data = file["events"][:]

with h5py.File("info/data/output_bg.h5", "r") as file:
    bg_data = file["events"][:]
```

[3]:
```python
# storing signal and background data in panda DataFrame
signal = pd.DataFrame(signal_data)
background = pd.DataFrame(bg_data)

# concatenating the data frames to be part of one big set
df = pd.concat([signal, background])

# reseting the indicies
df = df.reset_index()

# creating the labels for the data sets i.e; signal = 1, background = 0 for␣
 ↪classification
labels = np.concatenate([np.ones(signal.shape[0]), np.zeros(background.
 ↪shape[0])])
labels = pd.DataFrame({'ttZ': labels})

# adding labels as a column at the end of the DataFrame
df = df.join(labels)

# shuffling the DataFrame
df_shuffled = df.sample(frac=1, random_state=42)  # 'random_state' for␣
 ↪reproducibility
df_shuffled.head()

# splitting the labels from the rest of the dataset
y = df_shuffled['ttZ']

# we can check the class distribution in the subset
print('ttZ events: {:.2f}%'.format(np.sum(y)/len(y) * 100))
```

```python
print('WZ events: {:.2f}%'.format((1 - np.sum(y)/len(y)) * 100))
```

```
ttZ events: 68.65%
WZ events: 31.35%
```

2 Various Feature Lists

[4]:
```python
# base input list suggested by the project
input_list = [ "H_T",
               "jet_1_pt",
               "jet_2_pt",
               "lep_1_pt",
               "lep_2_pt",
               "n_bjets",
               "jet_1_twb",
               "jet_2_twb",
               "bjet_1_pt"]

# best input list suggested by SRS
input_list_2 = ['jet_1_pt',
                'jet_3_pt',
                'jet_1_eta',
                'jet_3_eta',
                'jet_1_twb',
                'jet_2_twb',
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets',
                'n_leptons']

# smallest input list that still has an accuracy >80%, suggested by SRS
input_list_3 = ['jet_3_pt',
                'jet_1_twb',
                'jet_2_twb',
                'jet_3_twb',
                'bjet_1_pt',
                'n_jets',
                'n_bjets']

input_lists = [input_list, input_list_2, input_list_3]
```

3 Defining Model Function

[5]:
```
def build_model(lr=0.002, layer1=25, layer2=12, layer3=5):
    model = K.Sequential([
        preprocessing_layer,
        K.layers.Dense(layer1, activation="relu"),
        K.layers.Dense(layer2, activation="relu"),
        K.layers.Dense(layer3, activation="relu"),
        K.layers.Dense(1, activation="sigmoid")
    ])
    model.compile(optimizer=K.optimizers.Adam(learning_rate=lr),␣
 ↪loss='binary_crossentropy', metrics=['accuracy'])
    return model
```

4 Importing Best Results

[6]:
```
# from model_selection.ipynb
results = pd.read_csv('model_selection.csv')
results
```

[6]:

	Unnamed: 0	base list	SRS: best list	SRS: best smallest list
0	batch_size	300.0000	100.0000	150.0000
1	model__layer1	50.0000	25.0000	50.0000
2	model__layer2	12.0000	25.0000	50.0000
3	model__layer3	10.0000	15.0000	5.0000
4	model__optimizer__lr	0.0020	0.0020	0.0002
5	best score	0.8296	0.8339	0.8270

5 Feature Importance through Permutations

[7]:
```
# Function to calculate permutation feature importance
def permutation_importance(model, X_valid, y_valid, metric=accuracy_score):

    # Store the baseline accuracy of the model on original data
    baseline_accuracy = metric(y_valid, model.predict(X_valid).round())

    # accuracy decreases will be stored here
    importances = []

    # iterations over each feature
    for i in range(X_valid.shape[1]):
        save = X_valid[:, i].copy()

        # shuffle individual feature
        X_valid[:, i] = shuffle(X_valid[:, i])
        m_accuracy = metric(y_valid, model.predict(X_valid).round())
```

```
        # restore original data
        X_valid[:, i] = save

        # store decrease in accuracy for feature i
        importances.append(baseline_accuracy - m_accuracy)

    return np.array(importances)
```

6 Running Best Models For Each Feature List And Ranking their Feature Importances

[8]:
```
# fig for all best model performances from each feature list
fig, axs = plt.subplots(3, 3, figsize=(12, 16), sharey='row')

#
fig2, axs2 = plt.subplots(3, 1, figsize=(12, 16))

for i, feature_list in enumerate(input_lists):
    names = ['base list', 'SRS: best list', 'SRS: best smallest list']

    ## train, test, val splits
    X = df_shuffled[feature_list]
    x_train, x_rem, y_train, y_rem = train_test_split(X, y, train_size=0.8)
    x_val, x_test, y_val, y_test = train_test_split(x_rem, y_rem, train_size=0.5)

    ## building model
    preprocessing_layer = K.layers.Normalization()
    preprocessing_layer.adapt(x_train)

    model = build_model(lr=results[names[i]][4],
                        layer1=int(results[names[i]][1]),
                        layer2=int(results[names[i]][2]),
                        layer3=int(results[names[i]][3]))

    # fitting model
    fit_history = model.fit(
        x_train,
        y_train,
        batch_size=int(results[names[i]][0]),
        epochs=100,
        validation_data=(x_val, y_val),
        verbose = 0)


    print("Printing summary of the trained model:")
```

```
    print(model.summary())

    titles = ['Base List', 'SRS: Best List', 'SRS: Smallest List with >80%␣
↪Accuracy']

    # plotting performance results
    axs[0, i].plot(fit_history.history["loss"], label="training")
    axs[0, i].plot(fit_history.history["val_loss"], label="validation")
    axs[0, i].legend()
    axs[0, i].set_title(titles[i])

    axs[1, i].plot(fit_history.history["accuracy"], label="training")
    axs[1, i].plot(fit_history.history["val_accuracy"], label="validation")
    axs[1, i].legend()

    _, bins, _ = axs[2, i].hist(model.predict(x_test[y_test.astype(bool)]),␣
↪bins=20, alpha=0.3, density=True, label="test signal")
    axs[2, i].hist(model.predict(x_test[~y_test.astype(bool)]), bins=bins,␣
↪alpha=0.3, density=True, label="test bg")
    axs[2, i].hist(model.predict(x_train[y_train.astype(bool)]), bins=bins,␣
↪density=True, histtype="step", label="train signal")
    axs[2, i].hist(model.predict(x_train[~y_train.astype(bool)]), bins=bins,␣
↪density=True, histtype="step", label="train bg")
    axs[2, i].legend()

    if i == 0:
            axs[0, i].set_ylabel("Loss")
            axs[1, i].set_ylabel("Accuracy")

    elif i == 1:
        axs[0, i].set_xlabel("Number of epochs")
        axs[1, i].set_xlabel("Number of epochs")
        axs[2, i].set_xlabel("NN output")


    # plotting feature rankings through the permutation method
    feature_importances = permutation_importance(model, x_test.to_numpy(),␣
↪y_test.to_numpy())

    # Sorting the features by importance
    df = pd.DataFrame({'Label': x_test.columns, 'Value': feature_importances})
    df = df.sort_values('Value', ascending=False)

    # Plotting the sorted data
    axs2[i].bar(df['Label'], df['Value'], color='blue')
    axs2[i].set_xticklabels(df['Label'], rotation=45)
```

```python
    axs2[i].set_title(titles[i])

    if i == 1:
        axs2[i].set_ylabel('Decrease in Accuracy')
    elif i == 2:
        axs2[i].set_xlabel('Features')

    # evaluating test sets
    probs = model.predict(x_test)
    y_pred = (probs > 0.5).astype(int)
    print(names[i])
    print(accuracy_score(y_test, y_pred))

fig.tight_layout()
fig.savefig("best_models.pdf")

fig2.tight_layout()
fig2.savefig("feature_importances.pdf")

plt.show()
```

```
Printing summary of the trained model:
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 9)                19
 n)

 dense (Dense)               (None, 50)                500

 dense_1 (Dense)             (None, 12)                612

 dense_2 (Dense)             (None, 10)                130

 dense_3 (Dense)             (None, 1)                 11

=================================================================
Total params: 1,272
Trainable params: 1,253
Non-trainable params: 19
_________________________________________________________________
None
1590/1590 [==============================] - 1s 371us/step
728/728 [==============================] - 0s 374us/step
12727/12727 [==============================] - 5s 409us/step
5812/5812 [==============================] - 2s 416us/step
2318/2318 [==============================] - 1s 447us/step
```

```
2318/2318 [==============================] - 1s 479us/step
2318/2318 [==============================] - 1s 453us/step
2318/2318 [==============================] - 1s 461us/step
2318/2318 [==============================] - 1s 441us/step
2318/2318 [==============================] - 1s 445us/step
2318/2318 [==============================] - 1s 527us/step
2318/2318 [==============================] - 1s 453us/step
2318/2318 [==============================] - 1s 491us/step
2318/2318 [==============================] - 1s 445us/step
 387/2318 [====>...] - ETA: 0s

/var/folders/3x/lv7sddxn2gg8mq0dwdcn1wg40000gn/T/ipykernel_79200/1070017733.py:7
5: UserWarning: set_ticklabels() should only be used with a fixed number of
ticks, i.e. after set_ticks() or using a FixedLocator.
  axs2[i].set_xticklabels(df['Label'], rotation=45)

2318/2318 [==============================] - 1s 402us/step
base list
0.8290854168352347
Printing summary of the trained model:
Model: "sequential_1"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_1 (Normalizat  (None, 11)               23
 ion)

 dense_4 (Dense)             (None, 25)                300

 dense_5 (Dense)             (None, 25)                650

 dense_6 (Dense)             (None, 15)                390

 dense_7 (Dense)             (None, 1)                 16

=================================================================
Total params: 1,379
Trainable params: 1,356
Non-trainable params: 23
_________________________________________________________________
None
1589/1589 [==============================] - 1s 371us/step
729/729 [==============================] - 0s 370us/step
12725/12725 [==============================] - 5s 367us/step
5814/5814 [==============================] - 2s 386us/step
2318/2318 [==============================] - 1s 372us/step
2318/2318 [==============================] - 1s 377us/step
2318/2318 [==============================] - 1s 369us/step
2318/2318 [==============================] - 1s 367us/step
```

```
2318/2318 [==============================] - 1s 610us/step
2318/2318 [==============================] - 1s 376us/step
2318/2318 [==============================] - 1s 370us/step
2318/2318 [==============================] - 1s 369us/step
2318/2318 [==============================] - 1s 367us/step
2318/2318 [==============================] - 1s 367us/step
2318/2318 [==============================] - 1s 417us/step
2318/2318 [==============================] - 1s 409us/step
 406/2318 [====>...] - ETA: 0s
```

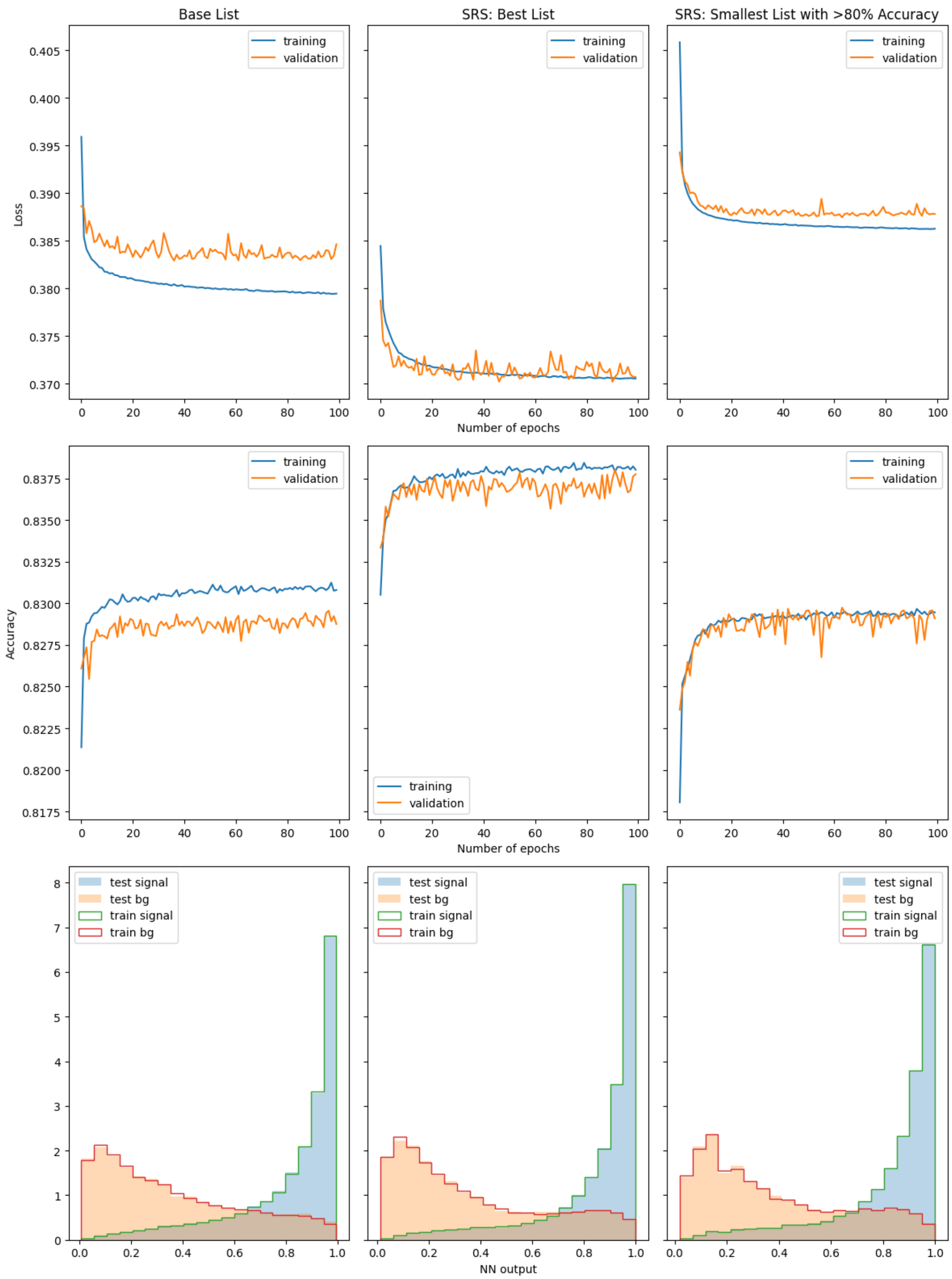
```
/var/folders/3x/lv7sddxn2gg8mq0dwdcn1wg40000gn/T/ipykernel_79200/1070017733.py:7
5: UserWarning: set_ticklabels() should only be used with a fixed number of
ticks, i.e. after set_ticks() or using a FixedLocator.
  axs2[i].set_xticklabels(df['Label'], rotation=45)
```

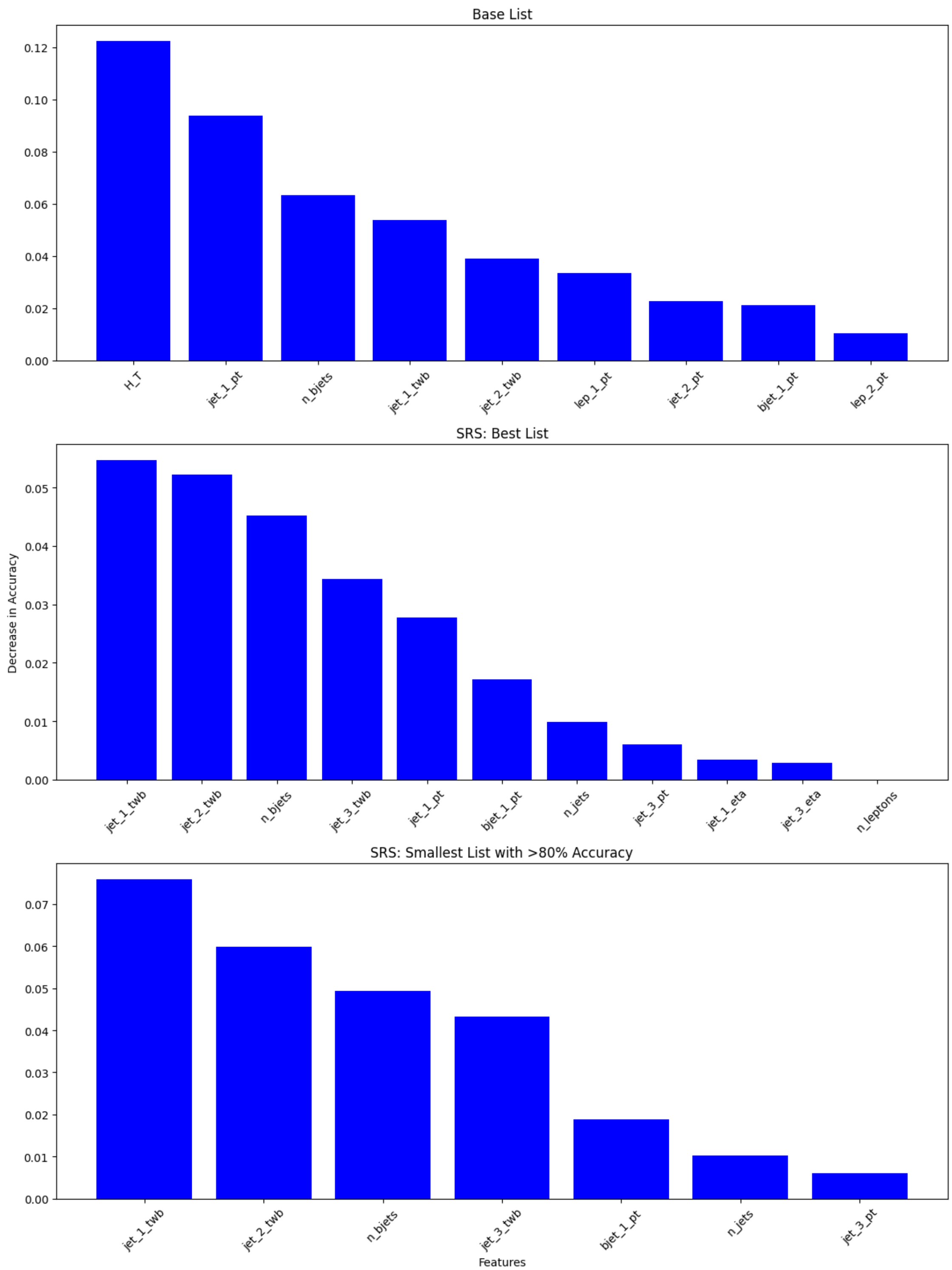
```
2318/2318 [==============================] - 1s 368us/step
SRS: best list
0.839482698168676
Printing summary of the trained model:
Model: "sequential_2"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization_2 (Normalizat  (None, 7)                15
 ion)

 dense_8 (Dense)             (None, 50)                400

 dense_9 (Dense)             (None, 50)                2550

 dense_10 (Dense)            (None, 5)                 255

 dense_11 (Dense)            (None, 1)                 6

=================================================================
Total params: 3,226
Trainable params: 3,211
Non-trainable params: 15
_________________________________________________________________
None
1595/1595 [==============================] - 1s 440us/step
723/723 [==============================] - 0s 472us/step
12721/12721 [==============================] - 5s 385us/step
5818/5818 [==============================] - 2s 387us/step
2318/2318 [==============================] - 1s 417us/step
2318/2318 [==============================] - 1s 374us/step
2318/2318 [==============================] - 1s 377us/step
2318/2318 [==============================] - 1s 375us/step
2318/2318 [==============================] - 1s 376us/step
```

```
2318/2318 [==============================] - 1s 375us/step
2318/2318 [==============================] - 1s 375us/step
2318/2318 [==============================] - 1s 374us/step
 400/2318 [====>...] - ETA: 0s
```

```
/var/folders/3x/lv7sddxn2gg8mq0dwdcn1wg40000gn/T/ipykernel_79200/1070017733.py:7
5: UserWarning: set_ticklabels() should only be used with a fixed number of
ticks, i.e. after set_ticks() or using a FixedLocator.
  axs2[i].set_xticklabels(df['Label'], rotation=45)
```

```
2318/2318 [==============================] - 1s 378us/step
SRS: best smallest list
0.8313240014024867
```


Base List
SRS: Best List
SRS: Smallest List with >80% Accuracy
training
validation
Loss
Number of epochs
Accuracy
test signal
test bg
train signal
train bg
NN output



Base List
H_T
jet_1_pt
n_bjets
jet_1_twb
jet_2_twb
lep_1_pt
jet_2_pt
bjet_1_pt
lep_2_pt
SRS: Best List
Decrease in Accuracy
jet_1_twb
jet_2_twb
n_bjets
jet_3_twb
jet_1_pt
bjet_1_pt
n_jets
jet_3_pt
jet_1_eta
jet_3_eta
n_leptons
SRS: Smallest List with >80% Accuracy
jet_1_twb
jet_2_twb
n_bjets
jet_3_twb
bjet_1_pt
n_jets
jet_3_pt
Features