Example of ML applications

In this example we will work with the public Top Quark Tagging Reference Dataset, which provides the following description:

A set of MC simulated training/testing events for the evaluation of top quark tagging architectures.

In total 1.2M training events, 400k validation events and 400k test events. Use “train” for training, “val” for validation during the training and “test” for final testing and reporting results.

Description

- 14 TeV, hadronic tops for signal, qcd diets background, Delphes ATLAS detector card with Pythia8
- No MPI/pile-up included
- Clustering of particle-flow entries (produced by Delphes E-flow) into anti-kT 0.8 jets in the pT range [550,650] GeV
- All top jets are matched to a parton-level top within ΔR = 0.8, and to all top decay partons within 0.8
- Jets are required to have |eta| < 2
- The leading 200 jet constituent four-momenta are stored, with zero-padding for jets with fewer than 200
- Constituents are sorted by pT, with the highest pT one first
- The truth top four-momentum is stored as truth_px etc.
- A flag (1 for top, 0 for QCD) is kept for each jet. It is called is_signal_new
- The variable "ttv" (= test/train/validation) is kept for each jet. It indicates to which dataset the jet belongs. It is redundant as the different sets are already distributed as different files.

With this dataset, which you can download from the provided link, we will exemplify one Machine Learning tasks: **Classification**.

To do so we will need to install different packages

```
import os
import numpy as np
import scipy
import matplotlib.pyplot as plt
import h5py
import pandas as pd
import sklearn as sk
import torch
```

```
import torch
```

Additionally, download and extract the Top_Quark_Tagging_dataset

```
path_train = "train.h5"
path_val = "val.h5"
path_test = "test.h5"
```

```
!wget -q -N https://zenodo.org/records/2603256/files/train.h5
!wget -q -N https://zenodo.org/records/2603256/files/val.h5
!wget -q -N https://zenodo.org/records/2603256/files/test.h5
```

```
def check_dataset_path(path):
    return os.path.isfile(path)
```

```
if (
    check_dataset_path(path_train)
    * check_dataset_path(path_val)
    * check_dataset_path(path_test)
    == 0
):
    print("Path not properly set")
else:
    print("All good here")
```

```
All good here
```

Data preprocessing

Let's load the datasets. These are a bit heavy, but things should be okay.

To be safe against overfitting, every operation should be decided on the training dataset and applied without changes to the validation and testing datasets.

Additionally, to save some memory we won't load the full training dataset

```
train = pd.read_hdf(path_train, key="table", start=0, stop=500000)
train.shape
```

```
(500000, 806)
```

```
val = pd.read_hdf(path_val, key="table", start=0, stop=100000)
val.shape
```

```
(100000, 806)
```

```
# test = pd.read_hdf(path_test,key='table')
# test.shape
```

Let's explore what the features are.

```
train.keys()
```

```
Index(['E_0', 'PX_0', 'PY_0', 'PZ_0', 'E_1', 'PX_1', 'PY_1', 'PZ_1', 'E_2',
       'PX_2',
       ...
       'E_199', 'PX_199', 'PY_199', 'PZ_199', 'truthE', 'truthPX', 'truthPY',
       'truthPZ', 'ttv', 'is_signal_new'],
      dtype='object', length=806)
```

```
train.head()
```

	E_0	PX_0	PY_0	PZ_0	E_1	PX_1	
375	474.071136	-250.347031	-223.651962	-334.738098	103.236237	-48.866222	-56.7
377	150.504532	120.062393	76.852005	-48.274265	82.257057	63.801739	42.7
378	251.645386	10.427651	-147.573746	203.564880	104.147797	10.718256	-54.4
379	451.566132	129.885437	-99.066292	-420.984100	208.410919	59.033958	-46.1
380	399.093903	-168.432083	-47.205597	-358.717438	273.691956	-121.926941	-30.8

5 rows × 806 columns

```
train.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 500000 entries, 375 to 706
Columns: 806 entries, E_0 to is_signal_new
dtypes: float32(804), int64(2)
memory usage: 1.5 GB
```

```
train.describe()
```

	E_0	PX_0	PY_0	PZ_0	E_1	
count	500000.000000	500000.000000	500000.000000	500000.000000	500000.000000	5
mean	233.519699	0.098696	-0.212851	0.242043	129.961075	
std	173.288330	121.672943	121.746933	234.344116	82.238289	
min	23.743198	-609.698792	-634.309448	-1939.883179	0.000000	
25%	124.773357	-82.606472	-82.834406	-97.847517	77.015837	
50%	182.505470	-0.094346	-0.194142	-0.051609	107.595936	

75%	280.929466	82.905062	82.645300	97.636534	156.691650
max	2183.859863	627.447693	592.888916	2094.136475	986.571777

8 rows × 806 columns

We see how we have a **balanced dataset** (the mean of "is_signal_new" is 0.5. Let's distinguish between features and labels. Also, truthE, truthpx, truthpy, truthpz should be apart since it's only valid for tops

```
train_features = train.drop(
    columns=["truthE", "truthPX", "truthPY", "truthPZ", "ttv", "is_signal_new"]
)
train_labels = train["is_signal_new"]
top_momenta = train[["truthE", "truthPX", "truthPY", "truthPZ"]][train_labels == 0]
print(train_features.shape, train_labels.shape, top_momenta.shape)
```

```
(500000, 800) (500000,) (250838, 4)
```

```
val_features = val.drop(
    columns=["truthE", "truthPX", "truthPY", "truthPZ", "ttv", "is_signal_new"]
)
val_labels = val["is_signal_new"]
val_top_momenta = val[["truthE", "truthPX", "truthPY", "truthPZ"]][val_labels == 0]
print(val_features.shape, val_labels.shape, val_top_momenta.shape)
```

```
(100000, 800) (100000,) (49810, 4)
```

```
np.sum(train_labels == 0), train_features[train_labels == 0].shape, np.sum(
    train_labels == 1
)
```

```
(np.int64(250838), (250838, 800), np.int64(249162))
```

```
train_features[train_labels == 0].describe()
```

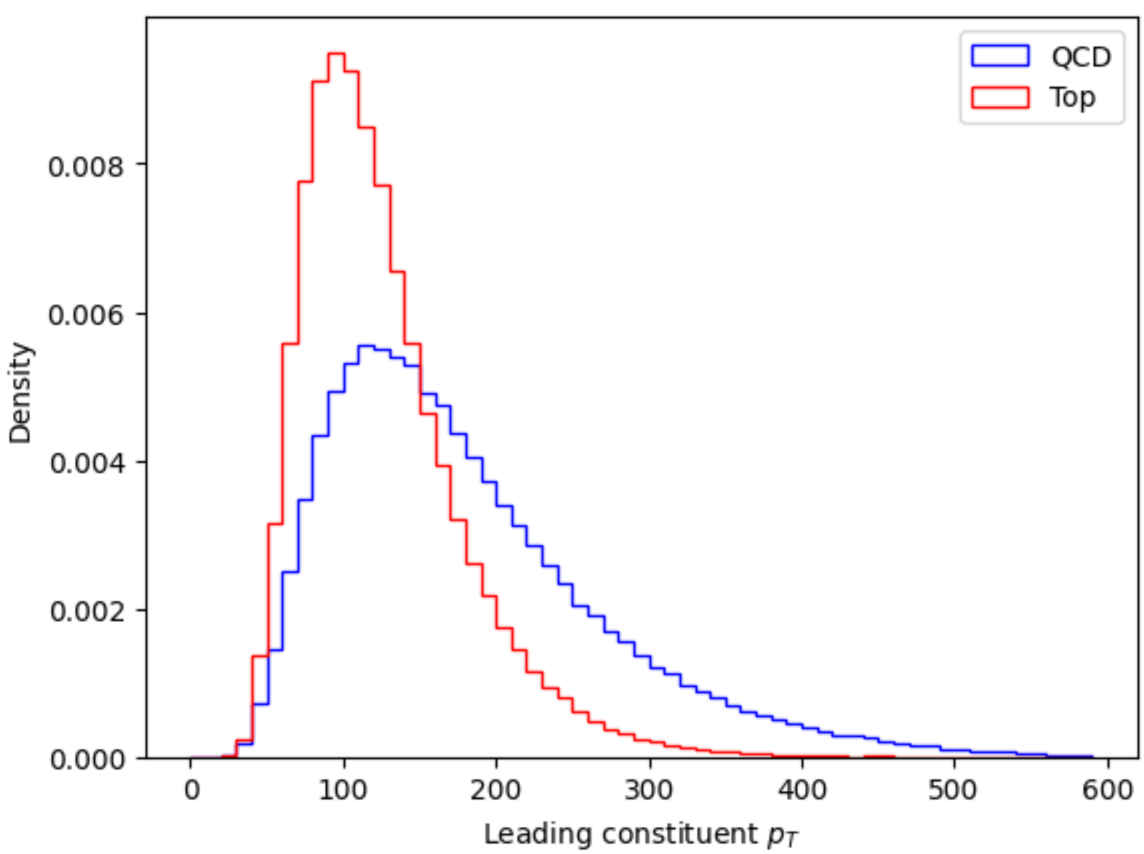
	E_0	PX_0	PY_0	PZ_0	E_1	
count	250838.000000	250838.000000	250838.000000	250838.000000	250838.000000	2
mean	287.215698	0.327478	0.064826	0.879631	151.365646	
std	207.589737	142.751984	142.665253	291.282715	96.555817	
min	23.743198	-609.698792	-634.309448	-1939.883179	0.000000	
25%	150.413422	-97.496674	-97.611715	-126.480492	87.534700	
50%	226.934143	0.198023	0.615853	0.255935	125.762245	
75%	354.181137	97.861605	97.628479	128.260685	185.753586	

max	2183.859863	627.447693	592.888916	2094.136475	986.571777

8 rows × 800 columns

We can start exploring the distributions to see how things look like. For instance, the p_T distribution of the leading constituent.

```
leading_pT = np.sqrt(train_features["PX_0"] ** 2 + train_features["PY_0"] ** 2)
plt.hist(
    leading_pT[train_labels == 0],
    bins=np.arange(0, 600, 10),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    leading_pT[train_labels == 1],
    bins=np.arange(0, 600, 10),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Leading constituent $p_T$")
plt.show()
```



Already we see a nice difference! The Top is softer than the background for the leading constituent. We can explain this by looking at the jet mass distribution. Because the cosntituents are zero-padded, we can obtain the total momentum by summing carefully. I prefer to work in numpy, so I'll transform everything to numpy.

```
train_features = train_features.to_numpy()
train_labels = train_labels.to_numpy()
top_momenta = top_momenta.to_numpy()
```

```
val_features = val_features.to_numpy()
val_labels = val_labels.to_numpy()
val_top_momenta = val_top_momenta.to_numpy()
```

```
totalE = np.sum(train_features[:, 0:801:4], axis=1)
totalPX = np.sum(train_features[:, 1:801:4], axis=1)
totalPY = np.sum(train_features[:, 2:801:4], axis=1)
totalPZ = np.sum(train_features[:, 3:801:4], axis=1)
print(totalE.shape, totalPX.shape, totalPY.shape, totalPZ.shape)
```

```
(500000,) (500000,) (500000,) (500000,)
```

```
total_mass = totalE**2 - totalPX**2 - totalPY**2 - totalPZ**2
total_mass = np.where(total_mass > 0, np.sqrt(total_mass), 0)
```

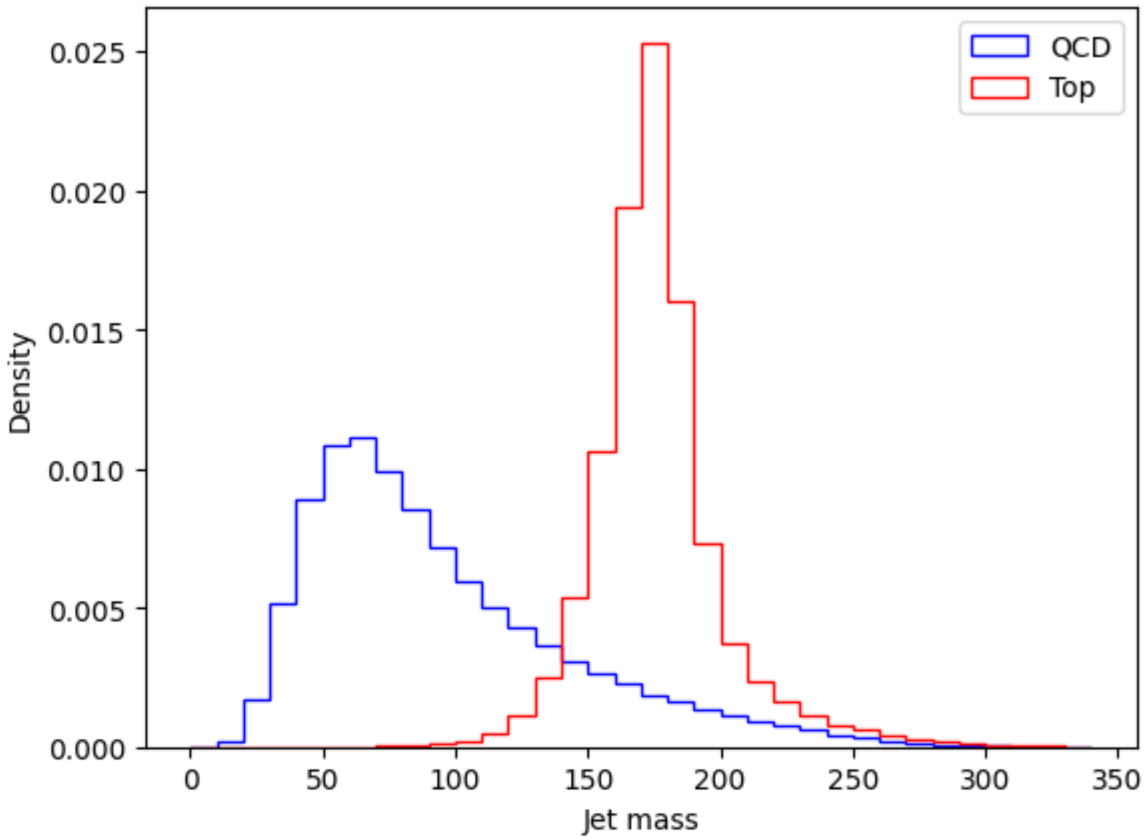
```
/tmp/ipython-input-31-327548360.py:2: RuntimeWarning: invalid value encountered in
  total_mass = np.where(total_mass > 0, np.sqrt(total_mass), 0)
```

```
total_mass
```

```
array([ 37.394016,  46.99734 ,  61.648197, ..., 172.09827 , 175.09676 ,
       198.52327 ], dtype=float32)
```

```
plt.hist(
    total_mass[train_labels == 0],
    bins=np.arange(0, 350, 10),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    total_mass[train_labels == 1],
    bins=np.arange(0, 350, 10),
    histtype="step",
    color="red",
    label="Top",
```

```
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Jet mass")
plt.savefig("mass.png")
plt.show()
```



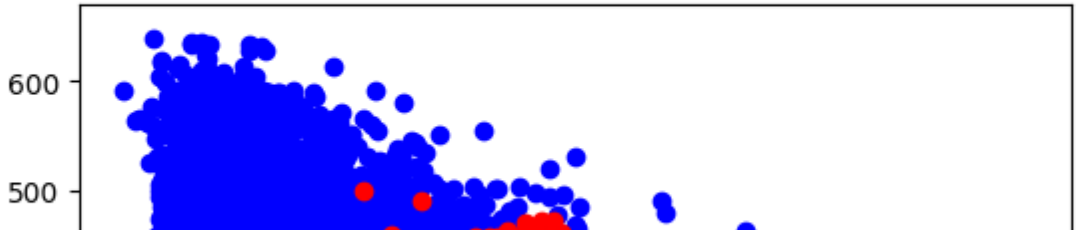
The jet mass is centered around the top mass for Top jets, while it's softer for QCD jets. Is there any relationship between mass and the leading constituent p_T?

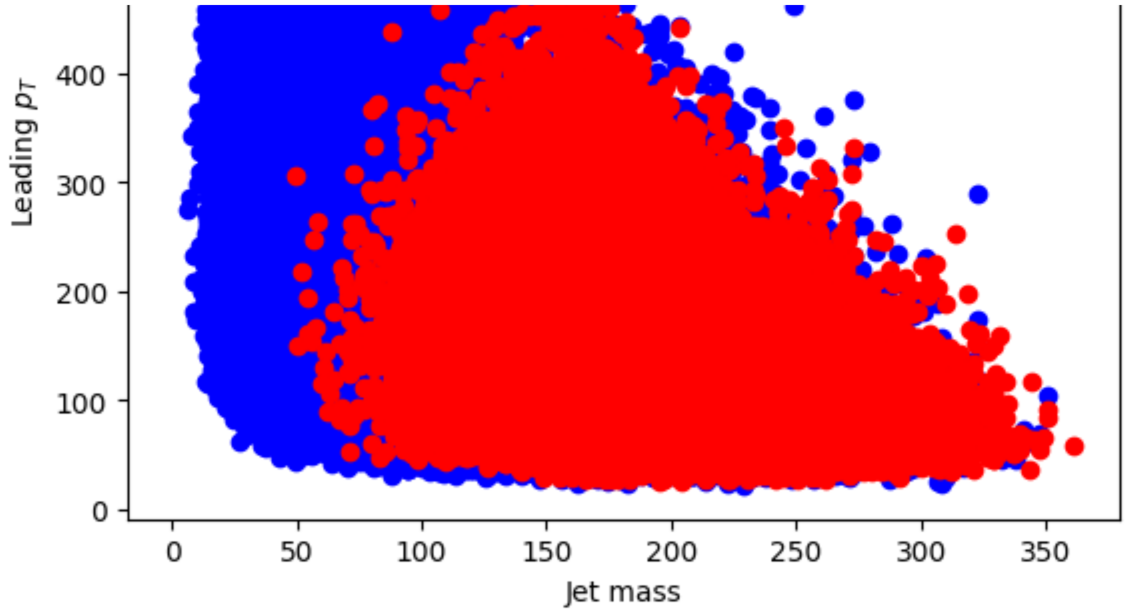
```
scipy.stats.pearsonr(total_mass, leading_pT)
```

```
PearsonRResult(statistic=np.float32(-0.47825938), pvalue=np.float64(0.0))
```

```
plt.scatter(total_mass[train_labels == 0], leading_pT[train_labels == 0], c="blue")
plt.scatter(total_mass[train_labels == 1], leading_pT[train_labels == 1], c="red")
plt.xlabel("Jet mass")
plt.ylabel("Leading $p_T$")
```

```
Text(0, 0.5, 'Leading $p_T$')
```





So, yes, but this doesn't look particularly useful. We can also look at other **global observables** . To do everything, its useful to compute the multiplicity. Because the energy is positive, we just need to check what's the first zero energy. We define a mask that can be used later on when using graphs.

```
train_mask = train_features[:, 0:801:4] > 0
multiplicity = np.argmin(train_mask, axis=1)
print(multiplicity.shape)
```

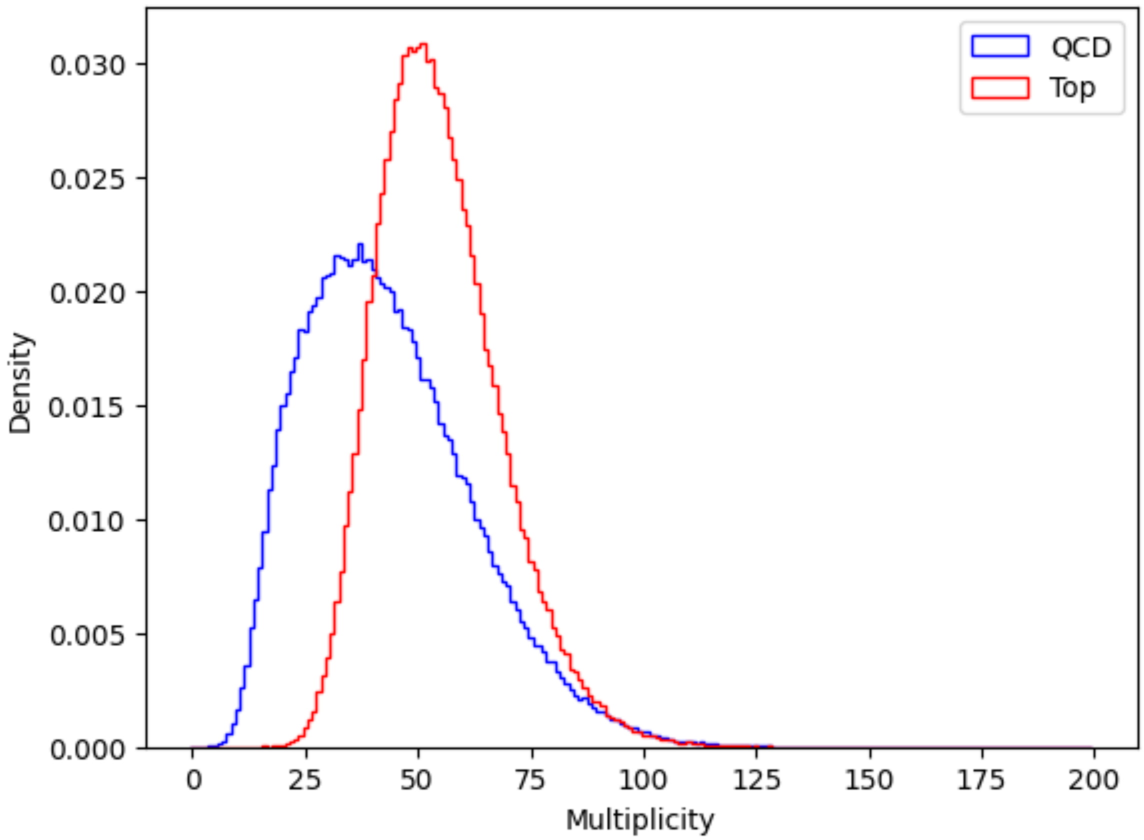
```
(500000,)
```

```
val_mask = val_features[:, 0:801:4] > 0
val_multiplicity = np.argmin(val_mask, axis=1)
print(val_multiplicity.shape)
```

```
(100000,)
```

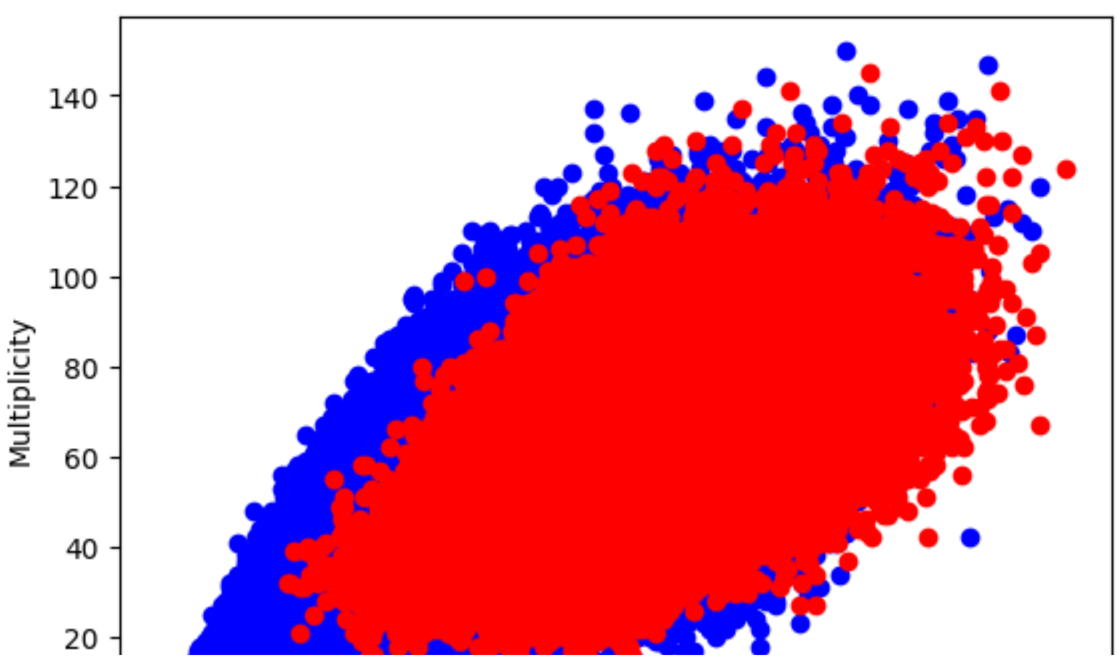
```
plt.hist(
    multiplicity[train_labels == 0],
    bins=np.arange(-0.5, 200.5, 1),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    multiplicity[train_labels == 1],
    bins=np.arange(-0.5, 200.5, 1),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
```

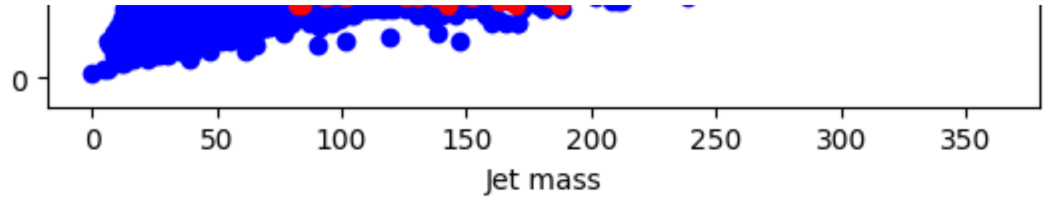
```
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Multiplicity")
plt.savefig("multiplicity.png")
plt.show()
```




```
plt.scatter(total_mass[train_labels == 0], multiplicity[train_labels == 0], c="blue")
plt.scatter(total_mass[train_labels == 1], multiplicity[train_labels == 1], c="red")
plt.xlabel("Jet mass")
plt.ylabel("Multiplicity")
```

```
Text(0, 0.5, 'Multiplicity')
```





Let's compute the average p_T (it's not the best observable but it's faster to compute). To do this, we need to move from (E,px,py,pz) to (pT,eta,phi,mass).

```
def Epxpypz_to_pTetaphimass(vec):
    E, px, py, pz = vec[0], vec[1], vec[2], vec[3]
    pT = np.sqrt(vec[1] ** 2 + vec[2] ** 2)
    phi = np.arctan2(vec[2], vec[2])
    mass = (
        np.sqrt(E**2 - px**2 - py**2 - pz**2)
        if E**2 - px**2 - py**2 - pz**2 > 0
        else 0
    )
    eta = np.arctanh(pz / np.sqrt(px**2 + py**2 + pz**2))
    return np.array([pT, eta, phi, mass])
```

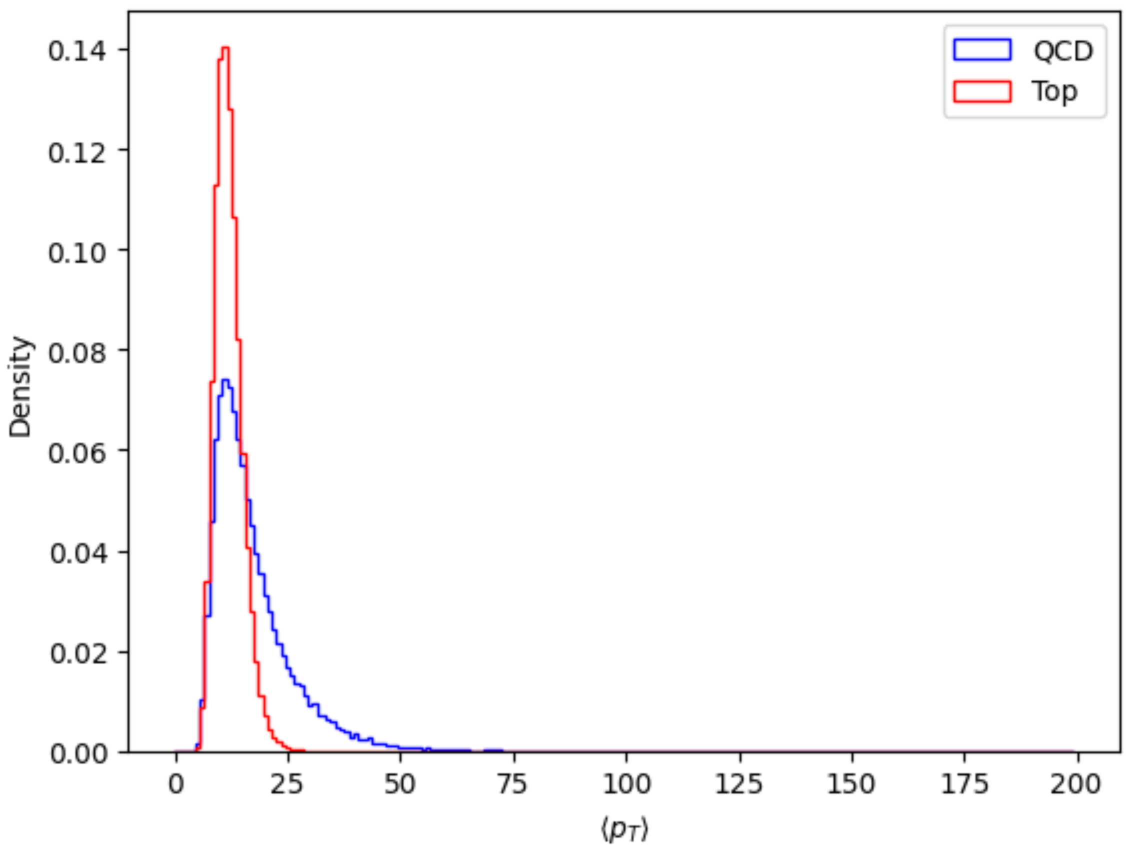
```
av_pT = np.zeros(len(train_features))
for nevent in range(len(train_features)):
    av_pT[nevent] = np.mean(
        np.sqrt(
            train_features[nevent, 1 : 4 * multiplicity[nevent] : 4] ** 2
            + train_features[nevent, 2 : 4 * multiplicity[nevent] : 4] ** 2
        )
    )
```

```
nevent, len(train_features)
```

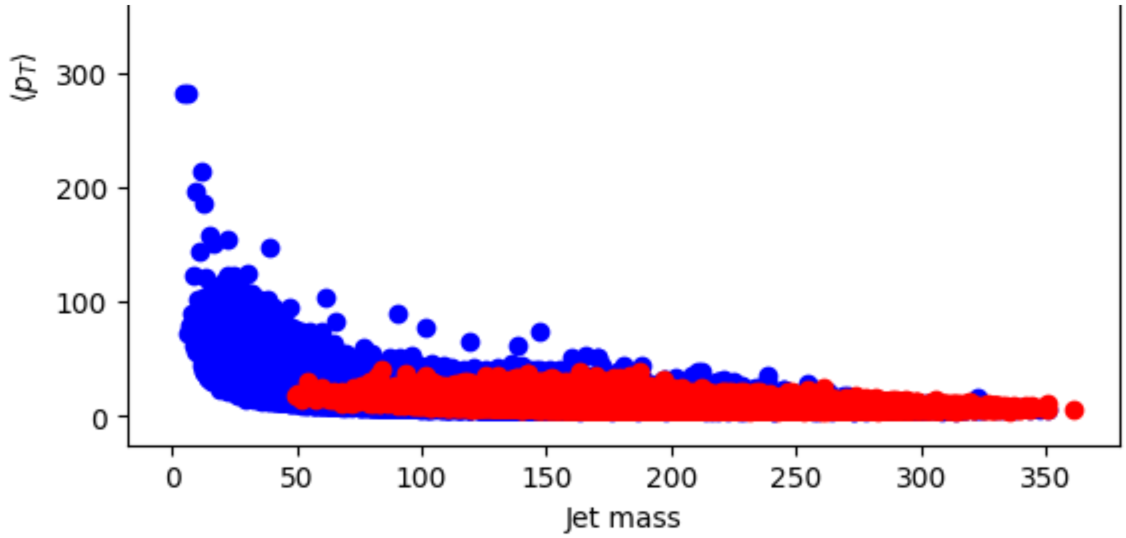
```
(499999, 500000)
```

```
plt.hist(
    av_pT[train_labels == 0],
    bins=np.arange(-0.5, 200.5, 1),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    av_pT[train_labels == 1],
    bins=np.arange(-0.5, 200.5, 1),
    histtype="step",
    color="red",
    label="Top",
    density=True,
```

```
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel(r"$\langle p_{T} \rangle$")
plt.savefig("av_pT.png")
plt.show()
```




```
plt.scatter(
    total_mass[train_labels == 0], av_pT[train_labels == 0], c="blue", label="QCD"
)
plt.scatter(
    total_mass[train_labels == 1], av_pT[train_labels == 1], c="red", label="Top"
)
plt.legend(loc="upper right")
plt.xlabel("Jet mass")
plt.ylabel(r"$\langle p_{T} \rangle$")
plt.legend(loc="upper right")
plt.savefig("mass_av_pT.png")
plt.show()
```



Baseline Classifier

We can use these two features to train a baseline classifier, let's use the simplest possible: a logistic regressor.

```
from sklearn.linear_model import LogisticRegression

lr = LogisticRegression()
```

```
X_train = np.vstack([total_mass, av_pT]).T
print(X_train.shape)
lr.fit(X_train, train_labels)
```

```
(500000, 2)
▾ LogisticRegression
LogisticRegression()
```

```
proba_lr = lr.predict_proba(X_train)[:, 1]
assignment_lr = lr.predict(X_train)  # it's just 0 if proba < 0.5 and 1 otherwise
```

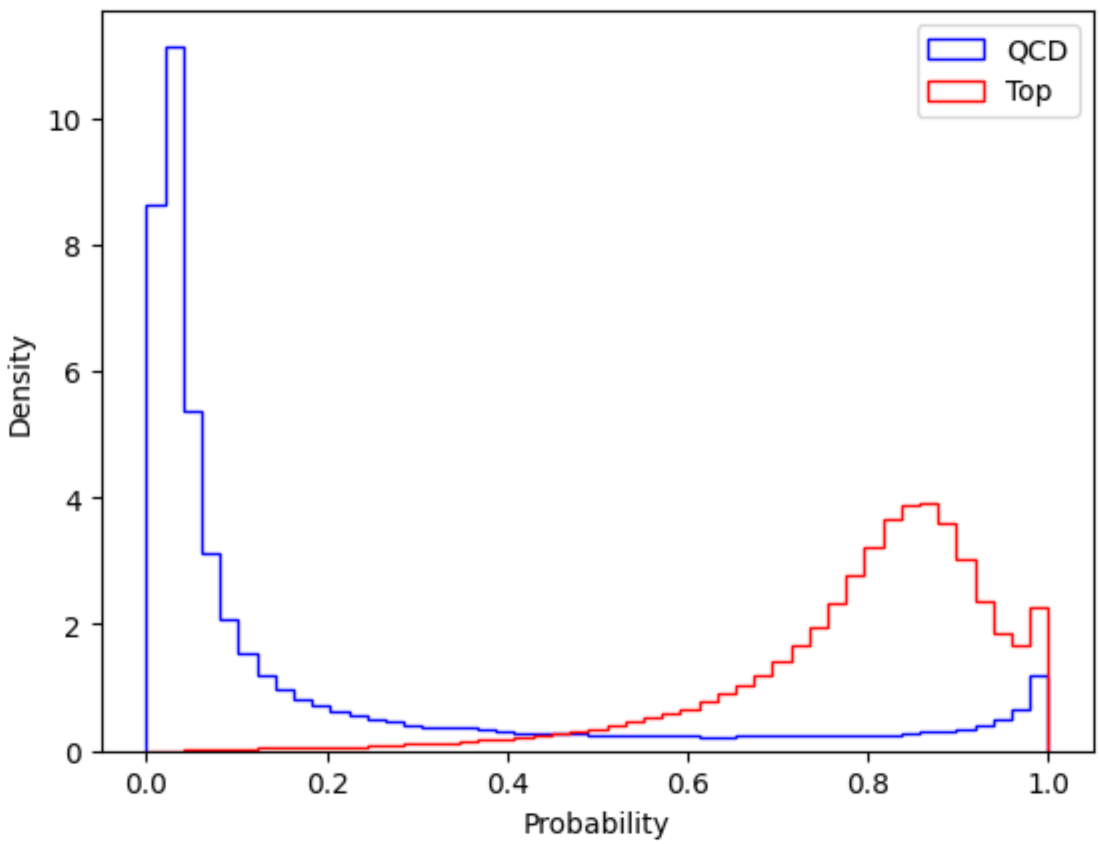
```
proba_lr
```

```
array([0.01346516, 0.00784004, 0.0170622 , ..., 0.88837949, 0.82817595,
       0.92391527])
```

Let's see how the probability region looks

```
plt.hist(
    proba_lr[train_labels == 0],
```

```
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    proba_lr[train_labels == 1],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Probability")
plt.savefig("proba_lr.png")
plt.show()
```

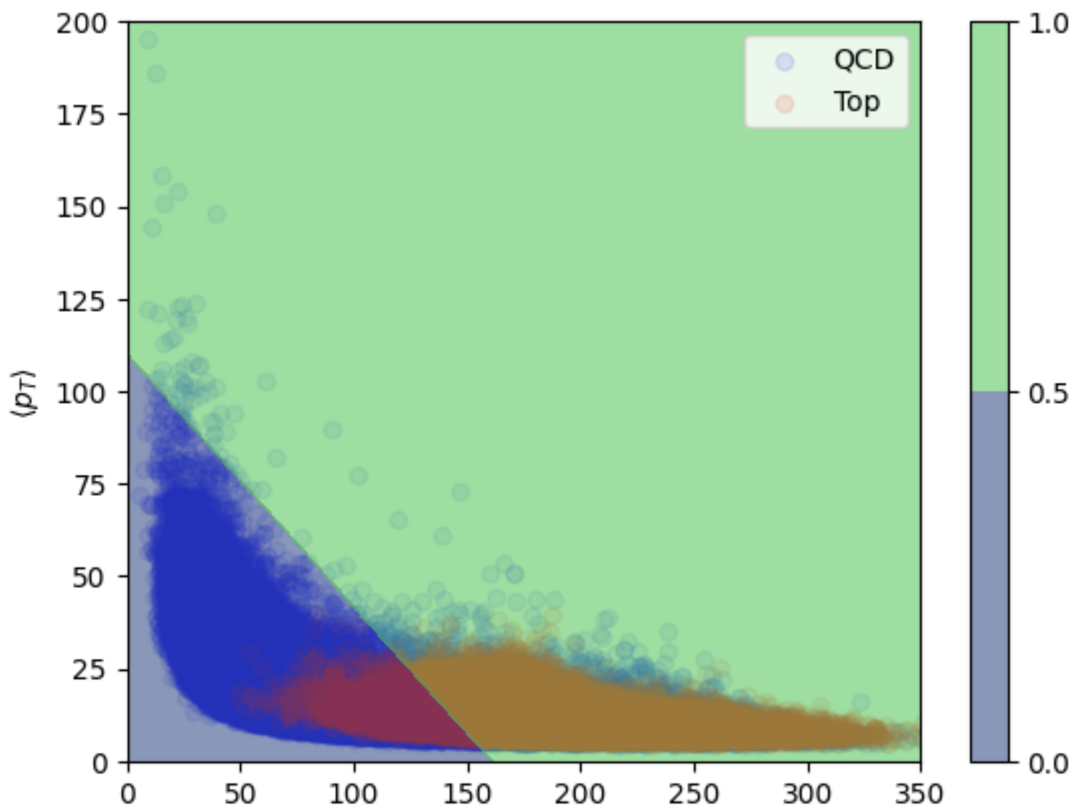



```
x1 = np.linspace(0, 350, 100)
x2 = np.linspace(0, 200, 100)
X1toplot, X2toplot = np.meshgrid(x1, x2)
# plt.xlim(0.0,0.2)
# plt.ylim(0.0,0.2)
plt.scatter(
    total_mass[train_labels == 0],
    av_pT[train_labels == 0],
    c="blue".
```

```
        alpha=0.1,
        label="QCD",
    )
    plt.scatter(
        total_mass[train_labels == 1],
        av_pT[train_labels == 1],
        c="red",
        alpha=0.1,
        label="Top",
    )
    Z = (
        np.asarray(
            [
                lr.predict_proba(np.asarray([el[0], el[1]]).reshape(1, -1))[0, 1]
                for el in np.c_[X1toplot.ravel(), X2toplot.ravel()]
            ]
        )
    ).reshape(X1toplot.shape)

    contour = plt.contourf(X1toplot, X2toplot, Z, levels=[0, 0.5, 1], alpha=0.6)
    plt.colorbar(contour)


    plt.xlim(0, 350)
    plt.ylim(0, 200)
    plt.xlabel("Jet mass")
    plt.ylabel(r"$\langle p_{T} \rangle$")
    plt.legend(loc="upper right")
    plt.savefig("classifier_space_lr.png")
    plt.show()
```



Jet mass

To evaluate the model, we need metrics. The logistic regressor outputs a probability and a hard assignment

```
from sklearn.metrics import accuracy_score, roc_auc_score, confusion_matrix

print(
    accuracy_score(train_labels, assignment_lr), roc_auc_score(train_labels, proba_lr)
)
```

```
0.891444 0.910334261676372
```

Let's show the confusion matrix: row is true class, column predicted class.

```
confusion_matrix(train_labels, assignment_lr)
```

```
array([[210189,  40649],
       [ 13629, 235533]])
```

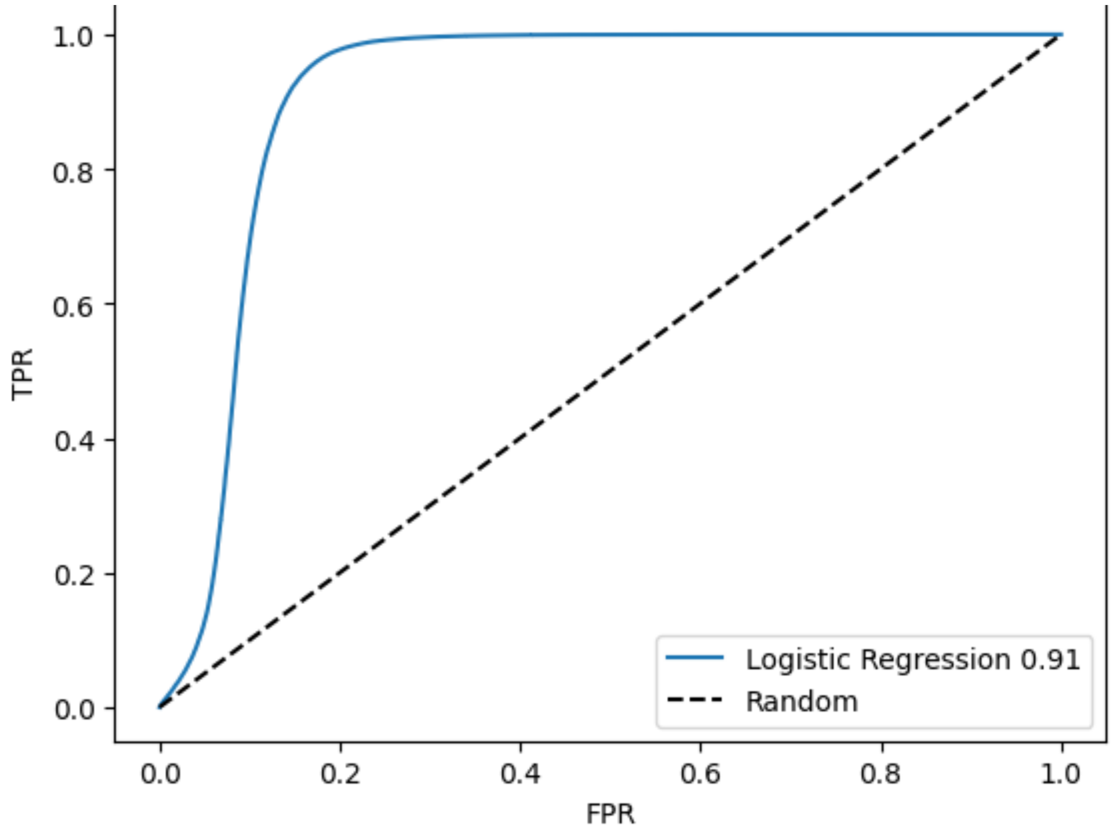
We see how many more QCD are tagged as tops than QCD as tops. This can be seen from the 2d plot above.

Let's plot the ROC Curve. There are many ways to plot, we'll do (FPR,TPR) so that up and left is better.

```
from sklearn.metrics import roc_curve

fpr_lr, tpr_lr, thr_lr = roc_curve(train_labels, proba_lr)


plt.plot(
    fpr_lr,
    tpr_lr,
    label="Logistic Regression " + str(round(roc_auc_score(train_labels, proba_lr), 3))
)
plt.plot(
    np.linspace(0, 1, 10),
    np.linspace(0, 1, 10),
    linestyle="dashed",
    color="black",
    label="Random",
)
plt.xlabel("FPR")
plt.ylabel("TPR")
plt.legend(loc="lower right")
plt.savefig("roc_curve.png")
```



Evaluate on validation

```
val_total_mass = (
    np.sum(val_features[:, 0:801:4], axis=1) ** 2
    - np.sum(val_features[:, 1:801:4], axis=1) ** 2
    - np.sum(val_features[:, 2:801:4], axis=1) ** 2
    - np.sum(val_features[:, 3:801:4], axis=1) ** 2
)
val_total_mass = np.where(val_total_mass > 0, np.sqrt(val_total_mass), 0)
```

```
val_total_mass
```

```
array([ 29.406233, 157.04945 , 226.96985 , ..., 173.36552 , 184.85028 ,
       130.6595  ], dtype=float32)
```

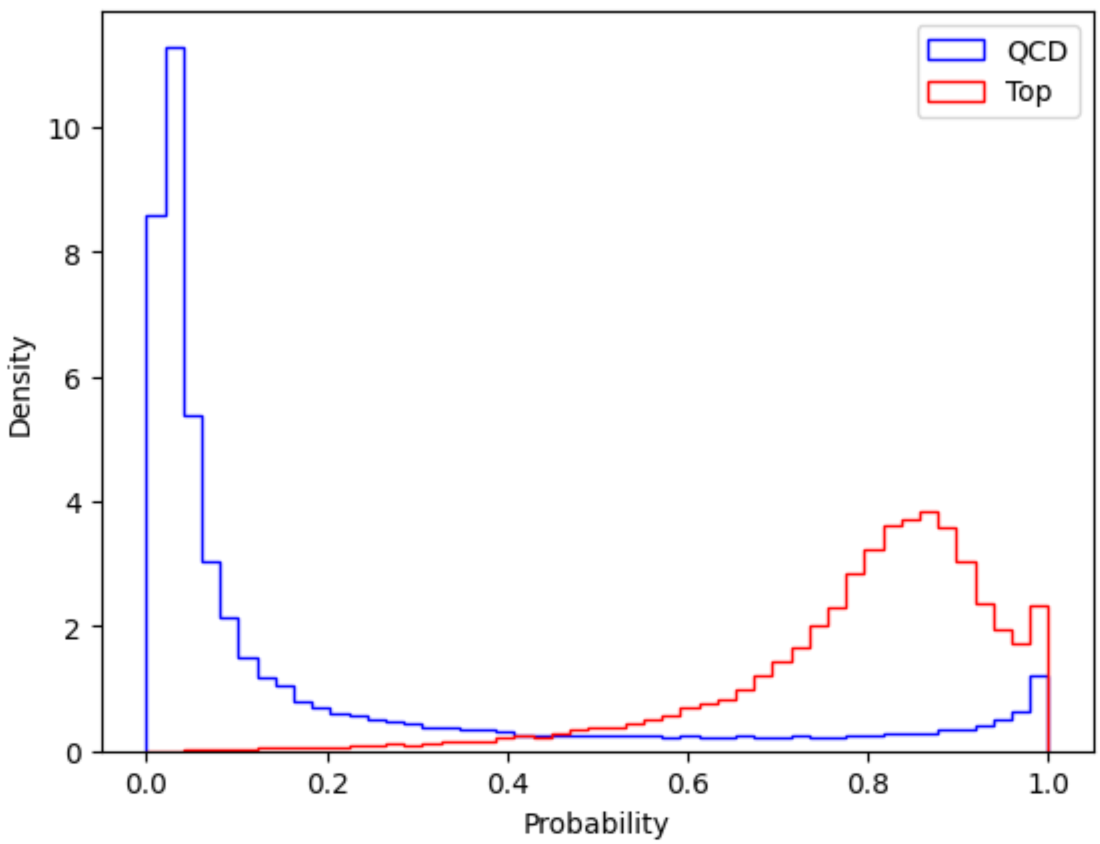
```
val_av_pT = np.zeros(len(val_features))
for nevent in range(len(val_features)):
    val_av_pT[nevent] = np.mean(
        np.sqrt(
            val_features[nevent, 1 : 4 * val_multiplicity[nevent] : 4] ** 2
            + val_features[nevent, 2 : 4 * val_multiplicity[nevent] : 4] ** 2
        )
    )
```

```
X_val = np.vstack([val_total_mass, val_av_pT]).T
print(X_val.shape)
val_proba_lr = lr.predict_proba(X_val)[:, 1]
```

```
val_proba_lr = lr.predict_proba(X_val)[:, 1]
val_assignmnet_lr = lr.predict(X_val)
```

```
    (100000, 2)
```

```
plt.hist(
    val_proba_lr[val_labels == 0],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    val_proba_lr[val_labels == 1],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Probability")
plt.show()
```




```
print(
    accuracy_score(val_labels, val_assignmnet_lr),
    roc_auc_score(val_labels, val_proba_lr),
```

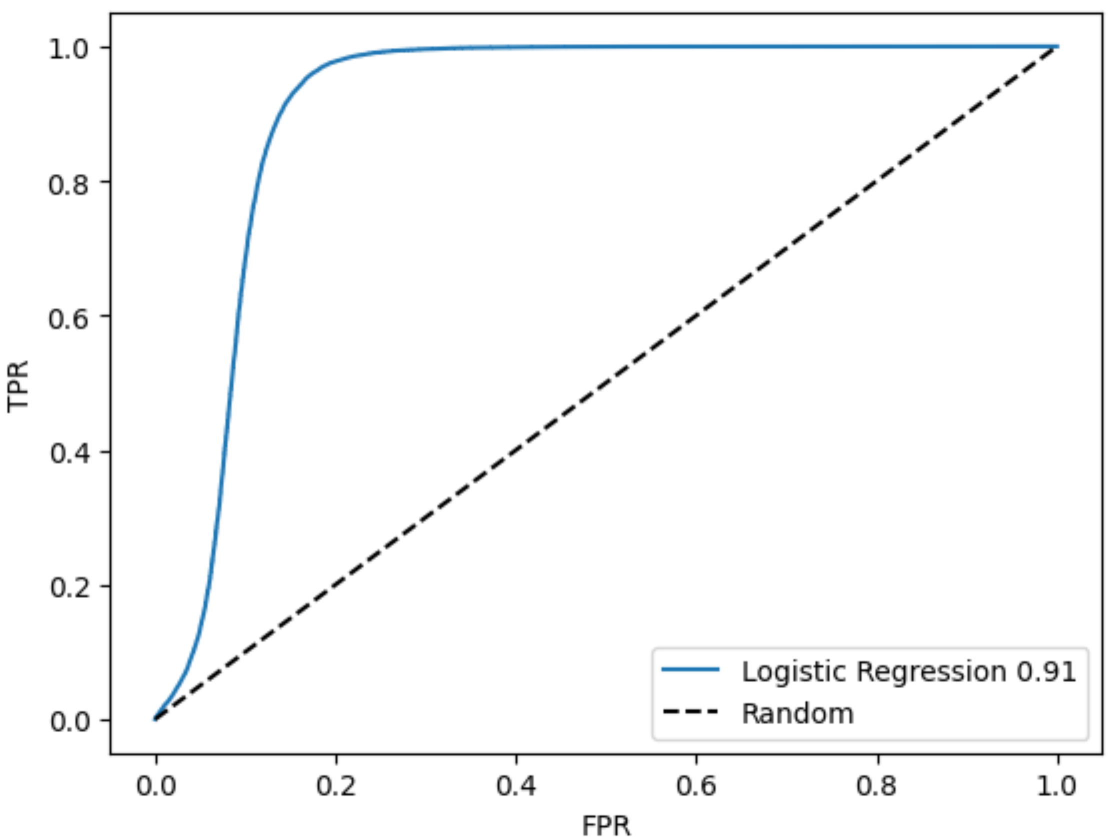
```
    roc_auc_score(val_labels, val_proba_lr),
)
```

```
    0.89114 0.9103360564526553
```

```
val_fpr_lr, val_tpr_lr, val_thr_lr = roc_curve(val_labels, val_proba_lr)
```

```
plt.plot(
    val_fpr_lr,
    val_tpr_lr,
    label="Logistic Regression "
    + str(round(roc_auc_score(val_labels, val_proba_lr), 3)),
)
plt.plot(
    np.linspace(0, 1, 10),
    np.linspace(0, 1, 10),
    linestyle="dashed",
    color="black",
    label="Random",
)
plt.xlabel("FPR")
plt.ylabel("TPR")
plt.legend(loc="lower right")
```

```
    <matplotlib.legend.Legend at 0x7da29e843c50>
```



Exercise:

Redo this using the C_3 coefficient defined here instead of the average p_T. It's much slower to compute, that's why we do not use it here.

A home-made DeepSets classifier: ParticleFlow Network

We will do a ParticleFlow network but in 4-momenta space, without using the (p_T,η,ϕ) representation. This will probably cost some performance, but it takes a bit longer to preprocess 1M events. You probably want to do that (and maybe try a CNN there as well!)

We'll define a custom Dataset and a custom Neural Network class in Pytorch.

Our dataset should have features, label and mask to indicate which particles are zero-padded

```
class CustomDataset(torch.utils.data.Dataset):
    """
    Joins the x and y into a dataset, so that it can be used by the pythorch syntax.
    """

    def __init__(self, x, y, m):
        self.x = torch.tensor(x).to(torch.float)
        self.y = torch.tensor(y).to(torch.float)
        self.m = torch.tensor(m).to(torch.float)

    def __len__(self):
        return len(self.x)

    def __getitem__(self, idx):
        if torch.is_tensor(idx):
            idx = idx.tolist()
        sample = [self.x[idx], self.y[idx], self.m[idx]]
        return sample
```

Let's standarize the dataset,otherwise the training gets really hard

```
maxE = np.max(train_features[:, 0:801:4])
maxPX = np.max(np.abs(train_features[:, 1:801:4]))
maxPY = np.max(np.abs(train_features[:, 2:801:4]))
maxPZ = np.max(np.abs(train_features[:, 3:801:4]))

meanE = np.mean(train_features[:, 0:801:4].flatten()[train_mask.flatten()])
meanPX = np.mean(train_features[:, 1:801:4].flatten()[train_mask.flatten()])
meanPY = np.mean(train_features[:, 2:801:4].flatten()[train_mask.flatten()])
meanPZ = np.mean(train_features[:, 3:801:4].flatten()[train_mask.flatten()])

stdE = np.std(train_features[:, 0:801:4].flatten()[train_mask.flatten()])
stdPX = np.std(train_features[:, 1:801:4].flatten()[train_mask.flatten()])
```

```
stdPX = np.std(train_features[:, 1:801:4].flatten()[train_mask.flatten()])
stdPY = np.std(train_features[:, 2:801:4].flatten()[train_mask.flatten()])
stdPZ = np.std(train_features[:, 3:801:4].flatten()[train_mask.flatten()])


print(maxE, maxPX, maxPY, maxPZ)
```

```
2183.8599 627.4477 634.30945 2094.1365
```

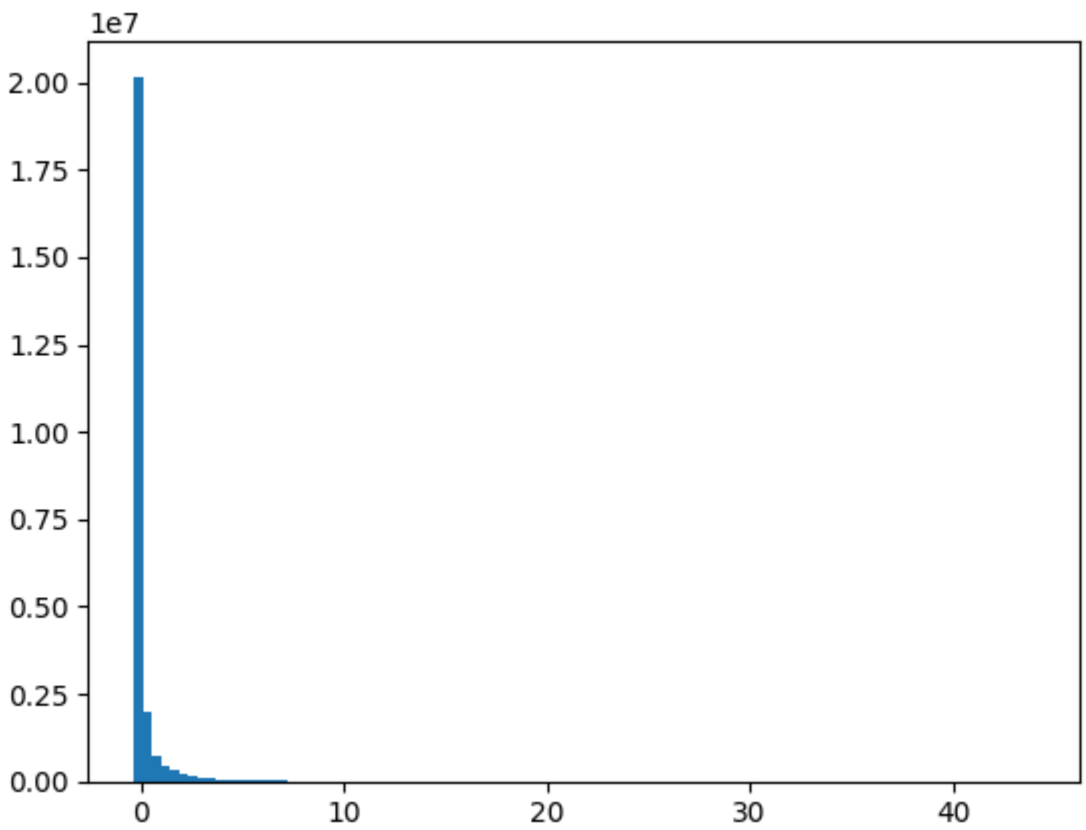
```
print(meanE, meanPX, meanPY, meanPZ)
print(stdE, stdPX, stdPY, stdPZ)
```

```
18.611986 -0.0044181882 -0.009700178 -0.00618418
49.125217 22.124771 22.137777 42.191326
```

```
"""
train_features[:,0:801:4]*=1/maxE
train_features[:,1:801:4]*=1/maxPX
train_features[:,2:801:4]*=1/maxPY
train_features[:,3:801:4]*=1/maxPZ
"""
train_features[:, 0:801:4] = (train_features[:, 0:801:4] - meanE) / stdE
train_features[:, 1:801:4] = (train_features[:, 1:801:4] - meanPX) / stdPX
train_features[:, 2:801:4] = (train_features[:, 2:801:4] - meanPY) / stdPY
train_features[:, 3:801:4] = (train_features[:, 3:801:4] - meanPZ) / stdPZ


plt.hist(train_features[:, 0:801:4].flatten()[train_mask.flatten()], bins=100)
plt.xlabel("Standarized Energy")
```

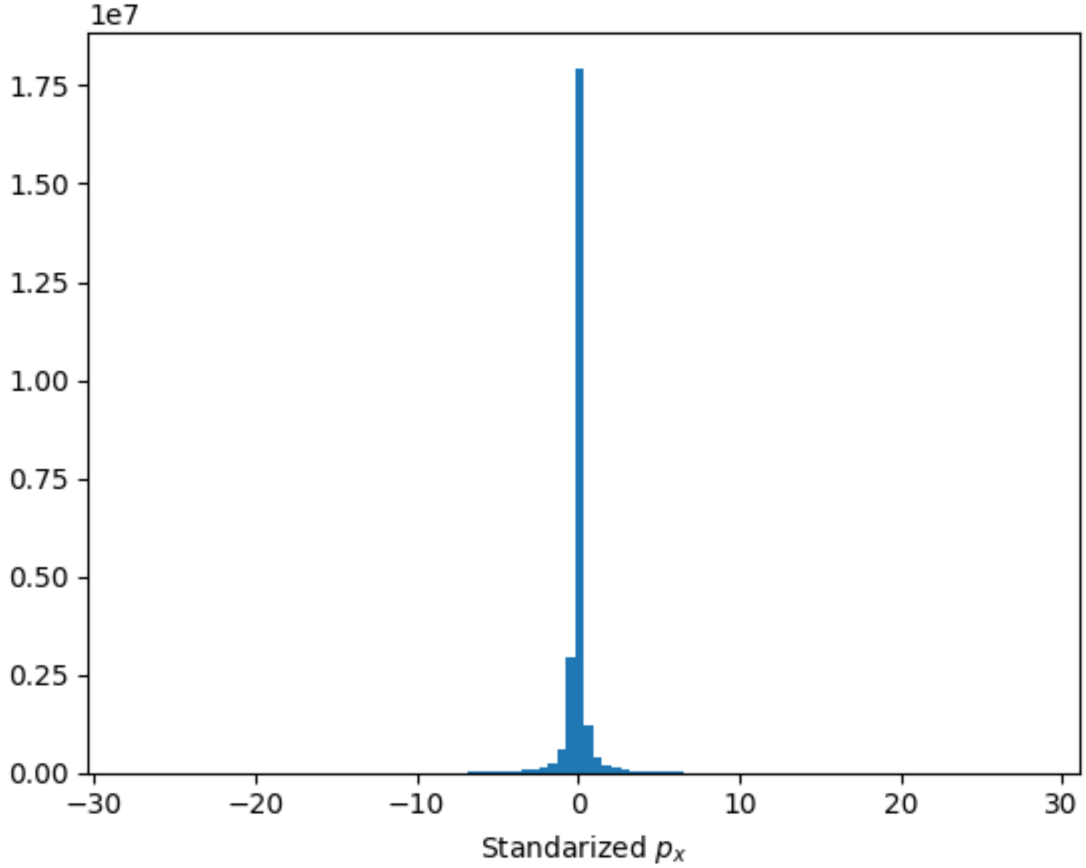
```
Text(0.5, 0, 'Standarized Energy')
```



Standarized Energy

```
plt.hist(train_features[:, 1:801:4].flatten()[train_mask.flatten()], bins=100)
plt.xlabel("Standarized $p_x$")
```

```
Text(0.5, 0, 'Standarized $p_x$')
```



We standarize the validation dataset using the same parameters

```
val_features[:, 0:801:4] = (val_features[:, 0:801:4] - meanE) / stdE
val_features[:, 1:801:4] = (val_features[:, 1:801:4] - meanPX) / stdPX
val_features[:, 2:801:4] = (val_features[:, 2:801:4] - meanPY) / stdPY
val_features[:, 3:801:4] = (val_features[:, 3:801:4] - meanPZ) / stdPZ
```

```
train_torch = CustomDataset(
    train_features.reshape((len(train_features), 200, 4)), train_labels, train_mask
)
val_torch = CustomDataset(
    val_features.reshape((len(val_features), 200, 4)), val_labels, val_mask
)
```

Let's free some memory

```
"""
del train
```

```
del X_train
del val
del X_val
del train_features
del val_features
del train_mask
del val_mask
"""
```

```
'\ndel train\ndel X_train\ndel val\ndel X_val\ndel train_features\ndel val_features
\ndel train_mask\ndel val_mask\n'
```

Our model consists of two neural networks, one evaluated per particle and one evaluated over all particles in an event

```
from torch import nn
from torch.nn.modules import Module
from torch.utils.data import DataLoader


# Define model
class PseudoParticleFlow(nn.Module):
    def __init__(
        self,
        dim_input=4,
        inner_dim=64,
        layers_Phi=[(64, nn.ReLU()), (64, nn.ReLU()), (64, nn.ReLU())],
        layers_F=[(64, nn.ReLU()), (64, nn.ReLU()), (64, nn.ReLU())],
    ):  # example of layers_data=[(layer1, nn.ReLU()), (layer2, nn.ReLU()), (output_siz
        super(PseudoParticleFlow, self).__init__()
        self.flatten = nn.Flatten()
        self.Phi = nn.ModuleList()
        self.F = nn.ModuleList()
        self.input_size = dim_input  # Can be useful later ...
        self.inner_dim = inner_dim  # Can be useful later ...
        input_size = dim_input
        for size, activation in layers_Phi:
            self.Phi.append(nn.Linear(input_size, size))
            input_size = size  # For the next layer
            if activation is not None:
                assert isinstance(
                    activation, Module
                ), "Each tuples should contain a size (int) and a torch.nn.modules.Modu
                self.Phi.append(activation)
        self.Phi.append(nn.Linear(input_size, inner_dim))

        input_size = inner_dim
        for size, activation in layers_F:
            self.F.append(nn.Linear(input_size, size))
            input_size = size  # For the next layer
            if activation is not None:
                assert isinstance(
                    activation, Module
```

```
                    activation, Module
                ), "Each tuples should contain a size (int) and a torch.nn.modules.Modu
                self.F.append(activation)
        self.F.append(nn.Linear(input_size, 1))
        self.F.append(nn.Sigmoid())

    def forward(self, x, m):
        output = x
        for layer in self.Phi:
            output = layer(output)
            # print(output.shape)
        ### this uses the mask to remove zero-padded particles when performing the aver
        output = torch.einsum("ijk,ij->ik", output, m) / (
            torch.einsum("ik,ik->i", m, m).unsqueeze(1)
        )
        # output = torch.stack((torch.masked.masked_tensor(output[:,:,0], m),torch.mask
        # print(output.shape)
        # output = torch.mean(output,1)
        # print(output.shape)
        for layer in self.F:
            output = layer(output)
            # print(output.shape)
        return output

    def latent(self, x, m):
        output = x
        for layer in self.Phi:
            output = layer(output)
            # print(output.shape)
        ### this uses the mask to remove zero-padded particles when performing the aver
        output = torch.einsum("ijk,ij->ik", output, m) / (
            torch.einsum("ik,ik->i", m, m).unsqueeze(1)
        )
        return output

    def proba_from_latent(self, ell):
        output = ell
        for layer in self.F:
            output = layer(output)
            # print(output.shape)
        return output

    def loss_function(self, y, t):
        # loss_fn = nn.MSELoss(reduction='mean')
        loss_fn = nn.BCELoss()

        return loss_fn(y, t)

    def reset_weights(self):
        for m in self.Phi:
            if isinstance(m, nn.Conv2d) or isinstance(m, nn.Linear):
                m.reset_parameters()
        for m in self.F:
            if isinstance(m, nn.Conv2d) or isinstance(m, nn.Linear):
```

```
        if isinstance(m, nn.Conv2d) or isinstance(m, nn.Linear):
            m.reset_parameters()
```

We can define training, testing and predicting functions

```
def train(model, optimizer, train_dataset, batch_size=1024):
    model.train()
    device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
    train_dataset_batched = DataLoader(
        train_dataset, batch_size=batch_size, shuffle=True
    )
    total_loss = 0
    for batch, (X, y, M) in enumerate(train_dataset_batched):
        X, y, M = X.to(device), y.to(device), M.to(device)
        # print(torch.mean(y))
        optimizer.zero_grad()  # Clear gradients.
        pred = model(X, M)[:, 0]  # Forward pass.
        # print(pred.shape,y.shape)
        loss = model.loss_function(pred, y)  # Loss computation.
        loss.backward()  # Backward pass.
        optimizer.step()  # Update model parameters.
        total_loss += loss.item()

    return total_loss / len(train_dataset_batched.dataset)


def test(model, test_dataset, batch_size=1024):
    model.eval()
    device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
    test_dataset_batched = DataLoader(
        test_dataset, batch_size=batch_size, shuffle=False
    )
    total_loss = 0
    for batch, (X, y, M) in enumerate(test_dataset_batched):
        X, y, M = X.to(device), y.to(device), M.to(device)
        pred = model(X, M)[:, 0]  # Forward pass.
        loss = model.loss_function(pred, y)  # Loss computation.
        total_loss += loss.item()

    return total_loss / len(test_dataset_batched.dataset)


def predict_proba(model, test_dataset, batch_size=1024):
    model.eval()
    device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
    test_dataset_batched = DataLoader(
        test_dataset, batch_size=batch_size, shuffle=False
    )
    truths = np.zeros(len(test_dataset))
    preds = np.zeros(len(test_dataset))
    initial_index = 0
    final_index = 0
```

```
    for batch, (X, y, M) in enumerate(test_dataset_batched):
        final_index += len(y)
        truths[initial_index:final_index] = y.detach().cpu().numpy()
        X, y, M = X.to(device), y.to(device), M.to(device)
        pred = model(X, M)[:, 0]  # Forward pass.
        preds[initial_index:final_index] = pred.detach().cpu().numpy()
        initial_index += len(y)
    return truths, preds


def predict(model, test_dataset, batch_size=1024):
    model.eval()
    device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
    test_dataset_batched = DataLoader(
        test_dataset, batch_size=batch_size, shuffle=False
    )
    truths = np.zeros(len(test_dataset))
    preds = np.zeros(len(test_dataset))
    initial_index = 0
    final_index = 0
    for batch, (X, y, M) in enumerate(test_dataset_batched):
        final_index += len(y)
        truths[initial_index:final_index] = y.detach().cpu().numpy()
        X, y, M = X.to(device), y.to(device), M.to(device)
        pred = model(X, M)[:, 0]  # Forward pass.
        preds[initial_index:final_index] = pred.detach().cpu().numpy()
        preds[initial_index:final_index] = np.where(
            preds[initial_index:final_index] > 0.5, 1, 0
        )
        initial_index += len(y)
    return truths, preds


def latent(model, test_dataset, batch_size=1024):
    model.eval()
    device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
    test_dataset_batched = DataLoader(
        test_dataset, batch_size=batch_size, shuffle=False
    )
    latent_variables = np.zeros((len(test_dataset), model.inner_dim))
    initial_index = 0
    final_index = 0
    for batch, (X, y, M) in enumerate(test_dataset_batched):
        final_index += len(y)
        X, y, M = X.to(device), y.to(device), M.to(device)
        pred = model.latent(X, M)  # Forward pass.
        latent_variables[initial_index:final_index] = pred.detach().cpu().numpy()
        initial_index += len(y)
    return latent_variables
```

With this, we initialize our model. We can save and load models

```
model = PseudoParticleFlow()
model_path = "saved_model.pth"
try:
    model.load_state_dict(torch.load(model_path))
    print("Loaded existing model")
except:
    print("New model")
device = torch.device("cpu")  # "cuda:0" if torch.cuda.is_available() else "cpu")
model.to(device)
```

```
New model
PseudoParticleFlow(
  (flatten): Flatten(start_dim=1, end_dim=-1)
  (Phi): ModuleList(
    (0): Linear(in_features=4, out_features=64, bias=True)
    (1): ReLU()
    (2): Linear(in_features=64, out_features=64, bias=True)
    (3): ReLU()
    (4): Linear(in_features=64, out_features=64, bias=True)
    (5): ReLU()
    (6): Linear(in_features=64, out_features=64, bias=True)
  )
  (F): ModuleList(
    (0): Linear(in_features=64, out_features=64, bias=True)
    (1): ReLU()
    (2): Linear(in_features=64, out_features=64, bias=True)
    (3): ReLU()
    (4): Linear(in_features=64, out_features=64, bias=True)
    (5): ReLU()
    (6): Linear(in_features=64, out_features=1, bias=True)
    (7): Sigmoid()
  )
)
```

You can always start over by resetting the weights as commented below

```
# model.reset_weights()
```

We define the optimizer that we'll use for training

```
learning_rate = 0.01
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

Now the epochs

```
nepochs = 30
npatience = 5
```

```
print(torch.einsum("ik,ik->i", train_torch[:2][2], train_torch[:2][2]))
print(
```

```
print(
    torch.einsum("ijk,ij->ik", train_torch[:2][0], train_torch[:2][2])
    / (torch.einsum("ik,ik->i", train_torch[:2][2], train_torch[:2][2]).unsqueeze(1))
)
```

```
tensor([23., 43.])
tensor([[ 0.3905, -0.8942, -0.8179, -0.6296],
        [-0.0974,  0.4896,  0.3201, -0.1127]])
```

```
# totalE[0]/(maxE*multiplicity[0]),totalE[1]/(maxE*multiplicity[1])
```

And let's train. We'll use the validation to test to avoid overfitting (this you shouldn't do if you're actually using the validation dataset to select the best model, you should either cross-validate or separate the training into actual training and evaluation datasets)

```
val_loss_aux = 1000
times = 0
for epoch in range(1, nepochs + 1):
    loss = train(model, optimizer, train_torch, batch_size=1024)
    val_loss = test(model, val_torch, batch_size=1024)
    print(
        f"Epoch: {epoch:02d}, Loss: {loss:.8f},Val Loss: {val_loss:.8f}, Learning Rate:
    )
    if epoch == 0:
        val_loss_aux = val_loss
        times = 0
        continue

    if loss < val_loss_aux:
        val_loss_aux = val_loss
        times = 0
    else:
        times += 1

    if times == npatience:
        learning_rate *= 0.1
        optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
    if times == 2 * npatience:
        break
    torch.save(model.state_dict(), model_path)
```

```
Epoch: 01, Loss: 0.00055325,Val Loss: 0.00053769, Learning Rate: 0.010000
Epoch: 02, Loss: 0.00053636,Val Loss: 0.00053611, Learning Rate: 0.010000
Epoch: 03, Loss: 0.00053108,Val Loss: 0.00052778, Learning Rate: 0.010000
Epoch: 04, Loss: 0.00052990,Val Loss: 0.00052990, Learning Rate: 0.010000
Epoch: 05, Loss: 0.00052862,Val Loss: 0.00053074, Learning Rate: 0.010000
Epoch: 06, Loss: 0.00052883,Val Loss: 0.00052731, Learning Rate: 0.010000
Epoch: 07, Loss: 0.00052855,Val Loss: 0.00052647, Learning Rate: 0.010000
Epoch: 08, Loss: 0.00052651,Val Loss: 0.00052854, Learning Rate: 0.010000
Epoch: 09, Loss: 0.00052678,Val Loss: 0.00052747, Learning Rate: 0.010000
Epoch: 10, Loss: 0.00052590,Val Loss: 0.00052737, Learning Rate: 0.010000
Epoch: 11, Loss: 0.00051027,Val Loss: 0.00047796, Learning Rate: 0.010000
```

```
Epoch: 12, Loss: 0.00043540,Val Loss: 0.00041100, Learning Rate: 0.010000
Epoch: 13, Loss: 0.00040730,Val Loss: 0.00041211, Learning Rate: 0.010000
Epoch: 14, Loss: 0.00040134,Val Loss: 0.00040576, Learning Rate: 0.010000
Epoch: 15, Loss: 0.00039876,Val Loss: 0.00040256, Learning Rate: 0.010000
Epoch: 16, Loss: 0.00039761,Val Loss: 0.00040467, Learning Rate: 0.010000
Epoch: 17, Loss: 0.00039761,Val Loss: 0.00040239, Learning Rate: 0.010000
Epoch: 18, Loss: 0.00039199,Val Loss: 0.00039126, Learning Rate: 0.010000
Epoch: 19, Loss: 0.00038687,Val Loss: 0.00038584, Learning Rate: 0.010000
Epoch: 20, Loss: 0.00038543,Val Loss: 0.00038601, Learning Rate: 0.010000
Epoch: 21, Loss: 0.00038581,Val Loss: 0.00038845, Learning Rate: 0.010000
Epoch: 22, Loss: 0.00038352,Val Loss: 0.00038383, Learning Rate: 0.010000
Epoch: 23, Loss: 0.00038394,Val Loss: 0.00039164, Learning Rate: 0.010000
Epoch: 24, Loss: 0.00038339,Val Loss: 0.00038396, Learning Rate: 0.010000
Epoch: 25, Loss: 0.00038267,Val Loss: 0.00039358, Learning Rate: 0.010000
Epoch: 26, Loss: 0.00038416,Val Loss: 0.00038505, Learning Rate: 0.010000
Epoch: 27, Loss: 0.00038284,Val Loss: 0.00038728, Learning Rate: 0.010000
Epoch: 28, Loss: 0.00038178,Val Loss: 0.00038556, Learning Rate: 0.010000
Epoch: 29, Loss: 0.00038196,Val Loss: 0.00038015, Learning Rate: 0.010000
Epoch: 30, Loss: 0.00038194,Val Loss: 0.00038180, Learning Rate: 0.010000
```

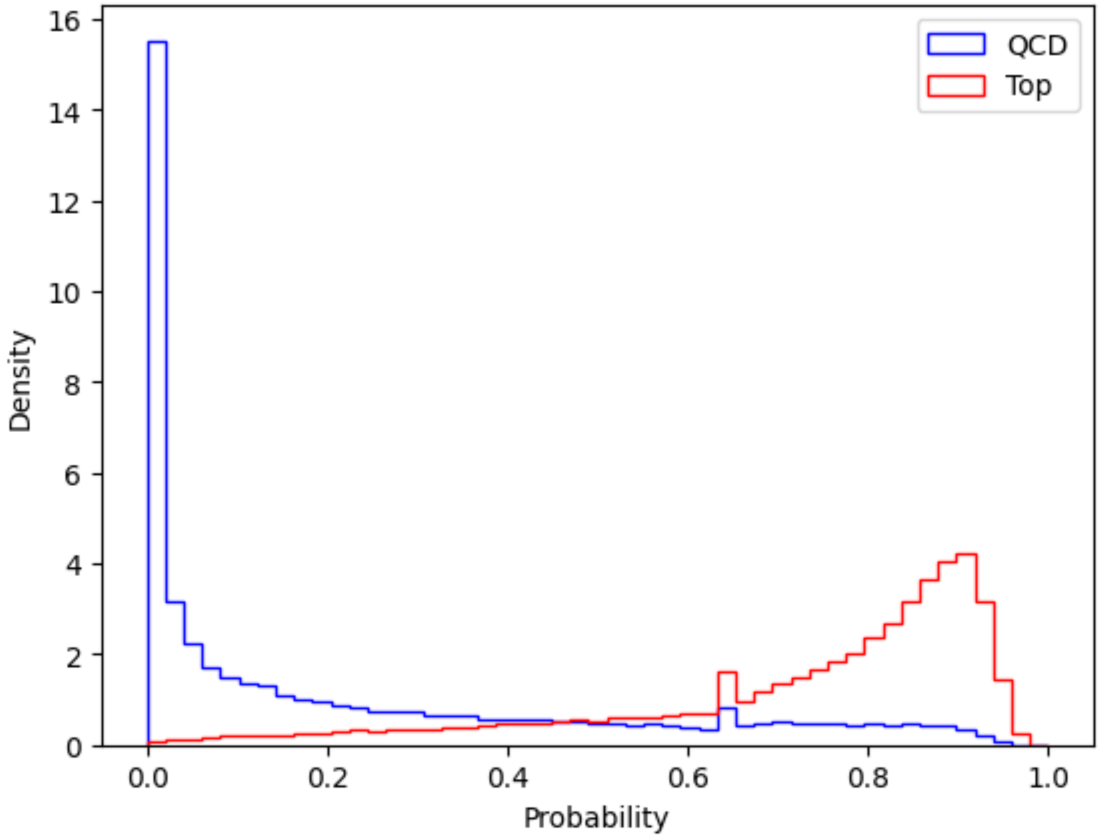
Once the model is slightly trained, we can obtain the predictions and do the same analysis

```
val_labels_NN, val_proba_NN = predict_proba(model, val_torch, batch_size=128)
val_assignmnet_NN = np.where(val_proba_NN > 0.5, 1, 0)
```

```
confusion_matrix(val_labels_NN, val_assignmnet_NN)
```

```
array([[39979,  9831],
       [ 7795, 42395]])
```

```
plt.hist(
    val_proba_NN[val_labels_NN == 0],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    val_proba_NN[val_labels_NN == 1],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Probability")
plt.savefig("proba_NN.png")
plt.show()
```



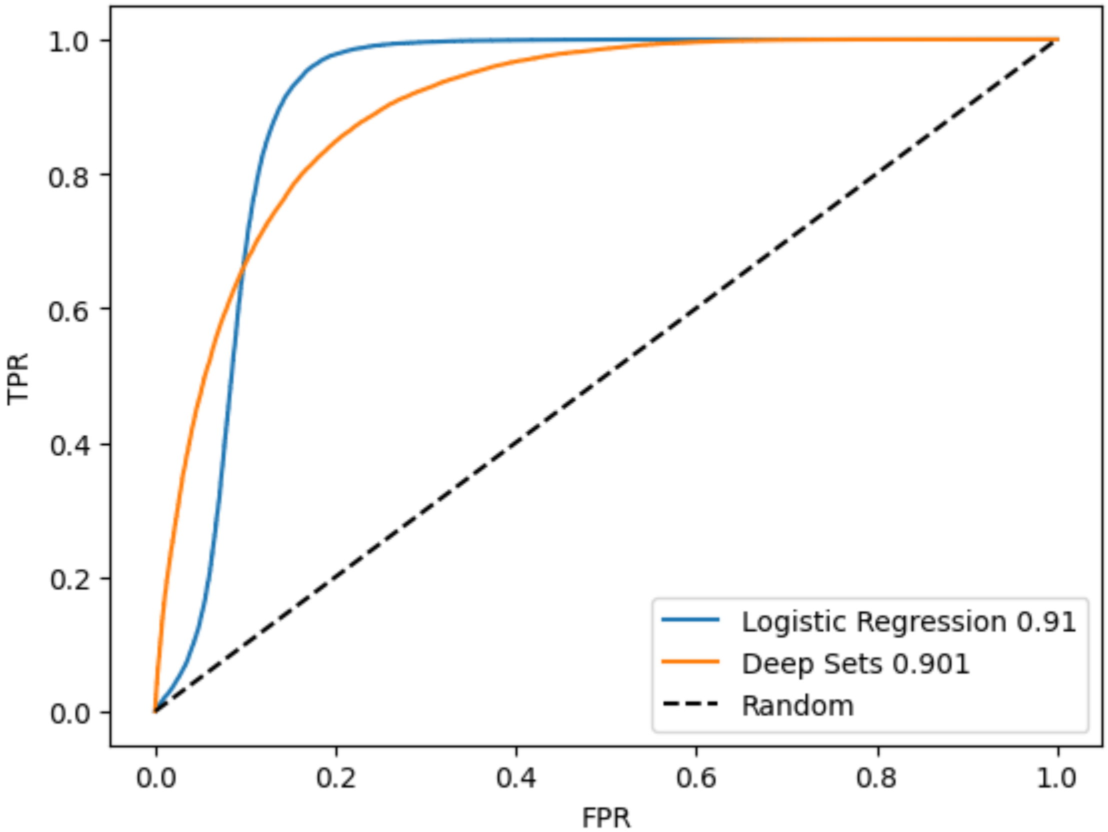

```
print(
    accuracy_score(val_labels_NN, val_assignmnet_NN),
    roc_auc_score(val_labels_NN, val_proba_NN),
)
```

```
0.82374 0.9010830212388268
```

```
val_fpr_NN, val_tpr_NN, val_thr_NN = roc_curve(val_labels_NN, val_proba_NN)
```

```
plt.plot(
    val_fpr_lr,
    val_tpr_lr,
    label="Logistic Regression "
    + str(round(roc_auc_score(val_labels, val_proba_lr), 3)),
)
plt.plot(
    val_fpr_NN,
    val_tpr_NN,
    label="Deep Sets " + str(round(roc_auc_score(val_labels_NN, val_proba_NN), 3)),
)
plt.plot(
    np.linspace(0, 1, 10),
    np.linspace(0, 1, 10),
    linestyle="dashed",
    color="black",
    label="Random",
)
plt.xlabel("FPR")
```

```
plt.xlabel("FPR")
plt.ylabel("TPR")
plt.legend(loc="lower right")
plt.savefig("roc_NN.png")
```



Here the performance is not that impressive. This is because the architecture is not huge and we are not using the full dataset and training for a long time.

Now the interpretation is more difficult of course...

We can try to interpret the latent space

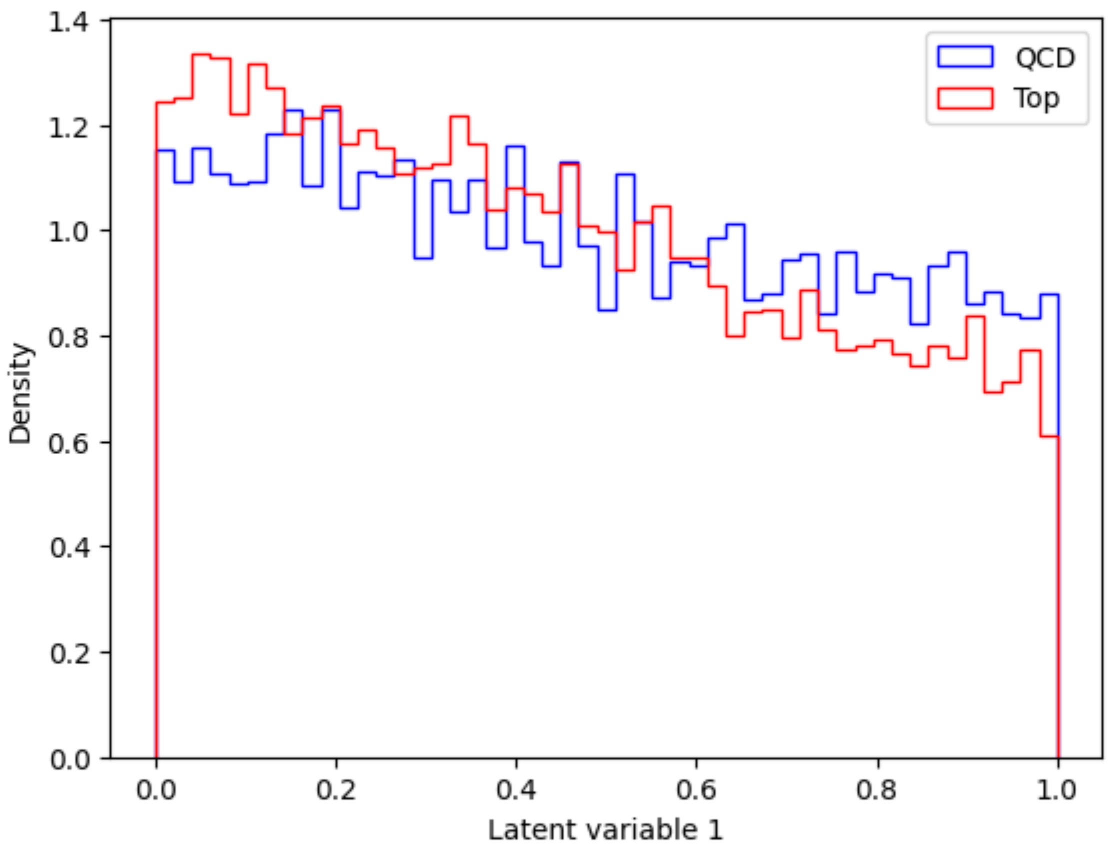
```
val_latent_variables_NN = latent(model, val_torch, batch_size=128)
```

```
val_latent_variables_NN.shape
```

```
(100000, 64)
```

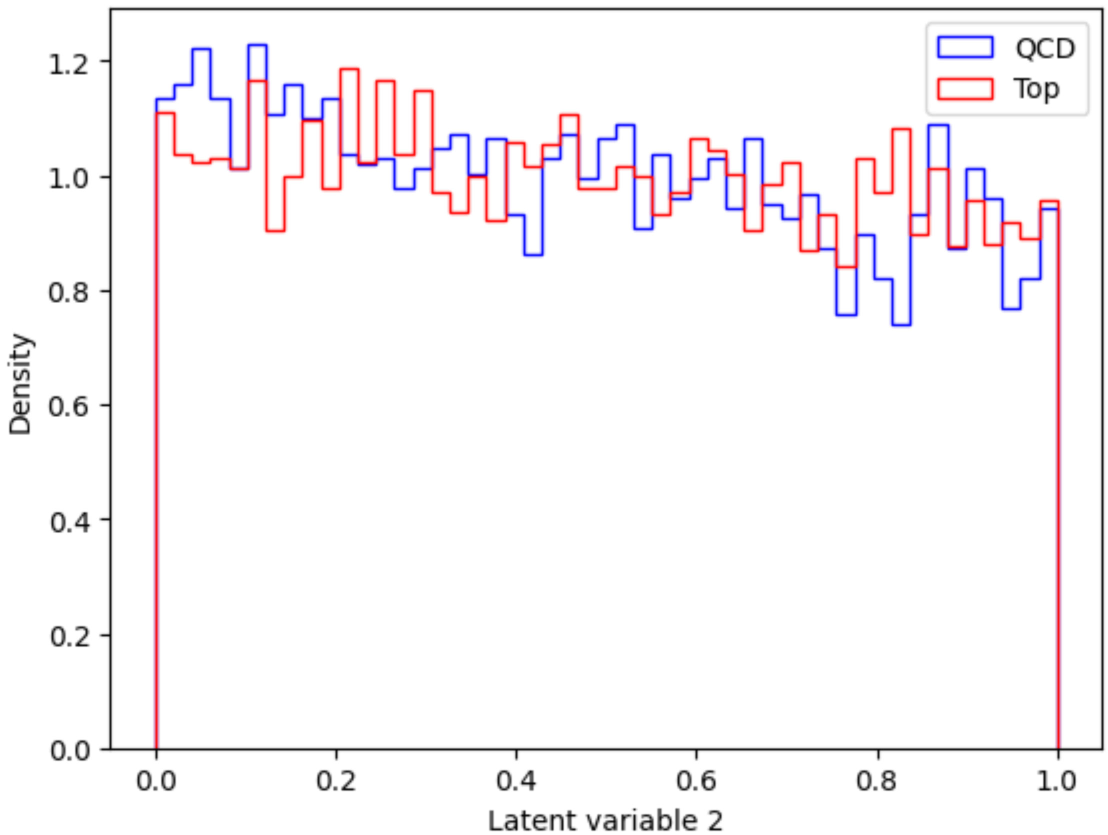
```
plt.hist(
    val_latent_variables_NN[val_labels_NN == 0, 0],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
```

```
    val_latent_variables_NN[val_labels_NN == 1, 0],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Latent variable 1")
plt.savefig("latent_1.png")
plt.show()
```




```
plt.hist(
    val_latent_variables_NN[val_labels_NN == 0, 1],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="blue",
    label="QCD",
    density=True,
)
plt.hist(
    val_latent_variables_NN[val_labels_NN == 1, 1],
    bins=np.linspace(0, 1, 50),
    histtype="step",
    color="red",
    label="Top",
    density=True,
)
```

```
,
plt.legend(loc="upper right")
plt.ylabel("Density")
plt.xlabel("Latent variable 2")
plt.savefig("latent_2.png")
plt.show()
```




```
for nlatent_dim in range(model.inner_dim):
    plt.hist(
        val_latent_variables_NN[val_labels_NN == 0, nlatent_dim],
        bins=np.linspace(0, 1, 50),
        histtype="step",
        color="blue",
        label="QCD",
        density=True,
    )
    plt.hist(
        val_latent_variables_NN[val_labels_NN == 1, nlatent_dim],
        bins=np.linspace(0, 1, 50),
        histtype="step",
        color="red",
        label="Top",
        density=True,
    )
    plt.legend(loc="upper right")
    plt.ylabel("Density")
    plt.xlabel("Latent variable " + str(nlatent_dim + 1))
    # plt.savefig('latent_'+str(nlatent_dim+1)+'.png')
    plt.clf()
```

```
/usr/local/lib/python3.11/dist-packages/numpy/lib/_histograms_impl.py:895: RuntimeW
  return n/db/n.sum(), bin_edges
<Figure size 640x480 with 0 Axes>
```

```
for nlatent_dim1 in range(model.inner_dim):
    for nlatent_dim2 in range(nlatent_dim1 + 1, model.inner_dim):
        if nlatent_dim1 > 2 or nlatent_dim2 > 3:
            break
        plt.scatter(
            val_latent_variables_NN[val_labels_NN == 0, nlatent_dim1],
            val_latent_variables_NN[val_labels_NN == 0, nlatent_dim2],
            c="blue",
            alpha=0.1,
            label="QCD",
        )
        plt.scatter(
            val_latent_variables_NN[val_labels_NN == 1, nlatent_dim1],
            val_latent_variables_NN[val_labels_NN == 1, nlatent_dim2],
            c="red",
            alpha=0.1,
            label="Top",
        )

        # plt.xlim(0,1)
        # plt.ylim(0,1)
        plt.xlabel("Latent variable " + str(nlatent_dim1 + 1))
        plt.ylabel("Latent variable " + str(nlatent_dim2 + 1))
        plt.legend(loc="upper right")
        # plt.savefig('classifier_space_NN'+str(nlatent_dim1+1)+'_'+str(nlatent_dim2+1)
        plt.clf()
```

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

If the latent dimension is equal to 2, we can do the same plots as before

```
if model.inner_dim == 2:
    x1 = np.linspace(0, 1, 100)
    x2 = np.linspace(0, 1, 100)
    X1toplot, X2toplot = np.meshgrid(x1, x2)
    # plt.xlim(0.0,0.2)
    # plt.ylim(0.0,0.2)
    plt.scatter(
        val_latent_variables_NN[val_labels_NN == 0, 0],
        val_latent_variables_NN[val_labels_NN == 0, 1],
        c="blue",
        alpha=0.1,
        label="QCD",
    )
    plt.scatter(
        val_latent_variables_NN[val_labels_NN == 1, 0],
        val_latent_variables_NN[val_labels_NN == 1, 1],
```

```
        val_latent_variables_NN[val_labels_NN == 1, 1],
        c="red",
        alpha=0.1,
        label="Top",
    )
    Z = (
        np.asarray(
            [
                model.proba_from_latent(
                    torch.tensor(
                        np.asarray([el[0], el[1]]).reshape(1, -1), dtype=torch.float
                    )
                )
                .detach()
                .numpy()[0]
                for el in np.c_[X1toplot.ravel(), X2toplot.ravel()]
            ]
        )
    ).reshape(X1toplot.shape)

    contour = plt.contourf(X1toplot, X2toplot, Z, levels=[0, 0.5, 1], alpha=0.6)
    plt.colorbar(contour)

    # plt.xlim(0,1)
    # plt.ylim(0,1)
    plt.xlabel("Latent variable 1")
    plt.ylabel("Latent variable 2")
    plt.legend(loc="upper right")
    plt.savefig("classifier_space_NN.png")
    plt.show()
```

Exercises

- Repeat this with different inner dimension (don't break your computer!). To explore the latent space, you can use tools like t-SNE or PCA
- Reframe this as a regression task, learn the C_3 coefficient from the constituents. This could use the same architecture but a different loss function.
- Use a similar architecture for a GAN to generate tops or QCD jets (or both! but you'll find differences).