02_Tabular_Data_BDT

February 19, 2026

1 Hands-on 02: Tabular data and BDTs: Classifying LHC collisions

1.1 XGBoost Tutorial

[1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import xgboost as xgb

%matplotlib inline
```

1.1.1 Data

Load data First, load in the data and look at it. We will download a 10k event subsample of the Kaggle training data. Then we'll put it in the right format for XGBoost.

[2]:
```
data = pd.read_csv("../data/training_10k.csv")
```

Let's see what the data looks like:

[3]:
```
print("Size of data: {}".format(data.shape))
print("Number of events: {}".format(data.shape[0]))
print("Number of columns: {}".format(data.shape[1]))

print("\nList of features in dataset:")
for col in data.columns:
    print(col)
```

```
Size of data: (10000, 33)
Number of events: 10000
Number of columns: 33

List of features in dataset:
EventId
DER_mass_MMC
DER_mass_transverse_met_lep
DER_mass_vis
DER_pt_h
```

```
DER_deltaeta_jet_jet
DER_mass_jet_jet
DER_prodeta_jet_jet
DER_deltar_tau_lep
DER_pt_tot
DER_sum_pt
DER_pt_ratio_lep_tau
DER_met_phi_centrality
DER_lep_eta_centrality
PRI_tau_pt
PRI_tau_eta
PRI_tau_phi
PRI_lep_pt
PRI_lep_eta
PRI_lep_phi
PRI_met
PRI_met_phi
PRI_met_sumet
PRI_jet_num
PRI_jet_leading_pt
PRI_jet_leading_eta
PRI_jet_leading_phi
PRI_jet_subleading_pt
PRI_jet_subleading_eta
PRI_jet_subleading_phi
PRI_jet_all_pt
Weight
Label
```

[4]:
```
# look at column labels --- notice last one is "Label" and first is "EventId"␣
  ↪also "Weight"
print(f"Number of signal events: {len(data[data.Label == 's'])}")
print(f"Number of background events: {len(data[data.Label == 'b'])}")
print(f"Fraction signal: {len(data[data.Label == 's'])/(len(data[data.Label ==␣
  ↪'s']) + len(data[data.Label == 'b']))}")
```

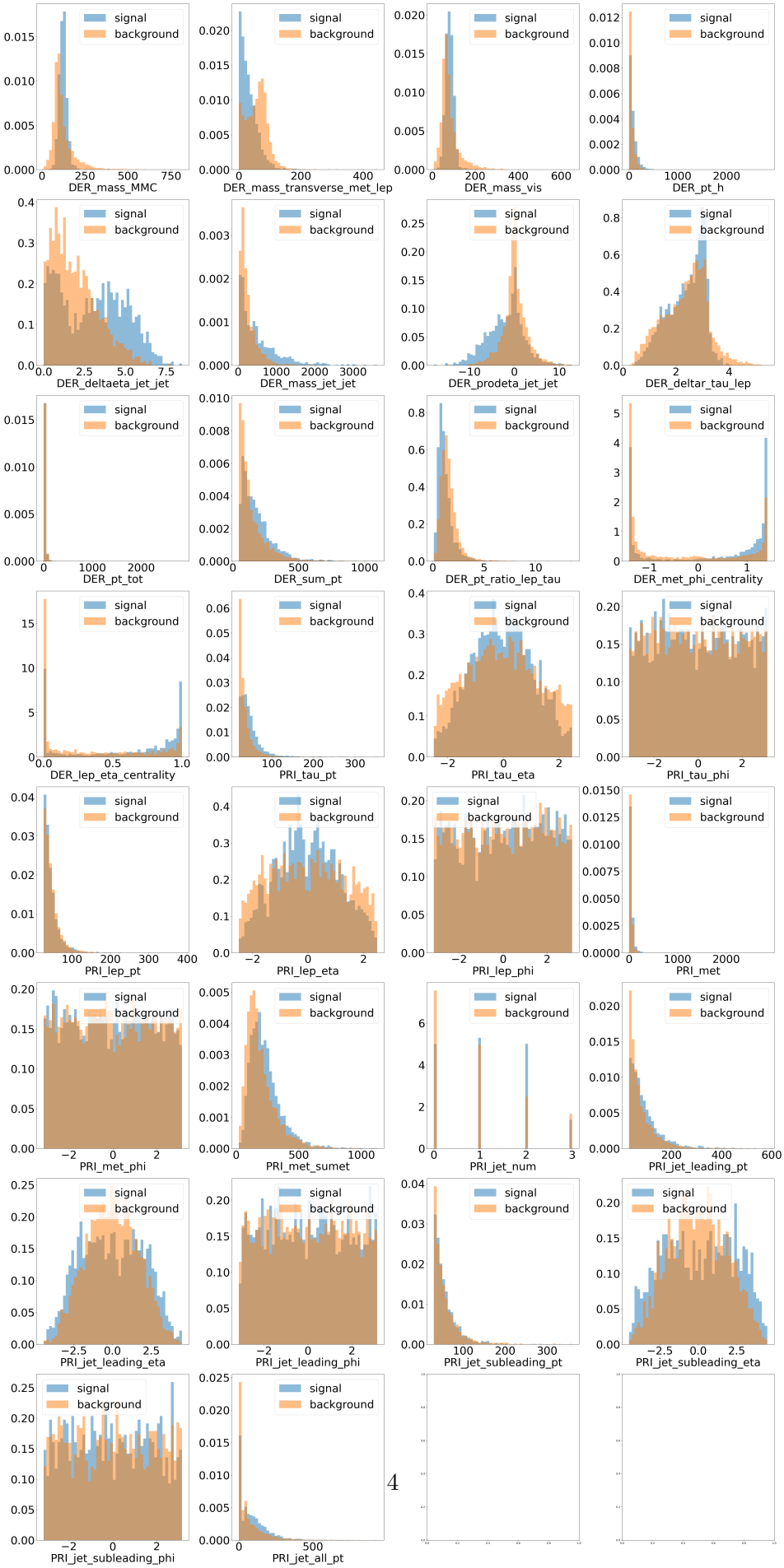
```
Number of signal events: 3372
Number of background events: 6628
Fraction signal: 0.3372
```

Visualize the features:

[5]:
```
plt.figure()


fig, axs = plt.subplots(8, 4, figsize=(40, 80))

for ix, ax in enumerate(axs.reshape(-1)):
    col = data.columns[ix + 1]
```

```
    if col == "Weight" or col == "Label":
        continue
    signal = data[col][data.Label == "s"].to_numpy()
    mask_signal = signal > -999
    background = data[col][data.Label == "b"].to_numpy()
    mask_background = background > -999
    xmin = min(np.min(background[mask_background]), np.min(signal[mask_signal]))
    xmax = max(np.max(background[mask_background]), np.max(signal[mask_signal]))

    ax.hist(signal[mask_signal], bins=np.linspace(xmin, xmax, 51), alpha=0.5,␣
 ↪label="signal", density=True)
    ax.hist(background[mask_background], bins=np.linspace(xmin, xmax, 51),␣
 ↪alpha=0.5, label="background", density=True)

    ax.set_xlabel(col, fontsize=40)
    ax.set_xlabel(col, fontsize=40)
    ax.tick_params(axis="both", which="major", labelsize=40)
    ax.legend(fontsize=40)
plt.tight_layout()
plt.show()
```

```
<Figure size 640x480 with 0 Axes>
```


signal
background
DER_mass_MMC
DER_mass_transverse_met_lep
DER_mass_vis
DER_pt_h
DER_deltaeta_jet_jet
DER_mass_jet_jet
DER_prodeta_jet_jet
DER_deltar_tau_lep
DER_pt_tot
DER_sum_pt
DER_pt_ratio_lep_tau
DER_met_phi_centrality
DER_lep_eta_centrality
PRI_tau_pt
PRI_tau_eta
PRI_tau_phi
PRI_lep_pt
PRI_lep_eta
PRI_lep_phi
PRI_met
PRI_met_phi
PRI_met_sumet
PRI_jet_num
PRI_jet_leading_pt
PRI_jet_leading_eta
PRI_jet_leading_phi
PRI_jet_subleading_pt
PRI_jet_subleading_eta
PRI_jet_subleading_phi
PRI_jet_all_pt

Format data: Now we should get the data into an XGBoost-friendly format. We can create DMatrix objects that will be used to train the BDT model. For now, we'll use all 30 of the features for training.

First, we'll slice up the data into training and testing sets. Here, we take 20% for the test set, which is arbitrary.

In this file, all samples are independent and ordered randomly, so we can just grab a chunk. Check out Scikit-learn Cross-validation for dividing up samples responsibly.

We can also change the data type of the `Label` column to the Pandas type `category` for easier use later.

[6]:
```
data["Label"] = data.Label.astype("category")
```

[7]:
```
data_train = data[:8000]
data_test = data[8000:]
```

Check to make sure we did it right:

[8]:
```
print(f"Number of training samples: {len(data_train)}")
print(f"Number of testing samples: {len(data_test)}")
print()
print(f"Number of signal events in training set: {len(data_train[data_train.
 ↪Label == 's'])}")
print(f"Number of background events in training set: {len(data_train[data_train.
 ↪Label == 'b'])}")
print(
    f"Fraction signal: {len(data_train[data_train.Label == 's'])/
 ↪(len(data_train[data_train.Label == 's']) + len(data_train[data_train.Label␣
 ↪== 'b']))}"
)
```

```
Number of training samples: 8000
Number of testing samples: 2000

Number of signal events in training set: 2688
Number of background events in training set: 5312
Fraction signal: 0.336
```

The `DMatrix` object takes as arguments: - `data`: the features - `label`: `1`/`0` or `True`/`False` for binary data (we have to convert our label to boolean from string `"s"`/`"b"`) - `missing`: how missing values are represented (here as `-999.0`) - `feature_names`: the names of all the features (optional)

[9]:
```
feature_names = list(data.columns[1:-2])  # we skip the first and last two␣
 ↪columns because they are the ID, weight, and label
```

```
print(len(feature_names))

train = xgb.DMatrix(
    data=data_train[feature_names], label=data_train.Label.cat.codes,␣
 ↪missing=-999.0, feature_names=feature_names
)
test = xgb.DMatrix(
    data=data_test[feature_names], label=data_test.Label.cat.codes,␣
 ↪missing=-999.0, feature_names=feature_names
)
```

```
30
```

Check if we did it right:

[10]:
```
print(f"Number of training samples: {train.num_row()}")
print(f"Number of testing samples: {test.num_row()}")
print()
print(f"Number of signal events in training set: {len(np.where(train.
 ↪get_label())[0])}")
```

```
Number of training samples: 8000
Number of testing samples: 2000

Number of signal events in training set: 2688
```

1.1.2 Make the model

Set hyperparameters: The XGBoost hyperparameters are defined here. For a nice description of what they all mean, and tips on tuning them, see this guide.

In general, the tunable parameters in XGBoost are the ones you would see in other gradient boosting libraries. Here, they fall into three categories: 1. General parameters: e.g., which booster to use, number of threads. We won't mess with these here. 2. Booster parameters: Tune the actual boosting, e.g., learning rate. These are the ones to optimize. 3. Learning task parameters: Define the objective function and the evaluation metrics.

Here, we will use the defaults for most parameters and just set a few to see how it's done. The parameters are passed in as a dictionary or list of pairs.

Make the parameter dictionary:

[11]:
```
param = {}

param["seed"] = 42  # set seed for reproducibility

# Booster parameters
param["eta"] = 0.1  # learning rate
param["max_depth"] = 10  # maximum depth of a tree
param["subsample"] = 0.8  # fraction of events to train tree on
```

```
param["colsample_bytree"] = 0.8  # fraction of features to train tree on

# Learning task parameters
param["objective"] = "binary:logistic"  # objective function
param["eval_metric"] = "error"  # evaluation metric for cross validation, note:␣
 ↪last one is used for early stopping
param = list(param.items())

num_trees = 100  # number of trees to make
```

First, we set the booster parameters. Again, we just chose a few here to experiment with. These are the parameters to tune to optimize your model. Generally, there is a trade off between speed and accuracy. 1. `eta` is the learning rate. It determines how much to change the data weights after each boosting iteration. The default is 0.3. 2. `max_depth` is the maximum depth of any tree. The default is 6. 3. `subsample` is the fraction of events used to train each new tree. These events are randomly sampled each iteration from the whole sample set. The default is 1 (use every event for each tree). 4. `colsample_bytree` is the fraction of features available to train each new tree. These features are randomly sampled each iteration from the whole feature set. The default is 1.

Next, we set the learning objective to `binary:logistic`. So, we have two classes that we want to score from 0 to 1. The `eval_metric` parameters set what we want to monitor when doing cross validation. (We aren't doing cross validation in this example, but we should be!) If you want to watch more than one metric, `param` must be a list of pairs, instead of a dict. Otherwise, we would just keep resetting the same parameter.

Last, we set the number of trees to 100. Usually, you would set this number high, and choose a cut off point based on the cross validation. The number of trees is the same as the number of iterations.

1.1.3 Now train!

[12]:
```
booster = xgb.train(param, train, num_boost_round=num_trees)
```

We now have a trained model. The next step is to look at it's performance and try to improve the model if we need to. We can try to improve it by improving/adding features, adding more training data, using more boosting iterations, or tuning the hyperparameters (ideally in that order).

Evaluate: First, let's look at how it does on the test set:

[13]:
```
print(booster.eval(test))
```

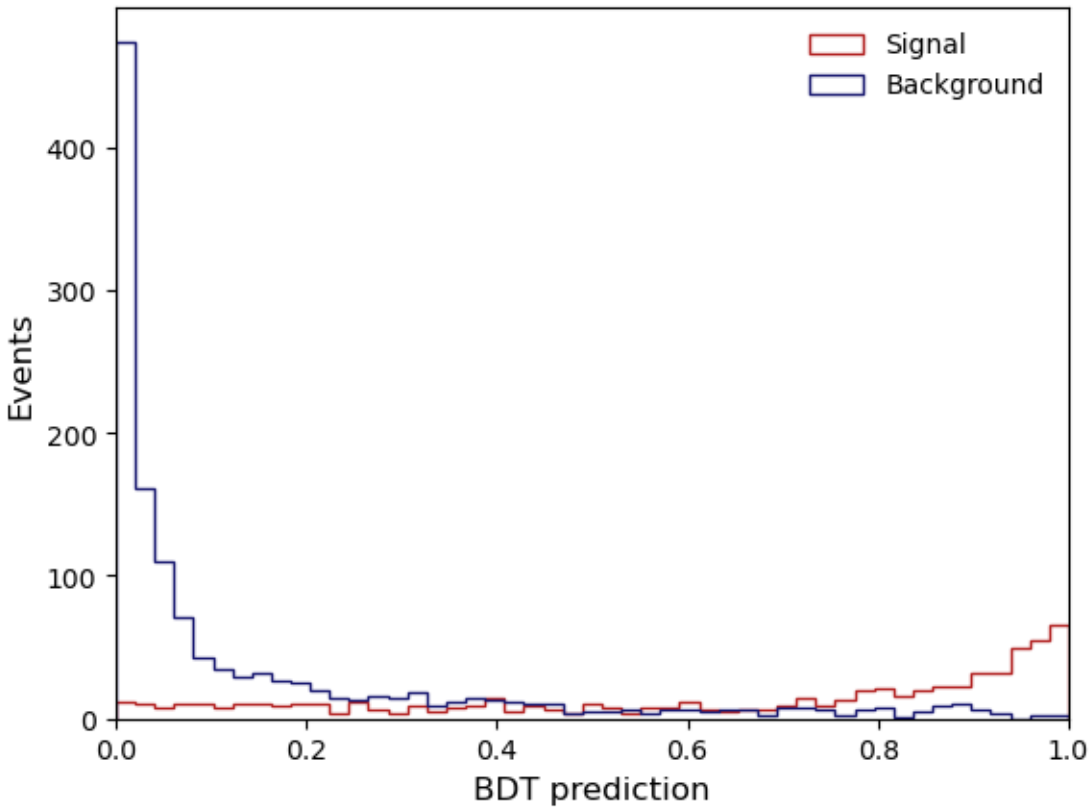
```
[0]     eval-error:0.17050000000000001
```

These are the evaluation metrics that we stored in the parameter set.

It's pretty hard to interpret the performance of a classifier from a few number. So, let's look at the predictions for the entire test set.

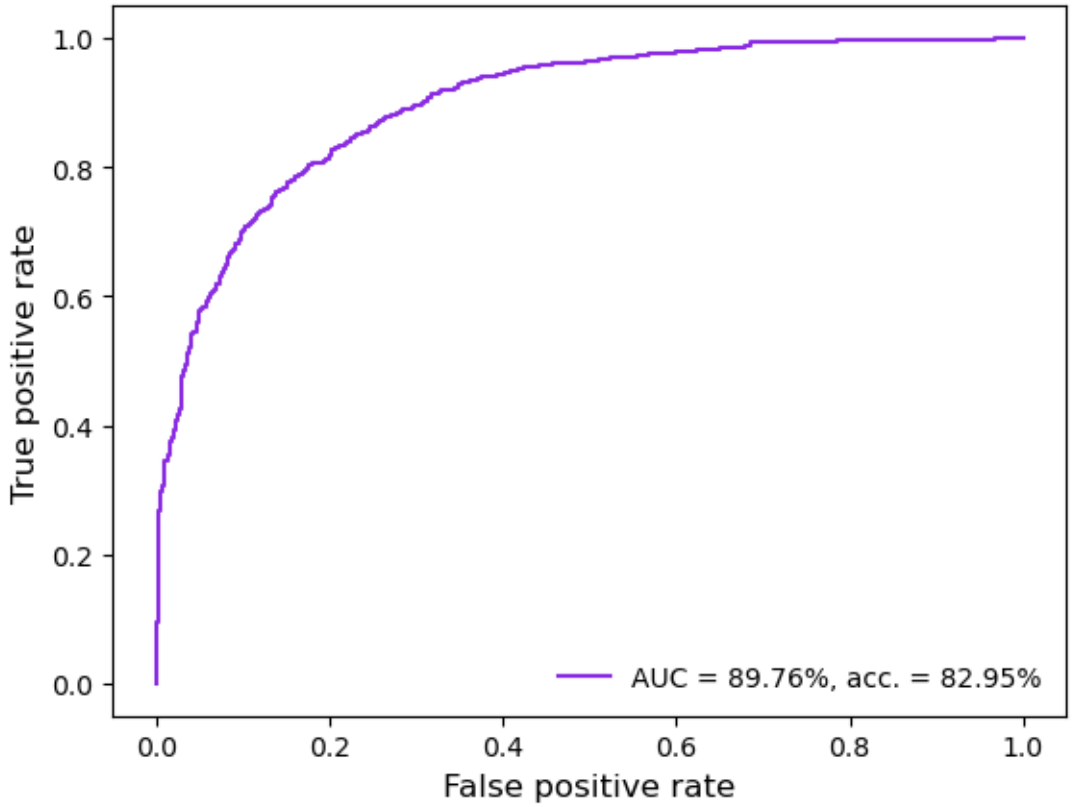
[14]:
```
predictions = booster.predict(test)
labels = test.get_label().astype(bool)
```

[15]:
```
# plot signal and background predictions, separately
plt.figure()
plt.hist(predictions[labels], bins=np.linspace(0, 1, 50), histtype="step",␣
 ↪color="firebrick", label="Signal")
plt.hist(predictions[~labels], bins=np.linspace(0, 1, 50), histtype="step",␣
 ↪color="midnightblue", label="Background")
# make the plot readable
plt.xlabel("BDT prediction", fontsize=12)
plt.ylabel("Events", fontsize=12)
plt.legend(frameon=False)
plt.xlim(0, 1)
plt.show()
```



[16]:
```
from sklearn.metrics import roc_curve, auc, accuracy_score

fpr, tpr, _ = roc_curve(labels, predictions)
auc_score = auc(fpr, tpr)
acc_score = accuracy_score(labels, predictions > 0.5)

# plot TPR vs. FPR (ROC curve)
```

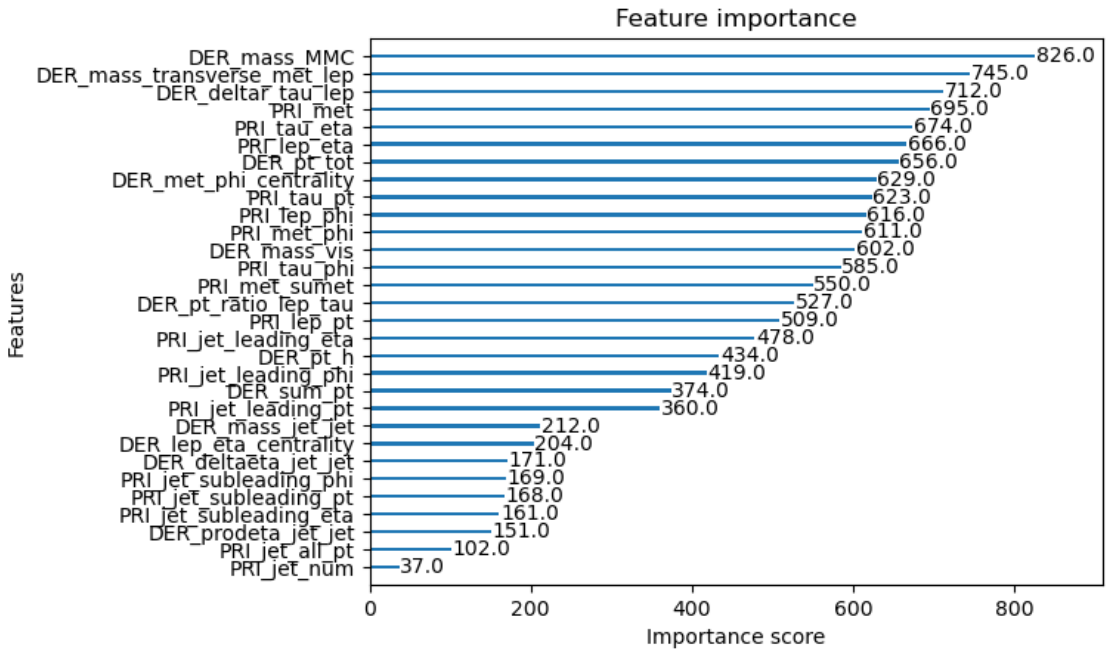
```
plt.figure()
plt.plot(fpr, tpr, color="blueviolet", label=f"AUC = {auc_score*100:.2f}%, acc.␣
  ↪= {acc_score*100:.2f}%")
# make the plot readable
plt.xlabel("False positive rate", fontsize=12)
plt.ylabel("True positive rate", fontsize=12)
plt.legend(frameon=False)
plt.show()
```



It's also very informative to look at the importance of each feature. The "F score" is the number of times each feature is used to split the data over all the trees (times the weight of that tree).

There is a built-in function in the XGBoost Python API to easily plot this.

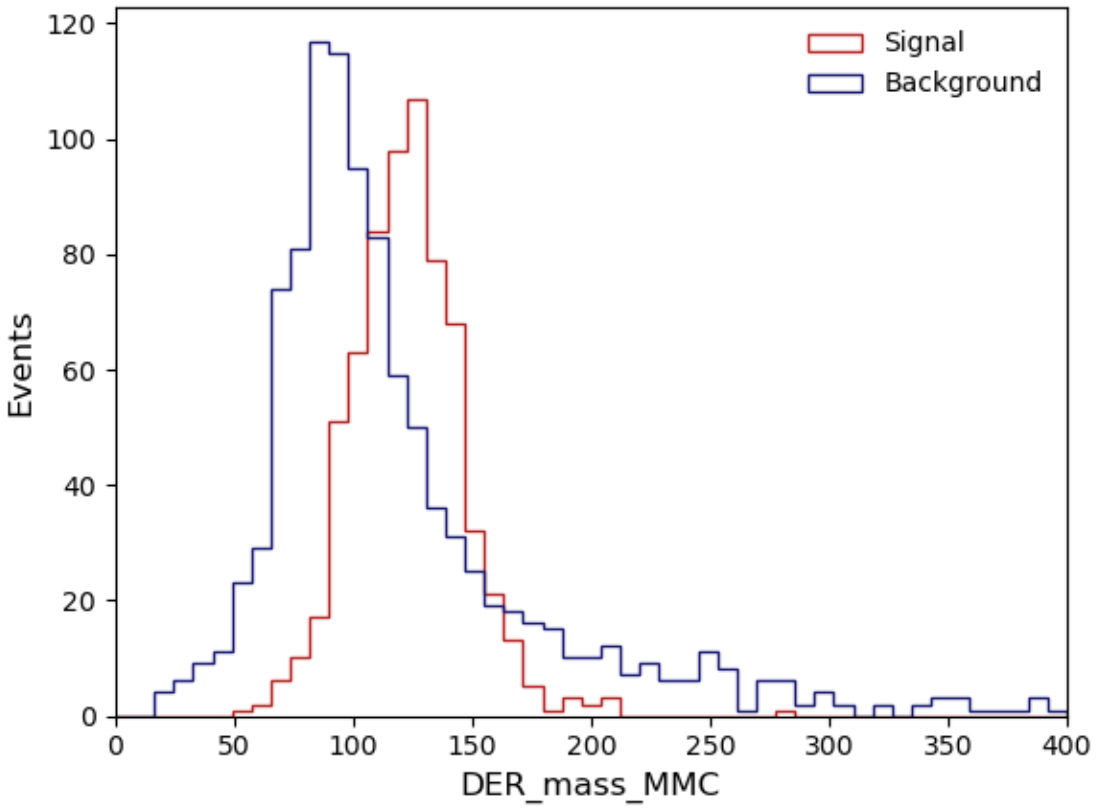
[17]:
```
xgb.plot_importance(booster, grid=False)
plt.show()
```



The feature that was used the most was `DER_mass_MMC`.

We can plot how this feature is distributed for the signal and background.

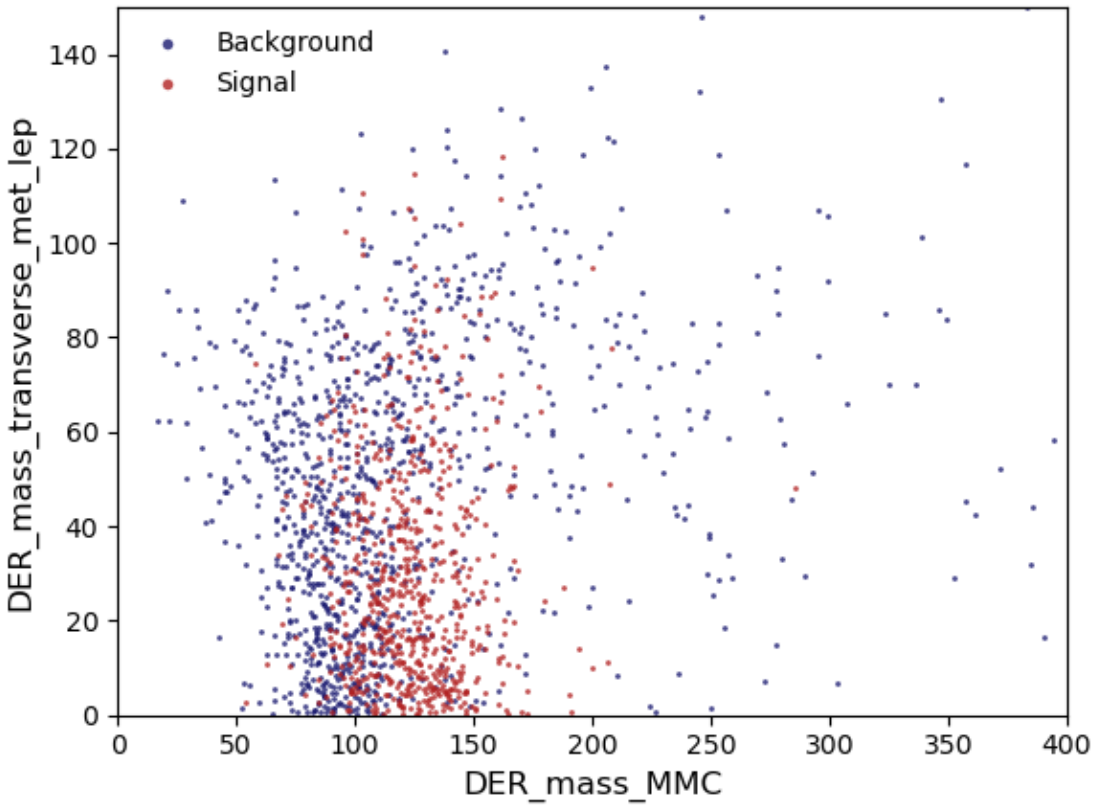
[18]:
```
plt.figure()
plt.hist(
    data_test.DER_mass_MMC[data_test.Label == "s"],
    bins=np.linspace(0, 400, 50),
    histtype="step",
    color="firebrick",
    label="Signal",
)
plt.hist(
    data_test.DER_mass_MMC[data_test.Label == "b"],
    bins=np.linspace(0, 400, 50),
    histtype="step",
    color="midnightblue",
    label="Background",
)

plt.xlim(0, 400)
plt.xlabel("DER_mass_MMC", fontsize=12)
plt.ylabel("Events", fontsize=12)
plt.legend(frameon=False)
plt.show()
```



This variable is physically significant because it represents an estimate of the Higgs boson mass. For signal, it is expected to peak at 125 GeV. We can also plot it with one of the next most important features `DER_mass_transverse_met_lep`. Note: the exact ranking of features can depend on the random seed and other hyperparameters.

[19]:
```
plt.figure()

mask_b = np.array(data_test.Label == "b")
mask_s = np.array(data_test.Label == "s")

DER_mass_MMC = np.array(data_test.DER_mass_MMC)
DER_mass_transverse_met_lep = np.array(data_test.DER_mass_transverse_met_lep)

plt.plot(
    DER_mass_MMC[mask_b],
    DER_mass_transverse_met_lep[mask_b],
    "o",
    markersize=2,
    color="midnightblue",
    markeredgewidth=0,
    alpha=0.8,
```

```
    label="Background",
)
plt.plot(
    DER_mass_MMC[mask_s],
    DER_mass_transverse_met_lep[mask_s],
    "o",
    markersize=2,
    color="firebrick",
    markeredgewidth=0,
    alpha=0.8,
    label="Signal",
)
plt.xlim(0, 400)
plt.ylim(0, 150)
plt.xlabel("DER_mass_MMC", fontsize=12)
plt.ylabel("DER_mass_transverse_met_lep", fontsize=12)
plt.legend(frameon=False, numpoints=1, markerscale=2)
plt.show()
```



1.2 Exercise: Retrain BDT with 2 features and plot decision boundary

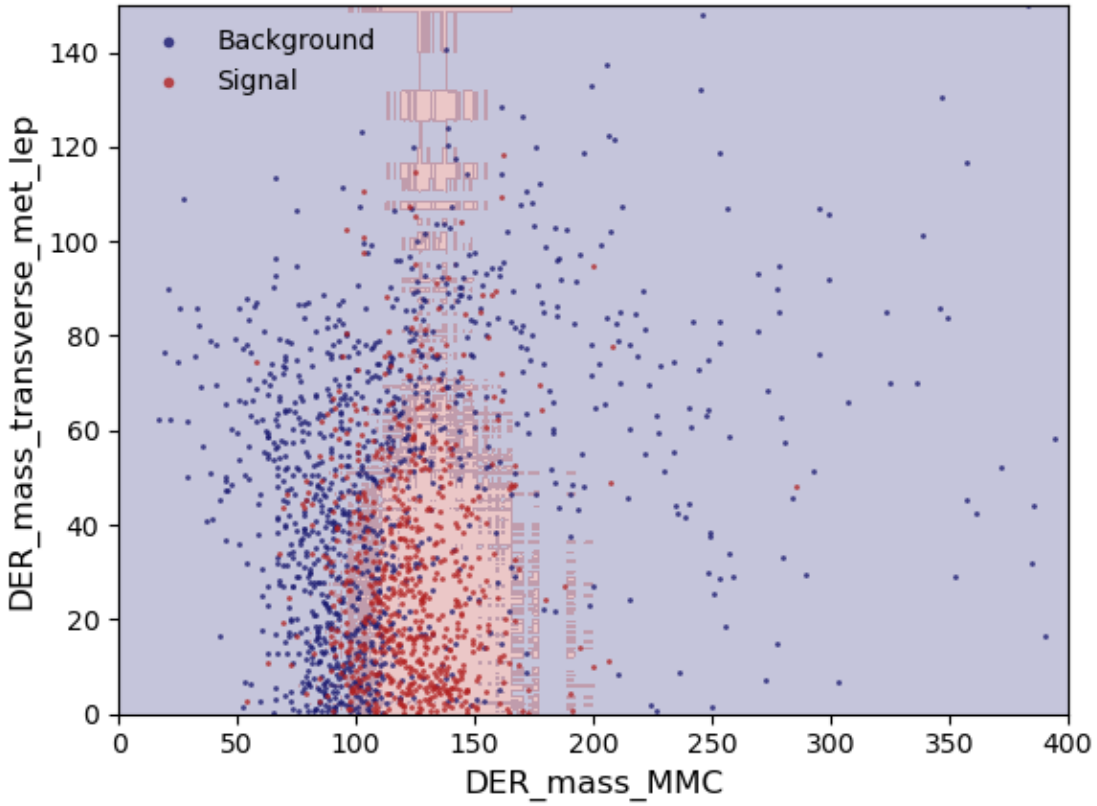
Repeat the steps above but manually set the features to just two of the most "important" ones: `feature_names = ["DER_mass_MMC", "DER_mass_transverse_met_lep"]`

Then use the code below to plot the decision boundary in 2D. 1) What do you notice about the shape of the decision boundary? 2) Do you see any evidence of overfitting? How can you prove it? (Hint: consider the training data)

[20]:
```
feature_names = ["DER_mass_MMC", "DER_mass_transverse_met_lep"]

train = xgb.DMatrix(
    data=data_train[feature_names], label=data_train.Label.cat.codes,␣
 ↪missing=-999.0, feature_names=feature_names
)

test = xgb.DMatrix(
    data=data_test[feature_names], label=data_test.Label.cat.codes,␣
 ↪missing=-999.0, feature_names=feature_names
)

booster = xgb.train(param, train, num_boost_round=num_trees)
```

[21]:
```
from matplotlib.colors import ListedColormap

# first get a mesh grid
x_grid, y_grid = np.meshgrid(np.linspace(0, 400, 1000), np.linspace(0, 150,␣
 ↪1000))
# convert grid into DMatrix
matrix_grid = xgb.DMatrix(
    data=np.c_[x_grid.ravel(), y_grid.ravel()], missing=-999.0,␣
 ↪feature_names=feature_names
)
# run prediction for every value in grid
z_grid = booster.predict(matrix_grid)
# reshape
z_grid = z_grid.reshape(x_grid.shape)


plt.figure()
# plot decision boundary
ax = plt.subplot(111)
cm = ListedColormap(["midnightblue", "firebrick"])
plt.contourf(x_grid, y_grid, z_grid, levels=[0, 0.5, 1], cmap=cm, alpha=0.25)
# overlaid with test data points
plt.plot(
    DER_mass_MMC[mask_b],
    DER_mass_transverse_met_lep[mask_b],
```

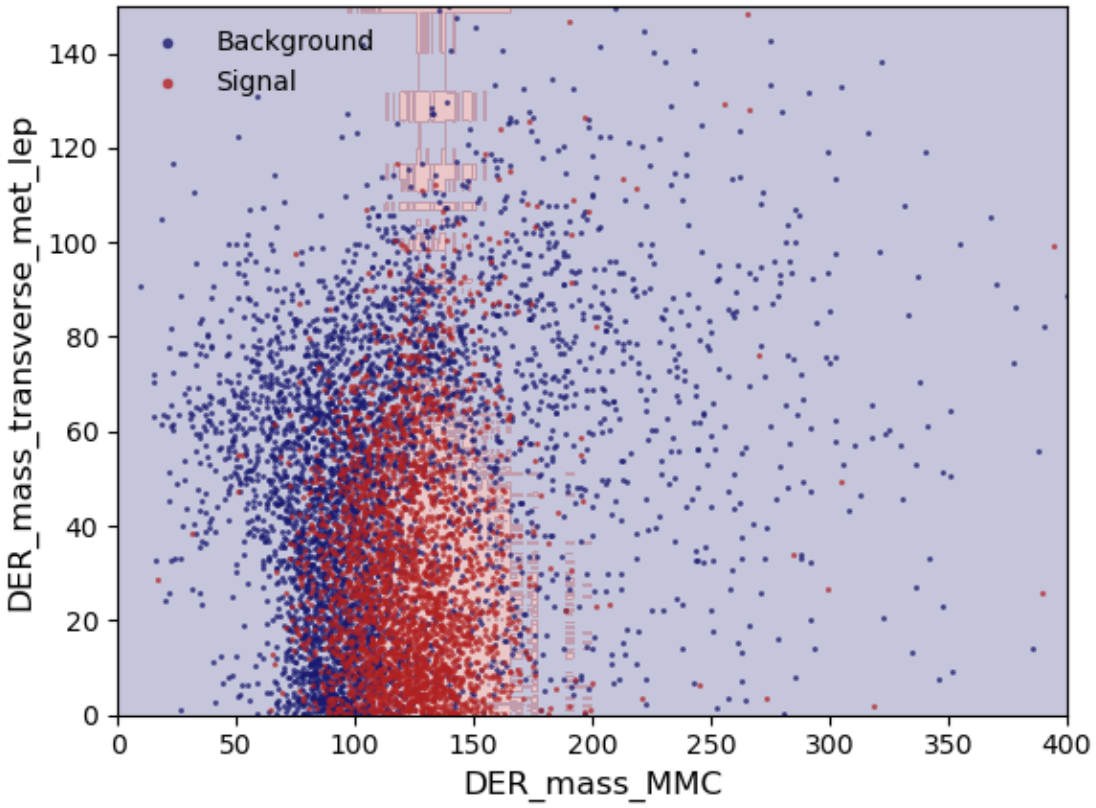
```
    "o",
    markersize=2,
    color="midnightblue",
    markeredgewidth=0,
    alpha=0.8,
    label="Background",
)
plt.plot(
    DER_mass_MMC[mask_s],
    DER_mass_transverse_met_lep[mask_s],
    "o",
    markersize=2,
    color="firebrick",
    markeredgewidth=0,
    alpha=0.8,
    label="Signal",
)
ax.set_ylim(0,150)
ax.set_xlim(0,400)
plt.xlabel("DER_mass_MMC", fontsize=12)
plt.ylabel("DER_mass_transverse_met_lep", fontsize=12)
plt.legend(frameon=False, numpoints=1, markerscale=2)
plt.show()
```



What I notice about the decision boundary is that it's made up of rectangles, not smooth at all. There is a concentrated mass around (x 100-150), (y 0-60). Which corresponds nicely with the 125 Gev mass of the Higgs Boson, fun fact.

I don't see real evidence of overfitting. Let's investigate a little:

[23]:
```
mask_b = np.array(data_train.Label == "b")
mask_s = np.array(data_train.Label == "s")

DER_mass_MMC = np.array(data_train.DER_mass_MMC)
DER_mass_transverse_met_lep = np.array(data_train.DER_mass_transverse_met_lep)

plt.figure()
# plot decision boundary
ax = plt.subplot(111)
cm = ListedColormap(["midnightblue", "firebrick"])
plt.contourf(x_grid, y_grid, z_grid, levels=[0, 0.5, 1], cmap=cm, alpha=0.25)
# overlaid with test data points
plt.plot(
    DER_mass_MMC[mask_b],
    DER_mass_transverse_met_lep[mask_b],
    "o",
    markersize=2,
    color="midnightblue",
    markeredgewidth=0,
    alpha=0.8,
    label="Background",
)
plt.plot(
    DER_mass_MMC[mask_s],
    DER_mass_transverse_met_lep[mask_s],
    "o",
    markersize=2,
    color="firebrick",
    markeredgewidth=0,
    alpha=0.8,
    label="Signal",
)
ax.set_ylim(0,150)
ax.set_xlim(0,400)
plt.xlabel("DER_mass_MMC", fontsize=12)
plt.ylabel("DER_mass_transverse_met_lep", fontsize=12)
plt.legend(frameon=False, numpoints=1, markerscale=2)
plt.show()
```



If there was widespread overfitting, I would expect to see a red dot in every rectangle. Looking at the plot with the training data instead of the test data, I can say that that is not the case. Therefore I proclaim: no overfitting!